

**Non-Energy Use and related CO₂ Emissions in
Germany: A Carbon Flow Analysis with the
NEAT Model for the Period of 1990-2003**

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Zusammenfassung

Die Erfassung von Emissionen aus der nichtenergetischen Nutzung fossiler Energieträger ist komplex und daher mit erheblichen Unsicherheiten behaftet. Um einen detaillierten Einblick in die Struktur des nichtenergetischen Verbrauchs und den daraus resultierenden Emissionen zu erhalten, wurde an der Universität Utrecht (Niederlande) das NEAT-Modell (NEAT steht für Non-energy Use Emissions Accounting Tables) entwickelt. NEAT berechnet mit Hilfe einer Massenbilanz- und Materialfluss-Analyse den nichtenergetischen Verbrauch fossiler Energieträger sowie die daraus resultierenden CO₂-Emissionen. Diese Berechnungen sind (weitestgehend) unabhängig von Daten aus der offiziellen Energiebilanz. Im Rahmen des Forschungsvorhabens zur Methodenaktualisierung für die Emissionsberechnung (F+E-Vorhaben 203 412 53/02 des UFOPLAN 2003) wurde das bereits existierende NEAT-Modell (Version 2.0) erweitert und für Deutschland im Zeitraum von 1990-2003 angewandt.

Für die Modellberechnungen wurden Produktions- und Außenhandelsdaten für mehr als 90 Chemikalien, Nichteisenmetalle, Ferrolegerungen und andere anorganische Produkte (z.B. Carbide und Phosphor) sowie detaillierte Informationen zu Produktionsrouten in der chemischen Industrie Deutschlands als Dateninput genutzt. Darüber hinaus wurden zwei zusätzliche Module in das bereits bestehende NEAT-Modell integriert, um Emissionen (i) aus der Abfall- und Abwasserbehandlung sowie (ii) aus Umwandlungsprozessen in der chemischen Industrie zu berechnen. Zusätzlich erfolgte eine Anpassung des NEAT-Modells, um den in Deutschland angewandten Prozessrouten Rechnung zu tragen.

Systemgrenzen des nichtenergetischen Verbrauchs in der deutschen Energiebilanz

Um die Resultate des NEAT-Modells mit offiziellen Daten vergleichen zu können, ist es wichtig, Kenntnis über die Systemgrenzen bzw. die Definition des nichtenergetischen Verbrauchs in der deutschen Energiebilanz zu haben. Im Rahmen dieses Projektes war es möglich, einen relativ detaillierten Einblick hinsichtlich Datenquellen und Methodik für die Erhebung des nichtenergetischen Verbrauchs in der Energiebilanz zu erhalten. Darüber hinaus verbleiben einzelne Unklarheiten, die im Rahmen zukünftiger Forschungsvorhaben abgeklärt werden sollten (siehe auch Kapitel 3.3).

Unsere Recherchen ergaben, dass in der deutschen Energiebilanz unterschiedliche Systemgrenzen für den nichtenergetischen Verbrauch verschiedener fossiler Energieträger verwendet werden. Für den Einsatz von Koks und anderer auf Kohle basierter Energieträger sowie für die Verwendung von Mineralölprodukten (z.B. Rohbenzin, Heizöle) wird der nichtenergetische Verbrauch als *Bruttoeinsatz* definiert; dies bedeutet, dass die Anteile an den Einsatzmengen, die (zum Beispiel beim Steamcracken von Rohbenzin) zur Erzeugung von Prozesswärme genutzt werden, in den Daten zum nichtenergetischen Verbrauch enthalten sind. Im Gegensatz dazu wird für den Erdgaseinsatz in der chemischen Industrie (z.B. zur Herstellung von Ammoniak und Methanol) eine *Nettodefinition* genutzt, wobei die Erdgasanteile, die zur Erzeugung von Prozesswärme verwendet werden, im nichtenergetischen Verbrauch *nicht* enthalten sind.

Diese Inkonsistenz liegt darin begründet, dass Organisationen, die an unterschiedlichen Stellen der Prozesskette operieren, Daten für die Arbeitsgemeinschaft Energiebilanzen bereitstellen. Informationen zur nichtenergetischen Nutzung von Kohle- und Mineralölprodukten werden zum Beispiel vom Bundesverband Braunkohle oder dem Mineralölwirtschaftsverband bereitgestellt. Beide Organisationen operieren *angebotsseitig*. Dies bedeutet, dass sie zwar Einblick in die Mengen an

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Energieträgern haben, die beispielsweise an die chemische Industrie geliefert werden, sich aber die weiteren Verwendungsstrukturen ihrer Kenntnis entziehen. Im Gegensatz dazu werden die Daten zum nichtenergetischen Verbrauch von Erdgas durch den VCI (Verband der Chemischen Industrie) an das DIW (Deutsches Institut für Wirtschaftsforschung) geliefert. Dieser Verband umfasst Firmen, die *verbrauchsseitig* operieren und daher detaillierte Angaben zum Einsatz der Erdgasmengen für bestimmte Verwendungszwecke machen können.

Eine eher indirekte Empfehlung, die aus unseren Arbeiten zum nichtenergetischen Verbrauch resultiert, wäre deshalb, die Systemgrenzen in der deutschen Energiebilanz für die unterschiedlichen Energieträger zu harmonisieren. Dazu sollte die Erstellung der Energiebilanz enger mit der Erarbeitung der Treibhausgasinventare koordiniert werden. Auf diese Weise könnte sichergestellt werden, dass die Qualität der Energiebilanz den Anforderungen genügt, die für die konsistente, genaue und vollständige Abschätzung der aus dem nichtenergetischen Verbrauch resultierenden Emissionen erforderlich ist.

Wichtige Details, wie zum Beispiel die Berechnungen zum nichtenergetischen Verbrauch von (i) Koks and anderen kohlebasierten Produkten, (ii) der Butadien- und Aromatenerzeugung in Raffinerien sowie (iii) die vielfältigen Butenströme zwischen Raffinerien und Crackanlagen, bleiben trotz aufwändiger Recherchen für dieses Forschungsvorhaben unklar und sollten im Rahmen zukünftiger Arbeiten untersucht werden.

Darüber hinaus zeigte sich, dass die deutschen Energiebilanzen im Hinblick auf die Produktion von Propylen (Propen) in Raffinerien sowie in Bezug auf den Verbrauch von Rohbenzol (Rohbenzol ist ein Produkt, das bei der Verkokung von Kohle entsteht) unvollständig sind. Für Rohbenzol wird höchstwahrscheinlich nur die Inlandsproduktion, nicht aber der Handel in die Energiebilanzdaten einbezogen. Aus diesem Grund ist die Menge an '*Anderen Steinkohleprodukten*', wie sie in der Energiebilanz für den nichtenergetischen Verbrauch ausgewiesen wird, unvollständig. Oder mit anderen Worten, die Menge an '*Anderen Steinkohle Produkten*' ist zu gering, gemessen an der Inlandsproduktion von Benzol.

Diskussion der NEAT-Ergebnisse in Bezug auf den IPCC-SA (IPCC-Sektorales Verfahren)

Mit NEAT werden Emissionen aus dem nichtenergetischen Verbrauch (ausgedrückt in CO₂-Äquivalenten) für alle relevanten Quellkategorien im IPCC-SA, d.h. für Energie, Industrieprozesse, Produktnutzung und Abfall berechnet.

Die mit NEAT berechneten Emissionen für die Produktion von Ammoniak (2,6-4,6 Mt CO₂ pro Jahr) sind deutlich höher als die IPCC-SA Berechnungen im Treibhausgasinventar des Jahres 2005 und etwas niedriger als die Werte im Inventar des Jahres 2006. Die niedrigeren NEAT Werte (verglichen mit dem 2006er Inventar) lassen sich damit erklären, dass in NEAT vergleichsweise effiziente Anlagen angenommen werden und darüber hinaus die Mengen an Kohlenstoff, die bei der Herstellung von Harnstoff eingesetzt werden, von den Prozessemissionen abgezogen werden. Im Gegensatz dazu wird im IPCC-SA (Inventar aus dem Jahr 2006) der IPCC-Standardemissionsfaktor von 1,5 kg CO₂/kg Ammoniak verwendet, welcher weder die Produktion von Harnstoff berücksichtigt noch die Emissionen aus der energetischen Nutzung von Teilen des gesamten Prozesseinsatzes von Erdgas und Schweröl beinhaltet. Im Gegensatz zum IPCC Standardemissionsfaktor folgen wir in NEAT den Systemgrenzen der Energiebilanz. Daher werden die aus der *energetischen* Nutzung von Teilen (30%) des *Erdgaseinsatzes* resultieren Emissionen aus den Prozessemissionen ausgeschlossen. Emissionen, die durch die Verwendung von *Schweröl* ebenfalls für energetische Zwecke bei der Ammoniaksynthese resultieren, sind demgegenüber im NEAT Emissionsfaktor enthalten. In diesem Zusammenhang ist es bedeutsam, dass UBA überprüft, in wieweit Emissionen aus der Ammoniakproduktion im 2006er Inventar korrekt bilanziert sind und ob

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Emissionen aus der energetischen Nutzung von Erdgas und Schweröl in der Quellkategorie 'Energie' angemessen berücksichtigt werden.

Die Emissionen, wie sie von NEAT für die Produktion von Aluminium berechnet werden (0,9-1,9 Mt CO₂ pro Jahr), sind wesentlich höher als die Werte aus dem IPCC-SA (0,7-1,0 Mt CO₂). Ein Hauptgrund für die Differenzen liegt darin, dass für die Emissionsberechnungen im IPCC-SA ein wesentlich niedriger Emissionsfaktor verwendet wird als in NEAT. Im Rahmen einer externen Inventarprüfung wurde der zu niedrige Emissionsfaktor bereits kritisiert (UNFCCC, 2005). Wir empfehlen daher, den derzeitigen IPCC-SA Emissionsfaktor noch einmal zu überprüfen und gegebenenfalls zu korrigieren.

Die NEAT-Abschätzung zu den Emissionen aus der Carbidproduktion (0,3-0,8 Mt CO₂ pro Jahr) übersteigt die Werte aus dem deutschen Treibhausgasinventar (0,0-0,4 Mt CO₂). Im Rahmen dieser Studie war es nicht möglich, die exakten Ursachen für die Differenzen zu identifizieren, da weder Aktivitäten noch Emissionsfaktoren für die Carbidherstellung im IPCC-SA gegeben sind. Ein mögliche Erklärung für die unterschiedlichen Emissionsabschätzungen könnte beispielsweise sein, dass bei den NEAT-Modellierungen über die Elektrodennutzung hinaus auch die Verwendung 'Anderer Kohleprodukte' als Reduktionsmittel für die Carbidproduktion in die Emissionsberechnungen einbezogen werden.

Neben den bisher genannten Prozessen werden im IPCC-SA aus dem Inventar des Jahres 2005 keine weiteren CO₂-Emissionen in der Quellkategorie 'Industrieprozesse' quantifiziert. Im Treibhausgasinventar aus dem Jahr 2006 werden demgegenüber auch CO₂-Emissionen für die Herstellung von Methanol, Ruß, Eisen und Stahl, Ferrolegierungen sowie aus Umwandlungsverlusten in der chemischen Industrie und dem Abbrand zum Regenerieren von Katalysatoren bilanziert. Die Kohlenstoffemissionen aus der Eisen- und Stahlerzeugung sowie aus der Regeneration von Katalysatoren ist nicht Bestandteil des nichtenergetischen Verbrauchs in der Energiebilanz und bleibt daher in den folgenden Diskussionen unberücksichtigt.

Gemessen an der physischen Produktion in Deutschland, sind die im IPCC-SA ermittelten Emissionen (aus der Oxidation von Elektroden und anderem Kohlenstoff) für die Herstellung von Ferrolegierungen zu niedrig. Die NEAT-Berechnungen ergeben Emissionen für der Herstellung von Eisenlegierungen, Nichteisen-Metallen und anderen Anorganika (ohne die Herstellung von Aluminium und Carbiden) zwischen 1,1-1,8 Mt CO₂ pro Jahr und sind damit um ein Vielfaches höher als in den Inventaren ausgewiesen. Wir empfehlen daher, die Emissionsschätzungen aus dem NEAT-Modell zu benutzen, um die Emissionsdaten im deutschen Inventar zu komplettieren.

In NEAT werden darüber hinaus auch Emissionen aus Umwandlungsverlusten in der chemischen Industrie berechnet (2,6-3,8 Mt CO₂-Äquivalente pro Jahr. Emissionen aus dieser Quelle umfassen direkte CO₂-Emissionen sowie darüber hinaus VOCs und NMVOCs (bilanziert als oxidiertes Produkt, d.h. als CO₂). UBA hat die NEAT-Werte bereits in das Inventar des Jahres 2006 integriert. Wir begrüßen diesen Schritt, der maßgeblich zur Vervollständigung der deutschen Treibhausgasinventare beiträgt, würden aber dennoch vorschlagen, Emissionen, die aus Umwandlungsverlusten resultieren, detaillierter darzustellen. Dazu könnten die NEAT Ergebnisse dieses Berichtes genutzt werden, welcher zwischen Emissionen aus der Herstellung von (i) Ethylenchlorid, (ii) Acrylnitril, (iii) Ethylenoxid sowie einer Kategorie 'andere Umwandlungsverluste' unterscheidet. Die NEAT-Emissionen aus Umwandlungsverlusten sind mit Unsicherheiten behaftet. Um diese zu verringern, empfehlen wir tieferegehende *bottom-up* Analysen.

NEAT berechnet darüber hinaus Emissionen für die Produktion von Methanol (0,8-2,2 Mt CO₂ pro Jahr) und Ruß (0,5-0,7 Mt CO₂ pro Jahr). Diese Emissionen stammen ausschließlich aus

der energetischen Nutzung der eingesetzten Energieträger. UBA nutzt diese Werte direkt für die Abschätzung von Prozessemissionen im IPCC-SA (Inventar aus dem Jahr 2006).

Emissionen, die aus dem *Steamcracken* resultieren (5,8-8,6 Mt CO₂, basierend auf NEAT-Berechnungen), werden demgegenüber nicht in der Quellkategorie '*Industrieprozesse*' im IPCC-SA aufgelistet. Diesbezüglich ist zu prüfen, ob die CO₂-Emissionen aus Steamcrackern bereits als energiebedingte Emissionen unter der Quellkategorie '*Energie*' im Inventar berücksichtigt sind.

Darüber hinaus ergeben sich Inkonsistenzen bei der Erfassung von Prozessemissionen im IPCC-SA (Inventar des Jahres 2006): Während die Emissionen aus der energetischen Nutzung von Energieträgern beim *Steamcracken* und zur Produktion von Ammoniak nicht als Prozessemissionen bilanziert sind, werden die energiebedingten Emissionen aus der Herstellung von Methanol und Ruß im IPCC-SA als Prozessemissionen betrachtet (für beide Prozesse sind die reinen Prozessemissionen aus der stofflichen Nutzung von Energieträgern null). Wir empfehlen daher, Emissionen aus der energetischen Nutzung von Energieträgern in Industrieprozessen nach einer einheitlichen Methodik zu erfassen und eine Entscheidung zu treffen, ob entweder alle Emissionen aus der energetischen Nutzung von Einsatzstoffen im IPCC-SA in der Hauptquellkategorie '*Energie*' erfasst werden sollen (in diesem Fall sollten die Emissionen aus der Herstellung von Methanol und Ruß aus der Kategorie '*Industrieprozesse*' entfernt werden und unter '*Energie*' aufgelistet werden) oder ob Emissionen konsistent mit den Systemgrenzen des nichtenergetischen Verbrauchs in der Energiebilanz zugeordnet werden sollen. In diesem Fall würden die Emissionen aus den *Steamcrackern* und aus der Produktion von Ammoniak, Methanol und Ruß, die aus dem Einsatz von kohle- und ölbasierten Energieträgern resultieren, unter der Quellkategorie '*Industrieprozesse*' erfasst und lediglich die energetisch genutzten Anteile des Erdgaseinsatzes (zur Herstellung von Ammoniak, Methanol und Ruß) der Quellkategorie '*Energie*' zugeordnet.

In den aktuellen Inventaren des Jahres 2006 werden fossile Kohlenstoffemissionen aus der Abwasserreinigung nicht berücksichtigt. Demgegenüber berechnen wir mit dem NEAT-Modell jährliche fossile Emissionen von 1,4-1,7 Mt CO₂-Äquivalenten basierend auf (i) dem chemischen Sauerstoffbedarf von Abwässern aus der chemischen Industrie sowie (ii) dem durchschnittlichen Tensidverbrauch in Deutschland. Die NEAT Werte repräsentieren überschlagsmäßige Schätzungen, die als Richtgrößen für detaillierte Abschätzungen verwendet werden können.

Im Unterschied zu den Prozessemissionen sind die NEAT-Berechnungen für die Emissionen aus der Produktnutzung mit großen Unsicherheiten behaftet. Die aus der Verwendung von Produkten resultierenden Emissionen werden mit dem NEAT-Modell auf minimal $6,9 \pm 2,7$ Mt CO₂ (im Jahr 1996) bis maximal $9,3 \pm 3,4$ Mt CO₂ (im Jahr 2000) geschätzt (vgl. 1.6-2.7 Mt CO₂-Äquivalente im IPCC-SA). Die Genauigkeit der NEAT-Berechnungen wird direkt durch die Qualität der verwendeten Produktions- und Außenhandelsdaten sowie der Richtigkeit der angenommenen Produktionsrouten bestimmt. Diese Parameter sind maßgeblich für die Ergebnisse der Massenbilanz im NEAT-Modell und damit, im Unterschied zur Berechnung von Industrieprozessemissionen (die getrennt von der Massenbilanz berechnet werden), ausschlaggebend für die Höhe der errechneten Produktnutzungsemissionen. Aus diesem Grund sind die mit NEAT berechneten Emissionen aus der Produktnutzung besonders sensitiv gegenüber Doppelzählungen in der Kohlenstoffbilanz, welche aus fehlerhaften Produktions- oder Außenhandelsdaten sowie ungenau definierten Produktkategorien resultieren können. Die Tatsache, dass NEAT in der Regel einen höheren nichtenergetischen Verbrauch (68-87 Mt CO₂) im Zeitraum von 1990 bis 1999 errechnet als im IPCC-RA (IPCC-Referenz Ansatz) angegeben wird (64-77 Mt CO₂), könnte einen Hinweis auf mögliche Doppelzählungen sein (siehe auch folgenden Absatz).

Zusammenfassung

Angesichts dieser Schwierigkeiten wurde eine *bottom-up* Berechnung zur unabhängigen Abschätzung der Produktnutzungsemissionen durchgeführt. Dabei wird zwischen (i) Lösemitteln, (ii) Pestiziden sowie (iii) festen paraffinischen Produkten als Emissionsquellen unterschieden (Emissionen für die Verwendung von Schmierstoffen als vierte Emissionsquelle können dem NEAT-Modell entnommen werden). Diese *bottom-up* Berechnung ist in verfeinerter Form Bestandteil eines deutlich vereinfachten NEAT-Modells (NEAT-SIMP), welches im Rahmen eines EU-Projektes (NEU-CO₂-III) erarbeitet wurde (siehe Anhang C).

Mit Hilfe des *bottom-up* Ansatzes errechnen sich Emissionen von 2,8-3,6 Mt CO₂-Äquivalenten pro Jahr (für einen Zeitraum am Ende der 1990er Jahre). Dieser Wert ist 60-70% niedriger als das NEAT Ergebnis für Produktnutzungsemissionen im Jahr 2000 (9,3 Mt CO₂-Äquivalente). Das Ergebnis unserer *bottom-up* Berechnung liegt damit deutlich unter den Emissionswerten, die NEAT für die Produktnutzung berechnet. Dieses Resultat erhärtet unsere Zweifel an der Genauigkeit der NEAT-Berechnungen bezüglich der Produktnutzungsemissionen. Aus diesem Grund raten wir davon ab, die NEAT Ergebnisse zur Verbesserung der Emissionsabschätzungen in der Hauptquellkategorie 'Lösemittel und andere Produktnutzung' zu verwenden. Wir empfehlen stattdessen, die Ergebnisse der unabhängigen *bottom-up* Berechnungen sowie die Daten aus dem in Anhang C näher beschriebenen NEAT-SIMP Ansatz zu verwenden, um eine detaillierte Berechnung der Emissionen aus der Produktnutzung für die einzelnen Emissionsquellen durchzuführen, wengleich dieses Vorgehen tendenziell die Gesamtemissionen unterschätzt. Für die *bottom-up* Berechnungen können die Daten von Theloke et al. (2000) und Jepsen et al. (2004) zu Lösemittlemissionen in Deutschland zusammen mit Berechnungen für die Emissionsquellen (i) Schmierstoffe, (ii) Wachse und wachshaltige Produkte sowie (iii) Pestizide kombiniert werden. Die Ergebnisse der unabhängigen *bottom-up* Berechnung (siehe Tabelle 15) sowie aus den Modulen des NEAT-SIMP Modells können diese Arbeiten unterstützen.

Diskussion der NEAT Ergebnisse in Bezug auf den IPCC-RA (IPCC-Referenz Verfahren)

Unter Berücksichtigung der Systemgrenzen, wie sie für den nichtenergetischen Verbrauch der einzelnen Energieträger in der deutschen Energiebilanz angewendet werden, **errechnet sich mit dem NEAT-Modell ein nichtenergetischer Verbrauch von 68-87 Mt CO₂-Äquivalenten pro Jahr im Zeitraum von 1990 bis 2003. Mit Ausnahme des Jahres 1990 liegen die NEAT-Werte damit um 1-12 Mt CO₂-Äquivalente über den Daten aus dem IPCC-RA (64-77 Mt CO₂-Äquivalente im Zeitraum von 1990-1999, Inventar aus dem Jahr 2005).** Wesentliche Gründe für die Unterschiede sind:

- Produktions- und Außenhandelsdaten sowie Informationen zu den Produktionsrouten in der chemischen Industrie Deutschlands sind mit Unsicherheiten behaftet. Dies könnte eine geringfügige Überschätzung des nichtenergetischen Verbrauchs im NEAT-Modell zur Folge haben.
- Die Daten zur Produktion von Buten sind mit Unsicherheiten behaftet. Darüber hinaus bleibt unklar, welche Anteile der Gesamtproduktion stofflich und welche energetisch, d.h. als Kraftstoffadditiv genutzt werden. Diese Unsicherheiten könnten eine Überschätzung des nichtenergetischen Verbrauchs in NEAT zur Folge haben.
- NEAT bezieht auch die Anteile von Erdgas in den nichtenergetischen Verbrauch mit ein, die zur Herstellung von Ruß eingesetzt werden (im Untersuchungszeitraum etwa 0,2 Mt CO₂-Äquivalente pro Jahr). Diese Mengen sind in den IPCC-RA Daten nicht enthalten.
- Der Verbrauch von 'Koks und anderen kohlebasierten Produkten' zur Herstellung von Nichteisenmetallen und Eisenlegierungen (1,1-1,8 Mt CO₂) wird bei den NEAT-

Zusammenfassung

Modellierungen dem nichtenergetischen Verbrauch zugerechnet. Trotz intensiver Expertenkontakte (DIW, 2005) konnte im Rahmen dieses Forschungsvorhabens nicht geklärt werden, ob diese Mengen auch in den Daten der Energiebilanz (bzw. des IPCC-RA) beinhaltet sind.

- Die Daten zum nichtenergetischen Verbrauch aus der Energiebilanz umfassen nicht die in Raffinerien erzeugten Mengen an Propylen (Propen). Dies führt zu einer deutlichen Unterschätzung des nichtenergetischen Verbrauchs von etwa 1,9 Mt CO₂-Äquivalenten pro Jahr. Darüber hinaus ist es wahrscheinlich, dass auch die Mengen an Aromaten und Butadien, die in Raffinerien erzeugt werden und einer stofflichen Verwendung zufließen, nicht als nichtenergetischer Verbrauch in der Energiebilanz berücksichtigt werden.
- Der nichtenergetische Verbrauch von *‘Koks und anderen Kohleprodukte’* beinhaltet unter anderem die Produktion und den Handel von Rohteer, allerdings nicht den Handel von Rohteer-Folgeprodukten, wie zum Beispiel Rohbenzol oder Pech. Wie bereits angedeutet, hat dies zur Folge, dass die Mengen an *‘Koks und anderen Kohleprodukten’*, die als nichtenergetischer Verbrauch in der Energiebilanz aufgeführt werden, für die Produktion von Benzol nicht ausreichen. Aus diesem Grund erachten wir die Mengen an *‘Koks und anderen Kohleprodukten’*, die in der Energiebilanz dem nichtenergetischen Verbrauch zugeordnet werden, als unvollständig.

Zusammenfassend stellen wir fest, dass die Energiebilanz (und folglich auch der IPCC-RA) den nichtenergetischen Verbrauch fossiler Energieträger in Deutschland mit hoher Wahrscheinlichkeit unterschätzen.

Außer dem soeben diskutierten Gesamteinsatz an nichtenergetisch genutzten fossilen Energieträgern berechnet NEAT auch die Mengen an Kohlenstoff, die pro Jahr in Produkten gespeichert werden und demzufolge nicht emissionsrelevant sind. Die Ergebnisse der NEAT-Berechnungen liegen diesbezüglich mit 40-54 Mt CO₂-Äquivalenten pro Jahr unter den Werten aus dem IPCC-RA (46-56 Mt CO₂-Äquivalente). Die auf dieser Grundlage mit NEAT berechneten Emissionen (27-34 Mt CO₂-Äquivalente) sind wesentlich höher als die Werte des IPCC-RA (14-22 Mt CO₂-Äquivalente). Wesentliche Gründe für die Unterschiede sind (i) der höhere nichtenergetische Verbrauch gemäß NEAT sowie (ii) inkompatible, weil auf unterschiedlichen Systemgrenzen beruhende, Korrekturfaktoren zur Kohlenstoffspeicherung (*‘carbon storage fractions’*). Der durchschnittliche NEAT-Korrekturfaktor für den Zeitraum 1990-2003 beträgt 61%. Demgegenüber werden im IPCC-RA durchschnittliche Korrekturfaktoren von 74% (im Zeitraum von 1990-1999, Inventar aus dem Jahr 2005) verwendet. Diese Unterschiede können durch systematische Abweichungen bei den Berechnungsmethoden der NEAT- und IPCC-RA-Korrekturfaktoren erklärt werden. **Während die IPCC-RA Korrekturfaktoren für die Kohlenstoffspeicherung lediglich Emissionen aus der energetischen Nutzung von Teilen der in der Kategorie nichtenergetischer Verbrauch zusammengefassten Energieträger berücksichtigen, werden die NEAT-Korrekturfaktoren in Anlehnung an die Systemgrenzen des nichtenergetischen Verbrauchs in der Energiebilanz berechnet (siehe Tabelle 45). NEAT berücksichtigt daher auch Emissionen aus der Produktnutzung sowie aus der stofflichen Verwertung von Energieträgern in industriellen Prozessen, so zum Beispiel bei der Ammoniaksynthese.**

Nichtsdestotrotz dürfen die mit NEAT berechneten Korrekturfaktoren nicht ohne weiteres im IPCC-RA genutzt werden, da der nichtenergetische Verbrauch (welcher zur Berechnung der Korrekturfaktoren in NEAT verwendet wird) von den Werten aus dem IPCC-RA abweicht. Um sicherzustellen, dass die Emissionen aus dem nichtenergetischen Verbrauch im IPCC-RA korrekt und konsistent mit den Systemgrenzen der Energiebilanzen berechnet werden,

empfehlen wir, die brennstoffspezifischen Mengen des gespeicherten Kohlenstoffs, wie sie mit NEAT berechnet werden, vom nichtenergetischen Verbrauch aus dem IPCC-RA abzuziehen, um auf diese Weise die Gesamtemissionen aus dem nichtenergetischen Verbrauch zu berechnen sowie konsistente Korrekturfaktoren für den gespeicherten Kohlenstoff (carbon storage fractions) für den IPCC-RA abzuleiten.

Schlussfolgerungen

Basierend auf den Ergebnissen unserer Modellierungen schließen wir, dass eine Stoff- und Materialflussanalyse, wie sie mit NEAT durchgeführt wurde, detaillierte Einblicke in die Struktur des nichtenergetischen Verbrauchs in Deutschland liefert. NEAT berechnet nicht nur die Höhe des nichtenergetischen Verbrauchs fossiler Energieträger, sondern auch im Detail die daraus resultierenden Emissionen. Die Ergebnisse dieses Projektes haben gezeigt, dass NEAT ein geeignetes Instrument ist, um die Qualität von Emissionsdaten zum nichtenergetischen Verbrauch in den offiziellen deutschen Treibhausgasinventaren zu überprüfen und zu verbessern. Auf den NEAT-Analysen basierend, hat das Umweltbundesamt im vergangenen Jahr große Anstrengungen unternommen und wesentliche Unsicherheiten bezüglich der wichtigsten Industrieprozessemissionen (z.B. Emissionen aus der Herstellung von Methanol und Ruß sowie Umwandlungsverluste), wie sie in den Jahre vor 2006 bestanden, im aktuellen Inventar korrigiert. Die Autoren begrüßen diese Anstrengungen des Umweltbundesamtes und empfehlen, auch zur Klärung derzeit noch bestehender Unsicherheiten (z.B. Emissionen aus Steamcrackern sowie bei der Herstellung von Ammoniak, Eisenlegierungen und Nichteisenmetallen) die Ergebnisse der NEAT-Modellierungen zu berücksichtigen. Auf diese Weise kann das Umweltbundesamt mit Hilfe der Ergebnisse aus diesem Forschungsvorschaben die derzeitig relativ gute Qualität der deutschen Treibhausgasinventare noch weiter verbessern.

Ein wesentlicher Nachteil des detaillierten NEAT-Modells ist es, dass in erheblichem Umfang Produktions- und Außenhandelsdaten sowie ein detaillierter Einblick in die Struktur der chemischen Industrie erforderlich ist. **Der zeit- und datenaufwändigste Teil der Modellberechnungen ist dabei das Erstellen einer geschlossenen Massenbilanz, welche ein zentraler Bestandteil der detaillierten NEAT-Modellierung ist. Dabei ist dieser Teil des NEAT-Modells zugleich auch der am meisten mit Unsicherheiten behaftetste.** Im Gegensatz dazu erfordert die Berechnung von industriellen Prozessemissionen wesentlich weniger Daten und generiert zuverlässige Ergebnisse. **Basierend auf diesen Erkenntnissen wurde ein vereinfachter NEAT-Modellansatz entwickelt (NEAT-SIMP, vgl. auch Anhang C), der ohne die aufwändige Massenbilanzierung auskommt. Die Ergebnisse aus den Berechnungen mit NEAT-SIMP können zukünftig zur Inventarverbesserung genutzt werden. Mit Ausnahme der Produktnutzungsemissionen, können wir darüber hinaus auch das detaillierte NEAT-Modell für die Fortschreibung der Inventare empfehlen.** Die Anwendung des Modells für die Folgejahre sollte weniger zeitaufwändig sein, da bereits wesentliche Informationen zu den Systemgrenzen des nichtenergetischen Verbrauchs in der Energiebilanz sowie zur Struktur der chemischen Industrie in Deutschland vorhanden sind.

Bereits in der gegenwärtigen Version geht die Qualität der Erfassung von CO₂-Emissionen aus dem nichtenergetischen Verbrauch im deutschen Emissionsinventar deutlich über das Niveau praktisch aller anderen Industrieländer hinaus. Dennoch empfehlen wir weitere Verbesserungen. Letztendlich gehen wir davon aus, dass mit Hilfe dieser Studie auch die wichtigsten Defizite und Unklarheiten, wie sie nach den Inventaranpassungen aus dem Jahr 2006 noch teilweise hinsichtlich der Erfassung von Emissionen aus dem nichtenergetischen Verbrauch bestehen, behoben werden können.

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Carbon emissions resulting from the non-energy use of fossil fuel are generally considered as uncertain part in the National GHG Inventories. To get a more detailed insight into this source of emissions the NEAT model (NEAT is an abbreviation for Non-energy Use Emissions Accounting Tables) was developed. NEAT calculates non-energy use of fossil fuels and related CO₂ emissions (nearly completely) independently from official energy statistics, based on a *bottom-up* material flow and carbon balance approach. For this study, an extended version of the NEAT model (NEAT 3.0) was developed and is applied to Germany for the period 1990-2003.

We used production and trade data for more than 90 chemical products, non-ferrous metals, ferroalloys and other inorganics as well as detailed information on chemical production routes were as core data inputs for the NEAT model. Two additional modules were implemented in NEAT in the context of this study in order to estimate emissions (i) from waste treatment and (ii) from chemical conversion losses. Moreover, several other adaptations were made (primarily in order to account for chemical production routes that are specific for Germany).

Systemboundaries of non-energy use in the German Energy Balances

Before calculating non-energy use and related CO₂ emissions, we investigated the exact definition of non-energy use in the German Energy Balance. Identifying the system boundaries of non-energy use is of crucial importance to ensure comparability between NEAT results and data as stated in the German GHG Inventory. Within the scope this study, it was possible to get a relatively detailed overview of the data sources and procedures used to calculate the non-energy use of fossil fuels in the Energy Balance. Uncertainties and open questions, however, remain and should be addressed by future research (for details see Section 3.3).

We found that the Energy Balance in Germany does not follow a consistent approach regarding the definition of non-energy use for all fossil fuels. In the case of coal/lignite and oil derived feedstocks, a *gross* definition of non-energy use is applied, thereby including the amounts of feedstock used for energy, i.e., fuel purposes. In contrast, a *net* definition of non-energy use is applied for natural gas, thereby excluding the fractions of natural gas used as fuel (e.g., in ammonia production) from the non-energy use.

The inconsistent definition of non-energy use is most likely caused by the fact that non-energy use data are delivered from companies, associations, and organizations operating at different stages of the process chain. While the ‘Working Group Energy Balances’ (Arbeitsgemeinschaft Energiebilanzen), which is in charge of preparation of the energy balance, obtains the non-energy use data of coal/lignite and oil based fuels from fuel *suppliers* (e.g., Mineralölwirtschaftsverband, Bundesverband Braunkohle), non-energy use data for natural gas are obtained from fuel *consumers*, i.e., the VCI (Verband der Chemischen Industrie). The latter have detailed insight into the consumption structure of feedstock. They can therefore provide detailed information on the *consumption* of natural gas used as chemical feedstock. The providers of non-energy data for coal/lignite and oil derived feedstocks lack this detailed knowledge. They can therefore only report the amounts of fossil fuels delivered to their customers without knowing the exact consumption pattern of fuels at the customers’ side.

Given this difference in definitions across the various types of fuels we therefore recommend supporting the harmonization of system boundaries for non-energy use. To this end, the process of preparing both the National GHG Inventory and the National Energy Balance

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should be closely related to each other. This would ensure that the Energy Balance better serves the needs of inventory makers who strive to prepare consistent, complete and accurate emission estimates for the non-energy use of fossil fuels.

Important details regarding non-energy use in the Energy Balance, such as accounting of (i) coke and other coal products, (ii) refinery butadiene and aromatics, and (iii) the various butene streams from refineries and steam crackers still remain unclear and deserve special attention in the future.

We further found that the energy balance is incomplete with respect to the production of refinery propylene and the consumption of crude benzene (crude benzene is a coal-derived product originating from coke making). For the latter, only domestic production seems to be accounted for, while trade is most likely neglected. For this reason, the final demand of '*other coal products*' as reported in the German Energy Balance is incomplete. Consequently, coal-derived feedstock reported in the Energy Balance is not sufficient to satisfy the requirements for benzene production in Germany.

NEAT and the IPCC-SA

The NEAT model calculates emissions for all IPCC-SA source categories that are relevant for non-energy use, i.e., *energy, industrial processes, product use, and waste*.

NEAT emission estimates for ammonia production (2.6-4.6 Mt CO₂ per year) are clearly above the IPCC-SA estimates (2005 submission) and slightly lower than the improved IPCC-SA estimates as given in the 2006 inventory submission. The lower NEAT values result from the fact that NEAT generates conservative estimates by assuming efficient plants and because NEAT accounts for the amount of carbon sequestered for urea production. In contrast the IPCC-SA uses the IPCC default emission factor, which does not account for urea production. It is furthermore important that the IPCC default value excludes all emissions resulting from the fuel use of parts of the feedstock, while NEAT follows the system boundaries of the Energy Balance and only excludes the fractions of natural gas used for fuel purposes while including the shares of heavy oil feedstock used for fuel purposes. Inventory makers should therefore check whether the inventory (2006 submission) correctly accounts for the fuel use emissions from ammonia production under the source category '*energy*'.

Emissions from aluminum production (0.9-1.9 Mt CO₂ per year) as calculated with NEAT clearly exceed estimates stated in the IPCC-SA (0.7-1.0 Mt CO₂). The main reasons for the deviations are different emissions factors, i.e., the emission factors used in the IPCC-SA are much lower than the ones used in NEAT. The problem of emission factors, which might be too low in the IPCC-SA, was also addressed during the in-country review of the German GHG Inventory (UNFCCC, 2005). We therefore recommend UBA to clarify and re-check the emission factors and to adapt them, if necessary.

Also NEAT emission estimates for carbides are higher (0.3-0.8 Mt CO₂ per year) than the ones stated in the IPCC-SA (0.0-0.4 Mt CO₂). It is not possible to identify the exact reason for this deviation because neither activity rates nor emission factors are given in the IPCC-SA. One possible explanation could, however, be that NEAT includes also '*other solid carbon*' sources (e.g., cokes and coal, next to electrodes consumed for carbide production), which might not be included in the IPCC-SA.

Apart from this, no emissions related to non-energy use are stated under the category '*industrial processes*' of the IPCC-SA (2005 inventory submission). In the 2006 submission, however, also emissions from the production of methanol, carbon black, iron and steel, and ferroalloys as well as chemical conversion losses and catalyst burning (i.e., regeneration) are stated. Iron and steel production as well as the regeneration of catalysts are not part of non-energy use in the National Energy Balances and are therefore not further discussed.

With respect to ferroalloy production, we argue that the values stated in the IPCC-SA are by far too low given the fact that we calculate in NEAT estimates for ferroalloy and other inorganics production (excluding the production of aluminum and carbides) of 1.1-1.8 Mt CO₂ per year. The NEAT results could therefore be used to improve the completeness of emission estimates in the IPCC-SA for this source category.

NEAT calculates chemical conversion losses, i.e., losses, off-gases and unspecified by-products to range between 2.6-3.8 Mt CO₂ equivalents per year. These emissions consists only partly of CO₂, while they may also contain the CO₂ equivalents of VOCs such as methane and NMVOCs. We support the decision of UBA to include these emissions in the IPCC-SA (2006 submission). However, we would recommend (i) presenting the estimates at a more disaggregated level, i.e., stating emissions from ethylene chlorine, acrylonitrile, and ethylene oxide production and remaining conversion losses. It is important to note that conversion losses as calculated with NEAT are subject to uncertainties and require more detailed bottom-up analysis.

With respect to emissions from methanol (0.8-2.2 Mt CO₂ per year) and carbon black production (0.5-0.7 Mt CO₂ per year), UBA adapted the IPCC-SA by using NEAT estimates to account for emissions from these processes under the category of *'industrial processes'*.

Emissions from steam cracking as they are calculated in NEAT (5.8-8.6 Mt CO₂ per year) are excluded from the industrial process section. It is therefore important to check whether these emissions are already included under the source category *'energy'* of the German GHG inventory.

Regarding the accounting of industrial process emissions, we furthermore identified inconsistencies in the IPCC-SA (2006 submission): While UBA excludes emissions resulting from the fuel use of feedstocks in steam crackers and for ammonia production, fuel use emissions are reported for methanol and carbon black production (for both processes pure feedstock use emissions are zero). UBA is therefore recommended to decide, whether all emissions resulting from fuel use of feedstocks should be uniformly allocated to the category *'energy'* (then also emissions from the production of methanol and carbon-black should be excluded from the *'industrial process'* section) or whether emissions should be reported according to the system boundaries of non-energy use in the German Energy Balance. In this case emissions from steam cracking as well as from ammonia, methanol, and carbon-black production should generally be stated under the category *'industrial processes'* and only the parts of natural gas feedstock used as fuel for ammonia, methanol, and carbon-black production have to be reported under *'energy'*.

The IPCC-SA does not account for fossil based emissions from wastewater treatment. The CO₂ emissions as calculated with NEAT (1.4-1.7 Mt CO₂) are rough estimates based on (i) the chemical oxygen demand in wastewaters from the chemical industry and (ii) the average surfactant consumption in Germany. The values, therefore, serve only as benchmark values for further, more detailed analysis.

A particularly difficult issue is the estimation of yearly product use emissions (ODU emissions), which have been calculated with NEAT to range between 6.9 ± 2.7 Mt CO₂ (in 1996) and 9.3 ± 3.4 Mt CO₂ (in 2000). The accuracy of the calculation of product use emissions in NEAT depends directly (i) on the quality of input data (from production and trade statistics) and (ii) on the correctness of production routes, while this is the case to a lesser extent for the emissions discussed above (source categories *'industrial processes'* and *'waste'*). Product use emissions as calculated in NEAT are particularly sensitive to possible double counting as a consequence of erroneous production data or widely defined product categories. The fact that NEAT also estimates a higher total non-energy use than stated in the IPCC-RA (68-87 Mt CO₂ versus 64-77 Mt CO₂ in the period 1990-1999, see text

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section below) is an indication that this might be the case. To check NEAT results for ODU emissions, *bottom-up* estimates for emissions from product use were calculated independently from NEAT. Thereby we account for the use of (i) solvents, (ii) pesticides, and (iii) solid paraffinic products (emission estimates for the fourth source category of product use emissions, i.e., lubricants can be obtained from the NEAT model calculations). This *bottom-up* calculation procedure (with some modifications) is part of a simplified version of the NEAT model (NEAT-SIMP), which we developed in the context of an EU-funded project (NEU-CO₂-III).

Applying the rough *bottom-up* approach leads to values of 2.8-3.6 Mt CO₂ per year (in the end of the 1990s), which is 60-70% smaller than the average NEAT estimate (9.3 Mt CO₂) for the year 2000. The product use emissions resulting from our bottom-up estimation are hence clearly below the NEAT estimates (slightly below the lower error range of NEAT estimates), which might also be partly explained by underestimating of emissions, caused by incomplete coverage of source categories. This substantiates the doubts about the reliability of NEAT estimates on product use emissions. Given the uncertainties with NEAT results, we cannot recommend using the NEAT product use emissions as direct input for the IPCC-SA. We recommend using the insight gained from the NEAT model and from the independent *bottom-up* calculations to develop more detailed (and hence more reliable) *bottom-up* estimates for product use emissions. To this end, UBA could use estimates for solvent use (Theloke et al., 2000, Jepsen et al., 2004) and add own estimates for the most prominent sources of product use emissions such as the consumption of (i) lubricants, (ii) waxes and paraffins, and (iii) pesticides. The model tool, which is delivered as part of the NEAT simplified approach (NEAT-SIMP), can assist this bottom-up estimating of product use emission.

NEAT and the IPCC-RA

Using the same system boundaries (as far as identifiable in this study) as the Energy Balance, NEAT calculates a total non-energy use of 68-87 Mt CO₂ equivalents per year in the period of 1990-2003. Except for the year 1990, the NEAT values are 1-12 Mt CO₂ equivalents higher than non-energy use according to the IPCC-RA (64-77 Mt CO₂ equivalents in the period of 1990-1999, 2005 inventory submission). The main reasons identified for this difference are:

- Production and trade data as well as information on chemical production routes are subject to uncertainties. This might result in a slight overestimation of non-energy use in the NEAT model.
- In particular, reporting of butene production in official production statistics and its unknown split regarding feedstock versus fuel use (as gasoline component) might result in a slight overestimation of non-energy use in NEAT.
- NEAT includes parts of the natural gas used as feedstock for carbon black production (roughly 0.2 Mt CO₂ equivalents per year) under non-energy use, whereas these amounts are excluded from non-energy use in the Energy Balance.
- The consumption of 'other cokes and coals' for the production of non-ferrous metals and ferroalloys (1.1-1.8 Mt CO₂ equivalents) is included in NEAT under non-energy use. It remains, however, unclear whether this is also the case in the Energy Balance.
- The non-energy use reported in the Energy Balance does not include refinery propylene although it is used as feedstock for chemical conversion processes. Already the omission of refinery propylene results in clear underreporting (roughly 1.9 Mt CO₂ equivalents) of non-energy use in the Energy Balance. Furthermore, it is questionable whether refinery aromatics and butadiene used for non-energy purposes are included under non-energy use in the Energy Balance.

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- The non-energy use of ‘*other coal products*’ includes (among other products) the production and trade of raw tars but not the trade of further downstream feedstocks produced from raw tar such as crude benzene or pitch. The amounts of chemical feedstock derived from raw tar and used for chemicals production (e.g., production of benzene) in Germany are therefore incomplete in the Energy Balance.

Given these findings, we conclude that the German Energy Balance and the current IPCC-RA underestimate non-energy use in Germany.

Carbon Storage as calculated with NEAT amounts to 40-54 Mt CO₂ equivalents per year and is considerably lower than carbon storage as stated in the IPCC-RA (46-56 Mt CO₂ equivalents). Consequently, emissions from non-energy use as calculated with NEAT (27-34 Mt CO₂) are considerably higher than the ones stated in the IPCC-RA (14-22 Mt CO₂). The reasons for this difference are (i) different estimates of total non-energy use and (ii) different carbon storage fractions as calculated with NEAT and as used in the IPCC-RA. The mean fraction of carbon stored as calculated with NEAT in the period 1990-2003 is 61%, whereas the average IPCC-RA storage fraction amounts to roughly 74% (period of 1990-1999, 2005 inventory submission). This deviation can be explained by systematic differences in the calculation of carbon storage fractions. **While the IPCC-RA storage fractions (calculated by Prognos (2000)) mainly account for emissions from the fuel use of hydrocarbons reported under non-energy use in the Energy Balance (i.e., emissions from pure feedstock use in industrial processes as well as NMVOC emissions from product use are treated as storage), the NEAT storage fractions are consistent with the definition of non-energy use in the Energy Balance and take also industrial process and product use emissions into account.**

The NEAT carbon storage fractions should not be used in the current IPCC-RA because total non-energy use as calculated with NEAT and as given in the IPCC-RA (which are used for calculating carbon storage fractions) differ from each other. To assure consistent accounting of non-energy use emissions in the IPCC-RA with the system boundaries in the National Energy Balances, we recommend using the fuel specific carbon storage as calculated with NEAT and subtracting it from the total non-energy use as stated in the IPCC-SA. This way, not only non-energy use emissions but also carbon storage fractions for use in the IPCC-RA can be calculated.

Final Conclusions

We finally conclude that a material flow analysis like the NEAT model is very useful in order to obtain a detailed insight in the structure of non-energy use in Germany. NEAT calculates the total non-energy use and related CO₂ emissions and provides furthermore an important consistency check for reported values on non-energy use in energy statistics. NEAT results proved to be useful in identifying errors and inconsistencies in both, the National Energy Balance (NEB) and the National GHG Inventory. Based on the NEAT calculations, the Germany Environmental Agency already corrected emission estimates for the production of methanol and carbon black in the current 2006 GHG inventory. These efforts are recognized by the authors. We recommend to use NEAT model results also for clarifying and correcting the remaining uncertainties in the 2006 inventory regarding, e.g., emissions (i) from steam cracking and (ii) from the production of ammonia, non-ferrous metals, ferroalloys, and inorganics. This way, the German Environmental Agency would be able to improve the already good quality of the German GHG inventory even further.

The requirement of considerable amounts of data and detailed insight in the German chemical industry remains a major drawback with respect to the applicability of the detailed NEAT model. It should be pointed out that by far the most time-consuming part of the NEAT model, requiring most of the data inputs, is the carbon mass balance, resulting in an estimate for product related emissions (ODU

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emissions). At the same time, the biggest uncertainty is related to this part. **To estimate industrial process emissions much less input data are required while nevertheless yielding reliable results. Baed on these insights a simplified NEAT model was developed (NEAT-SIMP, see also Appendix C), which does not include a complete mass balance. The results of the NEAT-SIMP model can be used for future improvements of the German GHG inventory. With the exception of product use emissions, we can also recommend using the detailed NEAT for updating data on non-energy use and related CO₂ emissions also for the years beyond 2003.** The application of NEAT for these years should be less time demanding because background information on the system boundaries of non-energy use in the German National Energy Balances as well as data on chemical production routes are already known from this research study.

Already in its current form, the quality of the German GHG inventory of CO₂ emissions from non-energy use goes beyond that of practically all other industrialized countries. Nevertheless we recommend further improvements. By implementing the recommendations given in this report most of the shortcomings related to non-energy use that were identified in this report and by the in-country review and which are not dealt with yet in the adapted 2006 inventory (UNFCCC, 2005) can be addresses in a satisfactory manner.

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Abbreviations and Units

a	-	year
ABS	-	Acrylonitrile B utadiene S tylene
BAFA	-	B undesamt für Wirtschaft und A usfuhrkontrolle
BMU	-	B undes <u>u</u> mwelt m inisterium
BREF	-	B est Available Technique R eference Document
C	-	C arbon
C ₄	-	organic molecules containing four carbon atoms
CFCs	-	C hloro f luoro c arbons
CH ₄	-	Methane
CO	-	Carbon monoxide
CO ₂	-	Carbon dioxide
COD	-	C hemical O xygen D emand
cont.	-	c ontinued
CRF	-	C ommon R eporting F ormat
EB	-	E nergy B alance
EF	-	E mission F actor
e.g.	-	exempli gratia (Latin, ‘for example’)
equ.	-	e quivalents
EU	-	E uropean U nion
e.V.	-	eingetragener V erein
excl.	-	e xclusive
GHG	-	G reenhouse G as
GJ	-	G iga J oule
GP	-	G üterverzeichnis für P roduktionsstatistiken
kJ	-	K ilojoule
kt	-	K ilotonne
i.e.	-	id est (Latin, ‘this means’)
IEA	-	I nternational E nergy A gency
IPCC	-	I ntergovernmental P anel on C limate C hange
IPCC-RA	-	I PCC- R eference A pproach
IPCC-SA	-	I PCC- S ectoral A pproach
l	-	L iter
LPG	-	L iquefied P etroleum G as
Max.	-	M aximum
mg	-	M illigramme
Min.	-	M inimum
Mt	-	M egatonne
m-xylene	-	m etha-xylene
NEAT	-	N on- E nergy use E mission A ccounting T ables
NEAT-SIMP	-	NEAT-S implified A pproach
NEB	-	N ational E nergy B alance
NEC	-	N et E nergy C onsumption
N ₂ O	-	N itrogen O xide
NGL	-	N atural G as L iquids

Abbreviation and Units

NMVOC	-	N on- m ethane volatile o rganic compound
NODU	-	N ot O xidized D uring U se
ODU	-	O xidized D uring U se
o-xylene	-	o rtho-xylene
%mas.	-	M ass Percentage
PE	-	P olyethylene
PET	-	P olyethylene therephthalate
PP	-	P olypropylene
ppm	-	p arts p er m illion
PS	-	P olystyrene
PUR	-	P olyurethane
PVA	-	P olyvinylacetate
PVC	-	P olyvinylchloride
p-xylene	-	p ara-xylene
TOC	-	T otal O rganic C arbon
UNFCCC	-	U nited N ation F ramework C onvention on C limate C hange
TJ	-	T errajoule
TPES	-	T otal P rimary E nergy S upply
UNFCCC	-	U nited N ations F ramework C onvention on C limate C hange
unsat.	-	unsaturated
VCI	-	V erband der C hemischen I ndustrie e.V. (Association of the Chemical Industry in Germany)
VCM	-	V inyl C hloride M onomer

1 Introduction

In the context of greenhouse gas (GHG) inventories, most attention is paid to anthropogenic CO₂ emissions originating from fossil fuel combustion. However, around 7.3% of the *total primary energy supply* (TPES) and 10.3% of the *final energy consumption* in Germany (in the year 2003) is not consumed for energy production but used for non-energy purposes. This is clearly above EU-19 average in the same year, where non-energy use represents 6.0% of total primary energy supply and 8.6% of final energy consumption (IEA, 2005a).

Non-energy use is defined as the sum of two parts:

- **The consumption of fossil fuels as *feedstock* in the chemical industry (e.g., the use of naphtha for the production of olefins or the consumption of natural gas for ammonia production)**
- **The consumption of the *non-energy use refinery and coke oven products* (e.g., consumption of lubricants and bitumen as well as the use of solid carbon for the production of non-ferrous metals and ferroalloys)**

Non-energy use is expected to grow in industrialized countries due to the increased use of polymers and other organic chemicals. Moreover, the *relative* importance of non-energy use is likely to increase, if countries successfully limit the rate of fossil fuel use for energy purposes.

The non-energy use of fossil fuels represents therefore an important source of CO₂ emissions because parts of the carbon are oxidized and emitted during the production and use phase of chemical and petrochemical products. To neglect non-energy use in official Greenhouse Gas Inventories can therefore easily lead to an underestimation of the total national CO₂ emissions by 1-2% in the IPCC Reference Approach (Patel et al., 2003). However, estimating non-energy use and related CO₂ emissions is not straightforward but complicated by the complexity and inter-linkages of energy and material flows in the chemical and petrochemical industry. The uncertainties related to emissions from non-energy use are therefore exceptionally high.

Against this background, the German Federal Environmental Agency (Umweltbundesamt – UBA) has chosen non-energy use as one of the key issues to be addressed in detail as part of their national emission inventory system NaSE (Nationales System Emissionen). This decision was driven not only by the general need for preparing complete, accurate, transparent, consistent and internationally comparable GHG emission inventories but also by additional and more specific reporting requirements set by the Executive Body of UN ECE Convention on Air Pollution Control (Luftreinhaltekonvention). As part of these requirements, the accuracy and the quality of emission data as well as underlying data used for estimation purposes must be reported for a total of 40 pollutants/groups of pollutants.

In order to improve the accuracy of German GHG inventories, UBA has commissioned Utrecht University to analyze in detail emissions resulting from the non-energy use of fossil fuels in Germany.

As part of the research contract, we contributed to a workshop on the national GHG inventory (Nationales System Emissionen) held on 8-9 November 2004 in Berlin. We showed that there is a major gap between the IPCC Reference Approach (IPCC-RA) and the IPCC Sectoral Approach (IPCC-SA) regarding non-energy use emission estimates (these methods are explained in Chapter 3.3).

Introduction

While the IPCC-SA, which is referred to as the ‘National Approach’ in the German GHG inventory, accounts only for around 2.6 Mt CO₂, the IPCC-RA implies 21.5 Mt CO₂ emissions from the non-energy use of fossil fuels (year 1999, based on the 2004 inventory submission (UNFCCC, 2004)). According to the preliminary analyses presented in Berlin it is very likely that the ‘National Approach’ as applied in Germany is incomplete (e.g., CO₂ emissions from the production of methanol, carbon black and olefins as well as emissions from product use are not taken into account¹). However, the decision about which source categories should be included in the ‘National Approach’ is partly determined by the system boundaries of non-energy use in energy statistics (AGE, 1990-1999). At the outset of this study, these are unclear, i.e., it is uncertain whether non-energy use data in energy statistics include or exclude fuel use for industrial processes (e.g., steam cracking and ammonia production).

This report is structured as follows: After the introduction and a short description of the report’s objective (Chapter 2), we give some background information on (i) the non-energy use of fossil fuels, (ii) the emissions reporting according to the German Greenhouse Gas Emissions Inventory, and (iii) the German Energy Balance as the main source of activity data for the energy as well as non-energy use of energy carriers in Germany (Chapter 3). We then describe the methodology of the applied NEAT (Non-energy Use Emissions Accounting Tables) model in Chapter 4. In the fifth Chapter, we present model results and compare them with official data from the National Greenhouse Gas Inventory and the German Energy Balance. Finally, we discuss the outcome of this research study with respect to sensitivity, uncertainties as well as further research requirements and we give recommendation on how to improve estimates of non-energy use and related emissions in the Greenhouse Gas Emissions Inventory of Germany (Chapter 6).

¹ Product use emissions are given in NMVOC equivalents but they are not included in the estimates of total non-energy use CO₂ emissions in the NIR (UBA, 2004a)

2 Objective

The objective of this study is to estimate non-energy use and resulting emissions in Germany for the period of 1990 to 2003 in order to improve the accuracy and reliability of the German Greenhouse Gas Inventory.

To meet this goal, we apply an improved version of the NEAT model, thereby adapting it to the specific situation in Germany. The model thereby allows crosschecking of official inventory data and, if necessary, the closing of gaps and inconsistencies between the 'National Approach' (i.e., the IPCC-SA) and the IPCC-RA in the current National GHG Inventory.

With NEAT we not only aim at calculating total non-energy use and resulting CO₂ emissions but also carbon storage and fuel-specific carbon storage fractions.

Another objective of this study is to study uncertainties related to both, NEAT model results and inventory data in order to assess the accuracy of the current emission accounting methods. Based on the experience gained regarding data availability and in view of uncertainties related to the generated NEAT results, recommendations will finally be made on how to improve estimates of CO₂ emissions from non-energy use in the German GHG inventory. Special attention will be paid to (i) completeness of emission estimates, (ii) improvement of default emission factors for the various industrial process emissions (e.g., ammonia, methanol or carbon black production) and (iii) the consistency of system boundaries for non-energy use. Next to the NEAT model we will also provide a simplified model version (NEAT-SIMP) for updating non-energy use emission estimates in future years.

It must be emphasized that the focus of this study is on CO₂ emissions from the non-energy use of fossil fuels. CO₂ emissions from the direct fuel combustion for energy production are therefore only of indirect interest. The scope of this analysis is hence limited to the chemical and petrochemical sector, excluding fuel products from refineries. We also exclude the use of carbon-feedstock in pig iron production, which is not reported as part of non-energy use in German energy statistics. In contrast, the use of electrodes for aluminum production is included in this study and so is the use of electrodes and other carbon sources used for the manufacture of other non-ferrous metals and in-organics such as ferroalloys and phosphorus.

This study makes use of the new insight gained during the third phase of the EU-funded network on 'Non-energy use and CO₂-emissions' (NEU-CO₂-III), which is coordinated by Utrecht University and runs from September 2004 until August 2006 (Patel et al., 2005/2006). Moreover, it accounts not only for the current 1996 IPCC GHG inventory guidelines but also for the changes made in the revised 2006 IPCC guidelines for National GHG Inventories (IPCC, 2006) in which Utrecht University is actively involved (Neelis, 2005).

3 Background Information

This chapter contains:

- **An introduction to the non-energy use and its relevance for emissions accounting**
- **A description of IPCC-RA and IPCC-SA in the German GHG Inventory and a discussion of major shortcomings regarding the accounting of non-energy use emissions**
- **An introduction to the German Energy Balance and the system boundaries chosen for non-energy use**

3.1 Non-energy Use of Fossil Fuels

Non-energy use is defined as the consumption of fossil fuels for feedstock purposes in the chemical industry and for the production of certain non-energy use refinery and coke oven products (e.g., lubricants and bitumen).

- The most important examples for *feedstock use* are the use of naphtha for the production of olefins and the use of natural gas for the production of ammonia. Feedstock use ultimately leads to the production of a large variety of products including plastics, fibers, lacquers and varnishes, solvents, fertilizers, greases, and waxes. Based on IEA (2005a), feedstock use exceeds the consumption of non-energy use refinery and coke oven products in Germany (2003) by around 4.5 times.
- Examples for non-energy use refinery products are bitumen used in the building industry and lubricants used for transportation. Compared to non-energy refinery products, coal and coke oven products used for non-energy purposes are in Germany of subordinate importance in terms of quantities. Coal, coke and pitch (pitch is a coal-derived product) are used directly or in the form of electrodes to produce non-ferrous metals, ferroalloys, and certain inorganic chemicals (pet coke, which is a refinery product is also used for this purpose). Coke-making results in the by-production of benzene and other aromatics, which are used for non-energy purposes (in addition to petrochemical benzene and aromatics).

Non-energy use of fossil fuels accounts worldwide for 5.9% of the TPES in 2003 (IEA, 2005b). This share differs from country to country, depending on the relative importance of refineries and basic chemical industries. Estimating CO₂ emissions resulting from the non-energy use of fossil fuels is not straightforward, because part of the carbon is first stored in chemicals that have lifetimes ranging from days to decades. These chemicals lead to emissions *during the use phase* (e.g., solvents) or at the end of their life cycle during *waste disposal* (e.g., surfactants). The applied waste treatment technology ultimately determines the amount of carbon released to the atmosphere. As an example, waste incineration results in the release of the full carbon content, whereas land filling does not lead to any product-related CO₂ emissions at all within the time span relevant for emission accounting. Apart from the emissions originating from the carbon embodied in synthetic organic chemicals, non-energy use may lead to *industrial process* emissions during the production of certain chemicals such as ammonia. In some processes, the hydrocarbon input is used *both as fuel and as feedstock* (e.g., in the steam cracking process for olefin production). Depending on the system boundary applied for non-energy use

in the energy statistics, part of the carbon embodied in feedstocks might therefore also lead to fuel combustion CO₂ emissions. The definition of non-energy use also determines to some extent whether *industrial process* emissions occur or whether these emissions are already accounted for as *energy* use emissions. In contrast, the definition of non-energy use has no influence on the allocation of emissions from waste incineration; these are reported as *energy* use in the German Greenhouse Gas Inventory because waste incineration facilities in Germany are generally operated with energy recovery.

3.2 Emissions Reporting in the German Greenhouse Gas Inventory

The Federal Environmental Agency (UBA) is responsible for greenhouse gas emission reporting in Germany. The overarching aim of emissions accounting is to apply a method, which generates transparent, comparable, complete, consistent and precise emissions estimates. In accordance with Article 5 of the Kyoto Protocol, UBA adopts the proposed IPCC methodologies to calculate anthropogenic greenhouse gas emissions for Germany.

In its guidelines, the IPCC introduces two different approaches for national greenhouse gas emissions reporting, the IPCC Sectoral Approach (IPCC-SA) and the IPCC Reference Approach (IPCC-SA) (IPCC, 1997). Like in most other industrialized countries, the IPCC-SA is applied in Germany as standard method to estimate greenhouse gas emissions. The IPCC-RA, in contrast, is mainly used as a validation tool for CO₂ emissions from fuel combustion obtained with the IPCC-SA.

3.2.1 The Reference Approach (IPCC-RA)

The principal idea behind the IPCC-RA is to estimate fossil-based greenhouse gas emissions by means of a *top-down* carbon balance, based on fossil fuel supply data as published in the National Energy Balance (NEB). The data requirements of this approach are therefore not as extensive as for the IPCC-SA. This makes the IPCC-RA (i) a suitable validation tool for fossil fuel use emissions as calculated with the IPCC-SA and (ii) a uniform method for emissions reporting throughout the international community.

Starting point of the IPCC-RA calculation is the TPES as it is determined in the NEB by (i) adding up the domestic production of primary energy carriers, imports of primary and secondary fuels, and international bunkers and net changes of fuel stocks, and (ii) deducting from that figure all exports of primary and secondary fuels (see Figure 1). The apparent fossil fuel consumption is equivalent to the total domestic CO₂ emission potential from the use of fossil fuels. The IPCC-RA distinguishes between one part of these fossil fuels, which is used for energy purposes (around 93% in Germany) and another part being used for non-energy purposes (e.g. as feedstock in the chemical industry or as non-energy use refinery and coke oven products). The fractions of fossil fuel used for energy purposes are multiplied with fuel specific emission factors (kt carbon/GJ) and subsequently converted into kt carbon dioxide equivalents² to calculate actual emissions from fuel combustion in the CRF Table 1.A(b) of the Germany GHG inventory.

² This conversion is done by simply using the ratio of the molecular weights of carbon dioxide and carbon, which is 44/12.

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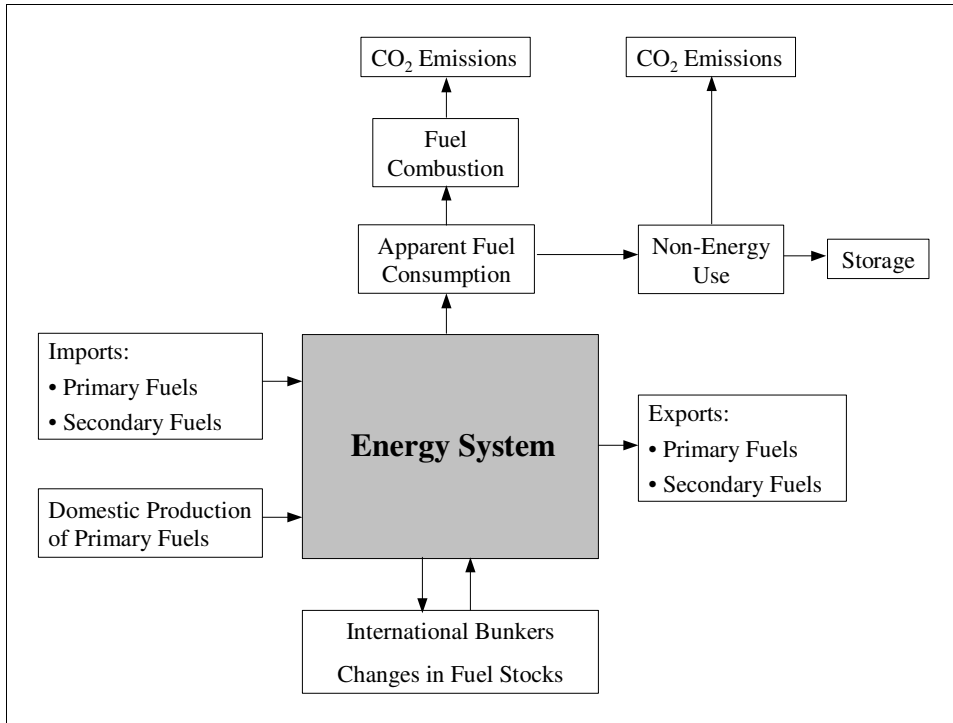


Figure 1: Basic principles of the IPCC-RA (after Prognos, 2000)

In the IPCC-RA of the German Greenhouse Gas Inventory, conversion factors of 100% are used for combustion processes. The total carbon initially contained in the fuel is therefore, assumed to be oxidized during combustion. The fraction of carbon remaining un-oxidized as combustion residue is thus zero. The CO₂ emissions from the combustion of individual fuels are summed up to estimate total CO₂ emission from fossil fuel combustion.

The non-energy use of fossil fuels and related CO₂ emission are dealt with by the IPCC-RA in Table 1.A(d) of the Common Reporting Format. The general aim of the calculations is to estimate the amount of carbon stored and the amount of carbon emitted from fuel-specific non-energy use. In a first step, the specific quantities of fossil fuels used for non-energy purposes (feedstock use and non-energy use refinery coke oven and refinery products) are obtained from the official National Energy Balance (Row 43). The non-energy use data are then multiplied with fuel specific emission factors and carbon storage fractions to calculate the amount of carbon, which remains stored in the economy.

If the carbon storage fractions f represent the share of non-energy use of a specific fuel, which remains un-oxidized, than $(1-f)$ represents the amount of non-energy use carbon which is oxidized. Using the latter term, it is possible to calculate actual CO₂ emissions from the non-energy use of fossil fuels:

$$EN_{NEU} = (1 - f) \times NEU \times EF_{CO_2}$$

where: EN_{NEU} - CO₂ emissions from non-energy use [t CO₂]
 f - Fraction of carbon stored [t/t]
 NEU - Non-energy use [PJ]
 EF_{CO_2} - CO₂ emission factor [1000 t CO₂/PJ]

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The 1996 IPCC guidelines (IPCC, 1997) provide default carbon storage fractions to be used for calculations, if no other reliable fuel-specific data are available. For Germany, country specific storage fractions based on the analyses of PROGNOS (2000) are used (Table 1).

Table 1: Carbon storage fractions according to the IPCC guidelines (IPCC, 1997) and as used in the German GHG inventory based on Prognos (2000)

Year	IPCC Default Values	PROGNOS Values				
		1990, 1991	1992	1993	1994	1995-1999
Naphtha	0.80	0.65	0.58	0.57	0.57	0.57
Lubricants	0.50	0.94	0.92	0.92	0.92	0.92
Bitumen	1.00	1.00	1.00	1.00	1.00	1.00
Coal Oils and Tars	0.75	0.74	0.74	0.74	0.74	0.74
Natural Gas	0.33	0.94	0.90	0.90	0.90	0.90
Gas/Diesel Oil	0.50	0.65	0.58	0.57	0.57	0.57
LPG	0.80	0.65	0.58	0.57	0.57	0.57
Butane	0.80	-	-	-	-	-
Ethane	-	-	-	-	-	-
Residual Fuel Oil	-	0.93	0.89	0.89	0.89	0.89
Petroleum Coke	-	0.88	0.84	0.84	0.84	0.84
Refinery Gas	-	0.65	0.58	0.57	0.57	0.57
Other Oil Products	-	0.86	0.77	0.77	0.77	0.77
Lignite	-	0.89	0.82	0.82	0.82	0.82
Coke (Hard Coal)	-	0.91	0.85	0.85	0.85	0.85
Coke (Lignite)	-	0.92	0.87	0.87	0.87	0.87
Tar	-	0.88	0.84	0.84	0.84	0.84
Coal (hard coal)	-	0.89	-	-	-	-
Other Fuels	-	-	-	0.65	0.57	0.57

The IPCC guidelines do not state carbon storage fractions for all fossil fuels that are relevant for Germany. The deviations between the IPCC default values and the storage fractions from PROGNOS (2000) are mainly explained by methodological differences. To determine carbon storage fractions, PROGNOS (2000) regards (i) all products, which are not oxidized during use, (ii) all products, which do not result in direct CO₂ emissions (e.g., solvents), and (iii) all carbon emissions (including CO₂) from industrial processes) as storage. Therefore, **only emissions related (i) to the combustion of fossil fuels, which are reported under non-energy use in the National Energy Balance (e.g., fuel use in steam crackers), (ii) to waste incineration, and (iii) to direct CO₂ emissions from product use are considered as emissions and are consequently excluded from the fractions of carbon stored.** In other words, all carbon that is emitted due to fuel use of feedstock and direct CO₂ emissions from product use are considered as emissions, the remainder is treated as carbon storage. Due to this approach, the IPCC-RA serves in the German GHG Inventory as validation tool for CO₂ emissions from the fuel use of fossil resources but not as validation tool for the *total* fossil-based emissions as determined with the IPCC-SA. The shortcomings associated with the PROGNOS storage fractions currently used in the IPCC-RA will be discussed in Section 5.4.2.

The IPCC default storage fractions, in contrast, originate from the work of Marland and Rotty (1984) and constitute only a rough estimate of carbon storage in chemical products. They represent the total share of non-energy use of fossil fuels, which remains un-oxidized over long periods of time. The use of these storage fractions in the IPCC-RA leads therefore to CO₂ emission estimates, which include fuel combustion, waste incineration and oxidation during product use (Patel et al., 2005).

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The discussions around carbon storage fractions reveal a major point of controversy regarding the general scope of the IPCC-RA. In Germany, the IPCC-RA is mainly used as a validation tool for the total of CO₂ emissions from fuel combustion. It remains, however, questionable, if (according to the current 1997 IPCC guidelines) the IPCC-RA should rather be used as validation for the total national fossil CO₂ emissions, regardless whether they originate from fuel combustion or from any other source (e.g., product use, industrial processes, waste treatment).

The CO₂ emissions related to non-energy use are calculated in the German Greenhouse Gas Emission Inventory only for the years 1990 to 1999. For the years after 1999, data for the non-energy use of fossil fuels are not available due to incomplete National Energy Balances. Independent of this specific situation for Germany, the work of the NEU-CO₂ network has further shown that the IPCC-RA in general suffers additional shortcomings caused by the unclear and diverse system boundaries of non-energy use data as published in the various national energy statistics (inconsistent definitions of energy versus non-energy use) (Patel et al., 2002). To ensure international comparability of emission estimates according to the IPCC-RA (for both total national CO₂ emissions and even more so, for emissions from non-energy use) it would hence be necessary to arrive at an internationally harmonized definition of non-energy use data in National Energy Balances (harmonization with regard to system boundaries). So far, the attempts made by the IEA in this direction have not been as fruitful as hoped (Reece, 2002).

In the final stage of IPCC-RA calculation, both emissions from fuel combustion and (fuel use) emissions from non-energy use are added together in order to determine total CO₂ emission from fossil fuel consumption in Germany.

3.2.2 The Sectoral Approach (IPCC-SA)

The IPCC-SA, also referred to in the German GHG inventory as the *National-Approach*, estimates total national greenhouse gas emissions separately for various economic and industrial sectors by means of a 'bottom-up' approach. It therefore allows tracing emissions back to the actual polluter. This information is indispensable for effective CO₂ emission mitigation strategies and cannot be obtained from the IPCC-RA.

The IPCC-SA distinguishes between 7 principle source categories: *energy, industrial processes, solvent and other product use, agriculture, land-use change and forestry, waste, and others*. These categories are further divided into various subcategories. For each of the subcategories, actual greenhouse gas emissions are estimated based on methods grouped into Tier 1, Tier 2, and Tier 3 according to the calculation's level of detail and complexity.

In order to focus the calculating and reporting of emissions in the principal emission sources, the IPCC has introduced the concept of *level key sources* and *trend key sources*. Those source categories responsible for 95% of the total national emissions (in CO₂ equivalents) are identified as *level key sources*. Source categories, which have made a particular contribution to *changes* in the total greenhouse gas emissions with respect to their contribution in 1990, are identified as *trend key sources*. Both *level key sources* and *trend key sources* are identified by Tier 1 level assessment (either for single years or for time series). The identified key sources require then detailed analyses on the level of Tier 2 or Tier 3 to determine the actual amount of greenhouse gas emissions. Following the inventory practice proposed by the IPCC, out of the total of 174 individual activities, 44 were identified either as *level key source* or *trend key source* for the year 2002 in Germany. These sources contribute together to around 96.3% of the total national greenhouse gas emission (UBA, 2004a).

Out of these level and trend key sources, none is related to CO₂ emissions from the non-energy use of fossil fuels. According to the current inventory report, ammonia production is the single most

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important source of non-energy use CO₂ emissions, accounting for around 1.8 Mt CO₂ equivalents and being included among the source categories responsible for 97.1% of Germany's greenhouse gas emissions.

Emissions from the non-energy use of fossil fuels can be reported by the IPCC-SA in the source categories of energy, industrial processes, solvent and other product use, and waste. Table 2 shows the relevant source categories for CO₂ emissions from non-energy use as reported in the Common Reporting Format (CRF) Tables in the German National Inventory.

Table 2: Relevant source categories for CO₂ emissions from the non-energy use of fossil fuels

1. Energy	1.A.1. Energy Industries 1.A.2. Manufacturing Industries and Construction
2. Industrial Processes	2.B. Chemical Industry
	2.C. Metal Production
	2.G. Other
3. Solvent and other product use	3.A. Paint Application
	3.B. Degreasing and Dry Cleaning
	3.C. Chemical Products, Manufacture and Processing
	3.D. Other
6. Waste	6.A. Solid Waste Disposal on Land
	6.B. Waste Water Handling
	6.C. Waste Incineration (without Energy Recovery)
	6.D. Other

The IPCC guidelines provide a large degree of freedom regarding the allocation of emissions to the various source categories as long as the chosen approach is transparent, the emission estimates are complete and double counting of emissions is avoided. The most recent CRF tables of the German Greenhouse gas Inventory for the year 2004 state non-energy use CO₂ emissions explicitly only for two *industrial processes* (i) ammonia production (CRF Table 2.B.1.) and (ii) aluminum production (CRF Table 2.C.3.).

Emissions from *solvent and other product use* are given as NMVOC equivalents but are neither converted into CO₂ equivalents nor are they included in the total emission estimates according to the *National Approach* of the German Greenhouse Gas Inventory. This procedure is consistent with the methodology described in the current 1997 IPCC guidelines (IPCC, 1997), which, however, seem to omit important source categories. This is being corrected in the revised 2006 IPCC guidelines for emission inventories (IPCC, 2006). The new guidelines include the indirect CO₂ emissions originating from complete oxidation of NMVOC emissions from the solvent and other product use.

The estimates for emissions from non-energy use of fossil fuels in the IPCC-SA of the **2005 inventory submissions** are partly incomplete and partly vague also for a number of other emission sources. The critical points can be summarized as follows:

- The **emission records for industrial processes are incomplete** (e.g., emissions from the production of carbon black, methanol and non-ferrous metals/ferroalloys, as well as from chemical conversion losses) are not accounted for.
- **Emission estimates for certain industrial processes (e.g., ammonia production) remain uncertain** because it is unclear, which parts of the hydrocarbon feedstock are allocated to either

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energy use or industrial process emissions. In particular, emissions from ammonia production are calculated by use of an emission factor, which is considerably lower than the IPCC default value (0.7 kg CO₂/kg NH₃ versus 1.5 kg CO₂/kg NH₃) without giving reasonable explanations in the NIR (UBA 2004a)³.

- **Emissions from solvent and other product use are not included in the calculation of total greenhouse gas emissions.**
- **Emission estimates for waste treatment** (e.g., waste water treatment) **are incomplete:** The German GHG Inventory only accounts for biogenic emissions from landfills. Emissions originating from petrochemicals in the wastewater of the chemical industry and in public wastewater treatment due to the private and commercial use of petrochemical surfactants have not been accounted for.
- It remains **unclear if and where CO₂ emissions from fuel use in steam crackers and for ammonia production are accounted for.**

Most of these shortcomings were also identified during the external review process of the German GHG Inventory (UNFCCC, 2005). Given the problems and uncertainties in the IPCC-SA calculation of the German Greenhouse Gas Inventory (2005 submission), an in-depth analysis of emissions resulting from the non-energy use of fossil fuels is necessary.

3.3 The German Energy Balance

3.3.1 General Information

The German Energy Balance as published yearly by the *Arbeitsgemeinschaft Energiebilanzen* is the single most important data source for emissions from fossil fuel consumption as stated in the National Greenhouse Gas Inventory. Within the German Energy Balance, energy use is given per sector and per energy commodity in either energy units (TJ and coal equivalents) or natural units (mass and volume). The Energy Balance is compiled using several data sources. The publication of German Energy Balances by AGE is delayed by some years, i.e., the most recent German Energy Balance is only available for the year 1999.⁴

According to UBA (2004a), data from the official Energy Balance is no longer sufficient to accommodate the diverse requirements of emissions reporting due to the following reasons:

- The Energy Balance combines fuel inputs for plants subject to different immission protection legislation and plants, which operate according to different technical principles (e.g. steam turbine power stations, gas turbine power stations, and engine power stations).
- The Energy Balance does not allow the accounting for regional differences regarding fuel composition and properties (e.g., as it is especially relevant for crude lignite).
- The Energy Balance combines fuel inputs, which are allocated to different source categories of the GHG inventory.

³ Such an explanation could be that parts of the emissions are allocated to urea production. However, even if this is taken into account, emission factors are considerably lower than the ones calculated with NEAT (see Section 5.2.2).

⁴ As part of their energy balances for OECD countries, the IEA (International Energy Agency) publishes energy balances for Germany with a delay of approximately 2 years. To this end, the IEA makes own assumptions.

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- The Energy Balance reports fuel use in various lines according to its intended purpose (for electricity in the conversion sector, for heat generation in the respective industrial sectors) even if the fuels are used in one single plant (e.g., combined heat and power plants).

Since all these factors have an influence on the estimates made for GHG emissions, UBA has developed a model entitled the ‘Balance of Emission Causes’ to disaggregate data as stated in the National Energy Balance (UBA 2004a).

3.3.2 Non-energy Use in the German Energy Balance

A particular fuel should be reported under non-energy use if the energy commodity is used to produce non-energy use products that are not included in energy statistics, i.e., (i) as feedstock (e.g., for the production of ethylene) or (ii) consumed for other non-energy purposes (e.g., use of bitumen as building material). The system boundary between commodities included versus excluded in the energy statistics is therefore important and should be clear in order to determine non-energy use in a consistent manner.

For the years 1990 to 1999 non-energy use is reported for the following energy commodities in the official German Energy Balance (AGE 1990-1999):

- Hard coal and lignite
- Coke (produced from hard coal and lignite)
- Other coal derivatives (hard coal and lignite)
- Gasoline and diesel fuels
- Naphtha
- Gas/Diesel oil
- Fuel oil
- Pet coke
- Other oil products (heavy oils)
- Natural gas
- Refinery gas
- LPG (liquid gas)

Unlike in international energy statistics (IEA, 2004a), the consumption of bitumen and lubricants is not given as separate items in the German Energy Balance but included under the category of *other oil products*. In the course of this study, we collected detailed information on the level of individual fuels and products/processes. This allowed us to specify the system boundaries for the most important fuels used for non-energy purposes. This insight is important also for accurate modeling with the NEAT model (Chapter 4 and 5).

The non-energy use of coal products includes the consumption of coal oils and tars, lignite, hard coal and derived cokes. The non-energy use of these products (e.g., for the production of pitch, naphthalene, or creosote oils) as stated in the German Energy Balance, is based on calculations by the DIW (Deutsches Institut für Wirtschaftsforschung) (DIW, 2005).

Background Information

In the scope of this study, it was not possible to get a detailed insight into all the calculation procedure regarding non-energy use. According to the general information provided by the DIW (2005), non-energy use of coal-derived products is calculated based on various different sources, including the Association of Coal and Lignite producers in Germany (Bundesverband Braunkohle, Gesamtverband des Deutschen Steinkohlenbergbaus). It remains unclear, which system boundary for non-energy use is chosen by the different companies and producer associations. It is hence possible that non-energy use is not defined in a uniform way by all data suppliers. However, since most of the data are provided by coal producers and since these cannot be assumed to be familiar with the details of how these supplies are used at their customers, it is plausible to assume that the non-energy use data for coal products in the German Energy Balance follows a *gross* definition of non-energy use, i.e., also including (partly or completely) the fuel use of these products during the manufacturing processes.

The use of solid coal products (e.g., coal and coke) for the production of non-ferrous metals and inorganic chemicals could be principally accounted for in the same way as the use of coke in blast furnaces, which is assigned to the conversion sector in the energy balance. However, contrary to blast furnaces, which produce substantial amounts of blast furnace gas (which is used in large quantities in the power sector and for steel production) the production of non-ferrous metals and inorganic chemicals is not accompanied with the production of meaningful amounts of combustible gasses. Moreover, the carbon input has its pure function as reducing agents and is not consumed for the parallel providing of process heat. It can therefore be assumed that the amounts of solid coal products, which are used for the production of non-ferrous metals and inorganic chemicals are accounted for as non-energy use.

We furthermore identify that the non-energy use of coal oils and tars as stated in the Energy Balance under other coal products is incomplete with respect to feedstock used for chemicals production. This is because values in the energy balance include only the consumption of raw tars but not the trade of further downstream feedstocks such as pitch or crude benzene. As a result, more coal-derived feedstock is used in Germany for benzene production than reported in the Energy Balance.

The non-energy use of oil products includes (i) naphtha and LPG consumption in steam crackers, (ii) the consumption of gas/diesel oils, residual fuel oils, refinery gas, light and heavy fuel oils for the production of e.g. ammonia, methanol and carbon-black, (iii) the non-energy use of bitumen and lubricants, and (iv) the consumption of petroleum coke for electrodes production. Bitumen and lubricants are not stated as separate items but are included in the National Energy Balance under *other oil products*. The data on the non-energy use of oil products in the NEB are derived from the official oil statistics (Amtliche Mineralölstatistik) as published by the Federal Office of Economics and Export Control (BAFA – Bundesamt für Wirtschaft und Ausfuhrkontrolle). The official oil statistics follow the streams of 21 different fuels types from gross refinery production to final domestic deliveries (Inlandsablieferungen), thereby including internal consumption of fuels in refineries, trade (import and export of refinery products), stock changes, rededication and backflows of fuels. The official oil statistics classify final domestic deliveries according to different economic sectors, which receive the individual fuels.

The quantities for fuel oils, LPG and refinery gas given in the category *deliveries for chemical processing* (Einsatz zur chemischen Weiterverarbeitung) are directly taken over in the Energy Balance as non-energy use of these fuels. In the case of lubricants and bitumen, the final domestic deliveries, as stated in the official oil statistics, are considered as non-energy use in the National Energy Balance of these items.

The non-energy use of naphtha as given in the Energy Balance is obtained by deducting backflows from the chemical industry to refineries from the deliveries to the chemical industry as given

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in the official oil statistics.⁵ The non-energy use of petroleum coke in the Energy Balance is simply calculated by deducting the amounts of petroleum coke used for energy purposes (mainly in the cement industry) from the final domestic deliveries as given in the official oil statistics.⁶

Due to the approaches described above, we conclude that for all fuels except for naphtha, a *gross* definition of non-energy use is followed in the National Energy Balance. Since the *gross* deliveries to the manufacturing industries (i.e., chemical industry and electrodes manufacturing) are reported, the parts of feedstocks used as fuels within those industries are included in the values for non-energy use as given in the German Energy Balance. In the case of naphtha consumption, a *semi-net* definition of non-energy use is followed, thereby excluding all backflows to refineries from the non-energy use but still including the part of naphtha feedstock, which is used for energy purposes in steam crackers.

It is important to note that the *total* amount of backflows from the chemical industry to refineries is allocated to *naphtha* consumption (and is hence deducted from the *gross* naphtha use) and not to other fuels (e.g., LPG, which is also consumed as feedstock in steam crackers). The reason for this approach is most likely that naphtha is by far the most important (with respect to total input) feedstock for the chemical industry in Germany. Allocating backflows entirely to naphtha avoids complicated allocations across the various fuels.

Unlike in the Netherlands, the flows of pure oil-derived aromatics are not given as separate items in the Energy Balance. Aromatics are included in the flows of the various fuel oils given in the official oil statistics. The trade of pure aromatic compounds (exclusively used for chemical purposes) is therefore not accounted for in the German Energy Balance (the consequences will be discussed in Section 5.4.1).

Due to the approach chosen for oil products in the Energy Balance, the conclusion seems justified that the total reported non-energy use of oil feedstocks reported in the German Energy Balance is significantly higher than the total of non-energy products produced from those feedstock. In Section 6.2.1, recommendations are given to improve the insight in the non-energy use accounting practice.

Within the course of this project we further identified, that the non-energy use of oil derived fuels in Energy Balance (i) is incomplete with respect refinery propylene and (ii) might be incomplete with respect to refinery aromatics and butadiene. This results in considerable under estimation of the non-energy use of oil-derived feedstock in the Energy Balance.

The non-energy use data in the Energy Balance for the consumption of natural gas originate from the Association of the Chemical Industry in Germany (VCI – Verband der Chemischen Industrie e.V.; VCI, 2005). Within the scope of this study, it was not possible to get a detailed insight in the underlying data for deliveries and consumption of natural gas by individual process. However, according to information from Rothermel (2004), we conclude that the consumption data for natural gas as stated in the German Energy Balances follows a *net* definition of non-energy use. Therefore, fuel use in the two most important industrial processes consuming natural gas, i.e., ammonia and methanol production is excluded from non-energy use as well as hydrogen produced in refineries, based on synthesis gas. According to Rothermel (2004), natural gas consumption for carbon black production is excluded from the non-energy use data. The fractions of natural gas feedstock consumed in this process

⁵ By deducting the backflows from the gross input as reported in the official oil statistics (Amtliche Mineralölstatistik) we calculate values, which do not coincide exactly with the data reported in the Energy Balances. However the differences are within approximately 5% for the years studied in this report.

⁶ The latter is not available from the official oil statistics and is determined by DIW (2005) based on other sources.

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is, however, negligible compared to the total natural gas consumption in the chemical industry. The VCI further assumes for a split of 65% feedstock, i.e. non-energy use, versus 35% fuel use (energy use of natural gas). The NEAT model, in contrast, uses a split of 70% versus 30% for feedstock versus fuel use for ammonia production and 78% versus 22% for feedstock versus fuel use for methanol production (see below, Section 4.2.1.2). NEAT might, hence, slightly overestimate non-energy use and slightly underestimate fuel use of natural gas (see also, Section 5.2.2 and Section 5.4.1).

The analysis of the system boundaries for the key feedstocks discussed above reveals that the German Energy Balance does not follow a consistent definition for non-energy use. The **non-energy use of natural gas** follows strictly a *net* definition of non-energy use, thereby **excluding all fuel use** of natural gas from the non-energy use data. In contrast consumption data for **naphtha** obtained by from the official oil statistics (published by BAFA, 1990-2003) follow a **semi-net definition, i.e. excluding backflows to refinery but including fuel use of naphtha** in steam crackers. **For all other oil-derived products a gross definition of non-energy use is chosen.** Given the information available from DIW (2005) **we assume also a gross definition to be followed for the non-energy use of coal-based products** in the Energy Balance. The main reason for the inconsistent definition of non-energy use in the German Energy Balance can be explained by the fact, that some of the data on non-energy use originate from *producers* of primary and secondary fossil fuels (e.g., refineries and coke producers) while other data originate from *consumers* of fossil fuels (e.g., the chemical industry, which delivers non-energy consumption of natural gas). The producers of fossil fuels only report the amounts of hydrocarbon delivered to their customers, i.e. the chemical and non-ferrous metals industry. They lack the detailed insight in the exact fate of fossil fuels delivered to those industries. The chemical industry, in contrast, can report the *net* non-energy use of natural gas because of detailed insight in the consumption of this feedstock by the various companies. One important goal for the future should therefore be to harmonize the definition of non-energy use for the variety of feedstock stated in the German Energy Balances. To this end, consumption data for the non-energy use of hydrocarbons should be obtained from either the producers (which would than report *gross* deliveries) or from the consumers (which would report more detailed *net* consumption) depending on the definition of non-energy use aimed for in the German Energy Balance.

The evaluation of the Energy Balance by UBA (2004a) and the findings of this research study clearly show the need to improve and adapt the German Energy Balance not only in order to account for non-energy use in a correct and consistent way but also to fulfill its requirements as principle data source for greenhouse gas emissions accounting.

4 Methodology

This chapter contains:

- Background information on economy wide energy flows and the modeling of non-energy use and related emissions
- A detailed description of approaches and assumptions chosen in NEAT
- A description of input data used to model non-energy use and related emissions with the NEAT model

4.1 Background

The flow chart in Figure 2 covers all activities, which add up to a country's Total Primary Energy Supply (TPES). The TPES of a country consist of all primary energy commodities (e.g., crude oil, lignite, natural gas) produced within the country minus exports and plus imports of primary and secondary energy commodities.

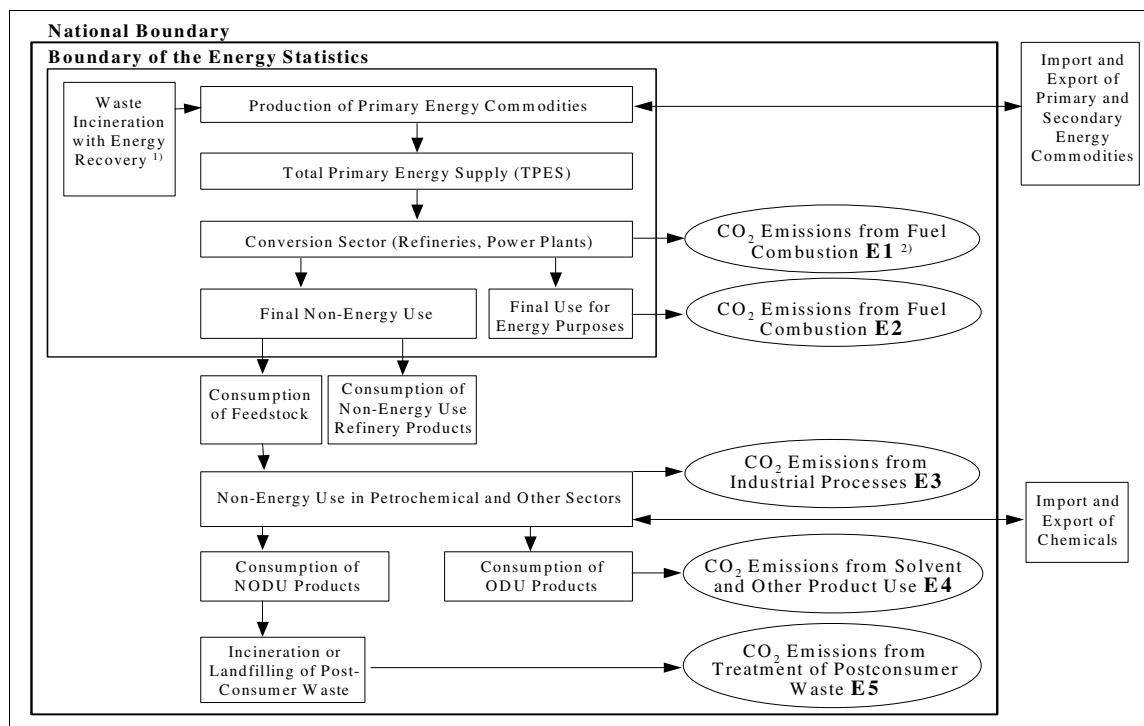


Figure 2: Overview of energy flows and fossil CO₂ emissions in the NEAT model

¹⁾ In line with the international energy balance of the IEA (2005a), waste incineration with energy recovery is assumed to be reported as energy commodity. The energy recovered from incineration is subsequently covered in the conversion sector and resulting CO₂ emissions are part of the emissions from fuel combustion (E1).

²⁾ Including emissions from waste incineration with energy recovery.

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The conversion of primary energy into secondary energy results in CO₂ emissions (E1). The resulting secondary energy commodities (e.g., fuel or electricity) are now available for final consumption. The majority of these commodities are consumed for energy purposes in the various economic sectors, leading to CO₂ emissions from fuel combustion (E2). A substantial fraction, however, is used for non-energy purposes, either as feedstock in the chemical industry (e.g., naphtha for olefin production or natural gas for the production of ammonia) or as non-energy refinery and coke oven products such as bitumen or lubricants. The secondary fuels used for non-energy purposes contain carbon. Parts of this carbon are oxidized during the production process of certain chemicals. The resulting emissions are referred to as industrial process emissions (E3). The remainder is embodied in chemical products.

With respect to CO₂ emissions, two major groups of chemical products can be classified. The first group comprises products such as solvents or detergents, which already oxidize partially or fully during their use phase. These chemicals are referred to as *oxidized during use* (ODU) products. The emissions from ODU products are assigned to the IPCC emission source category of *solvents and other products use* (E4)⁷. The second group comprises chemical products, which are *not* oxidized during their use phase. Such products are referred to as *not oxidized during use* (NODU) products.

The end-of-life waste treatment technology applied ultimately determines, which parts of the fossil carbon contained in NODU products is released as emissions. For example, in case of land filling the total amount of carbon remains stored in chemical products. In contrast, waste incineration leads to a 100% oxidation of carbon contained in the chemicals. According to the IPCC guidelines for emission inventories, waste that is incinerated with energy recovery is considered as fuel (IPCC, 1997). Since, in Germany, practically all waste incineration plants recover energy, waste incineration is defined as energy use, which leads to emissions from *fuel combustion* (E1). Emissions from incineration without energy recovery and from other waste treatment facilities like landfills or wastewater treatment plants are assigned to the emission category *waste* (E5). **All three source categories relevant for non-energy use emissions, i.e., industrial processes, solvent and other product use, and waste treatment are included in the NEAT model. NEAT further calculates fuel combustion emissions, if they are related to the non-energy use of fossil fuels, i.e., CO₂ emissions from the fuel use in steam crackers, from the fuel use for various industrial processes and from waste incineration.**

⁷ According to the 1996 IPCC guidelines, this holds also for emissions from urea consumption as fertilizer component. However, based on the revised 2006 IPCC guidelines, these emissions should be reported under the combined source category of *agriculture and land use change* (IPCC, 2006).

4.2 The NEAT Model Version 3.0

The NEAT (Non-Energy use Emission Accounting Tables) model was developed to improve the accounting for CO₂ emissions from non-energy use of fossil fuels. NEAT is a spreadsheet model (implemented in Microsoft Excel), which analyses the carbon flow through non-energy products and the main chemical and petrochemical processes. The model can be divided into three stages, with each stage consisting of one or more Excel-worksheets. Stage 1 of the model generates independent estimates for total CO₂ emissions from the non-energy use of fossil fuels. In stage 2, total non-energy use, carbon storage, fuel specific carbon storage fractions and total CO₂ emissions from the domestic use of fossil resources are calculated. All results can be used in stage 3 for comparisons with data from official sources such as the German GHG Inventory or the German Energy Balance. The calculation approaches and the key assumptions of the three stages are described in detail in the following sections.

4.2.1 Stage 1: Calculating CO₂ Emissions from the Non-energy Use of Fossil Fuels

Stage 1 represents the core of the NEAT model. Following the 1996 IPCC guidelines, the model distinguishes between the relevant source categories:

- Emissions from the use of solvents and other product use
- Industrial process emissions, which occur during the production of chemicals (e.g., ammonia, methanol or carbon black) and when fossil fuels are used as reducing agents for the production of non-ferrous metals, ferroalloys, and inorganic chemicals (depending on the definition chosen, also emissions from the partial oxidation of hydrocarbon feedstock in steam crackers might be accounted for in this category)
- Emissions from waste treatment, i.e., wastewater treatment
- Emissions from fuel combustion, i.e., emissions from waste incineration with energy recovery and, depending on the definition of non-energy use chosen, emissions from fuel use in steam crackers and the production of chemicals such as ammonia, methanol and carbon black

Especially with respect to direct CO₂ emissions from steam cracking there is some scope about whether to consider parts of the CO₂ as emissions from fuel combustion (E2 in Figure 2) or as industrial process emissions (E3 in Figure 2). Different allocation methods for the hydrocarbon input, either as energy use (emissions from fuel combustion) or non-energy use (industrial process emissions) are possible and have been included in the NEAT model.

4.2.1.1 Product Use Emissions

The concept of ODU and NODU products has been introduced above in Section 4.1. **ODU products are assumed to result in CO₂ emissions⁸** from product use within the inventory year. These emissions are also referred to as *product-related* emissions. Emissions from NODU products are dealt with in the category waste treatment (see Section 4.2.1.3).

The NEAT model calculates the quantities for ODU and NODU products by means of a carbon balance for the 80 most important chemical commodities.

⁸ This assumption in NEAT is a simplification, which might not hold in reality, as the majority of product use emissions are NMVOCs, which are only slowly degraded to CO₂ in the atmosphere.

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Model Input Data

The calculation of CO₂ emissions from product use is based on physical production and trade data [Mt/a] for 80 chemical products and product groups. These chemical core products consist of 22 basic chemicals, 35 intermediates, and 23 final products or product groups (see Table A1-A3 in Appendix A and Table B1 in Appendix B). In contrast to earlier model versions⁹, we introduce three new intermediate chemicals (i.e., acetaldehyde, adiponitrile, and hexamethylenediamine) to account for specifics of chemical production routes in Germany. We derive in NEAT domestic consumption of all chemicals by adding imports to and subtracting export from the production value¹⁰.

Among other basic chemicals, petroleum coke and pitch are included in NEAT. These chemicals are either used for energy purposes (e.g., in the conversion sector) or to produce electrodes, which are oxidized during the manufacture of non-ferrous metals and other inorganics (see Section 4.2.1.2). Data from the German Energy Balance confirm that the consumption of petroleum coke for electrode production covers the non-energy use of petroleum coke to around 100% (Table 3).

Table 3: Comparison of non-energy use of petroleum coke according to the German Energy Balance and NEAT¹¹

Year	Petroleum coke available for final use according to the NEB in Mt CO ₂	Total non-energy use of petroleum coke according to the NEB in Mt CO ₂	Petroleum coke used for electrode production according to NEAT in Mt CO ₂	Deviation in % [(NEAT-NEB)/NEB]
1990	2.58	1.76	2.18	24
1991	2.53	1.55	1.98	28
1992	2.66	1.59	1.85	16
1993	3.36	2.20	1.33	-40
1994	3.25	2.24	1.62	-28
1995	4.51	2.01	1.95	-3
1996	2.88	1.95	1.83	-6
1997	2.79	1.67	1.88	13
1998	3.09	1.88	1.95	4
1999	3.12	1.80	1.98	10

In order to avoid the accounting of emission from energy use, we assume that the consumption of petroleum coke and pitch for non-energy purposes other than electrode production is zero, i.e., we exclude both products from the calculation of product-related emissions. CO₂ emissions from the non-energy use of petroleum coke and pitch are hence only dealt with under industrial process emissions. A similar approach is chosen for ‘other tar products’, which are mainly used to produce carbon black, pitch and benzene. In NEAT, consumption of *other tar products* is excluded from the model in order to avoid double counting of feedstock use, i.e., once for producing *tar products* and again for the production of carbon black and benzene.

Based on their chemical composition, production, exports, and imports of chemicals can be expressed in Mt CO₂ equivalents for each year. For pure chemicals such as ethylene, the chemical

⁹ The older NEAT Model version 2.0 is explained in detail by Neelis et al. (2003, 2005a, and 2005b).

¹⁰ Exceptions from this are lubricants and bitumen for which consumption data are directly derived from the official mineral oil statistics.

¹¹ In some years, petroleum coke consumption for electrodes is higher according to NEAT than the feedstock available given in the German Energy Balance. The trade of electrodes, which we do not take into account here, could cause these discrepancies.

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composition is exactly known. Assuming 100% carbon efficiency, the CO₂ equivalents can be easily derived from the carbon content of the chemical substance. For other products and product groups such as *other tar products* or *polyamides*, which are less well defined, estimates for their chemical composition were used.

Carbon Balance

The purpose of the NEAT carbon balance is twofold. On the one hand, it gives an overview of the consumption structure of chemicals and forms therefore the basis for the allocation of product streams to the categories ODU and NODU. On the other hand, it serves as a valuable crosscheck for inconsistencies in the production and trade data used for NEAT calculations. Most basic chemicals are converted to a wide variety of intermediate and final products.

The carbon balance in NEAT contains conversion routs from 22 basic to 55 intermediate and final products. The principles of the mass balance are explained at the example of ethylene use as shown in Figure 3.

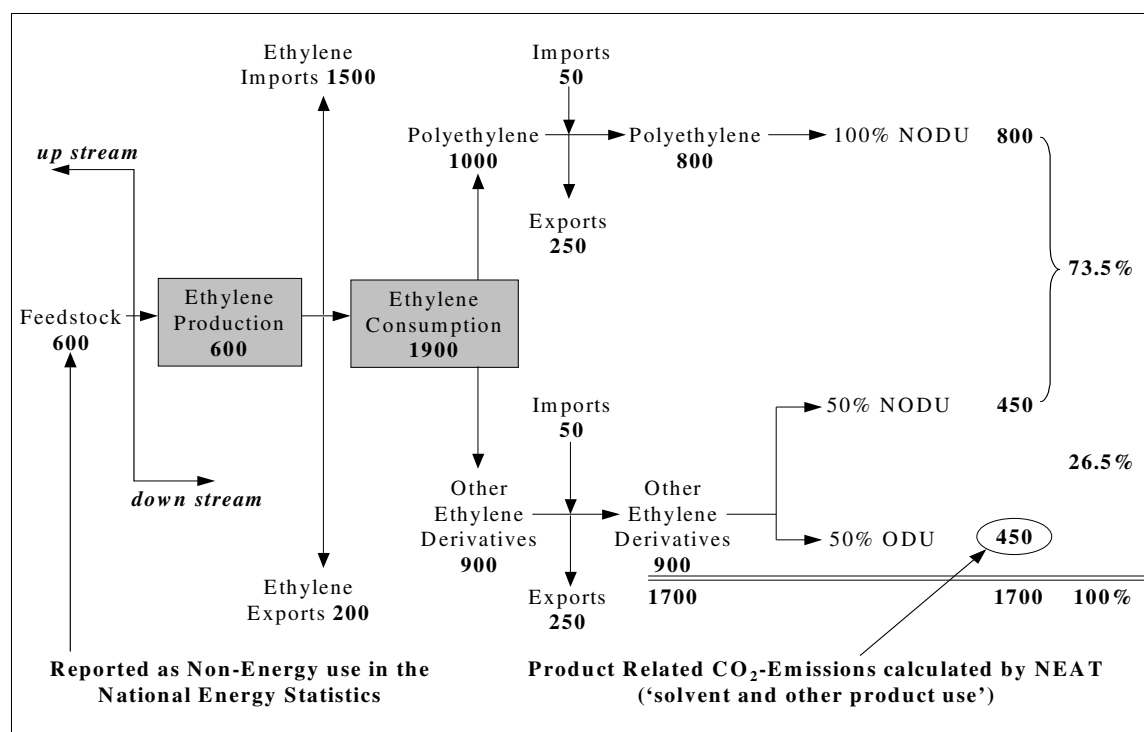


Figure 3: Calculating emissions from *solvent and other product use* in NEAT (simplified example after Neelis et al., 2003)

In this simplified example, ethylene is mainly used for the production of polyethylene. The remaining ethylene is consumed for producing e.g., synthetic ethanol, ethylene oxide, ethylbenzene, and other chemicals. If the mass balance is closed, the mass of carbon contained in ethylene equals the sum of (i) the carbon mass of polyethylene and (ii) the carbon mass of all other ethylene derivatives. In other words, the consumption of ethylene is completely used within the country for the production of ethylene derivatives modeled in NEAT.

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The difference between the basic chemical and its products is thus zero. Relatively high positive or negative deviations raise therefore serious doubts about the consistency of production and trade data used for NEAT calculations. In case of positive values, part of the consumption of ethylene is left for the production of other ethylene derivatives that are not explicitly modeled in NEAT. A negative NEAT carbon balance, on the other hand, indicates that there is not enough ethylene available to produce all ethylene derivatives. In this case, further investigations and data adjustments are required until the negative value becomes negligibly small. There are two main reasons for negative values in the NEAT mass balance:

- Errors in the apparent consumption: The production data used for a particular chemical might be too low and/or the trade data might be erroneous. Especially in the case of intermediates there is a risk that the production is not completely recorded or that it is not reported at all.
- Errors in stoichiometric factors: The derivative might be produced fully or partially from other raw materials (e.g., unlike in the Netherlands, cyclohexanone is in Germany not only produced from cyclohexane but partially also from phenol).

The carbon flow in the German chemical industry according to the NEAT mass balance is shown in Figure B1 in Appendix B. The figure is limited to all basic chemicals and intermediates explicitly modeled with NEAT. In order to keep the figure readable, two simplifications are made: (i) only the most important flows, accounting together for at least 80% of the carbon contained in products are shown and (ii) the production routes from intermediates to final polymers are not given individually. The carbon flows are not quantified for reasons of confidentiality of parts of the data used.

Oxidized During Use (ODU) Versus Not Oxidized During Use (NODU) Products

In the example from Figure 3, the total consumption of polyethylene and the total consumption of other ethylene derivatives are divided separately into ODU and NODU applications. This procedure is followed similarly for all other NEAT substances as well¹². The ODU versus NODU division is clear-cut for some commodities (e.g., all polymers are NODU products), for others, the fractions of ODU versus NODU products are estimated based on open literature (Weissermel and Arpe, 2003, Chauvel and Lefebvre, 1989). Special attention is given to lubricants because consumption patterns and final fate are complex. The division between ODU and NODU fractions for lubricants is based on data given in Table 4.

¹² An exception, however, is butene because parts of the butene production are used as fuel additive. Emissions from fuel consumption are not part of the non-energy use emissions but related to fuel use. We, therefore, divide only the part of butene used for non-energy purposes into fractions ODU versus NODU and regard the remaining fuel use butene as storage. Applying this approach, we avoid possible double counting of CO₂ emissions from butene, once as component in fuels and once as non-energy use.

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Table 4: Final fate of lubricants in Germany (Trischler, 1997)

Fate of waste lubricants (excluding water content)	in kt (1993)
Reprocessing	253
Fuel use in cement factories	109
Other fuel use	95
Other use and exports	20
Total reuse of waste lubricants	478
Storage in products	130
Fuel use in engines	165
Other losses	270
Total losses	564
Total waste lubricants	1042

Emissions from the fuel use of lubricants as well as exports of waste oils are regarded as storage due to the system boundaries of non-energy use. Therefore, only ‘*other losses*’ (see Table 4) are accounted for as ODU emissions in NEAT. The ODU versus NODU fractions for lubricants in NEAT is, hence, 26 versus 74% respectively. The split of lubricants into ODU and NODU remains, nevertheless, uncertain. Detailed research is highly recommended to determine consumption patterns, final fate and ultimately non-energy use emissions from lubricants more accurately.

The ODU and NODU fractions for all 80 NEAT products, including uncertainty ranges are given in Table B1 in the Appendix B. For commodities that are not (modeled to be) used as intermediates for the production of other NEAT chemicals (e.g., bitumen or carbon black), the total consumption is directly divided into ODU and NODU fractions. For commodities, which are (modeled to be) used for the production of other derivatives (e.g., acetylene or ethylene), the consumption of those other derivatives is divided into an ODU and NODU fraction and attributed to the initial product. These two cases are marked by the entries ‘*total*’ and ‘*other*’ in Table B1 (Appendix B). In the ‘*total*’ case, the chemicals consumption directly results from the production and trade statistics, whereas in the case of ‘*others*’, consumption values results from the carbon balance incorporated in the NEAT model. The calculation of emissions from the *solvent and other product use* with NEAT can be summarized with the following formula (Neelis et al., 2005a)¹³:

$$E_{tot} = \sum_{i=1}^{80} (P_i + I_i + E_i + C_{NEAT,i}) \times ODU_i [\%]$$

where:

E_{tot}	-	total emissions from solvent and other product use in CO ₂ equivalents
P_i	-	production of chemical i in CO ₂ equivalents
I_i	-	import of chemical i in CO ₂ equivalents
E_i	-	export of chemical i in CO ₂ equivalents
$C_{NEAT,i}$	-	consumption of chemical i for the production of other NEAT chemicals in CO ₂ equivalents
ODU	-	fraction of oxidize during use carbon
i	-	product index

¹³ Note that we include here also the emissions originating from urea consumption in fertilizers. However, according to the revised 2006 IPCC guidelines, these emissions should be reported separately, i.e., as emissions from agriculture and land use change.

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The restriction to 80 chemical key products results in the omission of imports and exports of some further downstream derivatives, which are covered as consumption for ‘other’ derivatives. This could lead to erroneous estimates for the consumption of ODU products in countries, which are either large *net* importers or *net* exporters. Neelis et al. (2003) found this effect to be significant for CO₂ emissions from the consumption of ODU products in the Netherlands.

We analyzed therefore additional trade data for around 450 chemical commodities in the year 2000. The results show that Germany is a *net* exporter of chemicals (-2.3 Mt CO₂ equivalents). However, compared to the domestic consumption of chemicals, which was around 65 Mt CO₂ equivalents in 2000, *net* trade of more downstream derivatives has a minor effect on CO₂ emissions from the consumption of ODU products in Germany (see also Section 5.1 for a more detailed discussion). Because this cannot be assumed to be the case for *all* countries, the NEAT model contains a separate sheet in order to account for additional trade (the sheet contains the names of the products/product groups, their product code and their carbon content).

The key simplifications and uncertainties inherent to the NEAT carbon balance are:

- NEAT assumptions about ODU versus NODU fractions are subject to uncertainties. These uncertainties are relatively high for products for which relatively little is known about the type and the exact use-structure of other derivatives. For this reason, a sensitivity analyses has been implemented in NEAT, covering also estimates for the minimum and maximum release of carbon during product use (see Table A1 in Appendix 1).
- All chemical conversions from basics to intermediates and final products are associated with carbon losses. The NEAT model accounts for carbon losses resulting (i) as direct CO₂ emissions and (ii) in form of unspecified by-products used, which are not used as fuels. This is a major improvement of the current NEAT model (Version 3.0) compared to earlier model versions (Version 2.0), where 100% carbon efficiency for all conversion processes was assumed, thereby overestimating emissions from *solvent and other product use*. The process specific carbon losses as used in the NEAT model are given in Table B2 in Appendix B; they are based on the work of Neelis et al. (2005c).
- The structure of the chemical industry is very similar throughout the world. Bulk chemicals are made via the same production routes and similar production processes everywhere (an important exception is South Africa with its coal-based chemical industry). However, some intermediates and final products can be made in more than one way. An example is again cyclohexanone, which can be made both from cyclohexane and phenol. Other examples are the mixed product groups like polyamides where the various representatives (e.g. polyamide 6 and polyamide 6,6) are manufactured from different raw materials. This leads to uncertainties regarding the production routes assumed in the NEAT mass balance approach.
- Because all calculations in NEAT are conducted in terms of CO₂ equivalents, the carbon content of all products must be known. While exact contents are available for pure components (e.g., ethylene), approximations must be made for other chemicals and mixed product groups (e.g., isocyanates, polyamides).

Beside inherent model uncertainties, there are uncertainties related to the extensive data requirements. Production and trade data for all 80 core-products are required for a correct application of the NEAT model. Those data are not always available for all core-products. Furthermore, data might be too aggregated for NEAT purposes due to pooling of different products under one single product code

in production and trade statistics. In those cases, data may have to be estimated on basis of capacity data or from mass balance calculations or enquiries at producer associations. Apart from non-existing data, values reported in the official statistics can also be erroneous. One typical reason is that intermediates that are converted further on the same site (e.g., ethylbenzene to styrene) may not always be reported in official production statistics.

A sensitivity analysis is conducted in order to account for the various types of data uncertainties related to the estimation of ODU products. To this end, ranges for (i) the total consumption of carbon embodied in chemicals, (ii) CO₂ emissions from product use, and (iii) the total amount of carbon stored in products are calculated (see Section 5.1). As explained by Neelis et al. (2005b), we assume the ranges for ODU versus NODU fractions (see Table B1 in Appendix B) to represent the 95% confidence interval of all ODU versus NODU fractions possible for a specific chemical. Uncertainties related to the consumption of chemicals are accounted for by assuming the 95% confidence interval of the consumption values of each chemical to represent 50% of the difference between the minimum and the maximum consumption between 1990 and 2003 of that chemical. We therefore attribute the full variation of consumption data in all years to the weak data situation. This approach might be questionable because parts of the data variability might be caused by an increased consumption of chemicals in Germany between 1990 and 2003. However, we consider this approach as suitable, due to the relatively high uncertainties associated with production data. Using standard error propagation rules, we calculate confidence intervals for total consumption of carbon contained in chemicals, ODU emissions, and NODU storage (for results see Table 12).

4.2.1.2 Industrial Process Emissions

Parts of the carbon embodied in fossil fuels used for feedstock purposes is directly oxidized to CO₂ during the production of chemical products, leading to industrial process emissions (E3 in Figure 2). The most important examples for industrial processes leading to non-energy use emissions are steam cracking as well as the production of ammonia and methanol. But also other processes, such as the production of carbon black, ethylene dichloride, ethylene oxide, and acrylonitrile, lead to relevant CO₂ emissions. Moreover, fossil carbon is used as reducing agent for the production of certain non-ferrous metals, ferroalloys, and other inorganic chemicals.

The carbon embodied in the feedstock is either not (ammonia, metals) or only partly (e.g., methanol, carbon black) embodied in the final product, while the remainder is emitted as CO₂.

According to the IPCC terminology (IPCC, 1997), steam cracking does not lead to ‘industrial process emissions’. Nevertheless, this process is one of the most important sources of CO₂ emissions among all industrial processes. Therefore and for practical reasons, it is dealt with under *industrial process emissions* here. Another, final reason is that this is in line with the newly proposed approach in the 2006 IPCC guidelines (IPCC, 2006).

NEAT contains a module to calculate industrial process emissions by multiplying the production volumes of products with specific emission factors.

Steam Cracking

Steam Cracking is by far the most important petrochemical process. It generates the key building blocks of the petrochemical industry, namely ethylene, propylene, butadiene, and aromatics. Roughly 40% of all bulk chemicals originate from steam cracking in industrialized countries (Patel et al., 1999). A variety of feedstock is used for steam cracking. In Germany, naphtha accounts for around

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three quarters of the total steam cracker input (IPTS, 2003), while plants operating on Natural Gas Liquids (NGL) and Liquefied Petroleum Gas (LPG) dominate in the USA (Weissermel and Arpe, 1998).

Steam cracking generates high value basic petrochemicals and low value by-products. The latter are either (i) used to fuel the steam cracking process, (ii) partly recycled back to refineries or (iii) used as fuels elsewhere in the petrochemical sector.

The yield data for all petrochemical products generated in steam crackers reported in literature typically represent the outcome of the first pass through the reactor, while not taking into account that unconverted raw materials are fed back to the steam cracker. The latter is the case for unconverted ethane, which is too valuable to be discarded to the fuel pool. Also propane is recycled in cases, where plants are designed to produce polymer grade propylene. Acetylene and propadiene are highly reactive species (e.g., poisoning of polyethylene catalysts) and are therefore removed by hydrogenation.

Taking these aspects into account, the ultimate yields of steam crackers are modeled in NEAT. The data are closely matched to the values reported in the IPTS (2003) because this document represents the most authoritative publicly available information source for steam cracking in Europe. The values given are used for further calculations and represent the state of technology as nowadays applied in Western Europe. The values from Table 5 represent the default data for steam cracking in the NEAT model.

Table 5 distinguishes between high value chemicals, fuel grade by-products, and backflows to refineries. High value chemicals are ethylene, propylene, butadiene, and aromatics. Other C₄ compounds apart from butadiene are generally not included in the group of high value chemicals. The steam cracking process yields also compounds such as butane-1 and isobutene but these are rarely extracted due to the large processing requirements for separation. Fuel grade products such as hydrogen and methane are consumed within the steam cracker to generate the required process heat. Finally, backflows are low-grade products, which are usually returned to the refineries.

An important indicator for the operation mode of a steam cracker is the so-called severity. The degree of severity describes the propylene/ethylene ratio of the steam cracker output. For naphtha steam crackers, P/E values around 0.7 indicate low severity and values below 0.5 high severity. Naphtha steam crackers in Western Europe have an average P/E value of 0.52. For the calculation of ultimate yields, we therefore assume the steam crackers to be operated under high severity. However, many of the older plants in Europe operate under low severity and even producers of modern plants may choose to crack at lower severity because it is often commercially more attractive. At lower severity, more propylene is produced per ton of ethylene but also more feedstock is required. The decision to crack at lower severity is thus determined by the relative market price and the demand of ethylene and propylene.

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Table 5: Ultimate yields of steam crackers as modeled with NEAT (based on IPTS (2003) and Neelis et al. (2003))

(kg product/1000 kg feedstock)	Feedstock				
	Naphtha	Gas oil	Ethane	Propane	Butane
High Value Chemicals	645	569	842	638	635
Ethylene	324	250	803	465	441
Propylene	168	144	16	125	151
Butadiene	50	50	23	48	44
Aromatics	104	124	0	0	0
Other (acetylene + propadiene)	0	0	0	0	0
Fuel Grade Products and Backflows	355	431	157	362	365
Hydrogen	11	8	60	15	14
Methane	139	114	61	267	204
Ethane and Propane after recycle cracking	0	0	0	0	0
Other C4	62	40	6	12	33
C5/C6	40	21	26	63	108
C7 + non-aromatics	12	21	0	0	0
<430C	52	26	0	0	0
>430C	34	196	0	0	0
Losses	5	5	5	5	5
Total	1000	1000	1000	1000	1000
Process Energy	264	261	314	249	242
Backflows to refineries (low value products only)	91	170	0	113	123

Using ethylene production data and the feedstock mix (e.g., naphtha, LPG, ethane) as model inputs, NEAT calculates the consumption of *net* feedstock and *net* energy use in steam crackers and the amount of backflows to refineries in CO₂ equivalents. For steam cracking, the allocation of carbon input to energy versus non-energy use is particularly problematic. When the hydrocarbon input as a whole is regarded as non-energy use, the backflows to refineries might be double counted in energy statistics, both as non-energy use and once more as inputs to refineries. Table 6 shows the key indicators used in NEAT to model the steam cracking process for Germany.

The energy use and related emissions (see Table 6) represent average values for operating a steam cracker. Depending on the type of feedstock and the operation mode there may be a deficit of heating gas (especially for gas oil and ethane crackers). This deficit is usually compensated by natural gas that has a higher CO₂ emission factor than the fuel gas recovered from the steam cracking process. Because the NEAT model only deals with CO₂ emissions from feedstock use, it is necessary to exclude emissions from external fuels from the model calculations. For this reason, emission factors (see Row 8 in Table 6) used in NEAT are 8-9% below the values stated by IPTS (2003).

As a further consequence, a factor indicating the share of the feedstock-specific process energy covered has been introduced in Row 14 of Table 6. We assume that the average naphtha steam cracker is operated on a self-sufficient basis. In contrast, gas oil and especially ethane crackers require fuel imports from external sources (Row 14 in Table 6). By multiplying these shares of total process energy covered by feedstock with the total values for energy and CO₂, feedstock-related energy use and CO₂ emissions are determined (see Row 16 and 17 in Table 6).

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Table 6: Key indicators for steam cracking (based on IPTS (2003) and Neelis et al. (2003))¹⁴

Row		Naphtha	Gas oil	Ethane	Propane	Butane	Others*	Total
1	Share ethylene from feedstock i divided by total ethylene production (%)	80.1	3.7	0.0	8.3	7.9	0.0	100
2	Share input feedstock i divided by total feedstock (%)	83.0	5.0	0.0	6.0	6.0	0.0	100
3	Heating value feedstock (GJ/t)	43.5	42.7	45	45	45	43.5	43.6
4	Total process energy (GJ/t ethylene)	35.5	47.0	22.0	24.1	24.7	35.5	34.1
5	Total process energy (GJ/t high value chemical)	17.8	20.7	21.0	17.6	17.1	17.8	17.9
6	Total process energy (GJ/t feedstock)	11.5	11.8	17.7	11.2	10.9	11.5	11.4
7	Total process energy (% of feedstock)	26.4	27.5	39.3	24.9	24.2	26.4	26.2
8	CO ₂ emission factor of fuel for steam cracking process (kg CO ₂ /GJ)	48.7	48.7	43.3	43.3	43.3	48.7	47.8
9	Specific CO ₂ emissions from fuel use steam crackers (Mt CO ₂ / Mt ethylene)	1.73	2.29	0.95	1.04	1.07	1.73	1.64
10	Specific CO ₂ emissions from fuel use steam crackers (Mt CO ₂ / Mt high value chemicals)	0.87	1.01	0.91	0.76	0.74	0.87	0.85
11	Specific CO₂ equivalents of backflows steam crackers (Mt CO₂ / Mt ethylene)	0.88	2.13	0.00	0.76	0.88	0.88	0.94
12	Tonnes of feedstock per tonne of ethylene	3.09	4.00	1.24	2.15	2.27	3.09	-
13	Tonnes of high value chemicals per tonne of ethylene	1.99	2.27	1.05	1.37	1.44	1.99	-
14	Estimated share of total process energy covered	1.00	0.95	0.80	1.00	1.00	1.00	-
15	Share of process energy originating from feedstock (GJ/t feedstock)	11.5	11.2	14.1	11.2	10.9	11.5	11.4
16	Share of process energy originating from feedstock (% of feedstock)	26.4	26.1	31.4	24.9	24.2	26.4	26.2
17	Specific CO₂ emissions from feedstock (Mt CO₂ / Mt ethylene)	1.73	2.17	0.76	1.04	1.07	1.73	1.64

As indicated above, severity is an important parameter for the yield pattern of a steam cracker. It has further also an impact on energy use in steam crackers. Low severity results in maximum ultimate yield of ethylene, but it requires more feedstock to be recycled. This would ultimately lead to higher energy consumption. **The choice of steam crackers operating under high severity results in a conservative estimate for CO₂ emissions.**

The part of feedstock that is not converted into high-value chemicals or combusted in the steam cracker itself is normally returned to refineries for further processing (see Row 11 in Table 6). However, there are some exceptions. The first one relates to potential losses in steam crackers, which add up to 0.5% at maximum and are therefore negligible. A more important exception could be that parts of the low value output that are used as fuel for industrial production processes or in cogeneration plants instead of being returned to refineries. Losses from steam crackers and exports of surplus fuel grade products especially from LPG steam crackers are not modeled explicitly in NEAT but are included in the backflows to refineries. Consequently, CO₂ emissions originating from feedstock, which are released in the chemical industry could be underestimated by NEAT.

¹⁴ The specific steam cracker feedstock composition is variable throughout the years studied. Therefore, values given in Table 6 are not fixed but vary depending on the specific year studied.

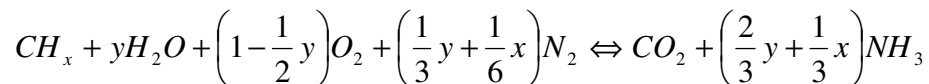
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Table 5 reports the total yield of aromatics that has been allocated to the category of *high value chemicals*. Those aromatics can either be extracted from the output stream in the separation unit of the steam cracker or in external refinery units. However, parts of the aromatics might end up in gasoline, which is used for energy purposes (i.e., the output of aromatics would be lower, while the backflows would be higher). As a consequence, the output of aromatics (for non-energy purposes) from steam crackers as stated in Table 5 may be too high. The aromatics balance becomes even more complicated due to the fact that part of the aromatics also originates from gasoline production in refineries and to a smaller extent also from coal. For these reasons, production data of benzene, toluene and xylene according to official production statistics are used to estimate CO₂ emissions from product use instead of using aromatics data from Table 5.

Ammonia Production

In industrialized countries, CO₂ emissions from ammonia production are comparable to or in some cases even higher than the CO₂ release from steam crackers (Patel et al., 1999). The hydrocarbon feedstock serves as source for hydrogen, which is then converted with nitrogen via the *Haber-Bosch* process into ammonia. Depending on the type of fuel, either steam forming or partial oxidation is applied to produce hydrogen from the fossil feedstock. In 2004, 67% of the German ammonia capacity is based on steam reforming of natural gas. The other 33% is driven by partial oxidation of heavy hydrocarbons (IPTS, 2004).

In principle, steam reforming can be applied to natural gas and to liquid hydrocarbons up to naphtha. The essential reactions are endothermic, converting methane or higher hydrocarbons to carbon monoxide and hydrogen. Additional hydrogen is formed via the water-gas shift reaction where carbon monoxide and water is converted to CO₂ and hydrogen. However, heavy hydrocarbons cannot be converted to synthesis gas by steam reforming because they contain too much sulfur (catalyst poisoning) and are difficult to vaporize. To avoid these problems, partial oxidation is applied to convert heavy hydrocarbons to carbon monoxide and hydrogen by reaction with oxygen and steam. Additional hydrogen is again formed by the water-gas shift reaction. The general idealized reaction equation for steam reforming and partial oxidation of hydrocarbon and the subsequent production of ammonia can be written as:



where: $2 \geq y \geq \frac{-x}{2}$

The above reaction is a strongly exothermic combustion of the fossil hydrocarbon feedstock when $y = -x/2$. If $y = 2$, the reaction equation represents the steam reforming of the hydrocarbons, which is endothermic.

Driven by thermodynamics and practical limitations, the process designs of steam reforming and partial oxidation combine the steam reforming-, partial oxidation-, and combustion-sections in a variety of configurations. In case of the conventional steam reforming process of natural gas, endothermic reforming and exothermic combustion take place separately in a catalytic reformer and in a furnace. The overall heat of reaction in methane steam forming is +119 kJ/mole. The necessary energy is supplied by burning parts of the feedstock in the furnace. Based on the LHV (lower heating

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value) of methane (891 kJ/mole), a theoretical amount of 0.13 mole methane has to be burned. As a result, the theoretical division between methane used as feedstock and methane used as fuel would be 88% versus 12% (1 mole versus 0.13 mole). Due to thermodynamic inefficiencies, the fraction of methane used as fuel is higher in practice than the calculated theoretical one. **Therefore, approximately 30% of the feedstock is burned and 70% is reformed to produce synthesis gas** in these processes (e.g., Hinderink et al., 1996). **This ratio is being used in the NEAT model.** The ratio differs slightly from the assumption of VCI according to which 35% of the natural gas use (for all processes, not only for ammonia production) is used as fuel (energy use) while 65% are considered as feedstock (Section 3.3.2).

In other process configurations, e.g., combined reforming, where combustion and reforming reactions take place in the same reactor, the division between input used as fuel and input used as feedstock cannot be determined in a straightforward way. It is therefore unclear from the outset, which part of the hydrocarbon input should be regarded as energy use and which part should be regarded as non-energy use.

The CO₂ emission factors for ammonia production chosen in the NEAT model are given in Table 7 and represent conservative estimates (i.e., for efficient plants) based on a literature survey done by Neelis et al. (2003). The emission factors used are on the lower side of possible ranges (compare IPTS (2004) and see also Table 18).

In the 1996 IPCC guidelines, a default emission factor of 1.5 kg CO₂/kg NH₃ is given (IPCC, 1997). This value excludes CO₂ emissions from fuel use. **In NEAT, we follow the definition of non-energy use in the German Energy Balance, thereby including the parts of heavy oils used as fuel but excluding the fuel use of natural gas. Therefore, CO₂ emissions from fuel use of heavy oil are zero.**

Table 7: Overview of CO₂ emission factors for ammonia production (based on Neelis et al. (2003))*

Feedstock	CO ₂ emissions from feedstock input in kg CO ₂ /kg NH ₃	CO ₂ emissions from input used as fuel in kg CO ₂ /kg NH ₃
Steam forming of natural gas ¹⁵	1.12	0.48
Partial oxidation of oil	2.50	0.00

* Emission factors before CO₂ sequestration for urea production, no emission factor for fuel use of oil is assumed due to gross definition of non-energy use for oil products in NEB

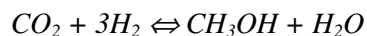
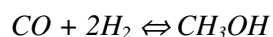
Methanol Production

Similar to ammonia, methanol is mainly produced from natural gas but depending on availability and prices of other raw material also oil products and coal may be used. Worldwide, almost 80% of the methanol is produced from natural gas (Chauvel et al., 1989). In that respect, methanol production in Germany is a strong exception. The methanol capacity is based to 73% on heavy oils, to 21% on acetylene gas, and to 5% on lignite (Patel et al., 1999). A negligible fraction of methanol is also produced from post-consumer plastic wastes. Depending on the feedstock used, either steam reforming or partial oxidation is applied. In a first step, the feedstock serves to produce synthesis gas (consisting

¹⁵ For natural gas, a split between feedstock use and fuel use of 70% versus 30% is assumed. The total emission factor of 1.6 kg CO₂/kg NH₃ originally implemented in NEAT is therefore split into 1.12 kg CO₂/kg NH₃ for feedstock use and 0.48 kg CO₂/kg NH₃ for fuel use of natural gas.

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of a mixture of hydrogen and carbon monoxide), which is then converted to methanol. The production is mainly based on the implementation of the following reactions:



Of the total feedstock used for methanol production, 1.38 t of CO₂ equivalents is embodied in each tonne of methanol, while the remainder being released as CO₂ during production. Contrary to ammonia production, the final objective in the production of synthesis gas is not to obtain a maximum hydrogen yield, but to obtain a hydrogen to carbon ratio between 2 and 3. In case of partial oxidation, the ideal H₂/CO ratio can be obtained by adjusting the oxygen content during the production process. In the steam reforming of natural gas, however, the hydrogen to carbon ratio needs to be adjusted by purging part of the excess hydrogen or by addition of CO₂ to the synthesis gas mixture. For methanol based on natural gas, the division between input used as feedstock and input used as fuel is not straightforward.

The CO₂ emission factors for methanol production as chosen for NEAT calculations base on literature study and assumptions made by Neelis et al. (2003) (Table 8). The total emission factors range by more than a factor of three depending on whether natural gas, oil, or coal is used as feedstock. In Table 8, the input to methanol production is given in CO₂ equivalents. That input is then corrected for the carbon contained in the methanol. The remaining carbon is considered to be emitted as CO₂. We again follow the definition of non-energy use in the German Energy Balance, i.e., **we choose a gross definition for oil and coal and a net definition for natural gas, thereby allocating the total amount of emissions from oil and coal input to industrial processes and the emissions from natural gas to fuel use**. Emissions from methanol consumption itself are not included in the emission factors but treated separately in the category of solvent and other product use. The data implemented as standard values in the NEAT model represent conservative emission estimates (i.e., assuming efficient plants).

Table 8: Overview of CO₂ emissions from methanol production (based on Neelis et al. (2003))

Feedstock	Total input (between brackets lowered by methanol's carbon content [CO ₂ equ.] of 1.38) in kg CO ₂ /kg CH ₃ OH	CO ₂ emissions from input used as feedstock in kg CO ₂ /kg CH ₃ OH	CO ₂ emissions from input used as fuel in kg CO ₂ /kg CH ₃ OH
Steam reforming of natural gas	1.80 (0.40)	0.00	0.40
Partial oxidation of coal	4.30 (2.90)	2.90	0.00
Partial oxidation of oil	2.80 (1.40)	1.40	0.00

Carbon Black Production

Carbon black is produced in Germany to 70% from heavy oil fractions and to 30% from carbon-black-oils ('Russöle') (Patel et al., 1999). A negligible amount of carbon black is also derived from acetylene. More than 95% of the world's carbon black production is produced in the furnace black process. The major advantage of the furnace black process its is great flexibility in manufacturing various grades of carbon black. However, also other processes can be used to produce small amounts of special grades of carbon black (Voll et al., 1997).

The heart of the furnace black process is a furnace in which the carbon black is formed. The oil feedstock is injected in a high temperature zone, which is achieved by burning fuel with air. The

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available oxygen is not sufficient for the complete combustion of fuel and feedstock. Therefore, the latter is pyrolysed and forms carbon black. During this process, 54-67% of the feedstock's carbon becomes embodied in the product, while the remainder is oxidized and results in CO₂ emissions. Natural gas is normally used as fuel for the furnace black process, but other gases (e.g., coke oven gas) are also occasionally used (Voll et al., 1997). The furnace black process also generates tail gas, which is available at high temperature and contains a certain amount of combustible gasses. The gas must be burned off for environmental reasons and the resulting energy can be used to generate steam or electricity. It is difficult to make a clear distinction between feedstock use and fuel use in the furnace black process, due to process configurations (i.e., oil and gas are fed into one single reactor) and due to the utilization of tail gas as energy source. Possible methods to allocate CO₂ emissions to either feedstock use (non-energy use) or fuel use are:

- The total carbon input is regarded as non-energy use or (ii) only the part of carbon-input, which is finally embodied in the product is regarded as non-energy use.
- Only the carbon input required for the production of energy (steam, electricity) is regarded as energy use.
- All natural gas is allocated to energy use and the input of heavy oils is allocated to feedstock use.

As for the other processes considered so far, we divide the inputs into partly feedstock use and partly energy use in accordance to the German energy statistics. As explained in Section 3.3.2, the total input of heavy oils is regarded as non-energy use. According to Rothermel (2004), natural gas consumption for carbon black production is excluded from the non-energy use data (Section 3.3.2) and the resulting emissions must consequently be allocated to fuel use. As a result of this approach, the industrial process emissions from natural gas consumption are zero. Table 9 gives an overview of typical feedstock use and emission factors for carbon black production. The data used in the NEAT model represent conservative estimates (i.e., assuming efficient plants).

Table 9: Overview of total CO₂ emissions from carbon black production (based on Neelis et al. (2003))

Feedstock	Industrial process emissions in kg CO ₂ /kg carbon black	CO ₂ emissions from feedstock used as fuel in kg CO ₂ /kg carbon black
Oil	1.77	0.00
Natural gas	0.00	0.15

The emission factor for the more efficient semi reinforced carbon black process is used as standard emission factor in the NEAT model. Comparing that value with data from other literature sources, it again becomes clear that the NEAT model generates conservative estimates for the total CO₂ emissions of carbon black production. If specific values for feedstock use in less efficient carbon black processes were used, the total process input would be around 20% higher. As a result, CO₂ emissions would be 60% higher than the emissions calculated by NEAT (Neelis et al., 2003).

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Chemical Conversion Losses due to the Production of Intermediate and Final Chemicals

The production of intermediate and final chemicals (e.g., ethylene dichloride, acrylonitrile, polyvinylchloride) leads to direct CO₂ emissions, off-gases, and non-specified by products due to incomplete conversion processes. Emissions result mainly either from direct carbon losses or partial oxidation of feedstock. The process specific CO₂ emissions as implemented in NEAT are given in Table B2 in Appendix B and base on the work of Neelis et al. (2005c).

Production of Non-ferrous Metals, Ferroalloys, and Other Inorganics

NEAT models also the use of solid carbon for the production of various metals, alloys, and inorganic chemicals. In these production processes, carbon is either used in form electrodes or as direct reducing agent. During metal and alloy production, the carbon becomes partially oxidized.

While there is no doubt that carbon used in electrodes represents a form of non-energy use, this is less obvious for carbon consumed as direct reducing agent because the latter could also be considered as fuel use. However, emissions from carbon use as reducing agent are generally small and can be neglected. The emission factors for all processes currently implemented in NEAT are based on IPTS (2001) and Ullmann (1997). **The use of coke and other reducing agents for the production of pig iron in blast furnaces is usually accounted for in the conversion part of energy balances (together with power production, refineries, and coke production) and is therefore not included in NEAT (Table 10).**

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Table 10: Overview of CO₂ emissions factors from the production of metals and inorganics (IPTs, 2001, Ullmann, 1997)

	Input raw materials in %			Specific CO ₂ emissions in kg CO ₂ /kg product
	Pet coke	Pitch	Coke/coal	
<i>Use of carbon electrodes</i>				
Primary aluminum	84	16	0	1.55
Electric steel	70	30	0	0.01
White phosphorus	72	28	0	0.18
Ferrosilicon	72	28	0	0.17
Silicon metal	85	15	0	0.36
Calcium silicon	85	15	0	0.32
Ferromanganese	72	28	0	0.04
Silicomanganese	72	28	0	0.09
Ferrochromium	72	28	0	0.06
Ferrochromiumsilicon	72	28	0	0.11
Magnesium	85	15	0	0.05
Ferronickel	72	28	0	0.01
Tin	85	15	0	0.04
<i>Use of other solid carbon</i>				
White phosphorus	6	0	94	4.18
Titanium dioxide	100	0	0	0.49
Ferrosilicon	0	0	100	2.75
Silicon metal	100	0	0	4.49
Calcium silicon	0	0	100	2.39
Ferromanganese	0	0	100	1.75
Silicomanganese	0	0	100	1.57
Ferrochromium	0	0	100	1.57
Ferrochromiumsilicon	0	0	100	2.71
Lead	0	0	100	0.64
Ferronickel	00	0	100	1.35
Tin	0	0	100	1.08
Zinc	0	0	100	0.43
Calcium carbide	15	5	80	1.10
Silicon carbide	100	0	0	2.30

General Uncertainties

All emission factors given for industrial process emissions are subject to various uncertainties. To discuss those in greater detail would go far beyond the scope of the NEAT model description. In general, emission factors, which represent the lower range of possible emissions are used for NEAT calculations. The model results for CO₂ emissions from industrial processes can therefore be regarded as estimates for efficient plants representing state-of-the-art technology. The choice for conservative emission factors was made to avoid overestimation of industrial process emissions in the NEAT model.

4.2.1.3 Emissions from Waste Treatment

The NEAT model contains a waste module for estimating both the amount of fossil carbon embodied in post-consumer wastes and the fossil-based CO₂ emissions originating from waste treatment (this is a new feature of NEAT 3.0, which was not yet available in Version 2.0). To this end, we distinguish between four categories of waste treatment:

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- Solid waste disposal on land (land filling)
- Incineration with energy recovery
- Wastewater treatment
- Other waste treatment

In the following, we describe methodology and main assumptions chosen for the various categories of waste treatment.

Land filling

According to UBA (2004b) there occurs virtually no oxidation of fossil-based carbon in landfills. Therefore, the amount of fossil-based CO₂ emissions originating from landfills is zero. An exception, however, are plasticizers (especially from PVC waste) and fuel or lubricant contaminated wastes. We assume, however, that the amounts of oxidized carbon from these sources are negligible.

Waste Incineration

In this category, we apply two approaches, a *top-down* and a *bottom-up* approach. Both approaches take into account that **there is no waste incineration without energy recovery in Germany** (UBA, 2004c). **The resulting CO₂ emissions from waste incineration should therefore be reported as secondary fuel use emissions in the source category ‘energy’ of the National GHG Inventory. The non-energy use emissions from waste incineration are thus zero.** In the *top-down* approach we multiply the total municipal waste incinerated (Destatis, 2002) with its average fossil carbon content (i.e., 8% based on Dehoust et al. (2002)). The average oxidation rate of fossil carbon containing products during incineration is assumed to be 99%. The amounts of emitted carbon are multiplied with a factor of 44/12 to convert the masses of carbon into CO₂ equivalents. Uncertainties related to the chosen approach concern the rather rough percentages regarding the shares of (i) incinerated municipal waste and (ii) fossil carbon content and furthermore the disregarding of industrial wastes.

To cross check the results of the *top-down* approach, a *bottom-up* approach was developed, which accounts for the incineration of (i) total plastics and (ii) *other chemicals*. The fractions of fossil-based carbon in plastics are readily available from the NEAT model and allow calculating the total weighted average carbon content of various polymers. Again, we assume that 99% of all carbon contained in plastics is oxidized during incineration. Based on the production ratios, we assume that *other chemicals* account for 30% of total plastics incineration. We furthermore make the rough assumption that 50% of the carbon contained in *other chemicals* is already oxidized during product use.

We include under *other chemical* products also the consumption of secondary fuels in the cement industry. The secondary fuels used in the cement industry are usually not part in the category of ‘*municipal waste incineration*’. However, overlapping with the former category might be possible. The emissions from incineration of secondary fuels are not accounted for under non-energy emissions as they are reported in the category of ‘*energy*’ in the National Greenhouse Gas Emission Inventories.

Wastewater Treatment

We distinguish in NEAT between two sources for emissions originating from wastewater treatment, i.e., ‘*domestic and commercial wastewaters*’ and ‘*wastewater from the chemical industry*’.

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We only account in NEAT for treated wastewaters. Unused water discharged from industry or untreated municipal and industrial wastewaters are excluded from our calculations. This is justified because the fossil carbon content in these waters is generally negligible.

We consider surfactants to be the main source of fossil carbon in *domestic and commercial wastewaters* and therefore limit our calculations to the study of emissions due to the oxidation of surfactants. To estimate the fossil carbon content and related emissions, we use the average consumption of surfactants in Germany (i.e., 450 kt per year), multiplied with their average fossil carbon content (data based on Patel (1999)). We assume further 100% oxidation of all surfactants contained in the wastewater. **We do not distinguish between oxidation, which occurs during the actual treatment of the wastewater and the subsequent processing of sewage sludge.** The data used on the domestic consumption of surfactants leads to an approximation of the *real* emissions, which are actually determined by the final consumption of surfactants in the form of end products such as shampoos and other detergents.

For explanation: The consumption of surfactants as determined based on data from industrial associations and foreign trade statistics represent the domestic input to the detergent industries, which makes final products by combining surfactants with scents, fillers, bleaching agents and other components. These final products are traded internationally. The quantities of final detergent products consumed domestically and their composition determine the emissions in the country studied. Since detailed data are not available at the level of final detergent products, we use data on domestic surfactant use as a first proxy.

Next to domestic and commercial wastewaters we also account for CO₂ that originates from wastewater from the chemical industry. The fossil carbon in the wastewater of the chemical industry originates from incomplete conversions and other losses that are discharged via the water phase. The absolute content of fossil carbon in industrial wastewaters is calculated by multiplying the total amount of wastewater with the average concentration of fossil carbon in industrial wastewaters. We assume a ratio between direct and indirect discharge of industrial wastewaters of 0.15. Therefore, 15% of all industrial wastewaters are treated in municipal wastewater treatment plants. The remaining 85% are treated directly in industrial wastewater treatment plants. The ratio of TOC to COD is assumed to be 0.375. We take into consideration that 8% of the discharged carbon is derived from renewable feedstock. We assume an oxidation rate for carbon containing chemicals of 100% (Patel et al., 1999). We do further not distinguish between oxidation, which occurs during the actual treatment of the wastewater and the subsequent processing of sewage sludge. **We thereby express the amounts of carbon emitted in CO₂ equivalents by simply multiplying the emitted carbon with a factor of 44/12. We hence assume, that all carbon released is oxidized instantaneously to CO₂ once entering the atmosphere. This is a simplification as fractions of carbon may be more persistently fixed in organic compounds (e.g., NMVOCs).**

Other Waste Treatment

NEAT does also account for other waste treatment such as the treatment of biological waste, contaminated soils, as well as biological-mechanical, and chemical-physical waste treatment, and waste treatment in shredding facilities. However, we assume that all of these waste treatment technologies do not result in fossil carbon emissions. That is because (i) biologic waste is assumed to contain no fossil carbon, (ii) shredding and biologic-mechanical waste treatment does not lead to oxidation of fossil carbon contained in products, and (iii) the chemical-physical waste treatment mainly aims at recycling

of wastes (e.g., waste oils). Fossil CO₂ emissions originating from *other waste treatment* are therefore negligible.

4.2.2 Stage 2: Calculating Total Non-energy Use, Carbon Storage, Carbon Storage Fractions and Total Fossil CO₂ Emissions

In the preceding Section, we have systematically dealt with all carbon flows related to the non-energy use of fossil fuels. **In NEAT, we use the previous results to estimate total non-energy use, carbon storage, and carbon storage fractions *independently* from official energy statistics.** Using data on the total primary energy supply as additional model input, we can furthermore calculate total CO₂ emissions from the consumption of fossil fuels in Germany. The following sections describe separately the methodology used to calculate each of the mentioned parameters.

4.2.2.1 Calculating Total Non-energy Use

As already mentioned in Chapter 3, total non-energy use of fossil fuels consists of two elements:

- the consumption of fossil fuels as feedstock
- the consumption of refinery and coke oven products for non-energy purposes (e.g., bitumen and lubricants)

The first element is estimated by adding (i) the CO₂ equivalents of all basic chemicals domestically produced from non-energy use feedstock in the chemical industry (excluding refineries) and (ii) the sum of all industrial process emissions resulting from feedstock use as calculated with NEAT.

The second part of non-energy use can be estimated by adding (i) the consumption of non-energy use refinery and coke oven products and (ii) the sum of all industrial process emissions resulting from the use of solid carbon for the production of metals and inorganic chemicals¹⁶.

The calculation of the total non-energy use can be summarized with the following formula:

$$NEU [CO_2] = \Sigma Feedstock\ use [CO_2] + \\ \Sigma Consumption\ of\ refinery\ and\ coke\ oven\ products [CO_2] + \\ \Sigma Industrial\ process\ emissions\ from\ solid\ carbon\ use [CO_2]$$

Feedstock Use

In Stage 1 of the model, we aimed at estimating emissions from *solvent and other product use* related to the final consumption of downstream chemicals (E4 in Figure 2). In contrast, an upstream carbon flow is now estimated to determine feedstock use in NEAT. This implies, that the carbon flow studied here differs from the one discussed in Stage 1 of the NEAT model. Now, we are interested in

¹⁶ Note that we distinguish here between industrial process emissions resulting from feedstock use and industrial process emissions resulting from the consumption of refinery products, i.e., electrodes, which are mainly produced from pitch and heavy tars. This distinction is, however, more of methodological importance and less relevant for actual emissions accounting.

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the equivalent feedstock requirements to produce all ODU products as well as all NODU products modeled in Stage 1.

Figure 4 shows the methodological differences at the example of ethylene derivatives: So far, it was our goal to estimate the amount of ethylene derivatives (such as polyethylene, ethylene oxide, or ethanol) used for the production of ODU products. Those products are oxidized during use and result in CO₂ emissions within the inventory year (450 kt in the example of Figure 4, *downstream* perspective). In contrast, we are now interested in the amount of feedstock used for total ethylene production (600 kt in the example of Figure 4, *upstream* perspective). To estimate the latter, it is not necessary to study all the downstream materials produced from ethylene. It is sufficient to know the amount of ethylene produced in the country of study. The value for the production of ethylene is obtained from official production statistics (in fact, the data has already been collected for Stage 1 of the NEAT model).

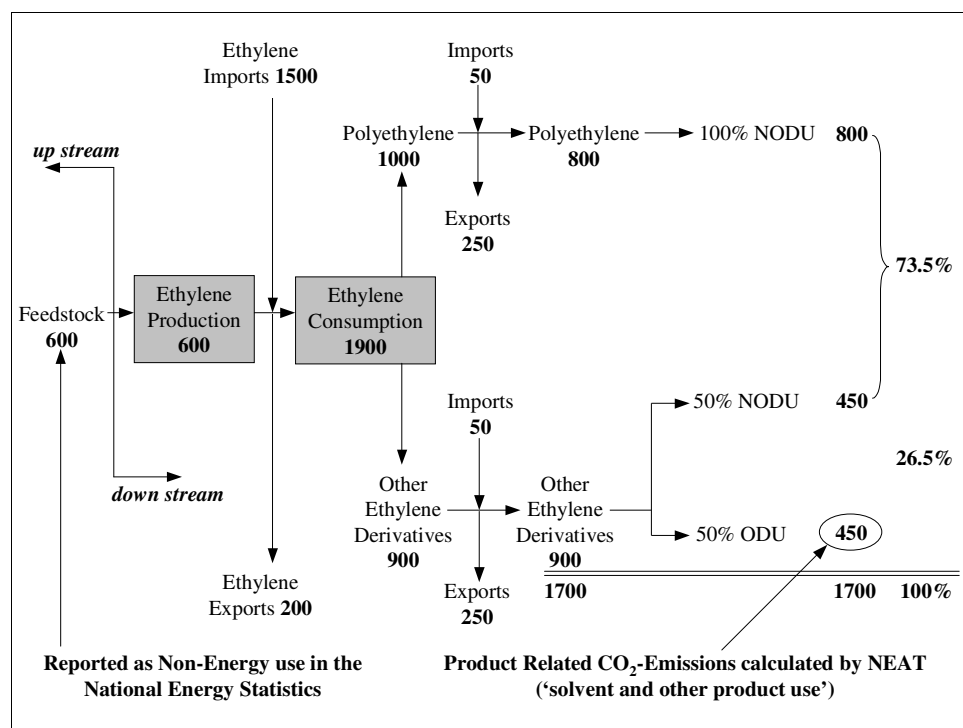


Figure 4: Hypothetical Example for ethylene production (Neelis et al., 2003)

In more general terms, estimates for total feedstock use can be obtained by adding up the CO₂ equivalents of *all* basic chemicals (not only ethylene) produced from hydrocarbon feedstock. The production values of the following chemicals thus be added: acetylene, benzene, butadiene, carbon black, other C₄ compounds, synthesis gas (CO), ethylene, methanol, propylene, toluene, urea and xylenes. In total, this yields an estimate for the (pure) *net* feedstock use.

Gross feedstock use includes (i) carbon losses during the production process, which are released as industrial process emissions, (ii) CO₂ emissions resulting from the combustion of parts of the feedstock for energy purposes, and (iii) backflows from steam crackers to refineries. Depending on the exact definition of non-energy use, which may be somewhere between pure *net* and pure *gross* depending on the fuel commodity and the country, industrial process emissions and CO₂ emissions from fuel combustion are added to the sum of CO₂ equivalents contained in basic chemicals in order to determine the amount of hydrocarbons used as feedstock (the first element of total non-energy use).

Refinery and Coke Oven Products

The second element of total non-energy use consists of the consumption of non-energy refinery and coke oven products. Of all NEAT core chemicals, bitumen, lubricants, petroleum coke, pitch, creosote oil, naphthalene, as well as waxes and paraffins are non-energy use refinery and coke oven products. In the energy statistics, the trade of these products is already taken into account. For this reason, the non-energy use of these products as reported in the energy statistics represents the *consumption* and not the *production*. In NEAT we therefore use consumption values for bitumen, lubricants, petroleum coke and waxes/paraffins to calculate total non-energy use.

Further Calculations

The total non-energy as calculated with NEAT can be allocated to the various fuels used for non-energy purposes as they are reported in the IPCC-RA of the National GHG inventory. For industrial process emissions and for some of the product-related non-energy use (e.g., bitumen or lubricants), the allocation is straightforward. The remainder of the product-related non-energy use is allocated to the mix of feedstocks from which the respective hydrocarbons are produced. The non-energy use resulting from ethylene production is, for example, allocated to the steam cracker feedstock given in Table 6. The NEAT results for non-energy use can therefore be compared with non-energy use data as stated in the Energy Balance and in the IPCC-RA in terms of totals and on a fuel-by-fuel basis (see Section 5.4.1).

4.2.2.2 Calculating Carbon Storage, Carbon Storage Fractions and Total Fossil CO₂ Emissions

Based on total non-energy use (in CO₂ equivalents) and the calculated emissions from non-energy use, the NEAT model provides estimates for carbon storage, carbon storage fractions, and the total CO₂ emissions from fuel combustion. An overview of the calculation procedures is given in Figure 5.

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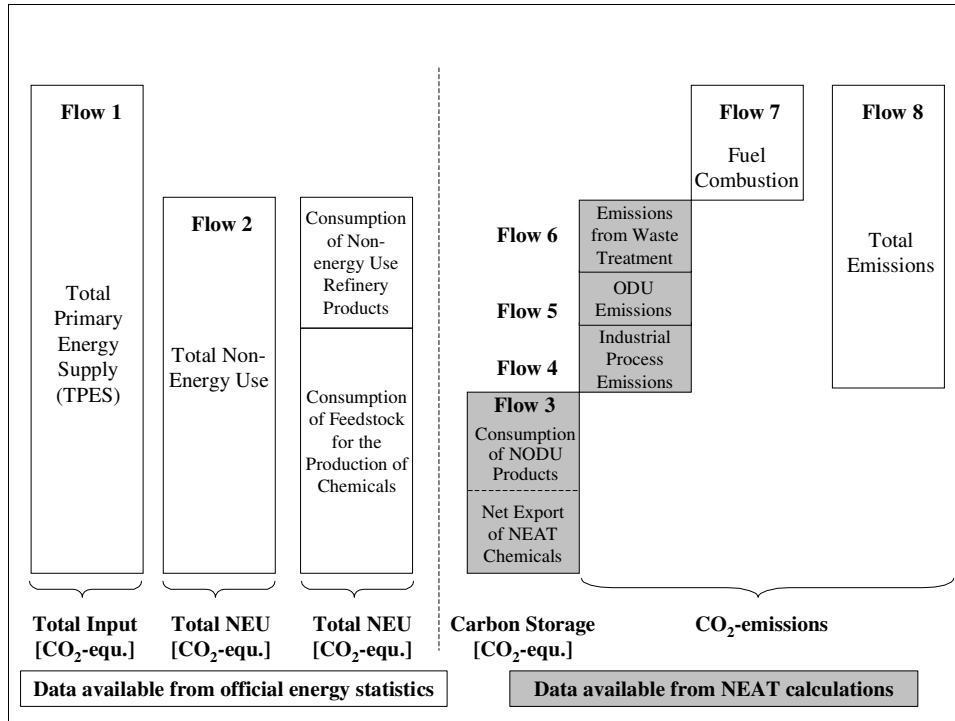


Figure 5: Storage and release of CO₂ according to NEAT (Neelis et al., 2003)

The total primary energy supply (TPES), multiplied with the CO₂ emission factors for the various fuels, yields a value for the total CO₂ emission potential of the country (Flow 1 in Figure 5). Part of this total CO₂ emission potential is used for non-energy purposes (Flow 2), the remainder is related to fuel combustion (Flow 7). The CO₂ equivalents of non-energy use are partly emitted as emissions from *solvent and other product use* (ODU products), partly as *industrial process emissions*, and partly as emissions from *waste treatment* (Flow 4-6)¹⁷. The remainder is stored and hence not emitted (Flow 3).

Carbon Storage

A further explanation of the carbon storage is given in Figure 6. Carbon storage according NEAT consists of two elements:

- the consumption of NODU products in Germany
- the *net* export of all basic chemicals, intermediates, and final products included in the NEAT model (excluding the non-energy use refinery and coke oven products for which trade is already accounted for in the energy statistics)

¹⁷ Only emissions released during wastewater treatment are regarded as non-energy use emissions. CO₂ resulting from waste incineration is generally reported as emissions from energy use in the National GHG inventories.

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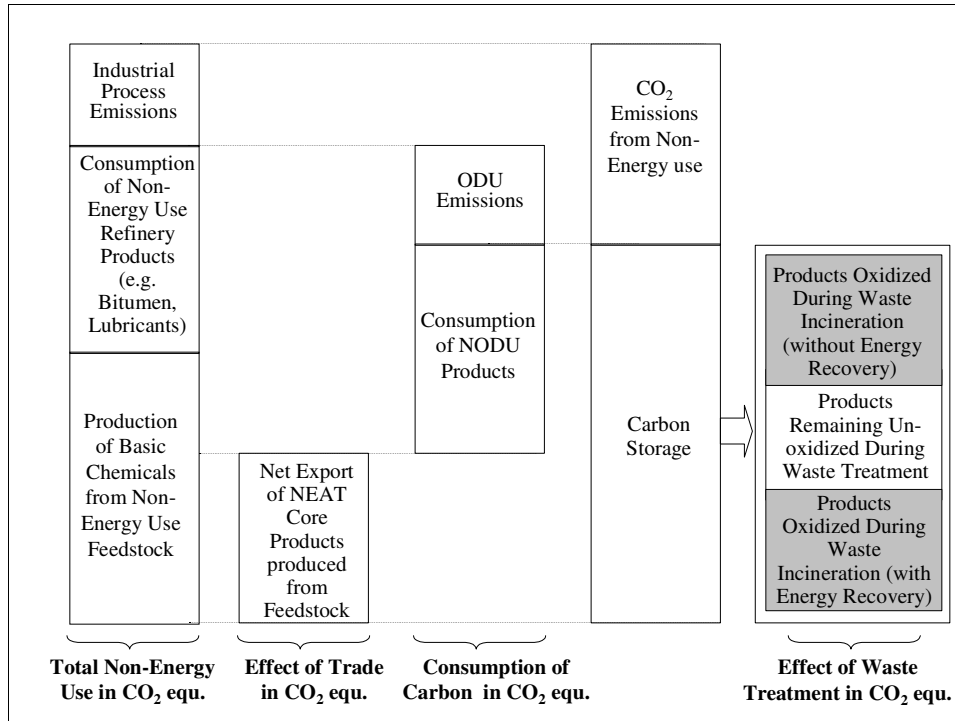


Figure 6: Carbon storage in the NEAT model (Neelis et al., 2003)

The ODU emissions and the consumption of NODU products are estimated in Stage 1 of the model (where we divide the consumption of end products and derivatives not used for other purposes into a part ODU and a part NODU, see Section 4.2.1.1). The *net* export of all basic chemicals is equal to the difference between the non-energy use (excluding industrial process emissions, see Figure 6) and the total consumption of carbon in Germany (ODU emissions and NODU products). It is important to note two important features of the carbon storage calculations:

- For *net* importing countries, *net* exports become negative. The resulting storage can therefore also be negative. Examples are countries without a basic chemical industry (i.e., no fossil fuels are used for non-energy purposes and the total non-energy use is zero), but with imports of chemicals that are oxidized during use. For such a country, the total emissions (Flow 8 in Figure 5) might exceed the total primary energy supply within the country (Flow 1 in Figure 5). Given is a hypothetical example a country without a basic chemical industry (non-energy use = 0) that imports 2 Mt CO₂ equivalents of ODU products. The first element of the carbon storage would be 0 Mt CO₂ equivalents and the second element would be -2 Mt CO₂ equivalents. This would result in an overall carbon storage of -2 Mt CO₂ equivalents.
- The carbon storage calculated with NEAT is independent from the definitions chosen for non-energy use. It only depends on the consumption for ODU and NODU products in NEAT. Therefore, NEAT estimates for the total CO₂ emissions within the country can be generated without knowing the definition of non-energy use in the German energy statistics.

Carbon Storage Fractions

Based on carbon storage and total non-energy use, NEAT also calculates carbon storage fractions for use in the IPCC-RA. The country-specific standard NEAT storage fractions for carbon are determined by dividing the carbon stored (Flow 3 in Figure 5) by the total non-energy use (Flow 2 in Figure 5). Both storage (Flow 3 in Figure 5) and emissions (Flows 4-6 in Figure 5) can be allocated to the various fuels that are used for non-energy purposes. For industrial process emissions, this allocation is relatively simple (e.g., CO₂ emissions from ammonia production are allocated to the feedstock used to produce ammonia). However, allocation is more complex for product-related emissions and carbon storage. There, the downstream emissions have to be allocated back to upstream fuels. As an example, all NEAT products derived from steam cracker outputs have to be allocated back to the feedstock used as steam cracker input. This allocation can be done by means of the mass balance prepared in Stage 1 of the NEAT model. A careful allocation to the various fuels finally allows the calculation of standard NEAT storage fractions by fuel types and makes it therefore possible to compare NEAT results with the values reported in the IPCC-RA on the level of individual fuels.

Total Fossil CO₂ Emissions

Deducting the carbon storage from the total CO₂ potential of all fossil fuels domestically consumed yields an estimate for the *total* fossil CO₂ emissions (see Flow 8 in Figure 5). This estimate for the *total* fossil CO₂ emissions includes both emissions from non-energy use and emissions from fuel combustion in all other sectors of the economy (direct fuel use in all industrial sectors, the service sector, households and transportation). The calculation procedure for the total fossil CO₂ emissions obtained with NEAT is identical to the one used for the total fossil CO₂ emissions according to the IPCC-RA. The two can therefore directly be compared with each other.

4.2.3 Stage 3: Comparison of NEAT Results with Data from Official Sources

Both NEAT and the IPCC-RA calculations start out with the total primary energy supply for calculating total fossil CO₂ emissions. Differences regarding emission estimates are therefore caused by:

- differences between total non-energy use as determined by NEAT (see Flow 2 und Figure 5) and the IPCC-RA
- the division between carbon stored (Flow 3 in Figure 5) versus carbon emitted (Flow 4-6 in Figure 5) in NEAT and in the IPCC-RA (This division is (i) calculated on basis of a material flow analysis in NEAT and (ii) based on storage fractions as determined by PROGNOSE (2000) in the IPCC-RA.

Referring to the first point, the total non-energy use as determined with NEAT is based on production and trade statistics. NEAT estimates are therefore fully or largely independent¹⁸ from the non-energy use as reported in energy statistics as well as in the IPCC-RA. A comparison between the

¹⁸ When applying the NEAT model to a given country it is sometimes turns out to be difficult or even impossible to ensure *full* independence from official energy statistics for *all* fuel commodities because the data derived from production and trade statistics may be erroneous for certain fuels, which in turn requires the using of other data sources for NEAT modeling.

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NEAT estimate for non-energy use and the non-energy use according to official energy statistics can hence serve several purposes:

- It serves as check for completeness and consistency of the material flow analysis in NEAT. If, for example the NEAT results for non-energy use are clearly higher than the values reported in the national energy statistics, this might be an indication of double counting in the model. The opposite could indicate that important products and processes have been overlooked in NEAT.
- It can help identifying erroneous non-energy use data as published in the national energy statistics.
- It can reveal information on the definition of non-energy chosen in the National Energy Balance.

Figure 7 shows several possible definitions for non-energy use as a function of system boundaries chosen. The decision about which system boundary to chose does obviously not influence the total CO₂ emissions but has an effect on the emissions allocated either to the categories *energy* or *non-energy use*. It hence also influences the value for non-energy use as estimated with the NEAT model. Therefore, the NEAT model allows calculating non-energy use in a very flexible way to account for the specific definition of non-energy use as chosen in the Nation GHG inventory.

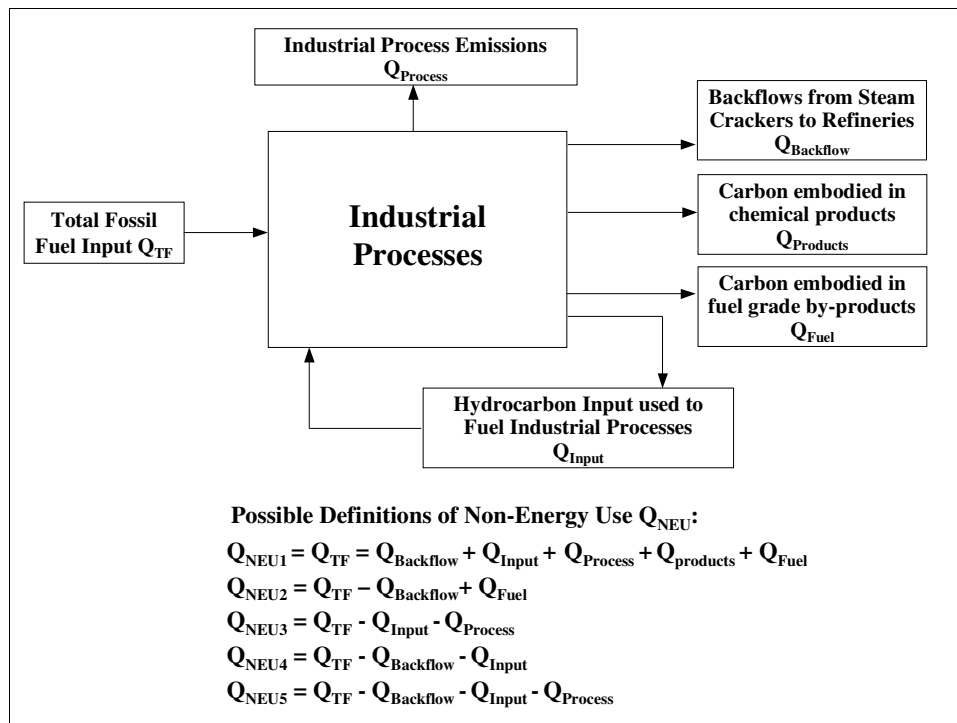


Figure 7: Overview of possible definitions for non-energy use (Neelis et al., 2003)

A detailed discussion of the definition chosen for non-energy use in the German Energy Balance can be found in Section 3.3. The NEAT results are shown and discussed in Chapter 5 of this report.

Elaborating the exact definition of non-energy use chosen in the Energy Balance is an iterative process in which the model user should use both NEAT results and the non-energy use data as given in the Energy Balance. If, for example, a country produces methanol from natural gas but does not report non-energy use of natural gas in the energy statistics, then this is an indication that this process is not properly accounted for in the Energy Balance. As a consequence, the CO₂ emissions according to the National GHG inventories would be too low. In reality, this situation is rather unlikely because fuel use is reported by companies and not per individual processes. It would hence be more likely that the natural gas use for methanol is allocated to energy use in the energy statistics instead of being assigned to non-energy use. As a consequence, CO₂ emissions would be overestimated in the National GHG inventories as fuel use results in direct emissions upon combusting the respective hydrocarbon.

When calculating carbon storage fractions, the carbon storage (Flow 3 in Figure 5) can either be based on the NEAT results for non-energy use (Flow 2 in Figure 5) or it can be based on non-energy use data as used in the IPCC-RA. The latter value can differ from the NEAT results. By dividing the carbon storage as calculated with NEAT by the total non-energy use from IPCC-RA (instead of Flow 2 in Figure 5 from NEAT), so-called *adapted* NEAT storage fractions can be determined. In the ideal case, where non-energy use calculated by NEAT equals the non-energy use in the IPCC-RA calculations, the storage fractions with and without adaptation are the same. Experience, however, shows that it is very difficult to arrive at identical values.

The NEAT model contains several elements that can be particularly useful for the preparation of CO₂ emission inventories in accordance to the IPCC-SA. Examples are the emission factors for steam cracking and for other industrial processes, i.e., production of ammonia, methanol, or carbon black. NEAT contains emission factors for individual types of feedstock, which are used as input for the respective industrial processes.

Furthermore, the NEAT results for product use emissions (use of ODU products) can be compared with product-related emissions as they are stated in the source category of *solvent and other product use* of the IPCC-SA.

It is important to keep in mind that the 1996 IPCC guidelines provide a large degree of freedom concerning the allocation of emissions to the various source categories. This is especially true for emissions resulting from the fuel use of feedstock in industrial processes, which can be allocated to the categories '*energy*' or '*industrial process emissions*' of the IPCC-SA.

4.3 Input Data for the NEAT Model

4.3.1 Production Data for 80 NEAT Core Products

The principal sources for production data of the 80 NEAT core chemicals (see Appendix A) are the official German production statistics as published by Destatis (1990-2003a). In all years, around 10-30% of the required production data are confidential because there are only 3 or less domestic producers of the relevant chemical. In these cases, confidential production data were made available to us from Destatis via confidentiality agreements with the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety ('Bundesumweltministerium', BMU).

Mainly in the case of final chemicals (e.g., polymers such as polyamides or polyethylene) total production data had to be calculated in NEAT by adding up the production values of several individual products.

Production data for the years 1990-1994 were classified in official production statistics according to the product classification of 1989, which is not always compatible to the product

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classification used for the years after 1994. Major difficulties can arise, if several individual chemicals are aggregated under one product code and if it remains unclear, (i) which chemicals are exactly included under the production code and (ii) what is the exact share of the relevant chemical product on the total production value stated. In the product classification from 1989, parts of the production of several polymers (e.g., polypropylene, polyacrylates and polystyrene) are grouped under one single number (i.e., No. 441410). In such cases it is only possible to estimate the share of individual products on the total production.

For the year 1990 production data were only available for former Western Germany. For the years 1991 and 1992, partly data from Western Germany were used if data for the reunified Germany were not available to us. In some cases the comparison of production data with confidential data provided by Destatis seems to indicate that production data given as *total production* do indeed refer to Western Germany only. It is therefore likely that NEAT underestimates non-energy use and related emissions in the years 1990-1993 because we at least partially neglect production in the former Eastern Germany.

A critical part with respect to the accounting of non-energy use, are C₄ chemicals, i.e., butenes and butadienes. The reason is that there are various inter-linkages in the production and use of these chemicals (details can be found in Section 5.4.1. under the subsection “Non-energy use of oil-based feedstock”). In view of limited insight we proceeded as follows: We assume that the production data for butenes according to Destatis (1990-2003a) represent accurate values for pure butenes, which are used for producing chemicals and gasoline additives. We estimate the quantities used for chemical purposes based on Patel et al. (1999) for the German chemical industry in 1995. We finally assume that the remainder is returned to the refinery sector for the production of gasoline additives¹⁹.

In several cases, the mass balance calculations in NEAT raise serious doubts about the correctness of certain values stated by the official production statistics. Production data are not always reliable, for several reasons:

- The registration of technical production of intermediates within a company requires insight into the production process. Furthermore, when an intermediate is immediately used in a subsequent process step, its production might not be reported. This might lead to underreporting of various intermediate chemicals such as styrene, ethylbenzene, or cyclohexanone.
- In some cases, double counting of production can occur. For example, chemical mixtures are sometimes delivered to customer sites where the formation of the final products takes place (e.g., production of polyurethanes). In such cases, it might be possible that polymer production is reported twice, once at the ‘technical’ production site and once again at the ‘customer’ site.

In all cases, where we seriously doubted official statistics, industrial experts were interviewed for additional information. These interviews proved to be very helpful and clarifying. In most cases, experts were capable of giving round-off production capacity numbers. In other cases, capacity data

¹⁹ We assume that backflows occur in the form of pure butenes, which are therefore not included in the backflows modeled for steam crackers. The chosen approach might explain to some extent why NEAT overestimates non-energy use (related to C₄). Further research on the accounting of production and fate of not only butene but also other C₄ chemicals is required in order to ensure correct accounting of these items under non-energy use.

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and mass balance principles were used to estimate production data. In total, about 20 (varying for individual years) production values of NEAT core products were corrected based on interviews and capacity data. As reliable source for production capacities in Germany we used Chemical Week (various years).

For the whole period of 1990-2003 data for lubricants and bitumen consumption as derived from production and trade statistics (Destatis, 1990-2003a,b) deviate considerably from the values stated in the Energy Balance (see Table B3 in Appendix B). The consumption of lubricants as derived from Destatis (1990-2003 a,b) is up to 64% higher than the consumption as stated by both the IPCC-RA²⁰ and the 'Mineralölstatistik'. There are several reasons why we consider the consumption data derived from Destatis to be at least partly unreliable:

- The data show implausibly large fluctuations for individual years.
- They show an increasing trend for, e.g., lubricants and bitumen consumption (while stabilization or even decrease would be expected) and too high overall consumption levels compared to the production of basic oils in refineries.

Since lubricants are produced and traded in various mixtures (while all products independent of their position in the process chain are referred to as lubricants), it is rather likely that double counting occurs. We therefore use as input for the NEAT model lubricant data as reported in the IPCC-RA, thereby accepting the fact that the goal of full independence from the NEB cannot be reached in this point.

Regarding bitumen consumption, Destatis data show both positive and negative deviations from the IPCC-RA and 'Mineralölstatistik' data. Although the relative deviations are clearly smaller for bitumen than for lubricants ($\pm 15\%$ for bitumen) we also choose for bitumen the data reported in the IPCC-RA as NEAT model input.

Further research should aim at harmonizing the Destatis (1990-2003a,b) and the 'Mineralölstatistik' data on lubricants and bitumen consumption to allow consistent and more accurate calculation of non-energy use and related emissions in the IPCC-RA. If double counting is indeed the reason for the larger value for lubricants according to Destatis (1990-2003a,b), a more detailed/suitable classification of product categories for lubricants in the production and/or trade statistics could allow improving data quality.

Data for the production of ethylene, propylene, butadiene, toluene, and xylenes were taken from VCI (1990-2004) because the outcome of NEAT mass balance calculations and expert interviews raised serious doubts about the reliability and consistency of production data from Destatis (1990-2003a) (Rothermel, 2004, VCI, 2005).

Furthermore, Destatis production data for polymers (e.g., polyamide, polyvinylchloride, or polypropylene) were too high in all years, compared to (i) the amounts of basic and intermediate chemicals available for the production of polymers according to the NEAT mass balance, (ii) data for German production capacities, and (iii) production data as published from Consultic (1997-2003). For around 6 polymers (polyethylene, polypropylene, polystyrene, polyvinylchloride, and polyamide) we therefore used data from Consultic (1997-2003) and not official data from the Destatis production

²⁰ In the German Energy Balance, the non-energy use of the oil products bitumen and lubricants is part of the category 'other oil products'. The IPCC-RA states data for the subcategories 'bitumen', 'lubricants', and 'coal oils and tars', which allows comparisons at a more detailed level.

statistics. Production values for adiponitrile were not available from Destatis (1990-2003a) in all years. We therefore used estimates, based on NEAT mass balance calculations.

4.3.2 Trade Data for 80 NEAT Core Products

The principal sources for trade data, i.e. exports and imports of the 80 NEAT core chemicals are the official trade statistics for Germany as published by Destatis (1990-2003b). In all years, around 20-40% of the required trade data are either confidential or only given as aggregated values, with the latter also including chemicals, which are not relevant as NEAT model input. In these cases, confidential trade data were made available to us from Destatis via confidentiality agreements with the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety ('Bundesumweltministerium, BMU). As is the case for production, also export and import values for many final chemicals (e.g., polymers such as polyamide or polyethylene) were calculated by adding up data of several individual chemicals. Trade data for adiponitrile were not available in all years. We therefore assumed imports as well as exports to be zero and the total consumption of this intermediate chemical to equal domestic production. Furthermore, for naphthalene und anthracene in the years 2001-2003, export data were not available. We used, therefore, the fraction of export/import in the year 2000 to calculate exports for the years 2001-2003.

Apart from NEAT core products, also the trade of around 450 additional chemicals is taken into account (see Table A7 in Appendix A). The additional trade data for Germany were obtained only for the years 1990, 1995, 2000 and 2003 from Destatis (1990-2003b).

4.3.3 Input Data for Industrial Processes

The only data input required in NEAT for the calculation of feedstock use and related CO₂ emissions of steam crackers are the production values of ethylene and the specific feedstock shares. Data for ethylene production in Germany were taken from VCI (1990-2004). Confidential data for the absolute amounts and the shares of specific steam cracker feedstock were obtained from the VCI (Rothermel 2004). Roughly two thirds of the steam cracker input in Germany is naphtha. The remaining one third comprises gas oil, ethane, propane and butane. The composition of steam cracker feedstocks in Germany is very similar to the European average and remains fairly constant over the years. Due to confidentiality of the data, the exact deliveries of feedstock in the individual years are not shown in this report.

Similar to steam crackers, only data on production volume and on specific feedstock composition are required in NEAT to model non-energy use and related CO₂ emissions from the production of ammonia and methanol. In both cases, production data were derived from Destatis (1990-2003a). The specific feedstock composition for ammonia production was estimated on the basis of personal communication with ammonia producers. Around 70% of the German production capacity for ammonia is based on natural gas while roughly 30% of ammonia is produced from heavy oils. The specific feedstock composition for methanol production was derived from Patel et al. (1999) (Table 11).

Methodology

Table 11: Specific feedstock composition for methanol production in Germany (Patel et al., 1999)

Feedstock	Heavy fuel oils	Natural Gas	Coal
Specific share	73%	22%	5%

To model non-energy use and related emissions for carbon black production, only production volumes of carbon black are needed as model input. These were derived from Destatis (1990-2003a).

Similarly, for modeling conversion losses in NEAT, no other data than production data of the 80 NEAT core is required.

To model electrode and solid carbon use for the production of non-ferrous metals, ferroalloys and other inorganic chemicals, production volumes of the respective materials are required as only model input in NEAT. These data were obtained from Destatis (1990-2003a). However, 20-30% of the required production data were confidential in the official production statistics. In these cases, confidential data were made available from Destatis via confidentiality agreement with the Federal Ministry for the Environment (BMU).

4.3.4 Input Data for Waste Treatment

Data for waste disposal in landfills were derived from Destatis (2002) and from personal communication with experts from UBA (2004b). The fractions of fossil carbon contained in the waste are calculated based on Dehoust et al. (2002). Data for *bottom-up* estimates of total plastics and other chemicals disposed in landfills are derived from APME (1991-2003). APME data refer only to typical plastics applications (e.g., moulding, thermo-forming) but neither include synthetic rubber materials nor textile fibers (APME, 2005). For the years before 1997, the exact data for plastic waste disposed on German landfills are not given explicitly in APME (1991-2003). We therefore estimated the amounts by assuming the same shares as in 1997. The fractions of fossil-based carbon in plastics are obtained from the NEAT model and represent the average of the carbon content of various polymers.

Data for waste incineration are derived from Destatis (2002). As in the case of waste disposed in landfills, the fractions of fossil carbon are calculated based on Dehoust et al. (2002). Data for plastics incineration are derived from APME (1991-2003). For the years before 1997, plastics incineration is not given directly but only the totals of plastics waste. We therefore apply the same share as in 1997 also to previous years. We included in NEAT also data for the consumption of secondary fuels in the cement industry, which were derived from VDZ (2004).

In the case of wastewater treatment, data on the amounts of surfactants consumed in Germany are derived from Patel (1999) and crosschecked with data given by Kaiser et al. (1998) and Assmussen (2000). Data on the amounts of industrial wastewater treated are derived from Destatis (1998, 2001, 2005). For years where no data were available, we estimated missing values by inter- and extrapolation. The average concentration of fossil carbon in industrial wastewaters is derived from VCI (2004a). For the years 1990-1994 estimates based on the value for 1995 are used because no other reliable data were available.

As bottom-up estimate for fossil carbon loads contained in wastewaters we used (i) data for surfactant consumption from UBA (2005) and (ii) data for surfactant production from Patel (1999) and TEGEWA (2005). The average content of fossil carbon in the various types of surfactants is derived from Patel (1999).

The data for other waste treatment technologies, e.g., treatment of biological wastes, shredding, biologic-mechanical as well as physical-chemical waste treatment, are derived from Destatis (2002). For years where no data were available, inter- and extrapolation was used to calculate estimates.

5 Results

This chapter presents:

- Emissions from product use as calculated with NEAT and as stated in the IPCC-SA
- Emissions resulting from industrial processes as calculated with NEAT and as stated in the IPCC-SA
- Fossil emissions resulting from waste treatment as calculated with NEAT and as stated in the IPCC-SA
- NEAT results on total non-energy use, carbon storage, and carbon storage fractions as well as a comparison of these results with the data given by the IPCC-RA

5.1 Product Use Emissions

In the NEAT model, emissions from product use are calculated based on the fraction of ODU (oxidized during use) products consumed. The complement of ODU emissions is the amount of carbon that remains stored in non-oxidized during use (NODU) products.

It is important to note that (unlike industrial process emissions) emissions from product use consist to a large extent not of direct CO₂ emissions but rather of NMVOCs. As NEAT is a carbon flow accounting model, we estimate the amount of carbon contained in emissions and express it uniformly (regardless whether emissions are actual CO₂ or NMVOCs) in CO₂ equivalents. The estimates for product use emissions as expressed here in CO₂ equivalents do not account for the higher greenhouse potential of NMVOCs relative to actual CO₂. They serve only as standard unit for carbon emissions accounting in NEAT.

An important new insight gained in this study is that the NEAT model calculations for product use emissions are highly uncertain. We observed a big gap between (i) the NEAT model calculations and (ii) our additional bottom-up estimate. However, there is no basis for considering one more reliable than the other. It is, however, very possible that the bottom-up calculations lead to underestimation, while the NEAT estimates lead to over-estimation of product use emissions. In the following we discuss first the results of NEAT model and afterwards the bottom-up estimate.

The total amount of carbon embodied in chemical products *consumed* in Germany (total of NODU products and ODU emissions) ranges from 49 to 60 Mt CO₂ equivalents in the years between 1990 and 2003. Of this total, around 40-49 Mt CO₂ is stored in products, which are not oxidized during use, while 9-11.5 Mt CO₂ (± 2.0 -3.3 Mt CO₂) are released as emissions during product use (*gross* ODU emissions in Table 12).

Results

Table 12: Results from the NEAT model and the IPCC-SA on German product use emissions in the period of 1990-2003*

Year	Total carbon embodied in products in Mt CO ₂	NODU in Mt CO ₂	Share NODU in %	Gross ODU emissions in Mt CO ₂	Share of fossil ODU emissions in %	ODU emissions from <i>net</i> exports of additional chemicals in Mt CO ₂	Fossil emissions due to wastewater treatment in Mt CO ₂	<i>Net</i> NEAT product use emissions in Mt CO ₂	IPCC-SA product use emissions in Mt CO ₂ (2005 inventory submission)**	IPCC-SA product use emissions in Mt CO ₂ (2006 inventory submission)**
1990	51.9	41.5 ± 4.3	80	10.4 ± 2.8	20	0.5 ± 0.23	1.7 ± 0.31	8.1 ± 2.8	2.68	2.68
1991	51.6	41.1 ± 4.4	80	10.5 ± 2.9	20	0.5 ± 0.23	1.7 ± 0.31	8.3 ± 2.9	2.62	2.62
1992	54.1	43.2 ± 4.4	80	10.9 ± 3.1	20	0.5 ± 0.23	1.7 ± 0.31	8.6 ± 3.1	2.52	2.52
1993	49.3	39.9 ± 4.4	81	9.4 ± 2.5	19	0.5 ± 0.23	1.7 ± 0.31	7.2 ± 2.5	2.52	2.52
1994	53.3	42.4 ± 4.4	80	10.8 ± 2.8	20	0.4 ± 0.23	1.7 ± 0.31	8.6 ± 2.8	2.52	2.52
1995	51.9	41.9 ± 4.4	81	10.0 ± 2.5	19	0.4 ± 0.23	1.7 ± 0.31	7.8 ± 2.5	2.43	2.43
1996	48.8	39.7 ± 4.5	81	9.0 ± 2.2	19	0.4 ± 0.23	1.6 ± 0.29	6.9 ± 2.2	2.33	2.33
1997	55.0	44.5 ± 4.5	81	10.4 ± 3.3	19	0.4 ± 0.23	1.6 ± 0.28	8.4 ± 3.3	2.33	2.33
1998	58.4	48.7 ± 4.5	83	9.7 ± 3.0	17	0.5 ± 0.23	1.5 ± 0.27	7.7 ± 3.0	2.31	2.31
1999	57.8	47.5 ± 4.7	82	10.2 ± 2.8	18	0.5 ± 0.23	1.5 ± 0.27	8.3 ± 2.8	2.17	2.17
2000	59.7	48.3 ± 4.9	81	11.4 ± 2.9	19	0.5 ± 0.23	1.5 ± 0.27	9.5 ± 2.9	2.02	2.02
2001	56.1	47.1 ± 4.8	84	9.0 ± 2.7	16	0.5 ± 0.23	1.4 ± 0.26	7.1 ± 2.7	1.88	1.88
2002	58.0	48.4 ± 4.8	84	9.6 ± 2.5	16	0.5 ± 0.23	1.4 ± 0.26	7.7 ± 2.5	1.73	1.75
2003	56.5	47.4 ± 4.7	84	9.1 ± 2.0	16	0.5 ± 0.23	1.4 ± 0.25	7.2 ± 2.0	-	1.57

* NEAT estimates include emissions resulting from the consumption of urea in artificial fertilizers.

** We assume here a conversion factor of 2.31 to convert NMVOC emissions into CO₂ equivalents (Schmidt-Stejskal et al., 2003).

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Throughout the years studied, the fractions of NODU versus (*gross*) ODU carbon remain fairly constant between 80-84% and 16-20% respectively (Table 12)²². In Table 12, a distinction is made between *gross* ODU emissions and *net* ODU emissions. *Net* ODU emissions are determined from *gross* ODU emissions:

- Firstly, by deducting approximately 1.4-1.7 Mt CO₂, which are released from the oxidation of surfactants and other chemicals during the treatment of wastewaters. These emissions are allocated to the source category *waste* of GHG inventory (see Section 5.3.2) and are therefore not accounted for as ODU emissions.
- Secondly, by accounting for 0.4-0.5 Mt CO₂ from *net* exports of chemical derivatives (additional trade) which are not included in the 80 NEAT core chemicals.

The second correction, which leads to an additional downward correction of ODU emissions by 0.4-0.5 Mt CO₂, is explained in more detail: The *gross* ODU emissions are calculated on the basis of the 80 NEAT core products. Since these products are converted to a myriad of other chemicals, which are imported and exported, emissions need to be corrected by the effect of the foreign trade with *derivatives* of the NEAT core products. To estimate the foreign trade with chemical derivatives, we studied about 450 chemicals for the years 1990, 1995, 2000 and 2003 (Table 13). Due to the large data requirements involved, the additional trade is not analyzed for all years covered in this study; instead, the missing values for the intermediate years are estimated by interpolation (with the exception of 1990, see below).

Table 13: Emission potential of 450 traded chemicals not included in NEAT

Year	Net export of carbon in Mt CO ₂			ODU emissions in Mt CO ₂		
	Mean	Min	Max	Mean	Min	Max
1990	0.63	0.49	0.76	0.13	0.06	0.20
1995	2.71	2.4	2.85	0.54	0.29	0.74
2000	2.3	2.06	2.52	0.46	0.25	0.66
2003	3.01	2.73	3.3	0.60	0.33	0.86
Average*	2.67	2.4	2.89	0.53	0.29	0.75

* In for the year 1990, not all trade data for the additional 450 chemicals were available. Therefore, values for this year are excluded from the average.

As Table 13 shows the mean net exports range from 0.6-3.0 Mt CO₂. The very low value of 1990 can be regarded as outlier, caused by the relatively low quality of available trade data in this

²² The ratio of ODU to NODU products according to Table 12 differs from the ODU to NODU fractions used as exogenous input to the NEAT model (see Table B1 in Appendix B) because the results in Table 12 account for the imports and exports of products. By accounting for trade, Table 12 gives the amounts of carbon oxidized during use (ODU) and the amounts of carbon stored (NODU) of chemical products *consumed* in Germany. These ODU versus NODU fractions differ from the amounts of carbon stored versus carbon oxidized from the *production* of chemicals. The difference between both considerations can be illustrated by the example of two countries, both consuming the same amounts and types of chemical products. Country A has a very large chemical industry. In contrast, country B has a very small chemical industry and imports the major part of its demand from country A. The NODU:ODU ratio for the *consumption* of chemicals is hence identical in both countries, while the NODU:ODU ratio at the level of *production* is larger for country A. The reason is that the amounts of carbon exported by country A are accounted for as being stored in country A.

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particular year. In order to understand the possible maximum effect of the additional trade we first consider the consequences of two extreme cases regarding ODU and NODU fractions: The largest influence on product-related emissions is obtained when the net value for additional trade is assumed to refer to ODU products only. In this case, disregarding the additional trade leads to an overestimation of ODU emissions in Germany by around 2.7 Mt CO₂. If, in contrast, the additional trade is assumed to refer exclusively to NODU products, then the influence on ODU emissions is zero. None of these two extreme cases is very likely. Since it is not possible to study in detail the fate of all 450 chemicals we assume (i) the same average ODU versus NODU fractions as well as (ii) the same error ranges of these fractions as used in the analysis of the 80 NEAT core products, i.e. a split into 20% ODU versus 80% NODU for the mean case is used. This leads to a downward correction of ODU emissions by 0.4-0.5 Mt CO₂ with an uncertainty range of around 0.23 Mt CO₂ (see Table 12 and Table 13).

The net emissions from product use ultimately amount to 7.1-9.5 Mt CO₂. The uncertainty ranges given in Table 12 for the *net* ODU emissions are based confidence intervals calculated with the higher and a lower ranges for the product-specific ODU/NODU ratios used in the NEAT calculations. According to our sensitivity analysis **the uncertainty of net ODU emissions ranges between 2.5 and 3.8 Mt CO₂** (Table 12). **Given this range, we cannot distinguish a clear trend for emissions from product use in the period of 1990-2003 in Germany** (in other words: the uncertainty range is clearly larger than the overall trend).

The uncertainties discussed so far do not cover possible errors related to false assumptions about production routes incorporated in NEAT. Errors related to the carbon content of aggregated NEAT core products (e.g., polyurethanes) are also not yet accounted for. An indication for the consistency of the data and model structure used is the closed NEAT carbon balance. Inconsistencies exist if the model determines higher amounts of carbon incorporated in intermediate and final chemicals than what is available for domestic consumption in basic chemicals according official production and trade statistics. This is the case for around 1-7% of the total consumption of chemicals modeled with NEAT in the period 1990-2003; the concomitant emission potential related to these inconsistencies is 0.7-4.3 Mt CO₂.

According to our NEAT model calculations, emissions originating from lubricants use account for around 10-15% of the total net ODU emissions (see Table 14).

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Table 14: Breakdown of NEAT *net* ODU emissions

Year	Net ODU	Of which:	
	Emissions in Mt CO ₂	Lubricants	Net ODU without lubricants
1990	8.1 ± 3.3	1.2 ± 0.4	6.9 ± 3.3
1991	8.3 ± 3.4	0.9 ± 0.3	7.4 ± 3.4
1992	8.6 ± 3.6	0.9 ± 0.3	7.7 ± 3.6
1993	7.2 ± 3.0	0.9 ± 0.3	6.3 ± 3.0
1994	8.6 ± 3.3	0.9 ± 0.3	7.7 ± 3.3
1995	7.8 ± 2.5	0.8 ± 0.3	7.0 ± 2.5
1996	6.9 ± 2.7	0.9 ± 0.3	6.0 ± 2.7
1997	8.4 ± 3.8	0.8 ± 0.3	7.6 ± 3.8
1998	7.7 ± 3.5	0.8 ± 0.3	6.9 ± 3.5
1999	8.3 ± 3.3	0.9 ± 0.3	7.4 ± 3.3
2000	9.5 ± 3.4	0.9 ± 0.3	8.6 ± 3.4
2001	7.1 ± 3.2	0.9 ± 0.3	6.2 ± 3.2
2002	7.7 ± 3.0	0.9 ± 0.3	6.8 ± 3.0
2003	7.2 ± 2.5	0.9 ± 0.3	6.3 ± 2.5

Based on Trischler (1997), the ODU:NODU ratio of 26:74 was determined for lubricants and used in NEAT by assigning the so-called ‘*other emissions*’ (270 kt) to ODU, while the remainder is considered as NODU (1042 kt – 270 kt = 772 kt). The fact that the exact fate of the release of lubricants is unknown gives an impression of the uncertainty of this assumption. For comparison, the consumption of ‘*on-purpose-release lubricants*’ (‘Verlustschmierstoffe’) in Germany is reported to range between 40 and at least 90 kt (data from literature are compiled in Patel et al. (1999); page A8-4). Subtraction of the value for ‘*on-purpose-release lubricants*’ (40-90 kt) from the value reported by Trischler (1997) (i.e., 270 kt) gives the amount of regular lubricants (engine lubricants, gearbox lubricants etc.), which we assume to be released to the environment. We consider this value to be uncertain and recommend further investigations on the fate of lubricants.

For comparison, the IPCC default storage fraction for lubricants is 50%, which translates to a release of around 500 kt (for a rounded lubricant use of 1000 kt per year). The storage fraction used in the IPCC-RA of the German Inventory Report (92%) is not comparable because it refers to different system boundaries (see Section 5.4.2). Actual emissions resulting from lubricant use in Germany are most likely higher than assumed in the IPCC-RA.

Bottom-up Estimate

Apart from lubricant use emissions, Table 14 reports also *net* ODU emissions without lubricants use. Since the uncertainty range of product use emissions is large, an attempt was made to develop an independent *bottom-up* estimate. To check plausibility of NEAT, we compare the data given in Table 12 with independent though rough *bottom-up* estimates for product use emissions. The *bottom-up* calculation adds the emission potential of all chemical components that are known to be released either directly or indirectly as CO₂ (Table 15).

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Table 15: Bottom-up estimation of emissions from product use (ODU emissions without lubricants); values for Germany in the end 1990s

	Quantity in Mt		Conversion factor in t CO ₂ /t	Quantity in Mt CO ₂		Source
	Lower value	Upper value		Lower value	Upper value	
Solvents	0.732	0.98	2.31	1.7	2.3	Jepsen et al., 2004; Theloke et al., 2000
Insecticides, Herbicides etc.	0.025		3.14	0.1		Theloke et al., 2000
Solid Paraffinic Products*)	0.117		3.14	0.4		Patel et al., 1999
Total				2.2	2.8	

* Lower value on quantity originates from Jepsen et al. (2004; Anhang I_Kurzfassung.pdf, p.12) for year 2000. Higher value from Theloke et al. (2000, see p. 299)

** E.g., protective coating cars, shoe creams, wood varnishes, cosmetic creams

*** Estimate by Patel et al. (1999) based on various sources

As shown in Table 15, product use emissions (excluding lubricants) according to our rough bottom-up estimate amount approximately to 2-3 Mt CO₂ equivalents. This is for all years lower than the possible range of NEAT values for ‘net ODU emissions without lubricants’ (compare Table 14 and Table 15)²³. One may conclude that the NEAT results for ‘net ODU emissions without lubricants’ (mean value) overestimate emissions by roughly 3-5 Mt CO₂ equivalents. However, the independent bottom-up estimate is subject to uncertainties itself. The real emissions could be higher, if several minor emission sources have been disregarded, which ultimately may add up to a sizable total.

Regardless of these uncertainties, NEAT results on product use emissions can be compared with estimates from the IPCC-SA. Emissions from the ‘*solvent and other product use*’ are only given in NMVOC equivalents in the IPCC-SA. We convert the IPCC-SA data into CO₂ equivalents (multiplying with a factor of 2.31 based on Schmidt-Stejskal et al. (2004)) and compare them afterwards with NEAT estimates²⁴.

NEAT values on product use emissions are clearly above the estimates stated by the IPCC-SA (see above, Table 12). Apart from uncertainties of NEAT results, differences are mainly a caused by the fact that product use emissions as stated in the IPCC-SA cover only solvent use emissions but exclude emissions from the consumption of lubricants as well as waxes and paraffins²⁵.

If emissions from the insecticides and paraffinic products (see *bottom-up* calculations in Table 15) and emissions from lubricant use according to NEAT (Table 14) were added to the IPCC-SA solvent emissions, total product use emissions would increase to around 3.1-4.4 Mt CO₂ equivalents (referred to as ‘*Bottom-up-IPCC-SA*’ in Figure 12). Taking the error ranges of NEAT product use

²³ This bottom-up estimate forms the basis of more detailed bottom-up estimations for product use emissions in a module of the NEAT simplified approach (NEAT-SIMP), which was developed in the course of the third phase of the EU-funded NEU-CO₂ Project and which are explained in more detail in Appendix C of this report.

²⁴ The conversion factor of 2.31 kg CO₂/kg NMVOC is uncertain itself. It assumes that NMVOC emissions in Germany consists of the same molecular composition as in Austria, for which Schmidt-Stejskal et al. (2004) prepared their study. Further research is therefore recommended to improve estimates on the actual carbon content of NMVOC emissions from product use.

²⁵ In the IPCC-RA, also emissions from lubricants consumption are calculated. These emissions are, however, not included under ‘product use’ in the IPCC-SA.

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emissions into account, the combined bottom-up-IPCC-SA values would still be slightly below the NEAT estimates (Figure 12).

A further reason to be cautious about the use product use emissions as calculated with NEAT is the fact that the non-energy use according to NEAT is larger than the quantities energy statistics (discussed in Chapter 5.4.1). While we were able to prove that this is partly caused by underreporting of non-energy use in the German Energy Balance (e.g., for coal and refinery products), we were not able to prove with certainty or with high probability that this explains the total gap. It is therefore possible that some double counting occurs in the detailed NEAT model, which could lead to overestimation of product use emissions.

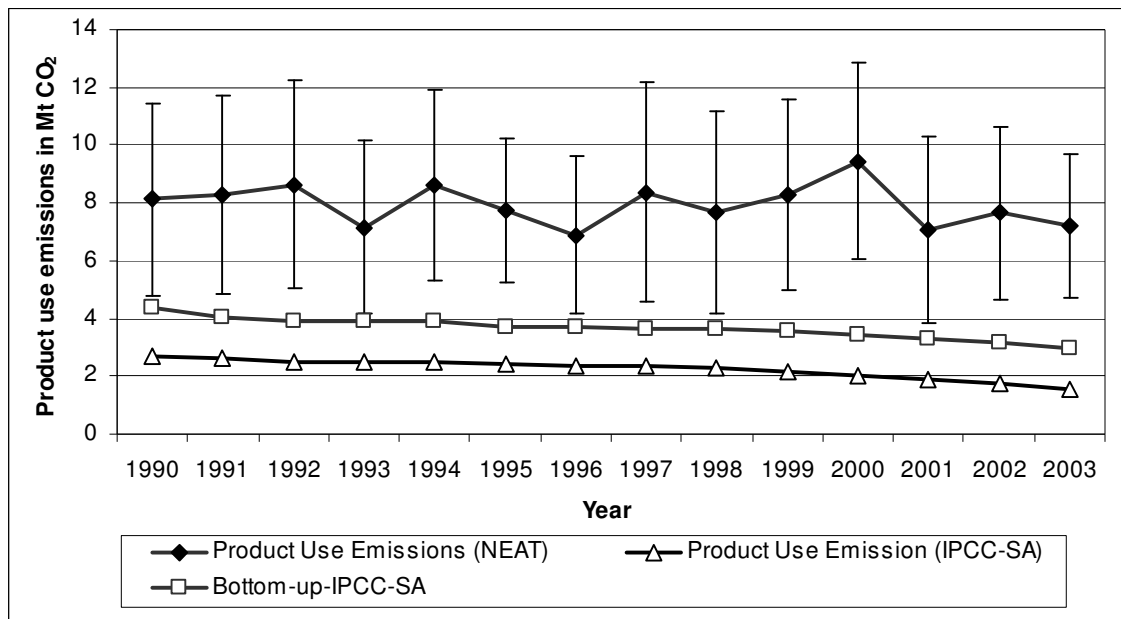


Figure 8: Comparison of NEAT and IPCC-SA data (2005 submission, except for the year 2003) on product use emissions

Combining the latter considerations with the insight gained from the comparison of NEAT results with the rough bottom-up estimate we conclude that NEAT estimates might overestimate the real product use emissions in Germany. **Given uncertainties associated with NEAT results and accounting also for differences between NEAT and the bottom-up IPCC-SA data, we cannot recommend using directly the NEAT results as estimates for solvent and other product use emissions in the IPCC-SA of the German GHG inventory.** The NEAT values might nevertheless serve as crosscheck for more detailed bottom-up calculation on product use emissions.

We can however recommend using the bottom-up calculations of product use emissions as performed with NEAT-SIMP, a simplified version of the detailed NEAT model, for crosschecking product use emission estimates in the IPCC-SA (see Appendix C) because the analysis of carbon emission factors for individual product groups is more detailed than in the bottom-up calculations, which are presented in Table 15.

Nevertheless, further research should address emissions resulting from product use in greater detail. This is especially true regarding fate and emissions from lubricants because this product group is (next to solvents) the most important source of product use emissions in Germany.

5.2 CO₂ Emissions from Industrial Processes

For the accounting of industrial process emissions it is crucial to clarify the system boundaries, i.e., to decide if and to what extent emissions resulting from the fuel use of feedstocks are regarded as industrial process emissions or whether they are treated as fuel use emissions and consequently being reported under the source category ‘energy’ in the GHG inventory. In that respect, different approaches can be followed by inventory makers, e.g., allocating all emissions resulting from the fuel use of feedstocks to energy use (as it is intended by UBA for the emissions accounting in the IPCC-SA), regarding all fuel use emissions as industrial process emissions, or even applying different system boundaries for the non-energy use of individual feedstocks as it is done in the National Energy Balance (NEB). In the following we generally follow the definition for non-energy use as it is applied in the NEB but discuss our results with respect to the approach chosen in the GHG inventory.

5.2.1 CO₂ Emissions from Steam Cracking

Around 17% (6-9 Mt CO₂ equivalents) of the feedstock input is used as fuel in German steam crackers is therefore directly emitted as CO₂ (Table 16)²⁶. Backflows to refineries account for around 10% (3-5 Mt CO₂ equivalents) of the carbon input in all years studied. The remaining carbon (73%) is incorporated in (i) high value chemicals used for further conversions within the petrochemical industry or (ii) low value fuels used for energy generation within and outside the chemical industry.

As discussed in Chapter 3.3.2, **the non-energy use data for steam cracker feedstock in the German Energy Balance include the fuel use in steam crackers but exclude backflows to refineries. Fuel-related CO₂ emissions from steam cracking are hence included in the data for feedstock use in the IPCC-RA but are not reported in the section of industrial process emissions according to the IPCC-SA.**

NEAT generates conservative estimates for fuel use emissions in steam crackers, while backflows tend to be overestimated (see Section 4.2.1.2). The NEAT data on CO₂ emissions from fuel use can therefore be considered as the lower boundary of possible values. Regarding the upper boundary it has been estimated that the CO₂ emissions from fuel use in steam crackers can be approximately 20% higher than the presented NEAT estimates from Table 16 (Neelis et al., 2003).

Comparing the NEAT results on CO₂ emissions (which are estimated from the fuel use of feedstocks in steam crackers) with inventory data, we find that **the IPCC-SA does not report any CO₂ emissions for steam cracking under the source category of industrial processes. This is because emissions from steam cracking are possible accounted for under the source category ‘energy’ in the CRF Table 1.A.2. This however needs to be verified by UBA in order to assure complete emissions accounting in the German GHG inventory.**

²⁶ Please note, that unlike emissions from product use, which consist mainly of NMVOCs, virtually all emissions from fuel use in steam crackers are pure CO₂ resulting from the combustion of parts of the feedstocks.

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Table 16: CO₂ emissions from steam cracking in the period 1990-2003 in Germany

Year	Total feedstock input in Mt	Total feedstock input in Mt CO ₂	Feedstock incorporated in products in Mt CO ₂	Backflows in Mt CO ₂	Emissions from fuel use of feedstock in Mt CO ₂	IPCC-SA, industrial process emissions from steam cracking in Mt CO ₂ (2005 and 2006 inventory submission)*
1990	10.43	33.31	24.17	3.35	5.79	-
1991	10.37	33.12	24.03	3.33	5.75	-
1992	11.06	35.30	25.65	3.51	6.14	-
1993	11.80	37.62	27.30	3.78	6.54	-
1994	12.48	39.71	28.79	4.02	6.91	-
1995	12.42	39.47	28.56	4.05	6.86	-
1996	11.82	37.60	27.27	3.79	6.54	-
1997	13.32	42.48	30.86	4.23	7.38	-
1998	14.06	44.86	32.59	4.47	7.80	-
1999	14.63	46.70	33.96	4.62	8.12	-
2000	15.08	48.09	35.00	4.73	8.36	-
2001	14.86	47.39	34.39	4.77	8.24	-
2002	15.03	47.89	34.74	4.82	8.32	-
2003	15.58	49.62	35.96	5.03	8.63	-

* As reported in the IPCC-SA under the source category of industrial processes (Table 2 in the CRF)

This accounting practice is in principle correct. We nevertheless have to stress in this respect the question of consistency of system boundaries for non-energy use. In the official National Energy Balance (NEB), a *gross* definition oil-based feedstock is used, thereby including the fuel use of these feedstocks in steam crackers into non-energy use data. The data from the NEB are directly used in the IPCC-RA of the German GHG inventory. To be consistent with the use of non-energy use data in the IPCC-RA, the IPCC-SA would have to report emissions from steam crackers in the source category of ‘*industrial processes*’ rather than ‘*energy*’. This is, however, solely a question of consistency rather than one of correct emissions accounting. Adapting methodologies, i.e., either adapting system boundaries of non-energy use in the IPCC-RA or changing emissions accounting in the IPCC-SA would allow a consistent accounting of non-energy use and resulting emissions and would hence reduce the risk of double counting or omission of relevant CO₂ emissions in the German GHG inventory.

In case UBA decides to crosscheck or adapt emission estimates for steam cracking, activity data for ethylene production and applied emission factors can be obtained from the NEAT models for the respective years, as they are delivered together with this project report.

5.2.2 CO₂ Emissions from Ammonia Production

Ammonia (NH₃) does not contain carbon itself. Hence, the entire carbon embodied in the feedstock, which is converted to synthesis gas is finally oxidized to CO₂ during the production process. One part of the emission is captured for urea production and therefore deducted from the total CO₂ emissions related to ammonia production.

As discussed in Section 3.3.2, the National Energy Balance does not follow a consistent approach with respect to the allocation of the different feedstocks (i.e., natural gas and gas/diesel oils) used for ammonia production: The fuel use of natural gas is excluded from the non-energy use data, whereas the fuel use of gas/diesel oils is included in the non-energy use data. **We therefore allocate in NEAT the total gas/diesel oil input for ammonia production to feedstock use and regard only**

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70% of the natural gas input as feedstock use, while 30% are regarded as fuel use, based on a split of 70% feedstock use versus 30% energy, i.e., fuel use. This results in a percentage of 17-18% for the overall weighted share of non-energy use that is used as fuel (Table 17).

According to NEAT, the total carbon input into ammonia production ranges from 3.8 Mt CO₂ in 1990 to 6.4 Mt CO₂ equivalents in 2003 (Table 17). Out of this input, a total of 0.7 to 1.1 Mt CO₂ equivalents result in emissions from fuel combustion, 2.6 to 4.6 Mt CO₂ equivalents are emitted as industrial process emissions and the remainder (0.5-0.7 Mt CO₂ equivalents) is embodied in urea. The NEAT results show that emissions from fuel use as well as feedstock use for ammonia production increased in the period between 1990 and 2003.

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Table 17: CO₂ emissions related to ammonia production in the period of 1990-2003 in Germany

Year	Total hydro-carbon input in Mt CO ₂	Input used as fuel in %	Input used as feed-stock in %	Emissions from energy use of feedstock in Mt CO ₂	Gross non-energy use emissions from feedstock use in Mt CO ₂	Carbon embodied in urea in Mt CO ₂	Net non-energy use emissions from feedstock use in Mt CO ₂ ¹⁾	Emissions from ammonia production ²		Absolute Difference (IPCC-SA ²⁾ - NEAT)	Ammonia Production in Mt		Implied Emission Factor in kg CO ₂ /kg ammonia		
								IPCC-SA ²⁾	IPCC-SA ³⁾		NEAT	IPCC-SA ²⁾	NEAT ⁴⁾	IPCC-SA ²⁾	IPCC-SA ³⁾
1990	3.80	18	82	0.68	3.13	0.50	2.63	1.75	4.60	-0.88	2.03	2.53	1.29	0.69	1.82
1991	4.83	18	82	0.86	3.97	0.48	3.50	1.46	3.85	-2.03	2.58	2.12	1.36	0.69	1.82
1992	4.81	18	82	0.86	3.95	0.45	3.50	1.46	3.83	-2.04	2.57	2.11	1.37	0.69	1.82
1993	4.78	18	82	0.85	3.93	0.53	3.40	1.45	3.84	-1.95	2.55	2.10	1.33	0.69	1.82
1994	4.94	18	82	0.88	4.06	0.70	3.36	1.50	3.94	-1.86	2.63	2.17	1.27	0.69	1.82
1995	5.73	18	82	1.02	4.71	0.89	3.82	1.79	4.71	-2.03	3.06	2.59	1.25	0.69	1.82
1996	5.66	18	82	1.01	4.65	0.96	3.69	1.77	4.66	-1.92	3.02	2.57	1.22	0.69	1.82
1997	5.62	18	82	1.00	4.62	0.86	3.76	1.76	4.62	-2.01	3.00	2.55	1.25	0.69	1.82
1998	5.67	18	82	1.01	4.66	0.90	3.76	1.77	4.64	-1.99	3.03	2.56	1.24	0.69	1.82
1999	5.48	18	82	0.98	4.50	0.86	3.64	1.70	4.48	-1.94	2.92	2.47	1.25	0.69	1.82
2000	5.91	18	82	1.05	4.86	0.97	3.89	1.82	4.78	-2.07	3.16	2.63	1.23	0.69	1.82
2001	5.74	18	82	1.02	4.72	0.85	3.87	1.80	4.72	-2.08	3.06	2.60	1.26	0.69	1.82
2002	5.88	17	83	1.01	4.87	0.75	4.12	1.83	4.81	-2.29	3.11	2.65	1.33	0.69	1.82
2003	6.44	17	83	1.10	5.34	0.71	4.62	-	5.25	-	3.40	-	1.36	-	1.82

¹⁾ Net emissions are calculated from gross emissions by deducting the amounts of carbon embodied in urea. Note that we allocate here the carbon, which is stored in urea entirely to the non-energy use emissions from ammonia production.

²⁾ 2005 submission (UNFCCC, 2005b).

³⁾ 2006 submission (UNFCCC, 2006).

⁴⁾ The NEAT emission factors account for urea production. The factors differ slightly from each other because urea production is not constant throughout the years studied.

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As data in Table 18 shows, the emission factors used in NEAT represent conservative estimates. For ammonia produced from natural gas and fuel oil, the *real* total feedstock input might be 6%-8% lower or 25%-32% higher than assumed in the NEAT model.

Table 18: Overview of CO₂ emission factors for ammonia production according to various sources (Neelis et al., 2003)

Feedstock	Source	Total input in kg CO ₂ /kg NH ₃	Minimum Deviation from NEAT in %	Maximum Deviation from NEAT in %
Steam reforming of natural gas	NEAT model	1.6	-	-
	IPTS, 2004 ¹⁾	1.6-1.7	0.0	6.3
	IPTS, 2004 ¹⁾	1.6-1.8	0.0	12.5
	Chauvel et al., 1989 ²⁾	1.5-1.8	-6.3	12.5
	de Beer, 1998 ³⁾	1.6-2.0	0.0	25.0
	Patel et al., 1999	1.6	0.0	0.0
Partial oxidation of oil	NEAT model	2.5	-	-
	IPTS, 2004 ¹⁾	2.5-2.8	0.0	12.0
	Chauvel et al., 1989 ²⁾	2.7-3.3	8.0	32.0
	Patel et al., 1999 ⁴⁾	2.3	-8.0	-

¹⁾ Steam reforming of natural gas: *Net* primary feedstock consumption is 22.1 GJ/t NH₃ for conventional steam reforming, 23.5 GJ/t NH₃ for excess air reforming and 24.8 GJ/t NH₃ for auto-thermal reforming; fuel use is 7-9 GJ/t NH₃ for conventional steam reforming, 5.5-7 GJ/t NH₃ for excess air reforming and 3.5-7 GJ/t NH₃ for auto-thermal reforming. Partial oxidation of fuel oil: *Net* primary feedstock consumption is 28.8 GJ/t NH₃; fuel use is 5.5-9 GJ/t NH₃. Assumed emission factors: 56 kg CO₂/GJ natural gas and 74 kg CO₂/GJ fuel oil (Patel et al., 1999).

²⁾ Steam reforming of natural gas: *Net* primary feedstock consumption is 23 GJ/t NH₃; fuel use is 4 GJ/t NH₃ for conventional process and 10 GJ/t NH₃ for improved processes. Partial oxidation of oil: Total input of 0.85-1.05 t oil/t NH₃. Assumed lower heating value for oil 43.0 GJ/t oil. Assumed emission factors, see note ¹⁾.

³⁾ Total input of 29-36.3 GJ/t NH₃. Values base on various literature sources. Assumed emission factor, see note ¹⁾.

⁴⁾ Steam reforming of natural gas: total input 28 GJ/t NH₃; partial oxidation of oil: total input 31 GJ/t NH₃. Assumed emission factors, see note ¹⁾.

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Given these uncertainties, a sensitivity analysis for emissions from ammonia production was performed in NEAT, assuming that specific feedstock input (i.e., natural gas and heavy fuel oils) could be 4% lower or up to 15% higher than NEAT averages. The results are given in Table 19.

Table 19: Uncertainty ranges for CO₂ emissions from ammonia production

Year	Net emissions from feedstock use in Mt CO ₂			Emissions from fuel combustion in Mt CO ₂		
	Min	Mean	Max	Min	Mean	Max
1990	2.52	2.63	3.02	0.65	0.68	0.78
1991	3.36	3.50	4.02	0.83	0.86	0.99
1992	3.36	3.50	4.03	0.82	0.86	0.98
1993	3.26	3.40	3.91	0.82	0.85	0.98
1994	3.22	3.36	3.86	0.84	0.88	1.01
1995	3.66	3.82	4.39	0.98	1.02	1.17
1996	3.55	3.69	4.25	0.97	1.01	1.16
1997	3.61	3.76	4.33	0.96	1.00	1.15
1998	3.61	3.76	4.32	0.97	1.01	1.16
1999	3.50	3.64	4.19	0.94	0.98	1.12
2000	3.74	3.89	4.48	1.01	1.05	1.21
2001	3.72	3.87	4.45	0.98	1.02	1.18
2002	3.96	4.12	4.74	0.97	1.01	1.16
2003	4.44	4.62	5.32	1.06	1.10	1.27

For both feedstock input and energy-related emissions, the NEAT estimates are on the lower side of possible values. Therefore, NEAT generates conservative emission estimates for ammonia production in Germany.

The NEAT estimates exceed the results of the IPCC-SA (2005 submission) as reported under the source category *industrial processes* by 0.9-2.3 Mt CO₂ in the period studied (Table 17). The following reasons for these substantial differences are identified:

- The values used for ammonia production in the IPCC-SA are lower than the values used in NEAT because **the IPCC-SA falsely states the mass of nitrogen contained in ammonia instead of accounting for the molar weight of the entire ammonia molecule**. This error might be caused by the fact that production statistics (Destatis, 1990-2003a) state only the mass of nitrogen contained in ammonia and not the absolute production value. UBA should correct this error and multiply the current ammonia production values by a factor of 17/14 kg ammonia/kg nitrogen.
- The **ammonia production value as used in NEAT** (based on data from Destatis (1990-2003a)) **for the year of 1990 is considerably lower than the one used in the IPCC-SA**.
- **The specific emission factor for ammonia production as used in NEAT is much higher than the 0.69 kg CO₂/kg ammonia stated in the IPCC-SA (2005 submission)**. The emission factor used in NEAT follows the definition of non-energy use chosen in the Energy Balances, thereby excluding CO₂ from the parts of natural gas consumed for fuel purposes (30% according to NEAT assumptions) but including the total emissions of heavy oils used for ammonia production (see Table 7). Multiplying the NEAT emission factor with values for ammonia production yields industrial process emissions from ammonia production, which comply with the definition of non-energy use in the NEB. From these, however, the amounts of CO₂ consumed for the production of urea are deducted to calculate *actual* emissions from ammonia production. The ‘*actual*’ emission factors stated in Table 17 are calculated by simply

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dividing the *actual* emissions by ammonia production. **The ‘actual’ emission factors for ammonia production in Germany vary between 1.2-1.4 kg CO₂/kg ammonia due to variations in yearly urea production.** As NEAT assumes rather efficient ammonia plants, we conclude that the emission factor used in the IPCC-SA (2005 submission) of 0.69 kg CO₂/kg ammonia underestimates CO₂ emissions from ammonia production substantially. This finding is also confirmed by the external expert review of the German Inventory (UNFCCC, 2005a) which states: “Emissions from ammonia production are estimated using an EF [emission factor] that is lower than the IPCC default and the lowest of all reporting parties, and is not well documented. The ERT [external review team] noted that Germany has planned to begin using the IPCC default value, which is recommended in the future.”

Meanwhile, **UBA accounted for the critics by using for their 2006 inventory submission the IPCC default emission factor of 1.5 kg CO₂/kg ammonia (equivalent to 1.82 CO₂/kg N contained in ammonia).**

It is important to note again, that **the IPCC default factor assumes natural gas being used as feedstock for ammonia production.** It furthermore **excludes the parts of feedstock used for fuel purposes.** The IPCC default emission factor follows thereby a *net* definition of non-energy use. It is valid to use this emission factor for the accounting of industrial process emissions resulting from ammonia production, if emissions from the fuel use, i.e., the share of the feedstock used for energy purposes is correctly reported under the source category ‘**energy**’ in the GHG inventory. Otherwise, the chosen approach leads very likely to an underestimation of total CO₂ emissions resulting from ammonia production in Germany.

We nevertheless want to stress two shortcomings of the current emission estimates for ammonia production in the inventory:

- The IPCC default emission factor assumes natural gas as the only feedstock. This assumption is not entirely correct as roughly 30% of ammonia is produced from heavy fuel oils in Germany. The IPCC emission factor therefore tends to underestimate actual emissions.
- The current approach of emissions accounting for ammonia production is partly inconsistent with the system boundaries chosen for non-energy use in the IPCC-RA. There, fuel use of natural gas feedstock is regarded as ‘*energy use*’ but the fuel use of oil-derived feedstock is considered as non-energy use.

In order to calculate emissions from ammonia production in the IPCC-SA we recommend therefore

- **to identify for each year the share of ammonia, which is produced from natural gas and heavy fuel oil.**
- **to apply for the shares of ammonia produced from the individual feedstocks the NEAT emission factors from Table 7, i.e., 1.6 kg CO₂/kg ammonia for natural gas and 2.50 kg CO₂/kg ammonia for heavy oils.**
- **to split emission factors and total emissions into 70% process emissions versus 30% energy use, depending on the choice of system boundaries for non-energy use and report the resulting estimates in the respective source categories of the German GHG inventory.**

5.2.3 CO₂ Emissions from Methanol Production

Methanol is produced in Germany from fuel oil, natural gas and lignite. **The major part of these feedstocks is embodied in the final product, while the remainder is emitted as direct CO₂.** Depending on the definition of non-energy use in energy statistics, either the whole input or certain parts of it might be allocated to either non-energy use or fuel use. From detailed information provided from experts involved in the preparation of the German Energy Balance we conclude, that a *net* definition is used for the non-energy use of natural gas (excluding natural gas used as fuel) but a *gross* definition for lignite and fuel oils is used (thereby including the amounts of these fuels used for energy purposes in the total feedstock use, Section 3.2.2). We therefore allocate emissions from the part of natural gas used for energy purposes to energy related emissions while the total of the remaining emission from lignite and fuel oil consumption is considered as feedstock emissions, i.e. industrial process emissions. **Based on the specific input of 2.8 kg CO₂ equivalents/kg methanol for fuel oil, 1.8 kg CO₂ equivalents/kg methanol for natural gas, and 4.3 kg CO₂ equivalents/kg methanol for lignite, 92% of the total carbon emissions are allocated to industrial process emissions and the remaining 8% to energy use (Table 20).**

Due to increased methanol production, the total hydrocarbon input increases from around 2 Mt CO₂ equivalents in 1990 to 5 Mt CO₂ equivalents in 2003. Consequently, the emissions from feedstock use (industrial process emissions) and fuel use for methanol production increase from 0.9 to 2.4 Mt CO₂ and from 0.1 to 0.2 Mt CO₂ respectively.

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Table 20: CO₂ emissions related to methanol production in the period of 1990-2003 in Germany

Year	Total hydrocarbon input in Mt CO ₂	Input embodied in methanol in Mt CO ₂	Process emissions in Mt CO ₂	Emissions allocated to feedstock use in Mt CO₂	Emissions allocated to energy use in Mt CO ₂	Emissions allocated to feedstock use in %	Emissions allocated to energy use in %	IPCC-SA, process emissions in Mt CO ₂ (2005 submission)	IPCC-SA, process emissions in Mt CO ₂ (2006 submission)
1990	1.93	1.03	0.90	0.83	0.07	92	8	-	0.83
1991	3.17	1.69	1.48	1.36	0.11	92	8	-	1.36
1992	3.32	1.78	1.55	1.43	0.12	92	8	-	1.43
1993	3.09	1.65	1.44	1.33	0.11	92	8	-	1.33
1994	3.70	1.98	1.72	1.59	0.13	92	8	-	1.59
1995	3.67	1.96	1.71	1.58	0.13	92	8	-	1.58
1996	3.98	2.13	1.85	1.71	0.14	92	8	-	1.71
1997	3.63	1.94	1.69	1.56	0.13	92	8	-	1.56
1998	4.11	2.19	1.91	1.77	0.14	92	8	-	1.77
1999	3.94	2.11	1.84	1.70	0.14	92	8	-	1.70
2000	4.85	2.59	2.26	2.09	0.17	92	8	-	2.09
2001	4.94	2.64	2.30	2.13	0.17	92	8	-	2.13
2002	4.74	2.53	2.21	2.04	0.17	92	8	-	2.04
2003	5.17	2.76	2.41	2.22	0.18	92	8	-	2.22

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As in the case of ammonia production, we again use conservative values representing the total carbon input and process specific CO₂ emission factors (Table 21). The *real* total process input for methanol production can be up to 17% higher for natural gas and up to 26% higher for lignite than assumed in NEAT (Neelis et al., 2003). In order to account for these variations, a sensitivity analysis was conducted in NEAT, assuming an average deviation of +10% for total feedstock.

Table 21: Overview of CO₂ emissions from methanol production according to various sources (Neelis et al., 2003)

Feedstock	Source	Total input in kg CO ₂ /kg methanol	Feedstock use in kg CO ₂ /kg methanol	Fuel use in kg CO ₂ /kg methanol
Steam reforming/partial oxidation of natural gas	NEAT model	1.8	1.4	0.4
	Hinderink et al., 1996 ¹⁾	1.9	1.4	0.5
	Hinderink et al., 1996 ¹⁾	1.8	1.4	0.4
	Hinderink et al., 1996 ¹⁾	1.8	1.4	0.4
	Chauvel et al., 1989 ²⁾	1.8-1.9	-	-
	Strucker et al., 1995 ³⁾	2.0-2.1	-	-
Partial oxidation of fuel oil	NEAT model	2.8	1.4	1.4
	Chauvel et al., 1989 ²⁾	2.8	-	-
	Patel et al., 1999 ⁴⁾	2.8	-	-
Partial oxidation of lignite	NEAT model	3.4	1.4	2.9
	Chauvel et al., 1989 ²⁾	-	5.1	1.6
	Patel et al., 1999 ⁴⁾	4.3		

¹⁾ Steam reforming of natural gas: *Net* primary feedstock consumption is 25.7 GJ/t methanol for conventional design with and without steam reforming and 25.6 GJ/t methanol for combined reforming; fuel use is 8.6 GJ/t methanol for conventional design, 7.7 GJ/t methanol for conventional design with primary reformer and 6.0 GJ/t methanol for combined reforming. Assumed emission factors: 56 kg CO₂/GJ natural gas and 74 kg CO₂/GJ fuel oil and 93 kg CO₂/GJ lignite (Patel et al., 1999).

²⁾ Steam reforming of natural gas: Total input is 32-33.5 GJ/t methanol; partial oxidation of coal: *Net* primary feedstock consumption of 2.0 t coal/t methanol; fuel use is 17 GJ/t methanol (assumed to be coal). Partial oxidation of residues: Total input of 0.90 t residues/t methanol. Assumed lower heating values: 27.3 GJ/t for lignite, 43.0 GJ/t for residues. Assumed emission factors, see note ¹⁾.

³⁾ Steam reforming of natural gas: Total input is 35.5-37.5 GJ/t methanol. Assumed emission factor, see note ¹⁾.

⁴⁾ Partial oxidation of lignite: *Net* feedstock consumption 2 t/t methanol; fuel use 19 GJ/t methanol for lignite. Partial oxidation of oil: Total input of 0.87 t/t methanol. Assumed heating value: 19.3 GJ/t for lignite (Patel et al. 1999), 43 GJ/t for fuel oil. Assumed emission factors: 111kg CO₂/GJ for lignite, 74 kg CO₂/GJ for fuel oil (Patel et al., 1999).

Because the NEAT data on specific feedstock consumption are already in the lowest possible range of values, only maximum estimates are presented in the sensitivity analysis. As Table 22 shows, NEAT might slightly underestimate the industrial process emissions and the emissions from fuel use for methanol production in Germany.

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Table 22: Uncertainty ranges for CO₂ emissions from methanol production

Year	Hydrocarbon input in Mt CO ₂		Industrial process emissions in Mt CO ₂		Fuel use emissions in Mt CO ₂	
	NEAT	Max	NEAT	Max	NEAT	Max
1990	1.93	2.13	0.83	1.01	0.07	0.08
1991	3.17	3.49	1.36	1.66	0.11	0.14
1992	3.32	3.65	1.43	1.74	0.12	0.14
1993	3.09	3.40	1.33	1.62	0.11	0.13
1994	3.70	4.07	1.59	1.94	0.13	0.16
1995	3.67	4.04	1.58	1.92	0.13	0.16
1996	3.98	4.38	1.71	2.08	0.14	0.17
1997	3.63	3.99	1.56	1.90	0.13	0.15
1998	4.11	4.52	1.77	2.15	0.14	0.18
1999	3.94	4.34	1.70	2.06	0.14	0.17
2000	4.85	5.34	2.09	2.54	0.17	0.21
2001	4.94	5.44	2.13	2.59	0.17	0.21
2002	4.74	5.22	2.04	2.48	0.17	0.20
2003	5.17	5.68	2.22	2.70	0.18	0.22

While the IPCC-SA of the 2005 inventory did not account for CO₂ emissions from methanol production, the 2006 inventory states estimates for this industrial process. For this purpose an emission factor of 1.11 kg CO₂/kg methanol is multiplied with physical methanol production. The average NEAT emission factor is 1.20 kg CO₂/kg methanol. Again the system boundaries of non-energy use are important when calculating industrial process emissions for methanol production. Two approaches for emissions reporting can be followed.

Approach 1:

If UBA follows the approach chosen for steam cracking and ammonia production, i.e., if all emissions, which result from fuel use of feedstocks should be allocated to the source category ‘energy’, then the total emissions resulting from methanol production should be reported in the chapter ‘energy’ and not as industrial process emissions in the IPCC-SA. This is because only the parts of feedstock carbon contained in the final product (i.e., methanol) are regarded (purely speaking) as non-energy use, while the remaining carbon is burned for energy purposes.

To be consistent with the approach chosen in the current IPCC-SA for steam cracking and ammonia production, we would suggest removing emissions, which result from methanol production from the inventory of industrial process emissions and include them under the source category ‘energy’.

As we already discussed, the approach chosen in the IPCC-SA for steam cracking and ammonia yields correct emission estimates but is not consistent with the definition of non-energy use in the IPCC-RA. To calculate emission estimates in the IPCC-SA, which are in line with IPCC-RA system boundaries for non-energy use, **we suggest following Approach 2:**

- **Identify the shares of methanol, which are produced from heavy oils, natural gas, and lignite.**
- **Multiply these shares with NEAT emission factors, i.e., 1.4 kg CO₂/kg methanol for heavy oils, 0.4 kg CO₂/kg methanol for natural gas, and 2.9 kg CO₂/kg methanol for lignite.**
- **Account the emissions according to the definition of non-energy use in NEB and IPCC-RA, i.e., include emissions from oil and lignite use as industrial process emissions (CRF**

Tables 2) and emissions from natural gas consumption as *energy* emissions (CRF Tables 1).

If UBA, however, wants to be consistent with the current accounting (in the 2006 inventory submission) of emissions from steam cracking and ammonia production, total emissions from methanol production must be removed from the industrial process section of the IPCC-SA and should be included in the source category 'energy' (CRF Table 1).

5.2.4 CO₂ Emissions from Carbon Black Production

From the total input for carbon black production (mainly heavy oils and tars derived from coal and crude oil) one part is embodied in the final product and the other part is emitted as CO₂. As described in Section 3.3.2, the German Energy Balance follows a *net* definition of feedstock use for natural gas and a *gross* definition for oil-derived feedstocks. We therefore consider only the carbon emissions resulting from the consumption of oil-derived feedstock to be industrial process emissions. All CO₂ released from natural gas consumption is considered as energy use emissions. **According to NEAT, around 66% of the total carbon input is contained in the final product and 34% is released as emissions**, based on a specific feedstock use of 5.2 kg CO₂/kg carbon black for heavy oils/tars and 0.4 kg CO₂/kg carbon black for natural gas. The total input for carbon black production varies between 1.7 Mt CO₂ in 1994 equivalents and 2.2 Mt CO₂ equivalents in 1990 (Table 23). Emissions from feedstock use vary between 0.5 and 0.7 Mt CO₂ and account for 92% of the total emissions released from carbon black production.

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Table 23: CO₂ emissions related to carbon black production in the period of 1990-2003 in Germany

Year	Total hydrocarbon input in Mt CO ₂	Input embodied in carbon black in Mt CO ₂	Total emissions in Mt CO ₂	Industrial process emissions in Mt CO ₂	Emissions from fuel use in Mt CO ₂	Emissions allocated to feedstock use in %	Emissions allocated to fuel use in %	IPCC-SA, process emissions in Mt CO ₂ (2005 submission)	IPCC-SA, process emissions in Mt CO ₂ (2006 submission)
1990	2.20	1.45	0.75	0.70	0.06	92	8	-	0.70
1991	2.12	1.39	0.73	0.67	0.06	92	8	-	0.67
1992	2.10	1.38	0.72	0.66	0.06	92	8	-	0.66
1993	1.87	1.23	0.64	0.59	0.05	92	8	-	0.59
1994	1.67	1.10	0.57	0.53	0.04	92	8	-	0.53
1995	1.85	1.21	0.63	0.58	0.05	92	8	-	0.58
1996	1.76	1.16	0.60	0.56	0.05	92	8	-	0.56
1997	1.88	1.24	0.65	0.60	0.05	92	8	-	0.60
1998	1.92	1.26	0.66	0.61	0.05	92	8	-	0.61
1999	1.89	1.24	0.65	0.60	0.05	92	8	-	0.60
2000	1.93	1.27	0.66	0.61	0.05	92	8	-	0.61
2001	1.94	1.28	0.67	0.62	0.05	92	8	-	0.62
2002	1.89	1.24	0.65	0.60	0.05	92	8	-	0.60
2003	1.94	1.28	0.67	0.62	0.05	92	8	-	0.62

Results

As for the other industrial processes discussed above, NEAT also generates conservative estimates for carbon black production with respect to total feedstock input and CO₂ emissions. The *real* process input of heavy oil fractions and natural gas might be about 20% and 25% respectively higher than assumed in NEAT (Neelis et al., 2003). In our uncertainty analysis we therefore assume that NEAT emission factors already represent the lower end of a possible value range and that the maximum value is 25% higher than currently used in NEAT²⁷ (see Table 24).

Table 24: Overview of total input and CO₂ emissions from carbon black production according to other sources (Neelis et al., 2003)

Feedstock	Source	Total input in kg CO ₂ /kg carbon black	Emissions from feedstock used as fuel in kg CO ₂ /kg carbon black*	Deviation total input in %	Deviation CO ₂ emissions in %
Natural gas	NEAT model	0.4	0.2	-	-
	Voll et al. 1997 ¹⁾	0.4	-	0	-
	Voll et al. 1997 ²⁾	0.5	-	25	-
Heavy oils	NEAT model	5.2	1.7	-	-
	Voll et al. 1997 ¹⁾	5.2	-	0	0
	Voll et al. 1997 ²⁾	6.2	-	19	-
Total	NEAT model	5.6	1.9	-	-
	Voll et al. 1997 ¹⁾	5.6	1.9	0	0
	Voll et al. 1997 ²⁾	6.7	3.1	20	63

* including feedstock that is not incorporated in carbon black

¹⁾ Average values for semi-reinforcing carbon black: Carbon black production 1750 kg/h, natural gas input 425 m³/h, oil input 2900 kg/h. Assumed heating values: 31.65 MJ/kg for heavy oils and 42.00 MJ/kg for natural gas. Assumed emission factors: 56 kg CO₂/GJ for natural gas and 74 kg CO₂/GJ heavy oils (Patel et al., 1999).

²⁾ Average values for reinforcing carbon black: Carbon black production 1250 kg/h, natural gas input 360 m³/h, oil input 2500 kg/h. Assumed heating values: 31.65 MJ/kg for heavy oils and 42.00 MJ/kg for natural gas. Assumed emission factors: 56 kg CO₂/GJ for natural gas and 74 kg CO₂/GJ heavy oils (Patel et al., 1999).

The results of our sensitivity analysis are shown in Table 25. Given the range of data found in literature on the specific feedstock input and CO₂ emissions from carbon black production (Table 25), the total emissions from carbon black production could be more than 60% higher than emissions as calculated with NEAT. Therefore, NEAT underestimates feedstock as well as fuel use emissions from carbon black production if the production processes are less efficient in Germany than assumed in NEAT.

²⁷ Here, we assume specific feedstock use for the less efficient reinforced carbon black process.

Results

Table 25: Uncertainty ranges for CO₂ emissions from carbon-black production

Year	Total hydrocarbon input in Mt CO ₂		Industrial process emissions in Mt CO ₂		Fuel use emissions in Mt CO ₂	
	Mean	Max	Mean	Max	Mean	Max
1990	2.20	2.75	0.70	1.20	0.06	0.10
1991	2.12	2.65	0.67	1.16	0.06	0.10
1992	2.10	2.63	0.66	1.15	0.06	0.10
1993	1.87	2.33	0.59	1.02	0.05	0.09
1994	1.67	2.09	0.53	0.91	0.04	0.08
1995	1.85	2.31	0.58	1.01	0.05	0.08
1996	1.76	2.20	0.56	0.96	0.05	0.08
1997	1.88	2.35	0.60	1.03	0.05	0.09
1998	1.92	2.40	0.61	1.05	0.05	0.09
1999	1.89	2.36	0.60	1.03	0.05	0.09
2000	1.93	2.41	0.61	1.06	0.05	0.09
2001	1.94	2.43	0.62	1.06	0.05	0.09
2002	1.89	2.36	0.60	1.03	0.05	0.09
2003	1.94	2.43	0.62	1.06	0.05	0.09

While of the IPCC-SA (2005 submission) does not report emissions from carbon-black production, industrial process emissions are reported in the 2006 submission of the German GHG inventory. The estimates used there seem to be derived from the NEAT analyses. We would therefore argue that **emissions reporting in the current IPCC-SA with respect to the production of carbon-black is correct, if not only industrial process emissions are accounted for but also the 0.04-0.06 Mt CO₂ emissions, which should be reported under the source category of ‘energy’²⁸.**

5.2.5 CO₂ Emissions from Conversion Losses

The conversion of basic chemicals to intermediates and final products is not 100% carbon efficient. Carbon losses occur (i) due to direct carbon losses from transportation and leakage and (ii) because the yield of chemical reactions is always lower than 100%, thereby creating by- and waste-products. **In our calculation of conversion losses we include direct CO₂ emissions as well as all emissions due to flaring of waste and off-gases from 37 different chemical conversion processes²⁹.** For the period 1990-2003, NEAT estimates conversion losses to rise from 2.6-2.7 Mt CO₂ equivalents to approximately 3.7 Mt CO₂ equivalents (Table 26). The main reason for the increase in losses is the rise in chemicals production.

²⁸ This accounting would be consistent with the definition of non-energy use in the IPCC-RA but it is not consistent with the current practice for the reporting of emissions from steam cracking and ammonia production. This is because for these industrial processes, the complete fuel use emissions are reported in the IPCC-SA as ‘energy’ use emissions. To follow this approach, the total emissions resulting from carbon-black production should be reported under the source category ‘energy’. Industrial process emissions would hence be zero.

²⁹ Note that CO₂ emissions from conversion losses do not include emissions from the use of waste- and by-products for energy purposes. It is furthermore important that **conversion losses consist not entirely of direct CO₂ but might also include methane, NMVOCs, and other organic substances. Expressing chemical conversion losses in CO₂ equivalents serves therefore only the correct accounting of carbon flows and does not express the specific greenhouse gas potential thereof.**

Results

Table 26: CO₂ emissions related to conversion losses of the chemical industry in the period of 1990-2003 in Germany

Year	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
Conversion-Losses in Mt CO ₂	2.70	2.66	2.60	2.66	2.91	2.93	3.21	3.35	3.54	3.59	3.76	3.5	3.73	3.68
IPCC-SA (2005 submission)	-	-	-	-	-	-	-	-	-	-	-	-	-	-
IPCC-SA (2006 submission)	2.70	2.66	2.60	2.66	2.91	2.93	3.21	3.35	3.54	3.59	3.76	3.5	3.73	3.68

The estimates for chemical conversion losses as calculated with NEAT are in range with results from other country studies (Tonkovich and Gerber, 1995, Theunis et al., 2003). Due to lack of other reliable information, the uncertainties related to conversion losses are not addressed explicitly. However, based on the insight gained in the study done by Neelis et al. (2005c) we conclude that the average uncertainty of conversion losses given in Table 25 is in the range of $\pm 10\%$. **Special attention should be drawn on the differentiation between energy use of by-products and simple carbon losses. While we assume that neither of the emissions resulting from chemical conversion losses originate from energy use of by-products, system boundaries are not always clear.** This particular point requires additional research in the future.

CO₂ emissions from chemical conversion losses, i.e., direct losses, off-gases, and non-specified by-products were not included in the 2005 submission, they have been taken into account by the 2006 submission of the IPCC-SA (Table 26). The IPCC-SA data are identical with our NEAT model results.

The chosen approach is correct but it is associated with uncertainties because it is not clear for all of the included conversion processes, whether CO₂ emissions from the fuel use of by-products is strictly excluded. We therefore present in Table 27 more detailed data for conversion losses resulting from the most important conversion processes. As shown in the column on the far right of Table 27, the *'remaining conversion losses'* represent a large share of the total conversion losses (76-82%). Further investigations would be required in order to reduce the uncertainties related to this rest category.

Results

Table 27: Activity data and CO₂ emissions from the production of ethylene dichloride, acrylonitrile, VCM, and other chemical processes³⁰

Year	Total conversion losses	Ethylene dichloride		Ethyleneoxide		Acrylonitrile		VCM (Vinyl-chloride-monomer) ²⁾		Remaining conversion losses ³⁾
	Emissions in Mt CO₂	Production in Mt	Emissions ¹⁾ in Mt CO ₂	Production in Mt	Emissions in Mt CO ₂	Production in Mt	Emissions in Mt CO ₂	Production in Mt	Emissions in Mt CO ₂	Emissions in Mt CO ₂
1990	2.70	2.21	-	0.63	0.28	0.28	0.20	1.44	0.10	2.12
1991	2.66	1.87	-	0.59	0.27	0.31	0.22	1.26	0.09	2.08
1992	2.60	1.93	-	0.63	0.28	0.31	0.22	1.29	0.09	2.01
1993	2.66	2.05	-	0.62	0.28	0.36	0.25	1.30	0.09	2.03
1994	2.91	2.39	-	0.66	0.30	0.41	0.29	1.52	0.11	2.21
1995	2.93	2.16	-	0.70	0.31	0.43	0.30	1.38	0.10	2.22
1996	3.21	2.24	-	0.69	0.31	0.44	0.32	1.45	0.10	2.48
1997	3.35	2.28	-	0.75	0.34	0.46	0.32	1.77	0.12	2.57
1998	3.54	2.53	-	0.84	0.38	0.43	0.31	1.86	0.13	2.73
1999	3.59	2.90	-	0.92	0.41	0.35	0.25	1.95	0.14	2.79
2000	3.76	2.90	-	0.92	0.41	0.37	0.26	2.00	0.14	2.95
2001	3.50	3.00	-	0.86	0.39	0.36	0.26	2.12	0.15	2.71
2002	3.73	3.19	-	0.72	0.32	0.33	0.23	2.19	0.15	3.02
2003	3.68	3.18	-	0.79	0.36	0.27	0.19	1.50	0.10	3.03

¹⁾ included in the production of VCM

²⁾ including losses from the production of ethylene dichloride

³⁾ excluding the production of ethylene dichloride, ethyleneoxide, acrylonitrile, and VCM

³⁰ The production values stated in Table 27 do not always comply with the data stated by Destatis (1990-2003a) because they are partly corrected to assure consistency of the NEAT carbon balance.

Results

Total emissions from conversion losses range from 2.6 to 3.7 Mt CO₂ in the period of 1990-2003. Out of these emissions, 0.3-0.4 Mt CO₂ result from the production of ethylene oxide, 0.2-0.3 Mt CO₂ are caused by acrylonitrile production and 0.1-0.2 Mt CO₂ are due to the generation of vinylchloride-monomer (VCM).

In the NEAT, we do not calculate emissions from ethylene dichloride and VCM production separately because the process of direct chlorination to produce ethylene dichloride and the ethylene dichloride cracking process to generate VCM are often combined to the so-called '*balanced process*'. This allows using the surplus of hydrogen chloride from the ethylene dichloride cracking directly as input for the oxy-chlorination of ethylene. Excluding these three production processes, the remaining emissions from other chemical conversions amount to 2.0-3.0 Mt CO₂ per year in the period of 1990-2003.

Regarding IPCC-SA emission estimates, **the NEAT values (Table 27) can be used directly by UBA (as it is done in the current 2006 inventory submission) or UBA might use only NEAT emission factors stated in Table 28 and multiply them with specific activity data for the three chemical conversion processes.** The remaining emissions from conversion losses, which do not originate from these three processes could than be taken from NEAT and stated as totals under '*remaining conversion losses*' in the IPCC-SA.

Table 28: Emission factors used in NEAT to calculate CO₂ emissions from chemical conversion losses

	Process Specific Emission Factor in kg CO ₂ /kg product		
	Ethylene oxide	Acrylonitrile	Vinylchloride Monomer (VCM)
NEAT	0.45	0.71	0.07
IPCC-SA*	0.35-0.86	0.79-1.00	0.29

* Emission factors as they are proposed in the revised 2006 IPCC inventory guidelines (IPCC, 2006)

The emission factors (Table 28) are on the lower side of possible value ranges and therefore represent conservative estimates. Depending on plant-specific process characteristics, emission factors might be higher or lower than the ones used in NEAT. For example, emission factors for acrylonitrile production might be lower than the ones stated in Table 28, if by-products such as acetonitrile and hydrogen cyanide are not flared but recovered and sold as products.

It is important to note that all process specific conversion losses are based on available literature data (i.e., on Neelis et al., 2005c). The data used, represent mainly average estimates for the most common production processes but do not account for specific settings on the level of individual chemical plants. The estimates of CO₂ emissions from chemical conversion losses are further complicated by the fact that only parts of the losses are directly emitted as CO₂, while other parts might be either flared with/without additional fuel input and with/without energy recovery or even sold as by-products. Moreover, the estimates on conversion losses are partly based on rather old process data, which might not represent the current industrial practice (Neelis et al., 2005c). Within the scope of this research study, it was not possible to elaborate in greater detail on the exact fate of the losses from the various chemical conversion processes. Further research is therefore recommended to increase the accuracy of estimates for this source of CO₂ emissions.

5.2.6 CO₂ Emission from the Production of Non-ferrous Metals, Ferroalloys, and Other Inorganics

Emissions from the production of non-ferrous metals, ferroalloys, and other inorganic materials result (i) from the consumption of electrodes made from petroleum coke, pitch, cokes or coal and (ii) from the consumption of other coke and coal products. Both are used as reducing agents (see Section 4.2.1.2).

The total emissions in the period of 1990-2003 range between 2.7 and 4.1 Mt CO₂ (Table 29). A clear trend towards either increasing or decreasing emissions cannot be observed. About 50-70% of the total CO₂ emissions from non-ferrous metals and ferroalloy production in all years originate from the use of electrodes while the remainder is caused by the oxidation of other solid carbon, i.e. cokes and coals.

As further explained in Section 3.3.2, we assume that the amounts of solid coal products (e.g., coal and coke) used for the production of non-ferrous metals, ferroalloys, and inorganic chemicals are accounted for as non-energy use in the National Energy Balance and IPCC-SA. The resulting emissions should hence be considered as industrial process emissions. This is also the case for electrode use. While we consider these allocations to be plausible, there is no absolute certainty in these points because it was not possible for us to obtain a written statement from the ‘Arbeitsgemeinschaft Energiebilanzen’ about the inclusion/exclusion of solid fuels used for non-energy purposes.

Due to lack of reliable information, we do not explicitly address uncertainties related to the use of *other carbon* sources for the production of non-ferrous metals, ferroalloys, and inorganics. Nevertheless, uncertainties are associated with the specific emission factors used in NEAT (see Table 10).

Due to the unclear position of *other solid carbon* in the Energy Balance (see Section 3.3.2) we also calculate with NEAT the **CO₂ emissions from electrode consumption only (1.2 to 2.5 Mt CO₂ per year). Comparing NEAT estimates with data from the IPCC-SA, we find that the latter reports much lower emissions (0.7-1.5 Mt CO₂) for the production of non-ferrous metals, ferroalloys, and other inorganics. The differences between NEAT and the IPCC-SA can be explained (i) by differencing emission estimates for aluminum and calcium carbide production between NEAT and the IPCC-SA and (ii) by the fact that the IPCC-SA is incomplete with respect to emissions from the electrode use for production of other non-ferrous metals and ferroalloys³¹.**

³¹ This statement refers the 2005 inventory submissions. In the 2006 GHG inventory, emissions from ferroalloy production are stated. These are, however, very low, given production volumes of ferroalloys in Germany.

Results

Table 29: CO₂ emissions related to the consumption of electrodes and other coke and coal as reducing agents for the production of metals, ferroalloys, and other inorganics during the period of 1990-2003 in Germany

Year	Total emissions from non-ferrous metals, ferroalloys, and inorganics production in Mt CO ₂			NEAT, emissions from electrode use in Mt CO ₂ ⁵⁾	NEAT, emissions from other carbon use in Mt CO ₂ ⁶⁾	Emissions from aluminium production in Mt CO ₂ ²⁾			Emissions from carbide production in Mt CO ₂				Emissions from the production of other non-ferrous metals, ferroalloys, and inorganics in Mt CO ₂			
	NEAT	IPCC-SA (2005 submission) ¹⁾	IPCC-SA (2006 submission) ¹⁾			NEAT	IPCC-SA (2005 submission)	IPCC-SA (2006 submission)	NEAT	NEAT ³⁾	IPCC-SA (2005 submission)	IPCC-SA (2006 submission)	NEAT	NEAT ³⁾	IPCC-SA (2005 submission) ⁴⁾	IPCC-SA (2006 submission) ⁴⁾
1990	4.14	1.45	1.88	2.31	1.83	1.80	1.01	1.01	0.81	0.34	0.44	0.44	1.53	0.17	0.00	0.43
1991	3.64	1.04	1.29	2.12	1.52	1.65	0.94	0.94	0.70	0.29	0.10	0.10	1.29	0.18	0.00	0.25
1992	3.53	0.90	1.07	1.92	1.61	1.54	0.82	0.82	0.66	0.28	0.08	0.08	1.33	0.10	0.00	0.16
1993	2.73	0.78	0.83	1.28	1.45	0.94	0.75	0.75	0.64	0.27	0.02	0.02	1.15	0.07	0.00	0.05
1994	3.00	0.71	0.73	1.64	1.36	1.30	0.69	0.69	0.61	0.26	0.03	0.03	1.09	0.08	0.00	0.01
1995	3.75	0.81	0.81	2.26	1.49	1.60	0.79	0.79	0.63	0.26	0.03	0.03	1.52	0.40	0.00	0.003
1996	3.63	0.81	0.81	2.26	1.37	1.54	0.79	0.79	0.51	0.21	0.02	0.02	1.58	0.51	0.00	0.003
1997	3.94	0.80	0.81	2.30	1.64	1.42	0.78	0.78	0.73	0.30	0.02	0.02	1.79	0.58	0.00	0.003
1998	3.85	0.86	0.86	2.27	1.58	1.57	0.84	0.84	0.66	0.28	0.02	0.02	1.62	0.42	0.00	0.002
1999	3.80	0.88	0.88	2.31	1.49	1.65	0.87	0.86	0.58	0.24	0.02	0.02	1.57	0.42	0.00	0.002
2000	4.11	0.90	0.90	2.54	1.57	1.75	0.88	0.88	0.61	0.26	0.02	0.02	1.75	0.53	0.00	0.002
2001	3.75	0.91	0.91	2.41	1.34	1.74	0.89	0.89	0.41	0.17	0.01	0.01	1.60	0.50	0.00	0.002
2002	3.52	0.91	0.91	2.41	1.11	1.76	0.89	0.89	0.27	0.11	0.02	0.02	1.49	0.54	0.00	0.002
2003	3.80	-	0.92	2.62	1.18	1.92	-	0.90	0.38	0.16	-	0.02	1.50	0.54	-	0.002

¹⁾ including the production of carbides, ferroalloys, and aluminium

²⁾ only electrodes but no *other solid carbon* is used for aluminium production

³⁾ only including electrode use but excluding emissions from *other solid carbon* use

⁴⁾ reported as emissions from ferroalloy production

⁵⁾ including the production of primary aluminium, electric arc furnace steel, white phosphorus, titanium dioxide, ferrosilicon, calcium carbide, silicon, and ferromanganese produced in electric arc furnaces

⁶⁾ including the production of ferrosilicon, ferromanganese, silicon manganese, ferrochromium, ferrochromium-silicon, chromium, secondary and primary lead magnesium, nickel, silicon, silicon carbide, tin, zinc, and calcium carbide

Results

The differences between NEAT and the IPCC-SA (2005 inventory submission) with respect to emissions from the electrode consumption for aluminum production arise from slight variations of activity data, i.e. values for aluminum production, and from the use of different CO₂ emission factors. In NEAT, a uniform emission factor of 1.5 kg CO₂/kg aluminum is used for all years. In contrast, emission factors used in the IPCC-SA vary throughout the years between 0.68 and 0.79 kg CO₂/kg aluminum. This variation of emission factors in the IPCC-SA can be explained by the fact that a *Tier 3a method* based on detailed company data is used to calculate emissions from aluminum production.

Data from literature (e.g., IPTS, 2001), however, suggests, that CO₂ emissions reported in the IPCC-SA are too low, given the aluminum production in Germany. We therefore recommend further research to verify the reliability of CO₂ emissions as stated by the German aluminum producers.

A detailed analysis of the differences between NEAT and IPCC-SA data on emissions from calcium carbide production is not possible because neither activity data nor emission factors are given in the IPCC-SA (2005 inventory submission). From the comparison of data given in Table 29, we however infer that only emissions from the electrode use for calcium carbide production are reported under '*industrial processes*' in the IPCC-SA (0.02-0.44 Mt CO₂) while emissions from other cokes and coal use are excluded.

To improve the IPCC-SA estimates for emissions from the non-ferrous metals and ferroalloy production we recommend to (i) improve estimates for emissions from aluminum production and to (ii) check completeness of emissions estimates from calcium carbide production and adjust data if necessary. Special attention should be paid to the position of '*other solid carbon*' used for the production of calcium carbide in the Energy Balance in order to avoid omission or possible double counting of emissions.

The expert review team (UNFCCC, 2005a) also recommended including estimates for CO₂ emissions from other ferroalloys and non-ferrous metals under the source category of '*industrial processes*' in the IPCC-SA. A first attempt could be to elaborate activity data for the various products (e.g., use production values as stated in NEAT) and multiply them with specific emission factors as stated by IPTS (2001), Ullmann (1997) or as they are implemented in the NEAT model (see Table 10 in Section 4.2.1.2). Special attention should be again paid to the position of '*other solid carbon use*'. If these carbon sources are excluded from the non-energy use and stated under final energy consumption in the Energy Balance, they must be excluded from the industrial process emissions. If that is the case, CO₂ emissions from non-ferrous metals and ferroalloys are calculated by:

$$CO_2 \text{ Emissions} = \text{Activity} \cdot \text{Specific Emissions from Electrode Use}$$

If the '*other solid carbon use*' is part of the non-energy use in the Energy Balance, emissions are calculated as:

$$CO_2 \text{ Emissions} = \text{Activity} \cdot \text{Specific Emissions from Electrode Use} + \\ \text{Activity} \cdot \text{Specific Emissions from Other Solid Carbon Use}$$

5.2.7 Final Conclusions on Industrial Process Emissions

The comparison between NEAT results and the IPCC-SA data has revealed shortcomings regarding estimates for industrial process emissions in the IPCC-SA. Some of these shortcomings were also identified during the external review of the German GHG Inventory in fall 2004 (UNFCCC, 2005a). With the 2006 inventory submission, UBA already accounted for parts of the criticism when estimating also emissions from methanol and carbon black production as well as chemical conversion losses based on NEAT calculations. We acknowledge these efforts but further recommend (i) to correct emission estimates, which are still incomplete (e.g., for the production of ferroalloys) and (ii) to pay special attention to the consistency of emission estimates for non-energy use as stated in the IPCC-RA and the IPCC-SA. This is especially relevant for the accounting of emissions resulting from steam cracking and from the production of ammonia, methanol, and carbon black either as *industrial process emissions* or as emissions from *energy* use. In this way, NEAT results can contribute to improve the accounting for industrial process emissions in the IPCC-SA of the German GHG inventory.

5.3 CO₂ Emissions from Waste Treatment

In this section, we give CO₂ emissions as calculated by NEAT for the relevant waste treatment categories. Landfills are excluded because there is virtually no oxidation of fossil-based carbon in landfills. It is important to note that we include only emissions originating from fossil-based carbon here. CO₂ released due to the oxidation of biogenic carbon (in landfills or during wastewater treatment) is, therefore, excluded.

5.3.1 CO₂ Emissions from Waste Incineration

NEAT calculates fossil CO₂ emissions from waste incineration with two approaches, (i) a *top-down approach* while taking into account the total amount of waste incinerated in waste incineration plants and the wastes' average carbon content and (ii) a *bottom-up approach* accounting for plastics and other chemicals waste incinerated (see Section 4.2.1.3). The results of both approaches are given in Table 30.

The CO₂ emissions from waste incineration as calculated with the *top-down* approach increase from around 2.8 Mt CO₂ in 1990 to 3.4 Mt CO₂ in the year 2003. In the same time period, the *bottom-up* estimates range between 1.6 and 2.4 Mt CO₂. The *bottom-up* approach as calculated in NEAT results, therefore, in emission estimates, which are 16 to 41% lower than the ones calculated with the *top-down* method.

The differences between the two approaches can be partly caused by incomplete accounting of emissions with the *bottom-up* method because (i) emission estimates for the incineration of *other chemicals* are only a very rough estimates based on Patel et al. (1999) and might therefore be incomplete and (ii) data for plastics incineration exclude synthetic rubber materials.

Results

Table 30: CO₂ emissions from waste incineration during the period of 1990-2003 in Germany*

Year	Top-down estimate of CO ₂ emissions from waste incineration in Mt CO ₂	Bottom-up estimate of CO ₂ emissions from waste incineration			Difference [(top-down – bottom-up)/top-down] in %	Non-energy use emissions in Mt CO ₂
		Emissions from plastics waste incineration in Mt CO ₂	Emissions from the incineration of other chemical waste in Mt CO ₂	Total bottom-up emissions in Mt CO ₂		
1990	2.76	1.54	0.10	1.64	41	0.00
1991	2.79	1.69	0.11	1.80	36	0.00
1992	2.83	2.09	0.13	2.22	22	0.00
1993	2.87	2.09	0.13	2.22	23	0.00
1994	2.86	2.25	0.14	2.40	16	0.00
1995	2.85	2.12	0.13	2.26	21	0.00
1996	2.83	1.78	0.11	1.89	33	0.00
1997	2.87	1.78	0.11	1.89	34	0.00
1998	2.91	1.72	0.11	1.83	37	0.00
1999	3.24	1.92	0.12	2.04	37	0.00
2000	3.45	2.11	0.13	2.24	35	0.00
2001	3.30	2.11	0.13	2.24	32	0.00
2002	3.42	2.15	0.14	2.28	33	0.00
2003	3.42	2.30	0.15	2.44	29	0.00

* Error ranges were not explicitly calculated because emissions from waste incineration are reported under ‘energy’ in the IPCC-SA and therefore beyond the scope of this study.

On the other hand, the *top-down* estimates may also be erroneous (i.e., too high) due to the fact that the average carbon content of incinerated wastes represents only a very rough estimate (small variations of the average carbon content can lead to significant changes of CO₂ emissions from waste incineration).

Due to lack of reliable information, the errors and uncertainties related to the *top-down* approach cannot be addressed explicitly. However, major uncertainties are associated (i) with the actual amounts of wastes incinerated and (ii) with the fossil carbon content of the different types of waste. Our NEAT calculations might therefore serve as a benchmark for a more detailed accounting of emissions from waste incineration (using either more accurate data for *Tier 1* estimates or *Tier 2* or *Tier 3* methodology).

All waste incineration plants in Germany recover energy from the incineration process. Greenhouse gas emissions resulting from waste incineration are consequently excluded from non-energy use and accounted for under ‘energy’ in the IPCC-SA. Non-energy use CO₂ emissions from waste incineration in Germany are thus zero. Emissions from waste incineration are therefore not addressed in the comparison of NEAT results and emission estimates as stated in the National GHG Inventory.

We finally want to stress that the source category of waste incineration is not clearly distinguished in the relevant CRF tables. To improve transparency of emission estimates on waste incineration, the external review team requested to indicate clearly where and to what extent emissions from waste incineration could be found in the IPCC-SA (UNFCCC, 2005). The NEAT data might be used as valuable crosscheck for emission estimates used for waste incineration under the category ‘energy’ in the IPCC-SA.

Results

5.3.2 CO₂ Emissions from Wastewater Treatment

Fossil-based emissions from wastewater treatment are calculated in NEAT based on (i) the chemical oxygen demand of wastewaters from the chemical industry and (ii) the domestic consumption of surfactants as proxy for the content of fossil-based carbon in municipal wastewater streams. **According to NEAT, the total fossil-based emissions from wastewaters decrease from 1.7 Mt CO₂ to 1.4 Mt CO₂ in the period of 1990-2003 (Table 31).**

Table 31: CO₂ emissions from wastewater treatment during the period of 1990-2003 in Germany

Year	NEAT, emissions from chemical wastewaters in Mt CO ₂	NEAT, emissions from surfactants consumption in Mt CO ₂ *	Total NEAT fossil-based emissions in Mt CO ₂	IPCC-SA, fossil based emissions from waste treatment in Mt CO ₂	IPCC-SA, fossil based emissions from waste treatment in Mt CO ₂
				2005 submission	2006 submission
1990	0.85	0.89	1.74 ± 0.31	-	-
1991	0.85	0.89	1.74 ± 0.31	-	-
1992	0.85	0.89	1.74 ± 0.31	-	-
1993	0.85	0.89	1.74 ± 0.31	-	-
1994	0.85	0.89	1.74 ± 0.31	-	-
1995	0.85	0.89	1.74 ± 0.31	-	-
1996	0.75	0.89	1.64 ± 0.29	-	-
1997	0.66	0.89	1.55 ± 0.28	-	-
1998	0.62	0.89	1.51 ± 0.27	-	-
1999	0.58	0.89	1.47 ± 0.27	-	-
2000	0.58	0.89	1.48 ± 0.27	-	-
2001	0.52	0.89	1.41 ± 0.26	-	-
2002	0.51	0.89	1.40 ± 0.26	-	-
2003	0.51	0.89	1.40 ± 0.25	-	-

* Estimates base on consumption data for one single year, i.e., 1996 (Patel, 1999).

We assume error ranges of 15% for wastewaters from the chemical industry based on expert judgement and 20% for emissions from surfactant consumption (based on Patel (1999), Assmussen (2000), Kaiser et al. (1998), and TEGEWA (2005)). The NEAT error ranges for total emissions from wastewater treatment amount to 0.25-0.31 Mt CO₂. As in the case of waste incineration emissions, the results obtained with the chosen methodology might serve as benchmark for more detailed calculations in the future.

The IPCC-SA states in the source category only CH₄ emissions from landfills, composting and mechanic-biological waste treatment as well as CH₄ emission from sewage sludge treatment. The latter emissions contain both, biogenic and fossil carbon.

Here it is important to note that NEAT emissions from wastewater treatment might contain CO₂ but also other components such as NMVOCs and CH₄. Our estimates serve therefore the correct accounting of fossil carbon emissions (expressed in CO₂ equivalents) but do not account for the specific greenhouse potential of emissions from wastewater treatment.

We furthermore do not distinguish between emissions from the actual treatment of wastewater and from the sludge treatment. This is important to note in order to avoid double counting of emissions resulting from the wastewater and sewage sludge treatment, i.e., either as CO₂ or as CH₄. Due to relatively high uncertainties associated with NEAT emission estimates, further research addressing fossil based emissions from wastewater treatment is strongly recommended. This is especially important in order to get a more detailed insight into the shares of biogenic and fossil-based emissions

on the totals. That way, NEAT result might serve as benchmark for estimating fossil-based emissions resulting from the treatment of wastewaters.

5.4 Total Non-energy Use, Carbon Storage, Carbon Storage Fractions, and Total Fossil CO₂ Emissions

5.4.1 Total Non-energy Use

In NEAT, total non-energy use is calculated (i) according to a *gross* definition (thereby including fuel use and backflows of feedstock) and (ii) in line with the definition of non-energy use as chosen in the German Energy Balance (i.e., a partial *net* definition which excludes backflows to refineries and the fuel use parts of natural gas feedstock). In order to obtain results, which are comparable to the data given in the IPCC-RA it is important to adopt the same system boundaries for non-energy use as chosen in the German Energy Balance. This means that we calculate the *net* non-energy use in NEAT as the sum of (i) the total carbon equivalents contained in the basic petrochemical products (i.e., synthetic organic chemicals and non-energy use refinery and coke oven products), (ii) the fuel use in steam crackers, (iii) the shares of non-energy use oil and coal feedstocks used as fuel and (iv) the pure industrial process emissions from the non-energy use of feedstocks (excluding emissions, which result from the share of feedstocks used for fuel purposes).

We refer to non-energy use with these system boundaries as *net* non-energy use. While purer (stricter *net*) definitions are possible, they have no practical relevance for Germany.

The total '*gross*' and '*net*' non-energy use as calculated with NEAT is given in Figure 10. Total non-energy use ranges between 72 and 93 Mt CO₂ adopting a '*gross*' definition and 68 and 87 Mt CO₂ using a '*net*' definition respectively. In all years, the difference between '*gross*' and '*net*' definition varies between 4 and 6 Mt CO₂. For the period of 1990-2003, total non-energy use according to both definitions shows an increasing trend, with the maximum being reached in the year 2000.

Table 32 gives an overview of total non-energy use and specific non-energy use of individual components as calculated according to both *gross* and *net* definitions. Table 33 shows total non-energy use based on a *net* definition for individual types of fuels. It is important to note that non-energy use related to products consumption (sum of storage and emissions) is not equal to the storage and emissions calculated in Section 5.1 because there we estimate emissions based on the total *domestic consumption* of basic, intermediate, and final chemical products. Here, in contrast, we estimate product-related emissions and storage based on the up-stream calculation of feedstock use for the *domestic production* of chemicals.

Results

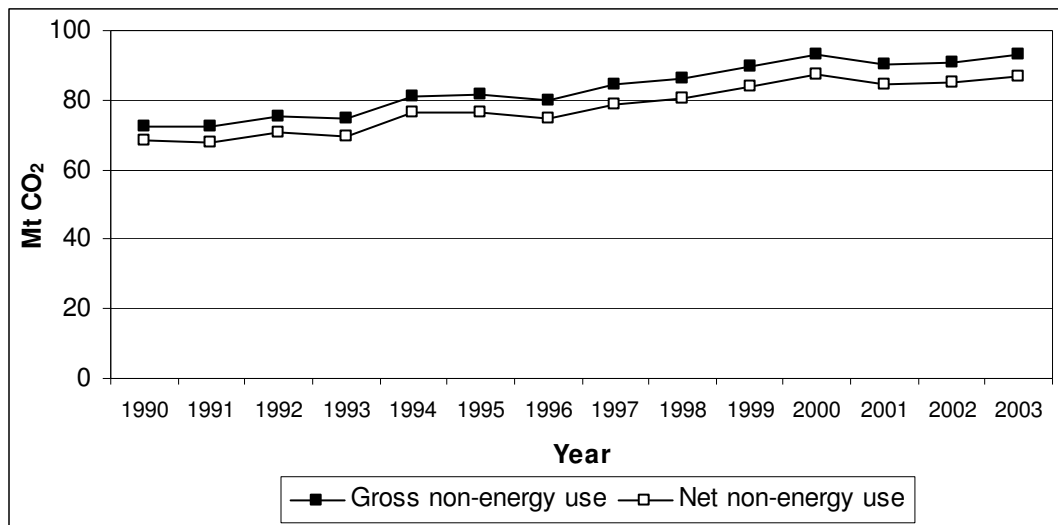


Figure 9: Non-energy use as calculated with NEAT according to a ‘gross’ and ‘net’ definition (the ‘net’ non-energy use as calculated with NEAT follows the system boundaries of the German Energy Balance)³²

The largest part of total non-energy use is related to the manufacture of products (total of ODU and NODU) according to both the ‘gross’ (in average 70%) and the ‘net’ definition (in average 74%).

The non-energy use reported in the German Energy Balance is directly used in the IPCC-RA (CRF Table 1.A(d)) of the German Greenhouse Gas Inventory. The value of non-energy use calculated with NEAT is expected to be in line with the system boundaries of non-energy use as chosen in German energy statistics and should therefore lead to identical values compared to those found in the official German Energy Balance (and hence also in the IPCC-RA of the National GHG Inventory) (Table 34). The preconditions for the consistency of the values are that

- the system boundaries for non-energy use must be absolutely identical in NEAT and in the German Energy Balance,
- no activities are overlooked neither in NEAT nor in the German Energy Balance, and
- no double-counting occurs in neither in NEAT nor in the German Energy Balance.

³² Due to the unclear position of ‘other solid carbon’ in the Energy Balance (the quantities might be included as final energy use in the Energy Balance), we exclude this carbon source from the non-energy data here.

Results

Table 32: Overview total non-energy use as calculated with NEAT according to a 'gross' and 'net' definition*

in Mt CO ₂	Year	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
Product use	Storage	41.21	39.80	42.05	43.16	47.09	46.93	46.40	47.90	49.52	51.94	53.00	53.33	53.00	54.23
	Emissions	10.35	10.52	10.87	9.41	10.83	10.00	9.04	10.41	9.67	10.24	11.43	8.98	9.56	9.10
Steam cracking	Emissions from fuel use of feedstock	5.79	5.75	6.14	6.54	6.91	6.86	6.54	7.38	7.80	8.12	8.36	8.24	8.32	8.63
	Backflows	3.35	3.33	3.51	3.78	4.02	4.05	3.79	4.23	4.47	4.62	4.73	4.77	4.82	5.03
Ammonia production	Net emissions from feedstock use	2.63	3.50	3.50	3.40	3.36	3.82	3.69	3.76	3.76	3.64	3.89	3.87	4.12	4.62
	Emissions from fuel use	0.68	0.86	0.86	0.85	0.88	1.02	1.01	1.00	1.01	0.98	1.05	1.02	1.01	1.10
Methanol production	Net emissions from feedstock use	0.83	1.36	1.43	1.33	1.59	1.58	1.71	1.56	1.77	1.70	2.09	2.13	2.04	2.22
	Emissions from fuel use	0.07	0.11	0.12	0.11	0.13	0.13	0.14	0.13	0.14	0.14	0.17	0.17	0.17	0.18
Carbon-black production	Net emissions from feedstock use	0.70	0.67	0.66	0.59	0.53	0.58	0.56	0.60	0.61	0.60	0.61	0.62	0.60	0.62
	Emissions from fuel use	0.06	0.06	0.06	0.05	0.04	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Non-ferrous metals and ferroalloy production	Emissions	4.14	3.64	3.53	2.73	3.00	3.75	3.63	3.94	3.85	3.80	4.11	3.75	3.52	3.80
Conversion-Losses	Emissions	2.70	2.66	2.60	2.66	2.91	2.93	3.21	3.35	3.54	3.59	3.76	3.50	3.73	3.68
Gross non-energy use		72.50	72.27	75.32	74.61	81.28	81.70	79.77	84.32	86.19	89.41	93.25	90.42	90.95	93.27
Net non-energy use		68.35	67.91	70.78	69.81	76.21	76.45	74.79	78.91	80.52	83.63	87.25	84.41	84.91	86.90
Difference		4.15	4.36	4.54	4.79	5.07	5.25	4.98	5.41	5.67	5.79	6.00	6.01	6.05	6.37

* The grey shaded columns are regarded as fuel use according to the definition of non-energy use in the Energy Balance and are therefore excluded from the calculation of total non-energy use according to the *net* definition.

Results

Table 33: Fuel specific *net* non-energy use as calculated with NEAT

Year	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
	in Mt CO ₂													
Naphtha	27.51	26.66	27.83	28.48	30.86	30.80	30.80	34.50	35.32	37.15	39.43	37.26	37.89	38.40
Lubricants	4.51	3.57	3.37	3.38	3.50	3.24	3.30	3.05	3.18	3.32	3.32	3.32	3.38	3.35
Bitumen	10.10	10.87	11.60	10.70	12.64	11.36	10.43	10.59	10.45	11.24	10.20	9.85	9.37	8.92
Coal Oils and Tars (from coking coal)	2.97	2.49	2.31	2.01	1.93	1.88	1.89	1.94	1.95	1.94	1.99	2.02	2.02	2.10
Natural gas	4.19	4.60	4.41	4.32	4.84	4.92	4.78	4.83	4.95	4.97	5.30	5.23	5.19	5.71
Gas/diesel oil (inc. residual fuel oil)	5.00	4.89	4.89	5.38	6.03	6.38	5.83	6.10	6.28	6.44	6.68	7.05	7.34	7.75
LPG	0.70	0.68	0.71	0.76	0.75	0.80	0.86	0.88	0.96	1.16	1.32	1.24	1.21	1.13
Butane	0.98	0.95	1.07	1.16	1.47	1.53	1.49	1.39	1.34	1.39	1.57	1.44	1.66	1.77
Ethane	0.95	0.98	1.10	1.21	1.53	1.58	1.54	1.43	1.38	1.44	1.62	1.48	1.60	1.71
Other														
-Residual fuel oil	4.66	6.00	6.06	5.71	6.17	6.53	6.66	6.43	6.86	6.63	7.56	7.58	7.56	8.18
-Petroleum Coke	2.18	1.98	1.85	1.33	1.62	1.95	1.83	1.88	1.81	1.98	2.13	1.99	2.27	2.11
-Refinery gas	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-Other oil products	2.71	2.59	3.91	3.90	3.42	3.69	3.60	3.88	4.04	4.21	4.17	4.18	4.13	4.08
-Coal	0.82	0.68	0.70	0.61	0.57	0.75	0.76	0.89	0.87	0.76	0.83	0.72	0.51	0.68
-Lignite	0.10	0.17	0.17	0.16	0.19	0.19	0.21	0.19	0.21	0.21	0.25	0.26	0.25	0.27
-Coke (Hard coal)	0.95	0.80	0.79	0.70	0.68	0.83	0.81	0.93	0.91	0.81	0.87	0.77	0.55	0.73
-Coke (Lignite)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-Tar	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	68.35	67.91	70.78	69.81	76.21	76.45	74.79	78.91	80.52	83.63	87.25	84.41	84.91	86.90

Results

Table 34: Fuel specific and total non-energy use as stated in the IPCC-RA of the German Greenhouse Gas Inventory (2005 submission)

in PJ in Mt CO ₂	EF in kt CO ₂ /PJ*	Year 1990		Year 1991		Year 1992		Year 1993		Year 1994		Year 1995***		Year 1996		Year 1997		Year 1998		Year 1999		
Coal	87.3	0.2	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lignite	113.1	3.4	0.4	4.5	0.5	4.3	0.5	3.3	0.4	3.4	0.4	0.2	0.0	0.0	0.0	0.2	0.0	0.3	0.0	0.3	0.0	0.0
Cokes (coal)	108.2	18.6	2.0	9.9	1.1	8.5	0.9	7.1	0.8	6.5	0.7	7.0	0.8	8.3	0.9	8.1	0.9	8.0	0.9	7.0	0.8	0.8
Cokes (lignite)	106.5	11.1	1.2	3.5	0.4	1.1	0.1	1.9	0.2	1.6	0.2	3.6	0.4	4.5	0.5	3.7	0.4	3.5	0.4	3.1	0.3	0.3
Petroleum coke	119.0	14.9	1.8	13.2	1.6	13.5	1.6	18.7	2.2	19.0	2.3	17.0	2.0	16.5	2.0	14.1	1.7	16.0	1.9	15.2	1.8	1.8
Coal oils and tars	87.6	18.8	1.6	19.8	1.7	21.6	1.9	14.7	1.3	13.1	1.1	11.1	1.0	17.0	1.5	12.4	1.1	10.8	0.9	7.0	0.6	0.6
Tar	87.6	12.2	1.1	5.9	0.5	4.5	0.4	6.2	0.5	7.6	0.7	5.5	0.5	8.5	0.7	6.2	0.5	5.4	0.5	3.5	0.3	0.3
Total solid fuels		79.2	8.1	56.6	5.8	53.5	5.4	52.3	5.4	51.7	5.4	44.5	4.7	54.7	5.6	44.7	4.6	44.0	4.6	36.2	3.9	3.9
Lubricants	73.3	61.5	4.5	48.7	3.6	45.9	3.4	46.0	3.4	47.7	3.5	44.2	3.2	45.0	3.3	41.5	3.0	43.3	3.2	45.3	3.3	3.3
Bitumen	80.7	125.1	10.1	134.6	10.9	143.7	11.6	132.5	10.7	156.5	12.6	140.7	11.3	129.2	10.4	131.1	10.6	129.5	10.4	139.2	11.2	11.2
Naphtha	74.4	357.5	26.6	364.7	27.1	368.3	27.4	379.4	28.2	408.7	30.4	419.6	31.2	422.2	31.4	472.9	35.2	499.4	37.2	491.0	36.5	36.5
Gas/Diesel oils	74.5	70.5	5.3	58.8	4.4	51.0	3.8	48.4	3.6	40.2	3.0	17.2	1.3	18.8	1.4	20.1	1.5	22.1	1.6	22.5	1.7	1.7
LPG	63.7	41.0	2.6	38.4	2.4	40.2	2.6	47.8	3.0	62.8	4.0	66.4	4.2	56.9	3.6	50.1	3.2	47.2	3.0	46.7	3.0	3.0
Residual fuel oils	78.8	75.0	5.9	67.1	5.3	70.6	5.6	61.8	4.9	75.4	5.9	-	-	90.6	7.1	80.5	6.3	91.1	7.2	87.7	6.9	6.9
Refinery gas	60.0	20.2	1.2	20.7	1.2	21.8	1.3	21.1	1.3	19.9	1.2	17.7	1.1	16.7	1.0	21.3	1.3	20.1	1.2	18.4	1.1	1.1
Other oil products	73.3	33.4	2.5	38.6	2.8	49.6	3.6	42.4	3.1	37.1	2.7	39.4	2.9	37.1	2.7	54.3	4.0	62.3	4.6	56.0	4.1	4.1
Total liquid fuels**		784.3	58.6	771.7	57.8	791.0	59.2	779.4	58.2	848.3	63.4	745.2	55.3	816.5	61.0	871.8	65.1	915.1	68.4	906.8	67.9	67.9
Natural gas	55.9	94.4	5.3	61.9	3.5	67.0	3.7	55.5	3.1	64.2	3.6	75.0	4.2	81.6	4.6	96.0	5.4	86.8	4.9	91.8	5.1	5.1
Total gaseous fuels		94.4	5.3	61.9	3.5	67.0	3.7	55.5	3.1	64.2	3.6	75.0	4.2	81.6	4.6	96.0	5.4	86.8	4.9	91.8	5.1	5.1
Total non- energy use		957.8	72.0	890.2	67.0	911.5	68.4	887.2	66.7	964.2	72.3	864.7	64.1	952.8	71.2	1012.4	75.1	1045.8	77.8	1034.8	76.8	76.8

* Emission factors obtained from CRF Table 1.A(d) of the German Greenhouse Gas Inventory ** Excluding petroleum coke

*** No data for 'residual fuel oils' are given; this is the explanation for the extreme low value for total non-energy use in 1995 compared to other years

Results

Since this list of requirements is not entirely fulfilled, total non-energy use according to NEAT and to both the National Energy Balance (NEB) and the IPCC-RA are not identical (compare Table 33 and Table 34 and see Figure 10). With the exception of 1990, the IPCC-RA (2005 submission) reports lower non-energy use than we estimate with the NEAT model. **While NEAT estimates range between 68 and 87 Mt CO₂ in the period of 1990-2003, the IPCC-RA data (64-78 Mt CO₂) are around 1-19% lower than the NEAT values (except for the year 1990). A clear exception is the year 1995, where IPCC-RA data are extremely low (64.1 Mt CO₂) as for this year no non-energy use of residual fuel oils is reported (Figure 10). Apart from that both the data from NEAT and the IPCC-RA show a good match regarding the overall trend and a clear increase of non-energy use in the period of 1991-1998.**

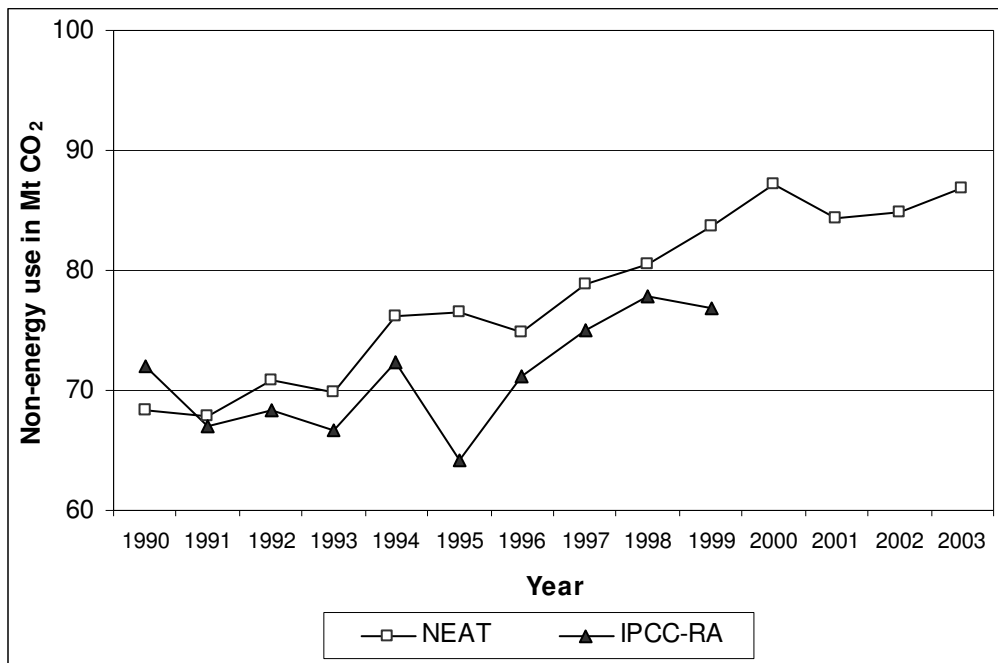


Figure 10: Total non-energy use according to NEAT and the IPCC-RA (2005 submission)

We discuss the differences between both data sources are in the following on the level of individual fuels. Table 35 gives an overview of 'net' non-energy use, thereby distinguishing between three different groups of fuels.

In all years studied, coke/other coal-derived products have a share of 7-10 % on the total non-energy use. Oil-derived fuels account for around 84-87% and natural gas for 6-7% respectively on the tot non-energy use as calculated with NEAT.

Results

Table 35: *Net non-energy use of individual fuels as calculated with NEAT*

Year	Non-energy use of cokes* and other coal products in Mt CO ₂	Non-energy use of oil products** in Mt CO ₂	Non-energy use of natural gas in Mt CO ₂	Total net non-energy use in Mt CO ₂
1990	7.03	57.13	4.19	68.34
1991	6.12	57.19	4.60	67.91
1992	5.82	60.55	4.41	70.78
1993	4.81	60.68	4.32	69.81
1994	5.00	66.37	4.84	76.21
1995	5.61	65.92	4.92	76.45
1996	5.50	64.51	4.78	74.78
1997	5.83	68.24	4.83	78.91
1998	5.75	69.82	4.95	80.51
1999	5.69	72.97	4.97	83.63
2000	6.07	75.87	5.30	87.24
2001	5.77	73.41	5.23	84.41
2002	5.59	74.13	5.19	84.91
2003	5.88	75.31	5.71	86.90

* including petroleum coke

** excluding petroleum coke

Non-energy Use of Coke and Other Coal/Lignite-based Feedstock

According to NEAT the non-energy use of cokes and other coal-derived products varies between 4.8 and 7.0 Mt CO₂ in the period of 1990-2003 (Table 36).

The major part of this non-energy use results from the consumption of cokes (including petroleum coke) and tars, while the use of coal and lignite contributes only a smaller share to the non-energy use of coke and other coal products. The total non-energy use of cokes and other coal products according to NEAT (values printed bold in Table 35) is sometimes larger and sometimes smaller than reported in the Energy Balances and according to the IPCC-RA (2005 inventory submission).

NEAT calculates the non-energy use of coke and other coal-derived feedstock as the sum of (i) coke, pitch and coal used to produce electrodes, (ii) other carbon sources used as reducing agent for the production of non-ferrous metals and ferroalloys and (iii) coal-based feedstock for the manufacture of chemicals such as benzene or methanol.

Results

Table 36: Non-energy use of cokes and other coal products according to NEAT and the NEB (IPCC-RA, 2005 submission)

Year		Coal/ Lignite	Cokes*	Tars**	Total	Absolute deviation (NEAT - NEB)	Relative deviation (NEAT/NEB)
						in Mt CO ₂	
1990	NEAT	0.92	3.13	2.97	7.03	-1.05	-13
	NEB	0.40	4.96	2.72	8.08		
1991	NEAT	0.85	2.78	2.49	6.12	0.36	6
	NEB	0.51	3.00	2.25	5.76		
1992	NEAT	0.87	2.64	2.31	5.82	0.41	8
	NEB	0.48	2.64	2.29	5.41		
1993	NEAT	0.77	2.03	2.01	4.81	-0.63	-12
	NEB	0.41	3.20	1.83	5.44		
1994	NEAT	0.76	2.31	1.93	5.00	-0.38	-7
	NEB	0.43	3.14	1.81	5.38		
1995	NEAT	0.95	2.78	1.88	5.61	0.96	21
	NEB	0.03	3.17	1.45	4.66		
1996	NEAT	0.97	2.64	1.89	5.50	-0.07	-1
	NEB	0.00	3.33	2.23	5.57		
1997	NEAT	1.08	2.82	1.94	5.83	1.24	27
	NEB	0.02	2.95	1.63	4.60		
1998	NEAT	1.08	2.72	1.95	5.75	1.16	25
	NEB	0.03	3.14	1.42	4.59		
1999	NEAT	0.97	2.79	1.94	5.69	1.83	47
	NEB	0.04	2.91	0.92	3.86		
2000	NEAT	1.08	3.00	1.99	6.07		
	NEB	-	-	-	-		
2001	NEAT	0.98	2.77	2.02	5.77		
	NEB	-	-	-	-		
2002	NEAT	0.75	2.82	2.02	5.59		
	NEB	-	-	-	-		
2003	NEAT	0.95	2.84	2.10	5.88		
	NEB	-	-	-	-		

* including cokes produced from coal and lignite as well as petroleum coke

** including tar and coal oil and tars

The NEAT approach may differ from the current accounting practice in the German Energy Balance. Within this research study, it was not possible to obtain detailed insight into the calculation practice of non-energy use of cokes and other coal-based feedstock in the German Energy Balance. It is, hence, not possible to identify the exact reason for the differences between NEAT and the IPCC-RA. Possible explanations could, however, be:

- In the German Energy Balance, the use of ‘*other solid carbon*’ consumed for non-ferrous metals and ferroalloy production might be reported as final energy use of the metal producing sector instead of being accounted for as non-energy use.
- The non-energy use of ‘*other coal products*’ in the Energy Balance may be too low: Table 37 shows data from VFT (1997), which is the only organization dealing with tar processing in Germany. According to this dataset, total input of tar (510 kt) is larger than the quantity reported as non-energy use in the energy balance (436 kt).

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Table 37: Tar processing in Germany 1995 (VFT, 1997; quoted in Patel et al. (1999))

Substance	Amount in kt
Crude benzene	6
Phenol	6
Creosote oils	8
Naphthalene	50
Anthracene	4
Chinoline and other substances	2.5
Other oils	183.5
Pitch	250
Total according to VFT	510
For comparison: 'Other coal products' according to energy balances for the year 1995 (AGE, 1990-1999)	436

Apart from tar processing, crude benzene originating from coke plants is used to produce chemical grade benzene. According to personal communication with industrial experts, a total of 250-300 kt of coal-derived crude benzene is processed in Germany. Of this total, around two thirds are imported while the remainder originates from domestic coke plants. Adding the 250-300 kt to the total tar processing as reported by VFT (i.e., 510 kt, Table 36) gives a value of around 760-810 kt, which is clearly beyond the value for *'other coal products'* as reported in the Energy Balance (while the values discussed refer to the year 1995, the overall picture has not changed since then).

Non-energy use of coke and other coal in the Energy Balance is a rather rough estimate (DIW, 2005). It can, therefore, be doubted that (i) a consistent system boundary for non-energy use of these products is chosen and that (ii) the Energy Balance take the further down-stream consumption of coke and coal-derived feedstock correctly into account.

In view of these findings, we highly recommend further research on the exact calculation procedure for the non-energy use of cokes and coal/lignite-based products in the German Energy Balance, not only to report non-energy use of these items in the IPCC-RA correctly but also to avoid double counting of process emissions in the IPCC-SA of the National GHG Inventory Report.

It is important to note that there is a risk of double counting of coke and other coal-derived non-energy use not only in energy statistics but also in the NEAT model. An example for a possible source of double count, which holds for both energy statistics and the NEAT model is the use of parts of the *'other oils'* in Table 37 to produce, carbon black in the petrochemical industry. Together with the coal-derived *'other oils'* also petroleum-derived heavy oils may be used, making it difficult to trace down individual feedstock flows. Further complications originate from the trade of finished and semi-finished products. Important examples are electrodes, for which we assume in NEAT that the quantities consumed for the production of non-ferrous metals and ferroalloys are also produced in Germany.

Specifically the deviation between the non-energy use data for petroleum coke in the German Energy Balance and the consumption values of petroleum coke for electrodes in NEAT (see Table 3) can be partly explained by trade of electrodes. Our assumption that the total amount of electrodes consumed domestically equals the amounts produced in Germany is justified because trade of electrodes is almost balanced in Germany (Destatis 1990-2003b). However, this might nevertheless be a source for minor errors, especially with respect to feedstock use for electrode production and could hence lead to underreporting or overreporting of non-energy use, depending on the magnitude of *net* trade.

While the examples given concern relatively small flows, which are difficult to follow, the rather obvious coal-derived flows used for non-energy purposes (tar and crude benzene) should be included in non-energy use data as reported in German energy statistics.

Non-energy Use of Oil-based Feedstock

The non-energy use of oil-based feedstock (excluding petroleum coke) varies according to NEAT between 57 and 76 Mt CO₂ and amounts to 84-87% of the total non-energy use in the period of 1990-2003. Table 38 shows that the NEAT estimates for the non-energy use of oil-based products are lower (up to 1.5 Mt CO₂) than according to the German Energy Balance in the years 1990, 1991 but higher (up to 5 Mt CO₂) in all years after 1991.

The relatively low NEAT values for non-energy use in 1990 and 1991 might be explained by the poor quality of chemicals production data due to the reunification of Germany in the same year. **It is likely that NEAT underestimates feedstock requirements for the period 1990-1992 because production data partly refer to Western Germany only and therefore exclude chemicals production in the former GDR.**

Parts of the difference between the non-energy use data according to NEAT and the Energy Balance can be explained by *bulk* chemicals produced in the refinery sector (e.g., propylene, butadiene and aromatics from refineries). **These bulk chemicals are part of the detailed mass balance in NEAT and they are therefore included in the NEAT estimates for non-energy use. In contrast, refinery propylene is excluded and refinery butadiene and aromatics are likely to be excluded from the non-energy use data as stated in the Energy Balance (Lorenz, 2005).**

Table 39 gives an overview of refinery streams in Germany (BAFA, 1990-2003). The estimates for refinery propylene (VCI, 1998) are in the range of 1.8 Mt CO₂ equivalents. These amounts are not included under non-energy use in the Energy Balance (Lorenz, 2005). Refinery propylene as well as butadiene, aromatics and sulfur from refineries are included under the category '*other refinery products*' in the mineral oil statistics (BAFA, 1990-2003).

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Table 38: Non-energy use due to consumption of oil-based feedstock

Year		Lubricants	Bitumen	Other oil-derived fuels*	Total	Absolute deviation (NEAT-NEB)	Relative deviation (NEAT-NEB)/NEB
		in Mt CO ₂					in %
1990	NEAT	4.51	10.10	42.51	57.13	-1.51	-2.58
	NEB	4.51	10.09	44.04	58.64		
1991	NEAT	3.57	10.87	42.75	57.19	-0.56	-0.97
	NEB	3.57	10.86	43.32	57.75		
1992	NEAT	3.37	11.60	45.58	60.55	1.33	2.24
	NEB	3.36	11.59	44.26	59.22		
1993	NEAT	3.38	10.70	46.61	60.68	2.50	4.30
	MEB	3.38	10.69	44.12	58.18		
1994	NEAT	3.50	12.64	50.23	66.37	2.99	4.71
	NEB	3.50	12.63	47.25	63.38		
1995	NEAT	3.24	11.36	51.32	65.92	2.86	4.54
	NEB	3.24	11.35	48.47	63.05		
1996	NEAT	3.30	10.43	50.77	64.51	3.49	5.72
	NEB	3.30	10.42	47.29	61.02		
1997	NEAT	3.05	10.59	54.61	68.24	3.15	4.85
	NEB	3.05	10.58	51.47	65.09		
1998	NEAT	3.18	10.45	56.18	69.82	1.43	2.09
	NEB	3.18	10.44	54.76	68.38		
1999	NEAT	3.32	11.24	58.41	72.97	5.11	7.54
	NEB	3.32	11.23	53.31	67.85		
2000	NEAT	3.32	10.20	62.35	75.87	-	-
	NEB	-	-	-	-		
2001	NEAT	3.32	9.85	60.23	73.41	-	-
	NEB	-	-	-	-		
2002	NEAT	3.38	9.37	61.38	74.13	-	-
	NEB	-	-	-	-		
2003	NEAT	3.35	8.92	63.03	75.31	-	-
	NEB	-	-	-	-		

* including naphtha, gas/diesel oils, LPG, butane, ethane, residual fuel oils, refinery gas and other oil products

It was not possible to obtain estimates for the amount of sulfur contained in the category of 'other refinery products'. We can therefore not exactly estimate the amount of refinery products, which are likely to remain unaccounted as non-energy use in the Energy Balance. However, taken only the amounts of refinery propylene into account, the gap of 1.3-5.1 Mt CO₂ between NEAT and the Energy Balance in the years 1992-1999 is reduced by around 1.8 Mt CO₂.

In spite of contacts with experts from the 'Mineralölwirtschaftsverband' and the developers of the National Energy Balance, it was not possible to get detailed insight into the accounting practice for butadiene and aromatics from refineries in the Energy Balance. Further research is therefore highly recommended to clarify if, to what extent, and where these refinery products are accounted for in the Energy Balance, i.e., under non-energy use or as part of energy conversions.

A critical part with respect to the accounting of non-energy use, are C₄ chemicals, i.e., butenes and butadienes. The reason is that there are various inter-linkages in the production and use of these chemicals. In Germany, butene and butadiene are exclusively produced from steam cracking and from

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fluid catalytic cracking of hydrocarbons.³³ Steam cracking is generally considered as process of the chemical industry while fluid catalytic cracking is a refinery process.

Table 39: Overview refinery streams

Year	Refinery propylene in Mt (VCI 1998)*	Refinery propylene in Mt CO ₂	Total of 'other refinery' products' in Mt (BAFA, 1990-2003)	Estimated amounts of refinery sulfur in Mt	Total of 'other refinery' products' in Mt CO ₂
1990	-	-	0.60	unknown	1.92
1991	-	-	0.80	unknown	2.54
1992	-	-	0.80	unknown	2.54
1993	-	-	0.86	unknown	2.76
1994	-	-	0.97	unknown	3.10
1995	0.56	1.76	0.97	unknown	3.10
1996	0.60	1.89	1.10	unknown	3.52
1997	0.60	1.89	1.15	unknown	3.68
1998	0.60	1.89	1.22	unknown	3.92
1999	0.60	1.89	1.48	unknown	4.74
2000	0.60	1.89	1.66	unknown	5.31
2001	-	-	1.59	unknown	5.08
2002	-	-	1.72	unknown	5.49
2003	-	-	1.63	unknown	5.21

* in italics: estimates

A large share of butene production is not used for chemicals production but (i) as direct fuel additive or (ii) as feedstock for the manufacture of anti-knock components for gasoline (Weissermel and Arpe, 2003). For the consumption of butene in fuels, various options exist. A mixed stream containing butene and butane from refineries can be used directly as gasoline component. Furthermore, refineries themselves can purify and separate butene from mixture streams and transform it in *on-site* units via dimerisation to diisobutene, which might be further transformed (via hydration and alkylation) into isobutane. Tracing the flows of butene is further complicated by the fact that some refineries operate *on-site* steam crackers.

Due to these rather complex process characteristics, it is was not possible within the scope of this study to elaborate the exact accounting practice of (i) butene production and (ii) the exact amount of butene (which is reported as such in the production statistics) used in fuels, as interviews with experts in industry did not yield useful results on the level of desired detail. This is partly because the accounting practice might vary between different companies depending on plant specific characteristics. **It remains therefore also unclear, whether the pure butenes produced in steam crackers as fuel additive are included in the backflows to refineries. If these butenes are regarded as backflows in the Energy Balance but not in NEAT, NEAT might overestimate non-energy use.**

³³ Butene and butadiene can also be produced via hydrogenation and dehydrogenation from each other. Neglecting these alternative production routes can result in overestimation of basic feedstock consumed to produce these C₄ chemicals. To date, butene production from butadiene is only performed in England by Exxon using a selective hydrogenation process in a 35,000 tones per year plant since 1993 (Weissermel and Arpe, 2003). Similarly, the production of butadiene from butene is negligible for Germany due to economic restrictions (at present, it is economically much more attractive to extract butene from refinery flows and steam cracker outputs than using relative expensive C₄ as feedstock). Production routes using butadiene, butanols, or acetylene for manufacturing butene are therefore insignificant for Germany. We hence conclude that, in Germany, butene and butadiene are exclusively produced from steam cracking and from catalytic cracking of hydrocarbons.

While research on the accounting of production and fate of butene and other C₄ chemicals is therefore strongly recommended, it is not clear whether such an effort can succeed due to its dependence on the availability of very detailed data from all refineries in Germany, which is hampered by data confidentiality and the complexity of hydrocarbon flows.

NEAT estimates non-energy use based on production data for 22 basic chemicals. Uncertainties and errors in the production data have a severe effect on the calculated non-energy use in NEAT. The accounting of non-energy use based on mass balance principles is further complicated by complex trade flows of basic chemicals. The difficulties can be illustrated by the example of Shell, which produces pyrolysis gasoline (mainly C₆-aromatics) in their steam cracker in Moerdijk, the Netherlands. Until 1999, this aromatics stream was transported to a benzene extraction unit owned by Shell in Germany. There, benzene was extracted from the pyrolysis gasoline. The pure benzene was then exported back to the Shell plant in Moerdijk, the Netherlands. This example shows the complexity of carbon flows in the chemical industry and the problems associated with correct accounting of these streams. The benzene, which is extracted in Germany, does very likely enter the German Production Statistic, but it is not clear whether the required feedstock enters the German energy statistics. If not, the reported non-energy use would be not sufficient to cover the entire benzene production in Germany. Due to these difficulties, NEAT might result in over- or underestimation of actual feedstock consumption in Germany.

Non-energy Use of Natural Gas

The non-energy use of natural gas as calculated with NEAT ranges from 4.2 Mt CO₂ in 1990 to 5.7 Mt CO₂ in 2003 (Table 40). The NEAT values exceed the non-energy use of natural gas as stated in the Energy Balance in all years except for 1990 and the period of 1997-1999. There are various possible explanations for the observed differences. Firstly, NEAT and the Energy Balance are not entirely consistent regarding the system boundary of non-energy use for natural gas. While NEAT includes natural gas consumed for carbon black production, the Energy Balance excludes this portion of natural gas from the non-energy use. The amounts of natural gas used for carbon black production are, however, minor compared to the total non-energy of natural gas (around 0.15 Mt CO₂ equivalents, see Table 40).

The relatively low natural gas consumption according to NEAT in 1990 might again be caused by the weak quality of production data in this particular year, i.e. the data refer to production in Western Germany only. Apart from these findings, also possible uncertainties associated with production and trade data as given by Destatis (1990-2003a,b) for other years can lead to deviating numbers for non-energy use as given by NEAT and the NEB. Especially the data quality for the years 1990-1994 is low due to (i) reunification of Germany and (ii) unclear product allocation as a consequence of incompatible production codes (i.e., change of product classification in 1995).

A further source of uncertainty is the allocation of feedstock versus energy use of natural gas for chemical processes. The NEB data are derived from the VCI, which assumes a split of roughly 65% versus 35% for feedstock versus energy use of natural gas consumption for ammonia production (VCI, 2004b). In contrast, NEAT uses a 70%:30% split, which might ultimately yield higher feedstock use, i.e., non-energy use of natural gas compared to the values stated in the NEB.

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Table 40: Non-energy use of natural gas

Year	NEAT	NEB	NEAT carbon black production	NEAT (excluding carbon black)	Absolute deviation (NEAT- NEB)*	Relative deviation (NEAT- NEB/NEB)*	Natural gas consumption according to VCI (2004b) compared to NEB**
	in Mt CO ₂					in %	
1990	4.19	5.28	0.18	4.01	-1.27	-24	-
1991	4.60	3.46	0.17	4.43	0.97	28	up to 25% higher
1992	4.41	3.75	0.17	4.24	0.49	13	
1993	4.32	3.11	0.15	4.17	1.07	34	
1994	4.84	3.59	0.13	4.71	1.12	31	
1995	4.92	4.19	0.15	4.77	0.58	14	
1996	4.78	4.57	0.14	4.63	0.07	1	
1997	4.83	5.37	0.15	4.68	-0.69	-13	up to 9% lower
1998	4.95	4.86	0.15	4.80	-0.06	-1	
1999	4.97	5.14	0.15	4.82	-0.32	-6	
2000	5.30		0.15	5.15			
2001	5.23		0.15	5.07			
2002	5.19		0.15	5.04			
2003	5.71		0.15	5.55			

* excluding natural gas consumed for carbon black production

** due to the confidentiality of data, exact values are not given here

A comparison of the non-energy use of natural gas from NEB and VCI (VCI, 2004b) revealed that VCI data are up to 17% higher than the NEB values in the period 1990-1995 and up to 18% lower in the years 1996-1999. Because the non-energy use data for natural gas are derived from the VCI (DIW, 2005), one would expect the differences between the data as stated by IPCC-RA and VCI to be small and constant throughout the years. This is, however, not the case, indicating that the data from VCI and the NEB are not entirely consistent. Comparing the NEAT data directly with values from VCI (2004b) shows that NEAT data are 5-26% higher than the estimates from VCI in all years studied. While the difference between NEAT and the VCI might be explained with the slightly different allocation of feedstock versus fuel use and the fact that natural gas used for carbon black production is excluded from the non-energy use of natural gas according to VCI (see above) the difference between NEB and the VCI data should be addressed by future research. Despite intensive contacts with experts from DIW (2005) and VCI (Rothermel, 2004) this open question could not be resolved in the course of this study.

In that respect, it is important to note that the statistical differences regarding non-energy use of total natural gas consumption as stated in the German Energy Balance exceeds for most of the years the reported non-energy use of natural gas. This finding is indicative not only for uncertainties associated with the non-energy use of natural gas but also for data related to non-energy use throughout the National Energy Balance.

5.4.2 Carbon Storage and Carbon Storage Fractions

Carbon storage is calculated in NEAT as the difference between two components (i) total non-energy use and (ii) the sum of product use and industrial process emissions. Total carbon storage as calculated with NEAT is independent from the definition of non-energy use and therefore only depends on the amount of NODU products domestically consumed and the total *net* exports of chemical

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products (see Section 4.2.2.2). The NEAT carbon storage for the period 1990-2003 is given by Table 41 and Table 42.

Table 41: Carbon storage and carbon emissions from the non-energy use of fossil fuels according to NEAT (total non-energy use according to the *net* definition)

Year	Carbon storage from cokes and other coal feed-stock* in Mt CO ₂	Carbon storage from oil feed-stock** in Mt CO ₂	Carbon storage from natural gas in Mt CO ₂	Total carbon storage in Mt CO ₂	Total emissions from non-energy use in Mt CO ₂	Total non-energy use in Mt CO ₂
1990	2.23	37.16	1.82	41.21	27.13	68.34
1991	1.84	36.23	1.73	39.80	28.10	67.91
1992	1.70	38.49	1.86	42.05	28.73	70.78
1993	1.65	39.72	1.79	43.16	26.66	69.81
1994	1.43	43.59	2.07	47.09	29.11	76.21
1995	1.38	43.70	1.85	46.93	29.52	76.45
1996	1.36	42.94	2.10	46.40	28.38	74.78
1997	1.41	44.42	2.08	47.90	31.00	78.91
1998	1.44	45.96	2.12	49.52	30.99	80.51
1999	1.38	48.37	2.19	51.94	31.69	83.63
2000	1.38	49.36	2.26	53.00	34.25	87.24
2001	1.47	49.67	2.18	53.33	31.08	84.41
2002	1.48	49.23	2.29	53.00	31.90	84.91
2003	1.50	50.37	2.36	54.23	32.67	86.90

* including petroleum coke

** excluding petroleum coke

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Table 42: Fuel specific carbon storage as calculated with NEAT

Year	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
	in Mt CO ₂													
Naphtha	16.46	15.56	16.68	17.97	19.15	20.06	20.07	21.75	22.76	23.93	25.12	25.37	24.94	25.83
Lubricants	3.34	2.65	2.49	2.50	2.59	2.40	2.44	2.26	2.35	2.46	2.46	2.46	2.50	2.48
Bitumen	10.10	10.87	11.60	10.70	12.64	11.36	10.43	10.59	10.45	11.24	10.20	9.85	9.37	8.92
Coal Oils and Tars (from coking oil)	2.12	1.72	1.59	1.54	1.31	1.26	1.24	1.30	1.33	1.28	1.26	1.35	1.35	1.35
Natural gas	1.82	1.73	1.86	1.79	2.07	1.85	2.10	2.08	2.12	2.19	2.26	2.18	2.29	2.36
Gas/diesel oil (inc. residual fuel oil)	2.99	2.81	2.95	3.46	3.74	4.09	3.83	3.92	4.15	4.27	4.48	4.95	4.94	5.37
LPG	0.58	0.53	0.56	0.60	0.58	0.63	0.68	0.68	0.76	0.93	1.06	0.99	0.96	0.88
Butane	0.58	0.55	0.63	0.75	0.89	0.96	0.94	0.88	0.89	0.91	1.02	1.02	1.07	1.18
Ethane	0.58	0.55	0.63	0.75	0.89	0.96	0.94	0.88	0.89	0.91	1.02	1.02	1.07	1.18
Other														
-Residual fuel oil	1.77	2.05	2.17	2.02	2.10	2.18	2.50	2.32	2.51	2.37	2.59	2.49	2.85	2.90
-Petroleum Coke	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-Refinery gas	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-Other oil products	0.78	0.67	0.78	0.97	1.01	1.06	1.12	1.14	1.21	1.35	1.41	1.53	1.53	1.62
-Coal	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-Lignite	0.04	0.06	0.06	0.06	0.07	0.08	0.08	0.07	0.08	0.08	0.09	0.09	0.11	0.11
-Coke (Hard coal)	0.07	0.06	0.05	0.05	0.06	0.04	0.03	0.03	0.03	0.03	0.03	0.03	0.02	0.03
-Coke (Lignite)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-Tar	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	41.21	39.80	42.05	43.16	47.09	46.93	46.40	47.90	49.52	51.94	53.00	53.33	53.00	54.23

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Carbon storage ranges between 41 and 54 Mt CO₂. A clear trend towards increasing carbon storage can be observed in the period of 1990-2003. As in the case of non-energy use, most carbon stored in chemical products is derived from oil feedstock (36-50 Mt CO₂).

In the IPCC-RA, carbon storage is calculated by multiplying non-energy use data for the various hydrocarbons with fuel specific storage fractions. The difference between NEAT and IPCC-RA regarding carbon storage decreases from 16 Mt CO₂ in 1990 to 3 Mt CO₂ in 1999 (Table 43) (note the exception from this in the year 1995).

Table 43: Carbon storage and emissions as given in NEAT and by the IPCC-RA

Year	Total non-energy use in Mt CO ₂		Carbon storage in Mt CO ₂			Carbon emissions in Mt CO ₂		
	NEAT	IPCC-RA	NEAT	IPCC-RA	Absolute difference NEAT-IPCC-RA	NEAT	IPCC-RA	Absolute difference NEAT-IPCC-RA
1990	68.35	72.00	41.21	57.05	-15.84	27.14	14.95	12.19
1991	67.91	66.97	39.80	52.53	-12.73	28.10	14.44	13.66
1992	70.78	68.38	42.05	50.49	-8.44	28.73	17.88	10.84
1993	69.81	66.72	43.16	48.34	-5.19	26.66	18.38	8.28
1994	76.21	72.35	47.09	52.87	-5.78	29.12	19.47	9.65
1995	76.45	64.12	46.93	45.72	1.21	29.52	18.40	11.12
1996	74.79	71.15	46.40	51.85	-5.45	28.39	19.30	9.09
1997	78.91	75.06	47.90	54.07	-6.17	31.01	20.99	10.02
1998	80.52	77.83	49.52	55.81	-6.29	30.99	22.02	8.97
1999	83.63	76.85	51.94	55.40	-3.46	31.69	21.45	10.24
2000	87.25	-	53.00	-	-	34.25	-	-
2001	84.41	-	53.33	-	-	31.08	-	-
2002	84.91	-	53.00	-	-	31.90	-	-
2003	86.90	-	54.23	-	-	32.67	-	-

The differences between IPCC-RA and NEAT data on carbon storage are caused by two factors, i.e., (i) differences of total non-energy use and (ii) differences with respect to fuel specific carbon storage fractions. Concerning the first factor (i), Table 43 shows that non-energy use as given by the IPCC-RA is considerably lower than the one calculated with NEAT (except for the year 1990, where the IPCC-RA value exceeds the NEAT estimates by 3.6 Mt CO₂). This explains one part of the differences. However, the reason explained is less important as, for example, the dataset for 1992 or 1998 show: for these years, total non-energy use according to NEAT and the IPCC-RA are very similar, while the difference in carbon storage is substantial. To explain the other part (ii), it is necessary to examine the specific storage fractions as calculated in NEAT and as given in the IPCC-RA (see Table 43). NEAT storage fractions were determined by dividing carbon storage according to Table 42 by the non-energy use as given in Table 33 (see also Section 4.2.2.2). While absolute carbon storage (in Mt CO₂) is independent from the definition of non-energy use, carbon storage fractions depend on the definition chosen (because the denominator, i.e., non-energy use depends on the definition chosen). For calculating carbon storage fractions with NEAT, we apply a *net* definition of non-energy use to assure consistency with the system boundaries chosen in the NEB.

It is important to note that the NEAT carbon storage fractions given in Table 44 should not be used to calculate storage or emissions in the IPCC-RA. This is because total non-energy use as calculated with NEAT differs from the one as reported in IPCC-RA and NEB. However, carbon storage as calculated with NEAT may be used in the IPCC-RA to determine carbon

storage fractions and non-energy use emissions, as carbon storage is independent from system boundaries of non-energy use.

Throughout the years studied overall NEAT carbon storage fractions vary between 59% and 63%. The overall NEAT storage fractions are 10-19% points smaller than the overall storage fractions as stated in the IPCC-RA of the German Greenhouse Gas Inventory.

For a discussion of these differences, it is important to recall the principle system boundaries used to calculate carbon storage fractions in NEAT and for the IPCC-RA. Due to delay of recent Energy Balances, storage fractions were not given for years after 1999 in the IPCC-RA (2005 inventory submission). The IPCC-RA storage fractions are, therefore, only given for the period of 1990-1999. The official storage fractions used for Germany in the IPCC-RA were calculated by PROGNOS (2000) and base on the following assumptions:

- Carbon is considered to be stored, if it is contained in chemicals with a lifetime of at least 20 years (long life products). If the lifetime of chemicals is shorter than 20 years (short life products), only the amount emissions released as direct CO₂ (i.e., due to incineration) are regarded as emissions. This means that NMVOC emissions from the consumption of short life products are regarded as storage.
- CO₂ released from the fuel use of non-energy use feedstock, i.e., energy use of hydrocarbons in chemical processes are accounted for as emissions. In contrast, emissions resulting from pure feedstock use, e.g., emissions from the steam reforming of natural gas for ammonia production, emissions from other industrial process, CO₂ emissions resulting from chemical conversion losses and emissions from the solvent and other product use are regarded as storage.
- CO₂ from waste incineration are regarded as emissions.
- The carbon contained in imported chemicals is completely excluded from the calculation of storage fractions.
- The carbon contained in exported chemicals is treated in the same way as the carbon contained in domestically produced and consumed chemicals, i.e. a split between short life products (lifetime shorter than 20 years) and long life products (lifetime equal or longer than 20 years) is made. Again, the carbon contained in short life chemicals is considered either to be released as CO₂ (emissions) or as NMVOC (storage).

Results

Table 44: Specific storage fractions as given in the IPCC-RA and as calculated by NEAT

Year	1990		1991		1992		1993		1994		1995		1996		1997		1998		1999		2000*	2001*	2002*	2003*
	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	IPPC-RA	NEAT	NEAT	NEAT	NEAT	NEAT
Naphtha in %	65	60	65	58	58	60	57	63	57	62	57	65	57	65	57	63	57	64	57	64	64	68	66	67
Lubricants in %	94	74	94	74	92	74	92	74	92	74	92	74	92	74	92	74	92	74	92	74	74	74	74	74
Bitumen in %	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
Coal Oils and Tars** in %	74	71	74	69	74	69	74	77	74	68	74	67	74	66	74	67	74	68	74	66	63	67	67	64
Natural Gas in %	94	43	94	38	90	42	90	41	90	43	90	38	90	44	91	43	91	43	91	44	43	42	44	41
Gas/Diesel Oil in %	65	60	65	57	58	60	57	64	57	62	57	64	57	66	57	64	57	66	57	66	67	70	67	69
LPG in %	65	82	65	78	58	78	57	78	57	77	57	78	57	78	57	78	57	79	57	80	80	80	79	78
Butane in %	-	59	-	58	-	60	-	65	-	61	-	63	-	63	-	63	-	66	-	66	65	71	64	67
Ethane in %	-	61	-	57	-	58	-	62	-	58	-	61	-	61	-	61	-	64	-	63	63	69	67	69
Other																								
Residual Fuel Oil in %	93	38	93	34	89	36	89	35	89	34	-	33	89	37	89	36	89	37	89	36	34	33	38	35
Petroleum Coke in %	88	0	88	0	84	0	84	0	84	0	84	0	84	0	84	0	1	0	84	0	0	0	0	0
Refinery Gas in %	65	0	65	0	58	0	57	0	57	0	57	0	57	0	57	0	57	0	57	0	0	0	0	0
Other Oil Products in %	86	29	86	26	77	20	77	25	77	30	77	29	77	31	77	29	77	30	77	32	34	37	37	40
Coal in %	89	0	-	0	-	0	65	0	57	0	-	0	-	0	-	0	-	0	-	0	0	0	0	0
Lignite in %	89	38	89	34	82	35	82	38	82	34	82	40	82	41	82	39	82	39	82	37	36	34	45	42
Coke (Hard Coal) in %	91	7	91	8	85	6	85	7	85	9	85	5	85	4	85	3	85	3	85	3	3	4	4	4
Coke (Lignite) in %	92	0	92	0	87	0	87	0	87	0	87	0	87	0	87	0	87	0	87	0	0	0	0	0
Tar in %	88	0	88	0	84	0	84	0	84	0	84	0	84	0	84	0	84	0	84	0	0	0	0	0
Total in %	79	60	78	59	74	59	72	62	73	62	73	61	73	62	72	61	72	62	72	62	61	63	62	62

* there are no IPCC-RA data available for the period of 2000-2003

** from coking coal

Results

We conclude that the fractions of carbon stored as calculated by PROGNOS (2000) contain (i) all long- and short-life products, which are not incinerated, and (ii) all industrial process emissions. The amount of carbon emitted (1-fraction of carbon stored) includes, therefore, (i) all emissions due to fuel use in industrial processes and (ii) direct CO₂ emissions from incineration of products, which have been domestically produced (domestic consumption plus *net* exports).

In contrast to the system boundaries chosen by PROGNOS (2000), NEAT storage fractions follow the system boundary of non-energy use chosen in the Energy Balance:

- All carbon contained in domestically consumed products (including imports), which do not oxidize during products' use phase and which might only be emitted during post consumer treatment is regarded as stored (fraction NODU products).
- All carbon contained in domestically consumed products (including imports), which is emitted during product use is regarded as emitted (fraction ODU products).
- CO₂ from industrial processes are regarded as emissions.
- Following the definition of non-energy use in the German Energy Balance, emissions from fuel use of coal and oil feedstock in industrial processes are taken into account, i.e., considered as CO₂ emissions.
- Emissions from the parts of natural gas feedstock used as fuel (e.g., during steam reforming for ammonia production) are completely excluded from the non-energy use and are therefore not part of the carbon emissions as calculated with NEAT storage fractions.
- NEAT follows a consumer approach, thereby regarding all exports of chemicals as carbon storage, regardless whether these products are oxidized or not oxidized during use in foreign countries.
- CO₂ emissions from the wastewater treatment. Emissions from waste incineration with energy recovery are part of the energy use emissions and therefore treated as storage. Waste incineration without energy recovery does virtually not occur in Germany.

The methodologies chosen by PROGNOS (2000) and in the NEAT model differ considerably with respect to scope and system boundaries (Table 45). **PROGNOS (2000) understands the IPCC-RA as validation tool for fuel combustion emissions only and generally regards emissions from product use and industrial processes as storage. PROGNOS (2000) follows a *producer approach*, thereby taking CO₂ emissions from exported chemicals into account but neglecting all emissions from chemical imports. NEAT follows a *consumer approach*, thereby regarding all exported chemicals as storage but all imported short-life products as well as industrial processes and domestic product use as relevant for CO₂ emissions. Due to these methodological differences, the storage fractions as calculated by PROGNOS (2000) and NEAT differ considerably and are not directly comparable with each other.**

In the following section, we discuss the storage fraction as calculated with NEAT and by PROGNOS (2000) for the three groups of feedstock (coal-derived, oil-derived, natural gas).

Results

Table 45: Comparison of methodologies for calculating carbon storage fractions in NEAT and by Prognos (2000)

	Prognos (2000)	NEAT model
Carbon emitted during product use	treated as storage	treated as emissions
Carbon emitted during waste incineration	treated as emissions	completely excluded from non-energy use emissions
Carbon contained in exported products	treated as domestic products, i.e., treated either as storage or in case of incineration as emissions	treated as storage
Carbon contained in imported products	completely excluded	treated as emissions if products oxidize during use, treated as storage else
Emissions from the fuel use of feedstock	treated as emissions	treated as emissions from coal and oil based feedstock treated as emissions, emissions from natural gas use completely excluded
Emissions from <i>pure</i> feedstock use	treated as storage	treated as emissions

Coke and Other Coal-derived Feedstock

The NEAT storage fractions for carbon contained in cokes and other coal-based feedstock (including petroleum coke and pitch) vary between 25 and 34% (Table 46). They are clearly below the storage fractions as calculated by PROGNOS (2000) for the IPCC-RA (see Table 45). The fact that the NEAT storage fractions are roughly half of the ones stated in the IPCC-RA can be explained by methodological differences. Cokes and pitch (along with other solid carbon produced from coal/lignite) are used to a large extent for the production of electrodes or as direct reducing agents during manufacturing of ferroalloys and non-ferrous metals. The resulting industrial process emissions are regarded as storage by the IPCC-RA storage fractions (PROGNOS 2000) but treated as emissions in NEAT.

Results

Table 46: Carbon storage fractions of coke and other coal-derived feedstock³⁴

Year	Carbon storage fraction of coke and other coal-derived feedstock* in %	
	IPCC-RA (2005 submission)	NEAT
1990	87	32
1991	85	30
1992	81	29
1993	82	34
1994	82	29
1995	83	25
1996	82	25
1997	82	24
1998	83	25
1999	83	24
2000	-	23
2001	-	25
2002	-	27
2003	-	25
Average	83	27

* including petroleum coke

Oil-derived feedstock

The carbon storage fractions as calculated by NEAT for oil-derived feedstock (excluding petroleum coke) range from 63% to 68%. The NEAT storage fractions are 10-15% points below the IPCC-RA values (Table 47) but slightly above the total NEAT storage fractions as calculated in Table 42. The fact that NEAT storage fractions are again lower than the ones stated by the IPCC-RA can be explained by methodological differences, i.e., NEAT regards CO₂ released from industrial processes as emissions, whereas PROGNOS (2000) treats these emissions as storage when calculating carbon storage fractions for the IPCC-RA. Moreover, industrial process emissions (e.g., conversion losses in the chemical industry) are regarded as storage in the IPCC-RA values (PROGNOS, 2000) but treated as emissions in NEAT.

The differences between NEAT and IPCC-RA values are smaller for oil-derived feedstock than for coke and other coal/lignite-based feedstock due to the following reasons:

- Oil-derived feedstock is mainly used to produce petrochemical products. Around 80% of these products are not oxidized during use. Both PROGNOS (2000) and NEAT treat the amounts of carbon contained in these products as storage.
- Oil-derived feedstocks are generally not used for producing synthesis gas (mainly used for ammonia and methanol production), which is an important source for industrial process emissions.
- A considerable amount of feedstock (mainly naphtha and LPG) is used in steam cracking for energy purposes. Due to the definition of non-energy use in the Energy Balance, NEAT treats the resulting CO₂ emissions as industrial process emissions and includes them therefore also as carbon emitted when calculating storage fraction. When calculating storage fractions for the

³⁴ The NEAT carbon storage fractions given here should *not* be used to calculate storage or emissions on the basis of non-energy use data as stated in energy balances (see text directly above Table 44).

Results

IPCC-RA, PROGNOS (2000) treats these emissions as fuel use emissions and similarly includes them in their calculations as emitted carbon.

Table 47: Carbon storage fractions of oil-derived feedstock³⁵

Year	Carbon storage fraction of oil-derived feedstock* in %	
	IPCC-RA (2005 submission)	NEAT
1990	77	65
1991	77	63
1992	72	64
1993	71	64
1994	71	66
1995	71	66
1996	71	67
1997	70	65
1998	70	66
1999	70	66
2000	-	65
2001	-	68
2002	-	66
2003	-	67
Average	72	66

* excluding petroleum coke

The fact that large fractions of feedstock end up in chemicals, which are not oxidized during their use phase also explains why the specific storage fractions for oil-derived feedstock are considerably higher than the ones for coke and other coal/lignite. The storage fractions for lubricants deserve special attention. While PROGNOS (2000) assumes that 92-94% of all lubricants consumed remain stored, NEAT only adopts a storage fraction of 74%.³⁶ The difference might partly be explained by emissions from lubricants use that are accounted for as storage by PROGNOS (2000) but as emissions in NEAT. However, **determining meaningful storage fractions for lubricants is by no means straightforward and requires detailed insight in the consumption patterns of lubricants.** Especially the combustion of lubricants in two stroke engines (motor scooters, power mowers, and other maintenance equipment) and the end-of-life treatment options of lubricants deserve special in-depth investigation to (i) generate more accurate estimates for the non-energy use of lubricants and (ii) calculate carbon storage and emissions for lubricants use correctly. We therefore consider also the NEAT storage fractions for lubricants as a rough estimate only. **Due to the complexity of this issue, further research on the consumption and fate of lubricants is highly recommended, in order to improve the understanding of emissions resulting from lubricants use in Germany.**

Natural gas

The NEAT carbon storage fractions for natural gas vary between 38 and 44% (Table 48). They are by more than a factor two smaller than the storage fractions as calculated by PROGNOS (2000) for use in the IPCC-RA (90-94%). The NEAT storage fractions for natural gas are in range with the ones calculated for coke and other coal/lignite feedstock but clearly below the ones for oil-derived feedstock. This finding and the huge difference between IPCC-RA and NEAT data can be explained by the fact,

³⁵ The NEAT carbon storage fractions given here should *not* be used to calculate storage or emissions on the basis of non-energy use data given in energy balances (see text directly above Table 44).

³⁶ This percentage is based on the data from Trischler (1997) as reported in Table 4 of this report, see Section 4.2.1.1) according to which 270 kt out of a total of 1042 kt waste lubricants represent 'other losses' of lubricants.

Results

that natural gas is mainly used for producing synthesis gas for ammonia and methanol production. Because no feedstock carbon is contained in the final ammonia, the production process yields substantial amounts of CO₂ emissions. PROGNOS (2000) treats these emissions as industrial process emissions and therefore as storage. According to the definition of non-energy use for natural gas in the Energy Balance, NEAT allocates 30% of the total feedstock input to fuel use and the remaining 70% to feedstock use. The feedstock input for fuel use is excluded from the non-energy use of natural gas. The remaining 70% are treated as emissions when calculating carbon storage fractions in NEAT. The very low NEAT storage fractions of natural gas are therefore caused by the fact that (i) the vast majority of carbon embodied in natural gas is oxidized during industrial processes and, therefore, (ii) only comparatively little feedstock carbon is finally incorporated in chemical products made from natural gas feedstock.

Table 48: Carbon storage fractions of natural gas³⁷

Year	Carbon storage fraction of natural gas in %	
	IPCC-RA (2005 submission)	NEAT
1990	94	43
1991	94	38
1992	90	42
1993	90	41
1994	90	43
1995	90	38
1996	90	44
1997	91	43
1998	91	43
1999	91	44
2000	-	43
2001	-	42
2002	-	44
2003	-	41
Average	91	42

Discussion of Carbon Storage Fractions Used in the IPCC-RA

The discussion in the previous section revealed severe methodological differences in the calculation of carbon storage fractions according to PROGNOS (2000) and NEAT. Although the current 1996 IPCC guidelines remain somewhat vague on the exact purpose of the IPCC-RA, many countries (including Germany) use the IPCC-RA as validation tool for emissions from fuel combustion and not as crosscheck for the total national CO₂ emissions as stated by the IPCC-SA. In that respect, the storage fractions as calculated by PROGNOS (2000) are not always consistent with their original purpose because (i) also direct CO₂ emissions from product use are taken into account and (ii) the system boundaries for non-energy use as defined by PROGNOS (2000) remain vague and seem not always properly defined. For example, PROGNOS (2000) regards the total amount of emissions from ammonia production as industrial process emissions and hence as carbon storage. This approach is correct for natural gas used to produce ammonia but not for the heavy oil fractions. For the latter, the

³⁷ The NEAT carbon storage fractions given below should not be used to calculate storage or emissions on the basis of non-energy use data given in energy balances. The reason is explained in the text directly above Table 44.

total oil feedstock is regarded as non-energy use in the Energy Balance but roughly 30% of the oil feedstock is used as fuel for ammonia production. The emissions from this fuel use should hence be accounted for as emissions and not as storage in the carbon storage fractions from PROGNOS (2000). Furthermore, PROGNOS (2000) follows a producer approach, thereby accounting for CO₂ emissions resulting from the consumption of exported chemicals but excluding imported chemicals from the calculation of storage fractions. This is inconsistent with the current IPCC guidelines, where a consumer approach is chosen as boundary principle to be applied in National GHG Inventories.

The NEAT storage fractions, in contrast, are calculated in order to use the IPCC-RA as a validation tool for the total national CO₂ emissions as calculated in the IPCC-SA. In that respect, the NEAT values are consistent with their purpose, i.e., excluding energy use of feedstock from the calculations completely and accounting for all emissions from industrial processes and product use. The NEAT system boundaries of non-energy use are consistent with the ones chosen in the German Energy Balance. The approach chosen by NEAT and consequently also the methodology to calculate storage fractions are based on the outcome of the work done in previous years by the NEU-CO₂ network. Although this network had an impact on the revision of IPCC guidelines, the draft 2006 IPCC guidelines (IPCC, 2006) clearly state the purpose of the IPCC-RA as reference tool for fuel combustion emissions only, which differs from earlier intentions of the NEU-CO₂ network. According to the new 2006 IPCC guidelines emissions from industrial processes, product use, as well as waste treatment without energy recovery (incineration without energy recovery, wastewater treatment) are excluded from the IPCC-RA emission estimates. **In order to calculate meaningful estimates for emissions resulting from the non-energy use of fossil fuels in the IPCC-RA, we would therefore recommend using NEAT carbon storage as presented in Table 42 and divide it by fuel specific non-energy use as stated in the IPCC-RA.**

If UBA decides at a later point to prepare the German Greenhouse Gas Inventory consistently with the updated 2006 guidelines, we recommend to apply a different approach as the 2006 guideline emphasize the IPCC-RA as validation tool for fuel combustion emissions only. We would therefore suggest to:

- Apply throughout the time series uniform storage fractions of 100% to the hydrocarbons listed in Table 1.(A)d (feedstock and non-energy use refinery products) (IPCC, 2006).
- Emissions from non-energy use, i.e., mainly industrial processes and solvent and other product use emissions, are then excluded from the IPCC-RA and should be only dealt with in the combined 'Industrial Processes and Product Use' chapter of the IPCC-SA (IPCC, 2006).

5.4.3 Total Fossil CO₂ Emissions

NEAT calculates total national CO₂ emissions by deducting NEAT carbon storage from the total consumption of fossil fuels as stated in the IPCC-RA (2005 submission, CRF Table 1.A(d)) (see Table 49; note that these emissions represent estimates for the *total* fossil CO₂ emissions in Germany, i.e., including emissions from energy and non-energy use of fossil fuels).

The total fossil-based emission decreased from 1034 Mt CO₂ in 1990 to 850 Mt CO₂ in 2003. This is equivalent to a reduction of emissions until the year 2003 by 18% compared to the base year 1990.

Results

Table 49: Total fossil-based CO₂ emissions in Germany as calculated by using total fossil fuel consumption according to the IPCC-RA and NEAT carbon storage*

Year	Total consumption of fossil fuels according to the IPCC-RA in Mt CO ₂	Carbon Storage according to NEAT in Mt CO ₂	Total fossil CO ₂ emission in Mt CO ₂	Emissions compared to 1990 in %	IPCC-RA, total fossil emissions in Mt CO ₂
1990	1076	41	1034	100	
1991	1034	40	994	96	
1992	985	42	943	91	
1993	973	43	930	90	
1994	960	47	913	88	
1995	948	47	901	87	
1996	975	46	928	90	
1997	946	48	899	87	
1998	937	50	887	86	
1999	902	52	850	82	
2000	-	-	-	-	
2001	-	-	-	-	
2002	-	-	-	-	
2003	-	-	-	-	

The results from Table 49 are discussed in greater detail in the next section, when discussing in detail the differences between IPCC-RA and IPCC-SA and the usefulness of NEAT results for improving emission estimates in the German GHG Inventory.

5.5 Comparing the results of IPCC-RA and IPCC-SA

5.5.1 Non-energy Use and Resulting Emissions in the IPCC-RA and IPCC-SA

The comparison of non-energy use CO₂ emissions as stated by the IPCC-RA and the IPCC-SA (mainly emissions from the source categories ‘*industrial processes*’ and ‘*solvent and other product use*’) is given in Table 50. The differences between both approaches range between 12 Mt CO₂ in 1990 and 19 Mt CO₂ in 1998 (2005 inventory submission). If NMVOC emissions from the ‘*solvent and other product use*’ are also included, the gap decreases to 8-16 Mt CO₂. It is important to note that NMVOC emissions are, however, not part of the total fossil CO₂ emission as stated by the IPCC-SA.

While the accounting of emissions from non-energy use in the IPCC-RA is entirely based on data from Energy Balances and therefore a rather straightforward procedure, this is not necessarily the case for the IPCC-SA. In the latter approach, emissions from non-energy use can possibly be omitted or double counted.

According to UBA (2004a), the German Energy Balances are also the most important data source for calculating emissions in the source category ‘*energy*’ of the IPCC-SA. The non-energy use emissions as calculated with the IPCC-RA and the IPCC-SA should be similar, (i) if IPCC-RA and IPCC-SA adopt the same system boundaries for non-energy use and (ii) if the carbon storage fractions used in the IPCC-RA reflect the amount of non-energy use carbon stored in the economy. **However, as outlined in Section 5.2, IPCC-RA, i.e., NEB and IPCC-SA are not consistent with respect to the system boundaries of non-energy use.**

Results

Table 50: Comparison of CO₂ emissions from the non-energy use of fossil fuels as stated by the IPCC-RA and the IPCC-SA of the German GHG Inventory (2005 submission)

Year	IPCC-RA			IPCC-SA		Absolute difference: IPCC-RA and IPCC-SA in Mt CO ₂	Absolute difference: IPCC-RA and IPCC-SA (including solvent emissions) in Mt CO ₂
	Non-energy use in Mt CO ₂	Storage in Mt CO ₂	Total emissions from non-energy use in Mt CO ₂	Total emissions from non-energy use in Mt CO ₂ ¹⁾	Total emissions from non-energy use including solvent emissions in Mt CO ₂ ²⁾³⁾		
1990	72.0	57.1	15.0	3.2	5.9	11.8	9.1
1991	67.0	52.5	14.4	2.5	5.1	11.9	9.3
1992	68.4	50.5	17.9	2.4	4.9	15.5	13.0
1993	66.7	48.3	18.4	2.2	4.7	16.2	13.7
1994	72.3	52.9	19.5	2.2	4.7	17.3	14.8
1995	64.1	45.72	18.4	2.6	5.0	15.8	13.4
1996	71.2	51.9	19.3	2.6	4.9	16.7	14.4
1997	75.1	54.1	21.0	2.6	4.9	18.4	16.1
1998	77.8	55.8	22.0	2.6	4.9	19.4	17.1
1999	76.8	55.4	21.4	2.6	4.8	18.9	16.6

¹⁾ Including emissions from the production of ammonia, carbides, and aluminium.

²⁾ Including emissions from the production of ammonia, carbides, aluminium, and the solvent and other product use.

³⁾ A conversion factor of 2.31 is used to convert NMVOC emissions into CO₂ equivalents (NMVOC emissions are not included in the total GHG emissions according to the current practice in the German GHG inventory).

Furthermore, also carbon storage fractions as used in the current IPCC-RA do not entirely reflect actual carbon storage correctly (see Section 5.4.2). Therefore, emissions as given in the IPCC-RA and IPCC-SA are not directly comparable with each other.

However, the fact that the IPCC-SA reports only 4.7-5.9 Mt CO₂ from non-energy use emissions (already including NMVOC emissions from '*solvent and other product use*') out of the total non-energy use of 64-77 Mt CO₂ raises the questions (i) whether emissions are simply forgotten in the IPCC-SA or (ii) whether parts of these emissions are accounted for in the IPCC-SA under the source category '*energy*'.

The fact that total emissions according to the IPCC-SA are 15-30 Mt CO₂ lower than in the IPCC-RA (see Table 51, 2005 inventory submission) strongly indicates that the non-energy use emissions in the source categories '*industrial processes*' and '*solvent and other product use*' of the IPCC-SA are incomplete.

Results

Table 51: Total fossil-based CO₂ emissions in Germany according to IPCC-RA and IPCC-SA (2005 inventory submission)*

Year	Total emissions from fossil hydro-carbon consumption in Mt CO ₂		Absolute difference in Mt CO ₂	Total emissions based on IPCC-RA and NEAT carbon storage in Mt CO ₂
	IPCC-RA	IPCC-SA		
1990	1018.6	988.9	29.7	1034
1991	981.2	953.6	27.5	994
1992	934.7	905.6	29.1	943
1993	924.4	896.1	28.3	930
1994	907.0	880.4	26.6	913
1995	895.7	876.1	19.6	901
1996	923.0	900.1	22.9	928
1997	892.4	868.1	24.2	899
1998	881.1	859.7	21.3	887
1999	846.6	832.1	14.5	850

* The data in this table do not refer to emissions from non-energy use only but to CO₂ from all sectors of the economy.

UBA explains two thirds of the differences between the IPCC-RA and IPCC-SA emission estimates in the National Inventory Report (UBA, 2004a), with different emission factors and carbon contents of the various fuels and only one third to systematic differences, e.g., system boundaries of carbon storage fractions as applied in the IPCC-RA.

In the 2006 inventory submission, UBA already accounted for parts of these inconsistencies by reporting next to emissions from ammonia and aluminium production also emissions from methanol, carbon black, and ferroalloy production under the source category of ‘industrial process emissions’ in the IPCC-SA. This closes the gap between the IPCC-RA and IPCC-SA non-energy use emission estimates to some extent. Remaining differences are caused by the applied IPCC-RA storage fractions, which do not account for all emissions from non-energy use and furthermore by the accounting practice for non-energy use emissions in the IPCC-SA, which is not in line with the IPCC-RA system boundaries for non-energy use (e.g., accounting emissions resulting from the fuel use in steam crackers under ‘energy’ and not as ‘industrial process emissions’, see Section 5.2).

5.5.2 Using NEAT Results to Explain Differences Between IPCC-RA and IPCC-SA

As indicated above, emissions from the non-energy use of fossil fuels according to IPCC-RA and IPCC-SA are not directly comparable. This is partly because the storage fractions as used in the IPCC-RA have been determined (by PROGNOS) to calculate mainly emissions from the fuel use of fossil energy carriers, which are reported as non-energy use in the Energy Statistics. We argue that the non-energy use emissions reported mainly in the source categories ‘*industrial processes*’ and ‘*solvent and other product use*’ of the IPCC-SA should additionally be taken into account (i) in order cover total emissions from the non-energy use of fossil fuels and therefore also (ii) to correctly estimate the amount of carbon actually stored in the economy.

In the ideal case, energy use (combustion) of fossil feedstocks would be completely excluded from the non-energy use in the Energy Statistics. If that were the case, fuel use of hydrocarbons reported as non-energy use would be zero. The source categories of ‘industrial processes’ and ‘solvent and other product use’ would in this case report pure non-energy use emissions. However, non-energy use data in the Energy Statistics (and hence in the IPCC-RA) include also the energy use of coal and oil derived feedstock, while excluding the fuel use parts of natural gas feedstock (see Section 3.3). This causes consistency problems, when reporting non-

energy use emissions in the respective source category of the IPCC-SA because parts of fuel use emissions from coal and oil feedstock in chemicals processes (e.g., steam cracking) should hence also be included under ‘*industrial processes*’ in the IPCC-SA.

Figure 11 compares non-energy use emissions as stated in the IPCC-RA and IPCC-SA (2005 inventory submission). The NEAT results are used to fill up missing emissions in the IPCC-SA (i.e., from industrial processes incl. conversion losses, product use, wastewater treatment). We made this choice in order to show how NEAT can be used to complement estimates, which are already part of the IPCC-SA.

Using NEAT results to close data gaps in the IPCC-SA (2005 submission) leads to emission estimates of 20.9 to 24.2 Mt CO₂ from non-energy use per year in the period of 1990-1999. The estimates would be around 2.0-3.5 Mt CO₂ higher if the IPCC-SA emission estimates for ammonia, aluminum, and carbides productions were replaced with NEAT estimates³⁸. The IPCC-RA values on non-energy use emissions are 1.7-6.4 Mt CO₂ per year lower than the combined IPCC-SA/NEAT estimates. As mentioned above, this is explained by methodological differences, i.e., the fractions of carbon stored in the IPCC-RA include emissions from feedstock consumption of industrial processes as well as from product use emissions. However, the results shown in Figure 11 give a valuable overview of the complete non-energy use emissions, as they should be reported in the various source categories of the IPCC-SA.

³⁸ This could be justified by the unexplainable low emission factors used in the IPCC-SA for ammonia and aluminum production in the IPCC-SA (2005 submission).

Results

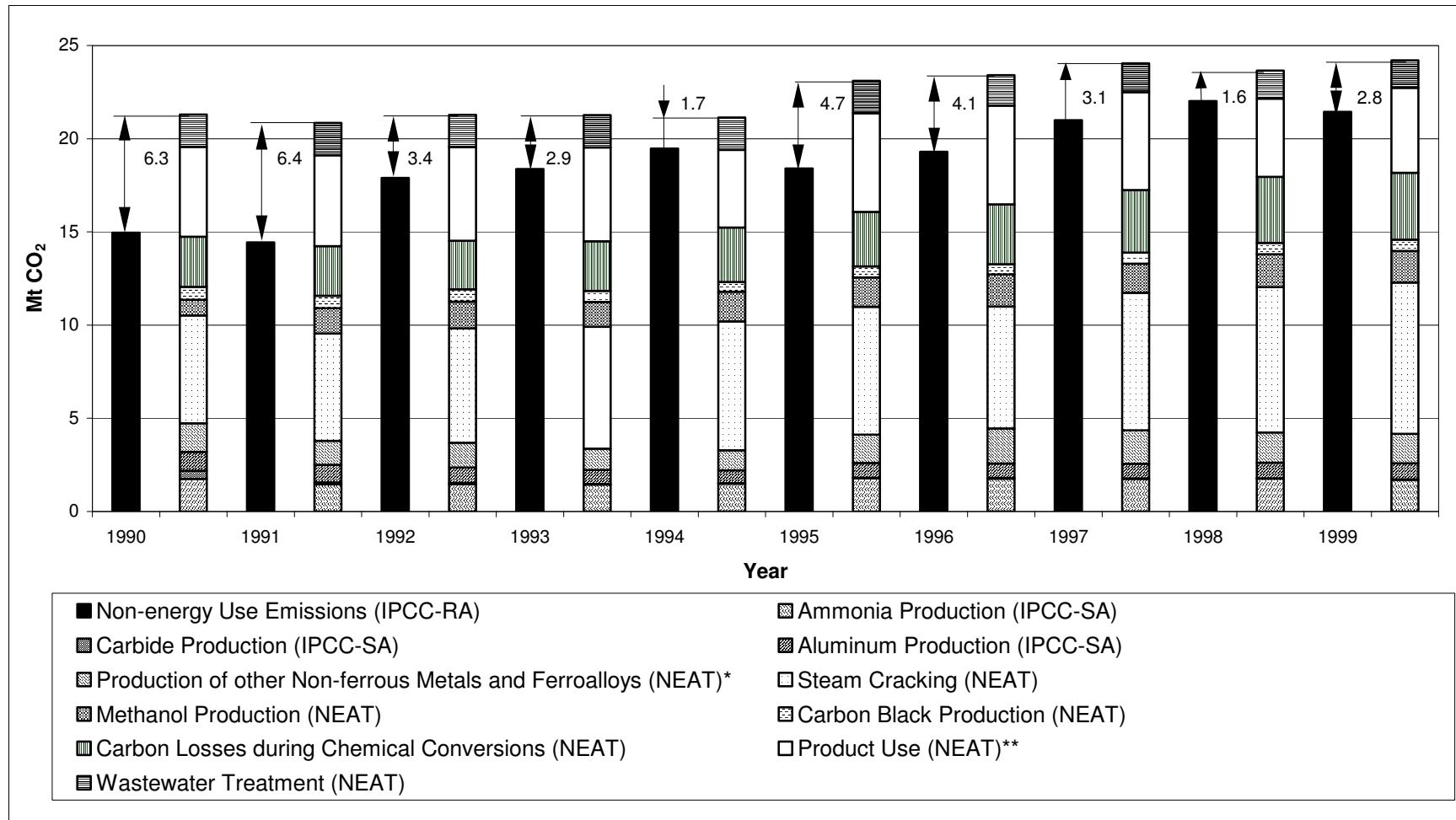


Figure 11: Comparison of non-energy use emissions as stated in the IPCC-RA and as calculated in the IPCC-SA/NEAT (2005 inventory submission)

* excluding aluminum and carbides production

** using lower end of possible values range

Results

It is important to note, that the previous discussion entirely refers to the German GHG Inventory as is was submitted in 2005. In the most recent 2006 inventory submission, IPCC-SA data are more complete (i.e., emissions from the production of methanol and carbon black as well conversion losses are included under the source category of '*industrial process emissions*'). The consistency problems associated with IPCC-RA and IPCC-SA of the current 2006 inventory submission will be discussed in the following section.

6 Conclusions and Recommendations

This chapter contains:

- **Conclusions regarding NEAT results and related uncertainties**
- **Recommendations for UBA regarding improvements of the current GHG inventory**
- **Recommendations on how to use NEAT estimates for inventory updates**

6.1 Conclusions on NEAT Results and the Related Uncertainties

The NEAT model calculates non-energy use and related CO₂ emissions based on a carbon flow and mass balance approach using production and trade data for the 80 most important chemical and petrochemical products consumed in Germany. The quality of production and trade data used as model input is crucial for the reliability of the model results. While trade data are generally considered to be reliable (because they are used for taxation purposes) this is not always the case for production data. **In the course of this study, major inconsistencies in the production data as stated by Destatis (1990-2003a) (e.g., for bitumen, lubricants, basic chemicals like butadiene, toluene or polymers like polyamide, polyurethane) were discovered³⁹.** Next to uncertainties related to input data, the assumed production routes for intermediate and final chemicals are critical for the accuracy of the NEAT model results on non-energy use and related emissions. Uncertainties arise because companies tend to give only vague information on production routes due to confidentiality reasons. To some extent, the production and trade data can be crosschecked by means of the mass balances implemented in NEAT: If production data are consistent with chemical production routes, there should be always sufficient amounts of basic or intermediate chemicals for the production of chemicals produced more downstream in the process chain. Regarding the NEAT model calculations for Germany, this is not always the case. In the period studied, deviations between chemical consumption and demand for further processing in the NEAT mass balance amount to 0.7-4.3 Mt CO₂ per year. These uncertainties amount to a maximum to 5% of the total non-energy use. **In general, we therefore consider the NEAT results as reliable, albeit with important differentiation for the various types results (see below). Further improvement in the accuracy of production and trade data as well as more detailed information on production routes in the chemical and petrochemical sector could, however, improve the NEAT estimates on non-energy use and related emissions.**

The main purpose of the NEAT model is to calculate non-energy use and resulting emissions independently (e.g., from the National Energy Balance) and to compare the model results with data from official sources, i.e. data from the National Energy Balance and the German GHG Inventory. **For these comparisons, it is of critical importance (i) to elaborate the precise system boundaries of non-energy use as stated in the Energy Balance and (ii) to apply the same system boundaries in the NEAT model calculations.**

Within the scope this study it was possible, to get an overview of the general data sources and procedures used to calculate the non-energy use of fossil fuels in the official Energy Balances. In communication with experts in the field (e.g., experts in charge of the oil statistics and experts in

³⁹ To correct for this, production data from producer associations (e.g., VCI (1990-2004), Consultic (1997-2003)) were used in some cases as model input.

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industry) the NEAT model has played a valuable role in pinpointing key issues (raw materials, products, processes, inconsistencies over time etc.). **However, important details, such as the accounting of (i) cokes and other coal products, (ii) refinery butadiene and aromatics, and (iii) the various butene streams from refineries and steam crackers still remain unclear and deserve special attention in the future.** Given the resolution of the model and the uncertainty of the data it uses, these points cannot easily be clarified. **Apart from these uncertainties, we conclude that the system boundaries of non-energy use as applied in NEAT are consistent with the ones used in the National Energy Balance.** Therefore, the NEAT results should be directly comparable with data from the official GHG Inventory of Germany.

Before applying the NEAT model to Germany, the former model version (version 2.0) was extended by a waste module and a module to calculate emissions from conversion losses in the chemical industry (i.e., direct CO₂ losses, off-gases and non-specified by-products) next to various other improvements (e.g., adaptation of chemical production routes). The new model version (NEAT version 3.0) ensures completeness and consistency of NEAT results with respect to the requirements for emissions reporting in accordance to the IPCC guidelines. NEAT calculates total non-energy use and related emissions for industrial processes, product use, and wastewater treatment.

NEAT results for yearly emissions from the production of ammonia (2.6-4.6 Mt CO₂), aluminum (0.9-1.9 Mt CO₂) and carbides (0.3-0.8 Mt CO₂) are above the IPCC-SA estimates (2005 inventory submission). This result can be explained with the very low emission factors used in the inventory for ammonia and aluminum production. IPCC-SA (2005 inventory submission) does not account for any other industrial processes. **The NEAT emission estimates for steam cracking (5.6-8.6 Mt CO₂), methanol production (0.8-2.2 Mt CO₂), carbon black production (0.5-0.7 Mt CO₂), chemical conversion losses (2.6-3.8 Mt CO₂) and the production of non-ferrous metals and ferroalloys other than aluminum and carbides (1.1-1.9 Mt CO₂) can hence be used to complete the estimates for product use emissions in the IPCC-SA. This was to some extent done in the 2006 inventory submissions, which report in addition to the 2005 inventory submission industrial process emissions for the production of methanol and carbon black, catalyst burning (i.e., regeneration) as well as for chemical conversion losses.**

The estimates for chemical conversion losses as calculated with NEAT for Germany are in range with results from other country studies (Tonkovich and Gerber, 1995, Theunis et al., 2003). Due to related uncertainties, we nevertheless recommend studying this particular source of CO₂ in more detail to improve the accuracy of emission estimates used in the IPCC-SA. In spite of remaining uncertainties, we regard the industrial process emissions as calculated with NEAT as reliable (with the exception of chemical conversion losses). We therefore recommend the use of these data to improve the emission estimates for industrial processes in the IPCC-SA.

The IPCC-SA does not account for fossil emissions from wastewater treatment. The CO₂ emissions as calculated with NEAT (1.4-1.7 Mt CO₂) are rough estimates based on (i) the chemical oxygen demand in wastewaters from the chemical industry and (ii) the average surfactant consumption in Germany and might therefore only serve as benchmark values for further, more detailed analysis.

Special attention needs to be paid to the product use emissions (ODU emissions) as calculated with NEAT ($7.2 \pm 2.5 - 9.3 \pm 3.2$ Mt CO₂ per year). As it is the case for the emissions discussed above, the calculation of product use emissions in NEAT (source categories industrial processes, waste and agriculture) depend on the quality of input data (from production and trade statistics). As important differences, the estimates for product use emissions additionally depend on the correctness of production routes. They require therefore much more interrelated data. Furthermore, many of the products causing ODU emissions are intermediates, which are particularly prone to double counting or

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non-reporting. The fact that NEAT estimates a higher total non-energy use than stated in the IPCC-RA (68-87 Mt CO₂ versus 64-78 Mt CO₂ in the period 1990-1999) might be an indication for double counting (this is on the other hand no proof because, as discussed in Chapter 5.4.1, several important products and processes seem to be missing in the non-energy use data according to the IPCC-RA. **The results for product use emissions based on additional *bottom-up* calculations are clearly below the NEAT estimates (slightly below the lower error range of NEAT estimates, see Figure 8). Although there is a chance that the *bottom-up* estimate is too rough and incomplete with respect to some emissions from product use, it raises doubts about the reliability of NEAT estimates on product use emissions. We can, therefore, not recommend using the product use emissions as calculated with NEAT as direct inputs for the IPCC-SA.**

NEAT calculates a total non-energy use of 68-87 Mt CO₂ per year in the period of 1990-2003. Except for the year 1990, the NEAT values are 1-7 Mt CO₂ higher than the IPCC-RA data on total non-energy use (64-77 Mt CO₂ in the period of 1990-1999, 2005 inventory submission). The differences between NEAT and the IPCC-RA data on total non-energy use are related to (i) incomplete accounting of non-energy use in the Energy Balance with respect to refinery propylene, downstream products of coal tars, i.e., crude benzene and very likely also regarding refinery aromatics and butadiene used for non-energy purposes and (ii) uncertainties related to NEAT model inputs on production/trade data and chemical production routes. Uncertainties are further related to the unclear position of '*other cokes and coals*' (used for non-ferrous metals and ferroalloy production) in the Energy Balance and due to the vague status of butene used as gasoline component in production statistics and in oil statistics.

We finally conclude that a material flow analysis like the NEAT model can be used to generate reliable (with some differentiation), useful, and independent estimates for non-energy use and related CO₂ emissions. The requirement of considerable amounts of data and detailed insight in the German chemical industry remains a major drawback with respect to the applicability of the NEAT model. It can therefore be doubted, whether the NEAT model can be applied in a short period of time by inventory experts (this holds for Germany and even more so for countries, where the data availability is considerably worse compared Western Europe standards). It should be pointed out that by far the most time-consuming part of the NEAT model, requiring most of the data inputs, is the *bottom up* carbon balance, resulting in an estimate for product related emissions. At the same time, the biggest uncertainty is in this part. Obtaining estimates for the industrial process emissions in the country of study requires much less data input and yields in turn more reliable results. Based on this insight, we developed in the context of the third phase of the NEU-CO₂ network a simplified version of the detailed NEAT model (NEAT-SIMP), which is shortly discussed in Appendix C of this report. We will revert to the NEAT-SIMP model while giving recommendations in the next chapter.

6.2 Recommendations

6.2.1 General Recommendations

The starting point of emissions accounting for the non-energy use of fossil fuels is the Energy Balance. Reliable estimates in the National GHG Inventory can only be obtained if the data in the Energy Balance are complete, accurate, transparent and reliable. Concerning these criteria, the official Energy Balance has severe shortcomings and inconsistencies. Many problems have been identified earlier by UBA (2004a) such as time-series inconsistencies due to the reunification of Germany in 1990. **In the case of data on non-energy use, the clear and consistent definition of system**

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boundaries is of crucial importance for the use of Energy Balance data in both, the IPCC-RA and the IPCC-SA. With this study, we found that for the non-energy use of natural gas, a *net* definition is applied, thereby excluding all industrial fuel use of feedstocks (e.g., for ammonia production) from the non-energy use data, while for coal/lignite and oil based products gross definitions are used, thereby including the fuel use of feedstock (e.g., in steam crackers) into the estimates for non-energy use. This inconsistency is caused by the fact that suppliers of data provide information at different stages of the fuel supply chain. While the non-energy use data of coal/lignite and oil products are obtained from feedstock *suppliers* (e.g., Mineralölwirtschaftsverband, Bundesverband Braunkohle), the data for natural gas are delivered by feedstock *consumers* (VCI – Verband der Chemischen Industrie). The fuel producers report fuel quantities, which they deliver for non-energy purposes to their customers. They therefore lack the detailed insight into the structure of final consumption. In contrast, the consumer side (VCI) knows relatively well what the fuels are used for in the facilities of the chemical industry. They can therefore differentiate between parts of the fuels used for feedstock, i.e., non-energy purposes and the parts of fuels, which are used for heat raising in production processes. The discrepancy in system boundaries for the non-energy use of the various types of fuels could be solved by, either using exclusively data from fuel suppliers (in that case non-energy use would follow a *gross* definition in the energy balance) or using more detailed data from the fuel consumers (in this case non-energy use would uniformly follow a *net* definition). As an intermediate step, non-energy use data from fuel suppliers and consumers could be crosschecked with each other, in order to obtain a consistent definition of non-energy use in the Energy Balance.

In order to progress on the issue of system boundaries, detailed information on the exact calculation procedure of non-energy use of coal/lignite-based fuels should be obtained. It remains especially questionable, whether solid carbon sources (cokes and coals), which are used as reducing agents for the production of non-ferrous metals and ferroalloys, are part of non-energy use or if these amounts are accounted for under final energy use.

The non-energy use in the Energy Balance is, furthermore, incomplete with respect to imports of coal-based aromatics and certain oil-based products. Apart from coal products, it was possible to pinpoint also concrete problems for oil products: Detailed analysis revealed that chemical grade refinery propylene is not included in the non-energy use data of the NEB (Lorenz, 2005). It is, moreover, likely that also other refinery products used for non-energy purposes (e.g., aromatics, butadiene) are excluded from the non-energy use in the German Energy Balance. It is of critical importance to address these points in the future because the unclear position of these hydrocarbons can easily lead to omission or double counting of emissions in the inventories.

To this end, a document prepared by the authors of the Energy Balance stating clearly and transparently all relevant items and calculation steps performed could decisively improve the understanding the reporting practice of non-energy use. A detailed analysis of questionnaires sent out by VCI and the '*Mineralölwirtschaftsverband*' to gather information on the production and consumption of fossil fuels in refineries and in the chemical industry can be a first step into that direction. UBA is therefore recommended (i) to play an active role in the development and improvement of the German Energy Balance and (ii) to deepen the understanding of non-energy use as it is reported in the Energy Balance. Especially the latter point is critical for reporting non-energy use and related emissions correctly in the German GHG Inventory.

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6.2.2 Recommendations for the IPCC-SA

Emissions from the non-energy use of fossil fuels should be ideally reported under the source categories of ‘*industrial processes*’, ‘*product use*’, and ‘*waste*’ in the IPCC-SA.

In the first step of non-energy use emissions reporting, an overview of relevant emission sources should be prepared (Table 52). We exclude emissions from iron and steel production as well as emissions from catalyst burning (i.e., catalyst regeneration), as the carbon sources of these emissions are not included under non-energy use in the NEB.

Table 52: Sources of non-energy use emissions in the IPCC-SA

Source Category	Source of Emission
Industrial Processes	Steam Cracking
	Ammonia Production
	Methanol Production
	Carbon Black Production
	Losses during Chemical Conversions
	- Production of Ethylene oxide
	- Production of Ethylene dichloride/VCM
	- Production of Acrylonitrile
	- Other Chemical Conversion Losses
	Production of Non-ferrous Metals, Ferroalloys and other Inorganics
	- Production of Aluminum
	- Production of Ferroalloys
	- Production of Carbides
- Production of other Metals and Inorganics	
Product Use	Emissions from Solvents
	Other Product Use Emissions
	- Emissions from Lubricant Use
	- Other Product Use (Pesticides, Waxes)
Waste	Treatment of Wastewaters

From this point onwards, there are two possible ways to proceed:

1. Calculating emissions for the various sources and allocating these emissions in line with the system boundaries for non-energy use in the IPCC-RA to either of the categories ‘*energy*’, ‘*industrial processes*’, ‘*product use*’, or ‘*waste*’.
2. Following the intentions of UBA and strictly allocate all emissions resulting from the fuel use of non-energy use feedstocks to the source category ‘*energy*’ in the IPCC-SA.

To be consistent with both the system boundaries of non-energy use in the NEB and IPCC-RA, UBA should only report emissions from the fuel use of natural gas under the source category ‘*energy*’. All other emissions, i.e., including the fuel use of coal- and oil-based feedstocks should be reported under industrial processes in the IPCC-SA. In practical terms, this would mean an allocation of emissions as given in Table 53.

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Table 53: Reporting of non-energy use emissions in the IPCC-SA, following the system boundaries for non-energy use as stated in NEB and IPCC-RA

Activity	Source Category in the IPCC-SA			
	Energy	Industrial processes	Product use	Waste
Industrial Processes				
Steam Cracking		total fuel use		
Ammonia Production	fuel use of natural gas	fuel use of oil feedstock and pure feedstock use of oils and natural gas		
Methanol Production	fuel use of natural gas	fuel use of oil and coal feedstock*		
Carbon Black Production	fuel use of natural gas	fuel use of oil and coal feedstock*		
Chemical Conversion Losses		total emissions		
- Production Ethylene oxide		total emissions		
- Production of Ethylene dichloride/VCM		total emissions		
- Production of Acrylonitrile		total emissions		
- Other Chemical Conversion Losses		total emissions		
Production of Non-ferrous Metals, Ferroalloys and Other Inorganics		total emissions		
- Production of Aluminum		total emissions		
- Production of Ferroalloys		total emissions		
- Production of Carbides		total emissions		
- Production of other Metals and Inorganics		total emissions		
Emissions from Solvent and Other Product Use				
Solvent Use			total emissions	
Lubricant Use			total emissions	
Other Product Use			total emissions	
Wastewater Treatment				
Treatment of Wastewaters				total emissions

*We only allocate the amount of carbon contained in the final product to pure feedstock use. Therefore, process emissions from feedstock use are zero.

The approach outlined in Table 53 is in line for the system boundaries chosen for non-energy use in the IPCC-RA. This would allow performing consistency checks between IPCC-RA and IPCC-SA emission estimates, which would be impossible, if UBA continues to follow the methodology as applied in the current IPCC-SA (2006 submission).

If UBA has the aim of strictly reporting emissions from fuel use of feedstocks under the source category ‘energy’, the approach presented in Table 54 should be followed.

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Table 54: Reporting of non-energy use emissions in the IPCC-SA, following a strict differentiation between fuel use and feedstock use of non-energy use hydrocarbons

Activity	Source Category in the IPCC-SA			
	Energy	Industrial processes	Product use	Waste
Industrial Processes				
Steam Cracking	total fuel use			
Ammonia Production	total fuel use	total feedstock use		
Methanol Production	total fuel use*			
Carbon Black Production	total fuel use*			
Chemical Conversion Losses		total emissions		
- Production Ethylene oxide		total emissions		
- Production of Ethylene dichloride/VCM		total emissions		
- Production of Acrylonitrile		total emissions		
- Other Chemical Conversion Losses		total emissions		
Production of Non-ferrous Metals, Ferroalloys and Other Inorganics		total emissions		
- Production of Aluminum		total emissions		
- Production of Ferroalloys		total emissions		
- Production of Carbides		total emissions		
- Production of other Metals and Inorganics		total emissions		
Emissions from Solvent and Other Product Use				
Solvent Use			total emissions	
Lubricant Use			total emissions	
Other Product Use			total emissions	
Wastewater Treatment				
Treatment of Wastewaters				total emissions

*We only allocate the amount of carbon contained in the final product to pure feedstock use. Therefore, process emissions from feedstock use are zero.

The current approach chosen in the IPCC-SA (2006 submission) is inconsistent with both of the methodologies outlined above (compare Table 54 and Table 55).

For example, emissions from steam cracking are excluded from ‘industrial processes’ in the IPCC-SA although it remains unclear if these emissions are correctly reported under ‘energy’. Following the system boundaries of non-energy use in the NEB, also the fuel use part of heavy oils resulting in ammonia emissions has to be excluded from ‘industrial processes’, e.g., by applying the IPCC default emission factor, which excludes fuel use. To be consistent with this approach also emissions from methanol and carbon black production should be excluded from the ‘industrial process’ section and should be reported under ‘energy’. In terms of consistency between IPCC-SA and NEB (IPCC-RA), we would therefore recommend to adapt the current IPCC-SA.

Three other points are important. **Firstly, it is not clear, if fuel use emissions from steam cracking and ammonia production are included under ‘energy’ in the IPCC-SA (2006 submission). This should be checked by inventory experts to assure completeness of the GHG**

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inventory. Secondly, NEAT estimates for emissions from chemical conversion losses are uncertain. We would therefore recommend removing the total estimates for chemical conversion losses from the inventory and state results in a more disaggregated way, i.e., as emissions from the production of ethylene oxide, ethylene dichloride/VCM, acrylonitrile, and for other chemical conversion losses. This would increase the transparency of the reported emission estimates. Finally, we would recommend to also include NEAT emission estimates for ferroalloy production under the source category of ‘*industrial processes*’ in the IPCC-SA.

Apart from this, UBA is recommended to clarify and if necessary justify the very low emission factors for aluminium production.

Table 55: Reporting of non-energy use emissions in the current IPCC-SA (2006 inventory submission)

Activity	Source Category in the IPCC-SA			
	Energy	Industrial processes	Product use	Waste
Industrial Processes				
Steam Cracking	total fuel use likely included here			
Ammonia Production	total fuel use most likely not included here	total feedstock use		
Methanol Production		total fuel use*		
Carbon Black Production		total fuel use*		
Chemical Conversion Losses		total emissions		
- Production Ethylene oxide		not specified		
- Production of Ethylene dichloride/VCM		not specified		
- Production of Acrylonitrile		not specified		
- Other Chemical Conversion Losses		not specified		
Production of Non-ferrous Metals, Ferroalloys and Other Inorganics				
- Production of Aluminum		total emissions		
- Production of Ferroalloys		emissions incomplete		
- Production of Carbides		total emissions		
- Production of other Metals and Inorganics		not given		
Emissions from Solvent and Other Product Use				
Solvent Use			total emissions	
Lubricant Use			not specified	
Other Product Use			not specified	
Wastewater Treatment				
Treatment of Wastewaters				not given

*We only allocate the amount of carbon contained in the final product to pure feedstock use. Therefore, process emissions from feedstock use are zero.

The discussion of results indicates that NEAT tends to overestimate emissions from product use (ODU emissions). This might be partly explained by NEAT overestimating non-energy use due to erroneous production data and shows the limited applicability of the NEAT mass balance approach for

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calculating product use emissions. **We, therefore, propose to apply the values at the lower error range of NEAT estimates for product use emissions only for validation purposes for more detailed bottom-up emission estimates. To develop such bottom-up emission estimates, UBA could use inventory data for NMVOC emissions (based on solvent estimates by Theloke (2000), Jepsen (2004)) and add separate estimates for the most prominent emission sources, i.e., the consumption of (i) lubricants, (ii) waxes and paraffins, (iii) creams and cosmetics, and (iv) pesticides. For this purpose, NEAT-SIMP estimates can be used as first estimate (see Appendix C).**

According to the 1996 IPCC guidelines, emissions from waste incineration are part of the fuel use, i.e., energy use emissions, if energy is recovered. This is the case in Germany, as waste incineration without energy recovery does not occur.

The NEAT results for emissions from wastewater treatment are regarded as rough estimates only. **The NEAT values could therefore be used in the IPCC-SA as a first approximation of fossil emissions from wastewater treatment.** Further research is required to obtain more accurate data on fossil based emissions from the wastewater treatment in Germany.

6.2.3 Recommendations for the IPCC-RA

While the status of the IPCC-RA remains unclear in the current 1996 IPCC guidelines, the revised 2006 IPCC guidelines clearly emphasize the purpose of the IPCC-RA as validation tool for emissions from fuel combustion only (IPCC, 2006). Emissions from the non-energy use of fossil fuels are therefore excluded from the IPCC-RA and should be only reported in the relevant source categories of the IPCC-SA. However, as stressed by UBA, the 1996 IPCC guidelines will remain relevant for calculating emissions in Germany. **We would therefore recommend UBA to follow the current approach, i.e., use non-energy use data from NEB directly for the IPCC-RA but to clarify the system boundaries of NEB data.**

For calculating non-energy emissions with the IPCC-RA we suggest removing PROGNOS (2000) storage fractions as these do not account for the actual amount of carbon stored but mainly for carbon, which is not emitted during fuel use of feedstock. We instead recommend using NEAT data on carbon storage (see Table 42) for the IPCC-RA and to calculate based on these calculations, fuel-specific carbon storage fractions. Ideally, this should be done by dividing the carbon storage for each fuel according to NEAT by *corrected* non-energy use data. If *corrected* non-energy use data are not available, the data as published in the NEB can also be used. In line with the definition of non-energy use in the NEB, the emissions as calculated with the IPCC-RA include then fuel use of coal- and oil-based feedstock but exclude the fuel use of natural gas feedstocks.

As stressed in the section above, it is important identify the system boundaries of non-energy use in the Energy Balances as exactly as possible. This is necessary to avoid omission or double counting of emissions in the National GHG Inventory. Special attention should be paid to the critical points mentioned in Section 6.2.1.

Additional uncertainties are related to the carbon storage in lubricants. Here we highly recommend further research activities to quantify (based on bottom-up analyses) the exact shares of lubricants, which are oxidized during use.

The NEAT results presented in this report have been used by the German inventory makers to improve emission estimates for industrial processes (e.g., emissions from methanol and carbon black productions as well as chemical conversion losses). We acknowledge this effort in further improving

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the already good quality of the German GHG inventory and recommend using NEAT and the NEAT-SIMP model (see Appendix C) for updating and adjusting emission estimates where necessary for both, the IPCC-SA and the IPCC-RA. To this end, NEAT might be a valuable tool for generating estimates of non-energy use and related CO₂ emissions also for the years beyond 2003. The application of NEAT for these years should be less time demanding because only the collection of input data is required, whereas background information on the system boundaries of non-energy use in the German Energy Balances as well as data on chemical production routes are already taken into account in the current NEAT model version, which was applied for Germany in this research study.

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Appendix A

Appendix A: Information on Chemicals Included NEAT

Table A1: Product codes (GP 95) and description of basic chemicals included in NEAT

Basic chemical	Production code	Product description	Combined Nomenclature Trade Code	Product description
Acetylene	24.14.11.90	Unsaturated acyclic hydrocarbons (excl. ethylene, propylene, butene, buta-1,3-diene and isoprene)	2901.29.80	Unsaturated acyclic hydrocarbons (excl. ethylene, propylene, butene, buta-1,3-diene and isoprene), for other use
Ammonia	24.15.10.75	Anhydrous ammonia (100% N)	2814.10.00 2814.20.00	Anhydrous ammonia (100% N) and in aqueous solution
Benzene	24.14.12.23	Benzene	2902.20.90	Benzene, for other use
Bitumen	23.20.32.50	Petroleum bitumen (black or dark brown solid and semi-solid thermo-plastic material with waterproofing and adhesive properties)	2713.20.00	Petroleum bitumen
Butadiene	24.14.11.65	Buta-1,3-diene	2901.24.19	Buta-1,3-diene, for other use
Other C4	24.14.11.50 24.14.11.67	Butene (butylene) and isomers thereof + isoprene	2901.23.19 2901.23.99 29.01.24.99	But-1-ene, but-2-ene and isoprene for other use + other butenes and isomers thereof, for other use
Carbon black	24.13.11.30	Carbon (carbon blacks and other forms of carbon, n.e.c.)	2803.00.10 2803.00.80	Carbon (carbon blacks and other forms of carbon, n.e.c.)
CO				
Ethylene	24.14.11.30	Ethylene	2901.21.90	Ethylene, for other use
Lubricants	23.20.18.30 23.20.18.50 23.20.18.70	Lubrication oils used as feedstock in refineries + Lubricants oils (liquid distillates, weight of petroleum oils >= 70%, extracted by distillation of crude oil; incl. motor oils, industrial oils and lubricating greases)	2710.19.71 2710.19.75 2710.19.80 2710.19.90	Lubrication oils (liquid distillates, weight of petroleum oils >= 70%, extracted by distillation of crude oil; incl. motor oils, industrial oils and lubricating greases) for specific treatment + Lubricants oils for chemical treatment different than treatment under 2710.19.71 + Lubrication oils for other use
Methanol	24.14.22.10	Methanol (methyl alcohol)	2905.11.00	Methanol
Petroleum coke	23.20.32.40	Petroleum coke (black solid product obtained mainly by cracking and carbonising residue feedstock, mainly 90 to 95% of carbon)	2713.11.00 2713.12.00	Petroleum coke, not calcined + Petroleum coke, calcined
Pitch	24.14.73.70	Pitch and pitch coke; obtained from coal tar or from other mineral tars	2708.10.00 2708.20.00	Pitch and pitch coke
Creosote oil	24.14.73.65	Creosote oils	2707.91.00	Creosote oils
Naphthalene	24.14.12.80	Naphtalene and anthracene	2902.90.10	Naphtalene and anthracene
Other tar products	24.14.73.67	Other oils and oil products, n.e.c.	2707.99.00	Other oils and oil products, n.e.c.
Propylene	24.14.11.40	Propene (propylene)	2901.22.90	Propylene, for other use
Toluene	24.14.12.25	Toluene	2902.30.90	Toluene for other use
Waxes, paraffins	23.20.31.00	Petroleum jelly, paraffin waxes and other waxes, incl. ozokerite (mixtures of saturated hydrocarbons, solid at ambient temperature)	2712.10.00 27.12.20.00 27.12.90.00	Petroleum jelly, paraffin waxes and other waxes, incl. ozokerite (mixtures of saturated hydrocarbons, solid at ambient temperature)
o-Xylene	24.14.12.43	o-Xylene	2902.41.00	o-Xylene
m-Xylene	24.14.12.47	m-Xylene and mixtures of xylene isomers	2902.42.00	m-Xylene
p-Xylene	24.14.12.45	p-Xylene	2902.43.00	p-Xylene

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Table A2: Product codes (GP 95) and description of intermediated chemicals included in NEAT

Intermediated chemical	Production code	Product description	Combined Nomenclature Trade Code	Product description
Acetaldehyde	24.14.61.13	Acetaldehyde (Ethanal)	2912.12.00	Acetaldehyde (Ethanal)
Acetic acid	24.14.32.71	Acetic acid	2915.21.00	Acetic acid
Acetone	24.14.62.11	Acetone	2914.11.00	Acetone
Acrylic acid	24.14.33.10	Acrylic acid and its salts and other monocarboxylic acid	2916.11.10 2916.11.90 2916.19.10 2916.19.30 2916.19.40 2916.19.80 2916.19.90 2916.20.00	Acrylic acid and salts, other acyclical mono-acids and derivatives and other mono-acids
Acrylonitrile	24.14.43.50	Acrylonitrile	2926.10.00	Acrylonitrile
Adipic acid	24.14.33.85	Adipic acid; its salts and esters	2917.12.10 2917.12.90	Adipic acid; its salts and esters
Adiponitrile	-	Adiponitrile	-	Adiponitrile
Aniline	24.14.41.51	Aniline and its salts (excl. derivatives)	2921.41.00	Aniline and its salts (excl. derivatives)
Bisphenol A	24.14.24.33	4,4-Isopropylidenediphenol (bisphenol A; diphenylolpropane) and its salts	2907.23.10 2907.23.90	4,4-Isopropylidenediphenol (bisphenol A; diphenylolpropane) and its salts
Butanol	24.14.22.30 24.14.22.40	Butan-1-ol (n-butyl alcohol) + Butanols (excl. butan-1-ol (n-butyl alcohol))	2905.13.00 1905.14.00	Butan-1-ol (n-butyl alcohol) + other butanols
Caprolactam	24.14.52.70	6-Hexanelactam (epsilon-caprolactam)	2933.71.00	6-Hexanelactam (epsilon-caprolactam)
Cumene	24.14.12.70	Cumene	2902.70.00	Cumene
Cyclohexane	24.14.12.13	Cyclohexane	2902.11.90	Cyclohexane for other use
Cyclohexanone	24.14.62.33	Cyclohexanone and methylcyclohexanones	2914.22.00	Cyclohexanone and methylcyclohexanone
Dimethylterephthalate	24.14.34.43	Dimethyl terephthalate	2917.37.00	Dimethyl terephthalate
Ethanol	15.92.12.05	Ethyl alcohol and other denatured spirits: synthetic	2207.20.00	
Ethylbenzene	24.14.12.60	Ethylbenzene	2902.60.00	Ethylbenzene
Ethylendichloride	24.14.13.53	1,2-Dichloroethane (ethylene dichloride)	2903.15.00	1,2-Dichloroethane (ethylene dichloride)
Ethylene glycol	24.14.23.10	Ethylene glycol (ethanediol)	2905.31.00	Ethylene glycol (ethanediol)
Ethylene oxide	24.14.63.73	Oxirane (ethylene oxide)	2910.10.00	Oxirane (ethylene oxide)
Formaldehyde	24.14.61.11	Methanal (formaldehyd)	2912.11.00	Methanal (formaldehyd)
Hexamethylenediamine	24.14.41.250	Hexamethylenediamine and its salts	2921.22.00	Hexamethylenediamine and its salts
MTBE	24.66.32.55 24.66.32.59	Anti-knock preparations based on lead compounds + Anti-knock preparations (excl. those based on lead)	3811.11.11 3811.11.19 3811.19.00	Anti-knock preparations
Higher alcohols	24.14.22.63 24.14.22.69	Octanol (octyl alcohol) and isomers thereof + Lauryl-, cetyl-, stearylalcohol and other saturated mono-alcohols	2905.16.10 2905.16.20 2905.16.80 2905.17.00 2905.19.10 2905.19.90	Octanol (octyl alcohol) and isomers thereof + Lauryl-, cetyl-, stearylalcohol and other saturated mono-alcohols
Orthophthalates	24.14.34.13 24.14.34.15 24.14.34.23 24.14.34.25	Dibutyl, dioctyl, dinonyl, diecyl and other esters of orthophthalic acid	2917.31.00 2917.32.00 2917.33.00 2917.34.00	Dibutyl, dioctyl, dinonyl, diecyl and other esters of orthophthalic acid
Phenol	24.14.24.15	Phenol (hydroxybenzene) and its salts	2907.11.00	Phenol (hydroxybenzene) and its salts
Phthalic anhydride PSA	24.14.34.33	Phthalic anhydride	2917.35.00	Phthalic anhydride
Polyether-polyols	24.16.40.15	Polyethylene glycols and other polyetheralcohols, in primary forms	3907.20.11 3907.20.12 3907.20.19 3907.20.21 3907.20.29	Polyethylene glycols and other polyetheralcohols, in primary forms

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Table A2 (cont.): Product codes (GP 95) and description of intermediated chemicals included in NEAT

Intermediated chemical	Production code	Product description	Combined Nomenclature Trade Code	Product description
n-Propanol and i-propanol	24.14.22.20	Propan-1-ol (propyl alcohol, n-propanol) and propan-2-ol (isopropyl alcohol)	2905.12.00	Propan-1-ol (propyl alcohol, n-propanol) and propan-2-ol (isopropyl alcohol)
Propylene oxide	24.14.63.75	Methyloxirane (propylene oxide)	2910.20.00	Methyloxirane (propylene oxide)
Styrene	24.14.12.50	Styrene	2902.50.00	Styrene
Terephthalic acid TPA	24.14.34.35	Terephthalic acid and its salts	2917.36.00	Terephthalic acid and its salts
Toluenediisocyanate	24.14.44.50	Isocyanates	2929.10.10 2929.10.90	Methylphenylene diisocyanates (toluenediisocyanates) + other isocyanates
Urea	24.15.30.13 24.15.30.19	Urea with less than 45% N and with more than 45% N	3102.10.10 3102.10.90	Urea with less than 45% N and with more than 45% N
Vinylchloride monomer VCM	24.14.13.71	Vinyl chloride (chloroethylene)	2903.21.00	Vinyl chloride (chloroethylene)

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Table A3: Product codes (GP 95) and description of final chemicals included in NEAT

Final chemical	Production code	Product description	Combined Nomenclature Trade Code	Product description
ABS	24.16.20.70	Acrylonitrile-butadiene-styrene (ABS) copolymers, in primary forms	3903.30.00	Acrylonitrile-butadiene-styrene (ABS) copolymers, in primary forms
BR	14% of: 24.17.10.50 24.17.10.90	Synthetic rubber	4002.20.00	Butadiene rubber (BR)
EPDM	10% of: 24.17.10.50 24.17.10.90	Synthetic rubber	4002.70.00	Ethylene-propylene-diene (non conjugated) rubber (EPDM)
Epoxy resin	24.16.40.30	Epoxy resins; in primary forms	3907.30.00	Epoxy resins; in primary forms
Melamine formaldehyde resin	24.16.55.70 24.16.56.30	Melamine resins; in primary forms + Amino resins; in primary forms (excl. urea, thiourea and melamine resins)	3909.20.00 3909.30.00	Melamine resins and other amino resins; in primary forms
Phenolic resin	24.16.56.50	Phenolic resins; in primary forms	3909.40.00	Phenolic resins; in primary forms
Polyacetals	24.16.40.13	Polyacetals; in primary forms	3907.10.00	Polyacetals; in primary forms
Poly-acrylates	24.16.53.50 24.16.53.90	Acrylic polymers; in primary forms (excl. polymethyl methacrylate) + Polymethyl methacrylate; in primary forms	3906.90.00 3906.10.00	Acrylic polymers; in primary forms (excl. polymethyl methacrylate) + Polymethyl methacrylate; in primary forms
Poly-acrylonitrile	Included under polyacrylates			
Polyamide 6,66	24.16.54.50 24.16.54.90	Polyamide -6, -11, -12, -6,6, -6,9, -6,10 of -6,12; in primary forms + other Polyamides; in primary forms	3908.10.00 3908.90.00	Polyamide -6, -11, -12, -6,6, -6,9, -6,10 or -6,12; in primary forms + other Polyamides; in primary forms
Poly-carbonate	24.16.40.40	Polycarbonates; in primary forms	3907.40.00	Polycarbonates; in primary forms
PE	24.16.10.35 24.16.10.39 24.16.10.50 24.16.10.70 24.16.10.90	Linear polyethylene having a specific gravity < 0.94; in primary forms + Polyethylene having a specific gravity < 0.94; in primary forms (excl. linear) + Polyethylene having a specific gravity >= 0.94; in primary forms + Ethylene-vinyl acetate copolymers; in primary forms + Polymers of ethylene; in primary forms (excl. polyethylene, ethylene-vinyl acetate copolymers)	3901.10.00 3901.20.00 3901.30.00 3901.90.00	Polyethylene having a specific gravity < 0.94 + Polyethylene having a specific gravity >= 0.94; in primary forms + copolymers of ethylene and vinylacetate, other polymers of ethylene, in primary form
PET	24.16.40.60	Polyethylene terephthalate, in primary forms	3907.60.00	Polyethylene terephthalate, in primary forms
PP	24.16.51.30 24.16.51.30	Polypropylene; in primary forms + Polymers of propylene or of other olefins; in primary forms (excl. polypropylene)	3902.10.00 3902.20.00 3902.30.00 3902.90.00	Polypropylene, polyisobutylene, copolymers of propylene, other polymers of propylene in primary form
PS	24.16.20.35 24.16.20.39 24.16.20.90	Expanded polystyrene; in primary forms + Polystyrene; in primary forms (excl. expandable polystyrene) + Polymers of styrene (excl. polystyrene, SAN and ABS)	3903.11.00 3903.19.00 3903.90.00	Expanded polystyrene + Polystyrene (excl. expandable polystyrene) + other polymers of Styrene (excl. SAN, ABS)
PUR	24.16.56.70	Polyurethanes; in primary forms	3909.50.00	Polyurethanes; in primary forms
PVA	24.16.52.30 24.16.52.50 24.16.52.70	Polymers of vinyl acetate, in aqueous dispersion; in primary forms + Polymers of vinyl acetate; in primary forms (excl. in aqueous dispersion) + Polymers of vinyl esters or other vinyl polymers; in primary forms (excl. vinyl acetate)	3905.12.00 3905.21.00 3905.19.00 3905.29.00 3905.30.00 3905.91.00 3905.99.00	Polymers of vinyl acetate, in aqueous dispersion; in primary forms + Polymers of vinyl acetate; in primary forms (excl. in aqueous dispersion) + Polymers of vinyl esters or other vinyl polymers; in primary forms (excl. vinyl acetate)

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Table A3 (cont.): Product codes (GP 95) and description of final chemicals included in NEAT

Final chemical	Production code	Product description	Combined Nomenclature Trade Code	Product description
PVC	24.16.30.10 24.16.30.23 24.16.30.25 24.16.30.30 24.16.30.40 24.16.30.50 24.16.30.90	Polyvinyl chloride; not mixed with any other substances; in primary forms + Non-plasticised polyvinyl chloride mixed with any other substances; in primary forms + Plasticised polyvinyl chloride mixed with any other substances; in primary forms + Vinyl chloride-vinyl acetate copolymers; and other vinyl chloride copolymers; in primaire vormen + Vinylidene chloride polymers; in primary forms	3904.10.00 3904.21.00 3904.22.00 3904.30.00 3904.40.00 3904.50.00 3904.90.00	Polyvinyl chloride; not mixed with any other substances; in primary forms + Non-plasticised polyvinyl chloride mixed with any other substances; in primary forms + Plasticised polyvinyl chloride mixed with any other substances; in primary forms
SAN	24.16.20.50	Styrene-acrylonitrile (SAN) copolymers; in primary forms	3903.20.00	Styrene-acrylonitrile (SAN) copolymers; in primary forms
Saturated polyester	24.16.40.90	Polyesters; in primary forms (excl. polyacetals, polyethers, epoxide resins, polycarbonates, alkyd resins, polyethylene terephthalate, other unsaturated polymers)	3907.99.10 3907.99.90	Polyesters; in primary forms (excl. polyacetals, polyethers, epoxide resins, polycarbonates, alkyd resins, polyethylene terephthalate, other unsaturated polymers)
SBR	58% of: 24.17.10.50 24.17.10.90	Synthetic rubber	4002.11.00 4002.19.00	Styrene-butadiene rubber (SBR)
Unsaturated polyester/alkyd resin	24.16.40.50 24.16.40.70 24.16.40.80	Unsaturated liquid polyesters; in primary forms (excl. polyacetals, polyethers, epoxide resins, polycarbonates, alkyd resins and polyethylene terephthalate) + Unsaturated polyesters; in primary forms (excl. liquid polyesters, polyacetals, polyethers, epoxide resins, polycarbonates, alkyd resins and polyethylene terephthalate) + Alkyd resins; in primary forms	3907.91.00 3907.50.00	Unsaturated liquid polyesters; in primary forms (excl. polyacetals, polyethers, epoxide resins, polycarbonates, alkyd resins and polyethylene terephthalate) + Unsaturated polyesters; in primary forms (excl. liquid polyesters, polyacetals, polyethers, epoxide resins, polycarbonates, alkyd resins and polyethylene terephthalate) + Alkyd resins; in primary forms
Urea formaldehyde resin UF	24.16.55.50	Urea resins and thiourea resins; in primary forms	3909.10.00	Urea resins and thiourea resins; in primary forms

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Table A4: Production Codes of NEAT basic chemicals according to German Production Statistics

Basic chemicals	Code (Year)		
	GP 89 (1990-1994)	GP 95 (1995-2000)	GP 02 (2001-2003)
Acetylene	422114 422117 422190	24.14.11.90	24.14.11.900
Ammonia	414200	24.15.10.75	24.15.10.750
Benzene	422410	24.14.12.23	24.14.12.230
Bitumen	227310	23.20.32.50	23.20.32.300
Butadiene	422114	24.14.11.65	24.14.11.650
Other C4	422116	24.14.11.50	24.14.11.500
	422119	24.14.11.67	24.14.11.670
Carbon black	411370	24.13.11.30	24.13.11.300
CO	-	-	-
Ethylene	421211	24.14.11.30	24.14.11.300
Lubricants	225100		
	225220		
	225250		
	225290		
	225510		
	225530	23.20.18.310	23.20.18.501
	225540	23.20.18.330	23.20.18.502
	225550	23.20.18.350	23.20.18.504
	225560	23.20.18.370	23.20.18.505
	225570	23.20.18.530	23.20.18.506
	225590	23.20.18.550	23.20.18.507
	225700	23.20.18.700	23.20.18.508
	227990	23.20.18.310	
	492210		
492290			
492310			
492400			
Methanol	423211	24.14.22.10	24.14.22.100
Petroleum coke	227700	23.20.32.40	23.20.32.400
Pitch	421800	24.14.73.70	24.14.73.700
Creosote oil	421210	24.14.73.65	24.14.73.650
Naphthalene	422490	24.14.12.80	24.14.12.800
Other tar products	421210		
	421290	24.14.73.67	24.14.73.670
Propylene	422113	24.14.11.40	24.14.11.400
Toluene	422420	24.14.12.25	24.14.12.25
Waxes, paraffins	212600		
	227120		
	227170	23.20.31.00	23.20.31.000
	227990		
o-Xylene	422433	24.14.12.43	24.14.12.430
m-Xylene	422438	24.14.12.47	24.14.12.470
p-Xylene	422438	24.14.12.45	24.14.12.450

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Table A5: Production Codes of NEAT intermediated chemicals according to German Production Statistics

Intermediated chemicals	Code (Year)		
	GP 89 (1990-1994)	GP 95 (1995-2000)	GP 02 (2001-2003)
Acetaldehyde	425540	24.14.61.13	24.14.61.130
Acetic acid	426121	24.14.32.71	24.14.32.710
Acetone	425720	24.14.62.11	24.14.62.110
Acrylic acid	426220 426260	24.14.33.10	24.14.33.100
Acrylonitrile	427651	24.14.43.50	24.14.43.500
Adipic acid	426375 426380 426391 426398	24.14.33.85	24.14.33.850
Adiponitrile	-	-	-
Aniline	427271	24.14.41.51	24.14.41.510
Bisphenol A	424241 424249	24.14.24.33	24.14.24.330
Butanol	423216 423217	24.14.22.30 24.14.22.40	24.14.22.300 24.14.22.400
Caprolactam	427550 429151 429155 429170 429180 429230	24.14.52.70	24.14.52.700
Cumene	422480	24.14.12.70	24.14.12.700
Cyclohexane	422440	24.14.12.13	24.14.12.130
Cyclohexanone	425730	24.14.62.33	24.14.62.330
Dimethylterephthalate	426458	24.14.34.43	24.14.34.430
Ethanol	423212	15.92.12.05	15.92.12.000
Ethylbenzene	422470	24.14.12.60	24.14.12.600
Ethylendichloride	422822	24.14.13.53	24.14.13.530
Ethylene glycol	423241	24.14.23.10	24.14.23.100
Ethylene oxide	425310	24.14.63.73	24.14.63.730
Formaldehyde	425520	24.14.61.11	24.14.61.110
Hexamethylenediamine	427230	24.14.41.25	24.14.41.250
MTBE	493100	24.66.32.55 24.66.32.59	24366.32.550 24366.32.590
Higher alcohols	423222 423229	24.14.22.63 24.14.22.69	24.14.22.630 24.14.22.690
Orthophthalates	426451 426452 426453 426454	24.14.34.13 24.14.34.15 24.14.34.23 24.14.34.25	24.14.34.130 24.14.34.150 24.14.34.250
Phenol	424212 424219	24.14.24.15	24.14.24.150
Phthalic anhydride PSA	426455	24.14.34.33	24.14.34.330
Polyether-polyols	441315	24.16.40.15	24.16.40.150
n-Propanol and i-propanol	423215	24.14.22.20	24.14.22.200
Propylene oxide	425350	24.14.63.75	24.14.63.750
Styrene	422460	24.14.12.50	24.14.12.500
Terephthalic acid TPA	426458	24.14.34.35	24.14.34.430
Toluenediisocyanate	427691	24.14.44.50	24.14.44.500
Urea	431117	24.15.30.13 24.15.30.19	24.15.30.130 24.15.30.190
Vinylchloride monomer VCM	422837	24.14.13.71	24.14.13.710

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Table A6: Production Codes of NEAT final chemicals according to German Production Statistics

Final chemicals	Code (Year)		
	GP 89 (1990-1994)	GP 95 (1995-2000)	GP 02 (2001-2003)
ABS	441448	24.16.20.70	24.16.20.700
BR	14% of: 441940 445200 445600	14% of: 24.17.10.50 24.17.10.90	14% of: 24.17.10.500 24.17.10.900
EPDM	10% of: 441940 445200 445600	10% of: 24.17.10.50 24.17.10.90	10% of: 24.17.10.500 24.17.10.900
Epoxy resin	441330	24.16.40.30	24.16.40.303 24.16.40.305 24.16.40.309
Melamine formaldehyde resin	441251 441253 441255 441258 441261 441269	24.16.55.70 24.16.56.30	24.16.55.700 24.16.56.300
Phenolic resin	441231 441233 441235 441237 441239	24.16.56.50	24.16.56.500
Polyacetals	441311	24.16.40.13	24.16.40.130
Polyacrylates	441410 441471 441474 441478	24.16.53.550 24.16.53.575 24.16.53.579 24.16.53.950 24.16.53.975 24.16.53.977 24.16.53.979	24.16.53.500 24.16.53.901 24.16.53.905 24.16.53.907 24.16.53.909
Polyacrylonitrile	included under Polyacrylates		
Polyamide 6,66	441370 441100	24.16.54.503 24.16.54.509 24.16.54.950 24.16.54.975 24.16.54.979	24.16.54.503 24.16.54.509 24.16.54.900
Polycarbonate	441351	24.16.40.40	24.16.40.400
Polyethylene PE	441431 441433 441435 441410	24.16.10.35 24.16.10.39 24.16.10.50 24.16.10.70 24.16.10.90	24.16.10.350 24.16.10.390 24.16.10.500 24.16.10.700 24.16.10.900
Polyethyleneterephthalate PET	441355	24.16.40.60	24.16.40.620 24.16.40.640
Polypropylene PP	441410 441437 441439	24.16.51.350 24.16.51.370 24.16.51.500	24.16.51.350 24.16.51.370 24.16.51.500
Polystyrene PS	441410 441442 441448	24.16.20.350 24.16.20.390 24.16.20.500 24.16.20.900	24.16.20.350 24.16.20.390 24.16.20.500 24.16.20.900 24.16.20.350
Polyurethane PUR	441290	24.16.56.705 24.16.56.709	24.16.56.705+709
Polyvinylacetate	441410 441462 441468 441469	24.16.52.305 24.16.52.309 24.16.52.505 24.16.52.509 24.16.52.703 24.16.52.705 24.16.52.709	24.16.52.305 24.16.52.309 24.16.52.500 24.16.52.702 24.16.52.709

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Table A6 (cont.): Production Codes of NEAT final chemicals according to German Production Statistics

Final chemicals	Code (Year)		
	GP 89 (1990-1994)	GP 95 (1995-2000)	GP 02 (2001-2003)
Polyvinylchloride PVC	441410	24.16.30.10	24.16.30.10
	441452	24.16.30.23	24.16.30.23
	441454	24.16.30.25	24.16.30.25
	441456	24.16.30.30	24.16.30.30
	441457	24.16.30.43	24.16.30.400
	441489	24.16.30.45	24.16.30.500
		24.16.30.50	24.16.30.900
SAN	441448	24.16.20.500	24.16.20.500
Saturated polyester	441395	24.16.40.90	24.16.40.900
SBR	58% of: 441940	58% of: 24.17.10.50	58% of: 24.17.10.500
	445200	24.17.10.90	24.17.10.900
	445600		
Unsaturated polyester/alkyd resin	441353	24.16.40.50	24.16.40.500
	441357	24.16.40.70	24.16.40.700
		24.16.40.80	24.16.40.800
Urea formaldehyde resin UF	441241	24.16.55.575	24.16.55.500
	441243	24.16.55.577	
	441245	24.16.55.579	
	441248		

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Table A7: Chemicals included in the additional trade module of NEAT

HS/CN code	Description	Carbon content (kg CO ₂ / kg product)		
		MEAN	MIN	MAX
29021910	Cycloterpanes	3.45	2.42	4.49
29021930	Azulene and its alkyl derivatives (Azulene)	3.44	3.44	3.44
29021999	Other cyclic hydrocarbons	3.45	2.42	4.49
29029010	Naphthalene and anthracene	3.45	3.44	3.46
	Naphthalene	3.44	3.44	3.44
	Anthracene	3.46	3.46	3.46
29029030	Biphenyl and terphenyls	3.44	3.43	3.44
	Biphenyl	3.43	3.43	3.43
	Terphenyls	3.44	3.44	3.44
29029050	Vinyltoluenes	3.36	3.36	3.36
29029060	1,3-Diisopropylbenzene	3.26	3.26	3.26
29029080	Other	3.26	2.26	4.24
29029090	Other	3.26	2.26	4.24
2903	Saturated chlorine derivatives of acyclic hydrocarbons	0.00	0.00	0.00
29031100	Chloromethane (methyl chloride) and chloroethane (ethyl chloride)	1.12	0.87	1.36
	Methyl chloride	0.87	0.87	0.87
	Ethyl chloride	1.36	1.36	1.36
29031200	Dichloromethane (methylene chloride)	0.52	0.52	0.52
29031300	Chloroform (trichloromethane)	0.37	0.37	0.37
29031400	Carbon tetrachloride	0.29	0.29	0.29
29031600	1,2 Dichloropropane and dichlorobutanes	1.28	1.17	1.39
	1,2 Dichloropropane	1.17	1.17	1.17
	Dichlorobutane	1.39	1.39	1.39
29021900	Other	0.00	0.00	0.00
29031910	1,1,1-Trichloroethane (methylchloroform)	0.66	0.66	0.66
29031990	Other	0.66	0.46	0.66
	Unsaturated chlorine derivatives	0.00	0.00	0.00
29032200	Trichloroethylene	0.67	0.67	0.67
29032300	Tetrachloroethylene (perchloroethylene)	0.53	0.53	0.53
29032900	Other	0.53	0.37	0.69
290330	Fluor-, Bromo- en Iodine derivatives of acyclic hydrocarbons	0.00	0.00	0.00
29033010	Fluoromethane	1.29	1.29	1.29
29033031	Diffuoromethane	0.85	0.85	0.85
29033033	Bromomethane (methyl bromide)	0.46	0.46	0.46
29033035	Dibromomethane	0.25	0.25	0.25
29033037	Iodine methane	0.31	0.31	0.31
29033038	Diiodine methane	0.16	0.16	0.16
290330390	Other bromides of acyclic hydrocarbons	0.00	0.00	0.00
29033090	Other	0.16	0.11	0.21
	Halogenes derivatives of acyclic hydrocarbons with two or more different halogenes	0.00	0.00	0.00
29034100	Trichlorofluoromethane	0.32	0.32	0.32
29034200	Dichlorodifluoromethane	0.36	0.36	0.36
29034300	Trichlorotrifluoroethanes	0.47	0.47	0.47
290344	Dichlorotetrafluoroethanes and chloropentafluoroethane	0.00	0.00	0.00
29034410	Dichlorotetrafluoroethanes	0.51	0.51	0.51
29034490	Chloropentafluoroethane	0.57	0.57	0.57
290345	Other derivatives perhalogenated only with fluorine and chlorine	0.00	0.00	0.00
29034515	Pentachlorofluoroethane	0.57	0.57	0.57
29034525	Heptachlorofluoroethanes	0.43	0.43	0.43
29034540	Tetrachlorotetrafluoroethanes	0.52	0.52	0.52
29034590	Other	0.40	0.28	0.52
290346	Bromochlorodifluoromethane, bromotrifluoromethane and dibromotetrafluoroethanes	0.00	0.00	0.00
29034610	Bromochlorodifluoromethane	0.27	0.27	0.27
29034620	Bromotrifluoromethane	0.30	0.30	0.30
29034690	Dibromotetrafluoroethanes	0.34	0.34	0.34
29034700	Other perhalogenated derivatives	0.40	0.28	0.52
290349	Other	0.00	0.00	0.00
	Halogenated only with fluorine and chlorine	0.00	0.00	0.00
29034910	Of methane, ethane or propane	0.47	0.47	0.47
29034920	Other	0.40	0.28	0.52
	Halogenated only with fluorine and bromine	0.00	0.00	0.00
29034930	Of methane, ethane or propane	0.27	0.27	0.27
29034960	Other	0.27	0.19	0.35
29034990	Other	0.27	0.19	0.35
	Halogenated derivatives of cyclanic, cyclenic or cycloterpenic hydrocarbons	0.00	0.00	0.00
29035100	1,2,3,4,5,6-Hexachlorocyclohexane	0.00	0.00	0.00
29035110	1,2,3,4,5,6-Hexachlorocyclohexane	0.91	0.91	0.91
29035190	Other	0.90	0.63	1.17
29035900	Other	0.82	0.57	1.07
29035910	1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane	0.82	0.82	0.82
29035990	Other	0.82	0.57	1.07
	Halogenated derivatives of aromatic hydrocarbons	0.00	0.00	0.00
29036100	Chlorobenzene, o-dichlorobenzene and p-dichlorobenzene	2.07	1.80	2.35
	Chlorobenzene	2.35	2.35	2.35
	o- and p-dichlorobenzene	1.80	1.80	1.80
29036200	Hexachlorobenzene and DDT (1,1,1-trichloro-2,2-bis(p-chlorophenyl)ethane)	1.26	0.93	1.69
	Hexachlorobenzene	0.93	0.93	0.93
	DDT	1.59	1.59	1.59
	Other	0.70	0.49	0.91
29036910	2,3,4,5,6-Pentabromoethylbenzene	0.70	0.70	0.70
29036990	Other	0.70	0.49	0.91
2904	Sulphonated, nitrated or nitrosated derivatives of hydrocarbons	0.00	0.00	0.00
29041000	Derivatives containing only sulpho groups, their salts and ethyl esters	0.27	0.21	0.32
29042000	Derivatives containing only nitro or only nitroso groups	0.27	0.21	0.32
290490	Other	0.00	0.00	0.00
290490100	Sulfohalogenederivatives	0.27	0.21	0.32
29049030	Sulfohalogenederivatives	0.27	0.21	0.32
29049040	Trichloronitromethane (chloropicrin)	0.27	0.27	0.27
29049085	Other	0.27	0.21	0.32
	Acyclic alcohols and their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
29051500	Pentanol (amyl alcohol) and isomers thereof	2.50	2.50	2.50
29051700	Dodecan-1-ol, hexadecan-1-ol and octadecan-1-ol	2.84	2.84	2.84
29051910	Other saturated monoalcohols	2.50	1.75	3.25
29051990	Other saturated monoalcohols	2.50	1.75	3.25
	Unsaturated monohydric alcohols	0.00	0.00	0.00

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Table A7 (cont.): Chemicals included in the additional trade module of NEAT

290522	Acyclic terpenealcohols	0.00	0.00	0.00
29052210	Geraniol, citronellol, linalol, rhodinol and nerol	2.87	2.82	2.97
	Geraniol (trans-3,7-dimethyl-2,6-octadien-1-ol)	2.86	2.86	2.86
	Citronellol	2.86	2.86	2.86
	Linolol(3-Di-methyl-1,6-octadien-3-ol)	2.86	2.86	2.86
	Rhodinol (mixture of terpene alcohols consisting principally of l-citronello)	2.82	2.82	2.82
	Nerol (3,7,11-trimethyl-1,6,10-dodecatrien-3-ol)	2.97	2.97	2.97
29052290	Other	2.80	1.96	3.64
290529	Other	2.28	1.82	2.73
29052910	Allyl alcohol	2.28	2.28	2.28
29052990	Other	2.28	1.82	2.73
29053200	Propylene glycol (propane-1,2-diol)	1.74	1.74	1.74
290539	Other	0.00	0.00	0.00
29053910	2-Methylpentane-2,4-diol (hexylene glycol)	2.24	2.24	2.24
29053920	Butane-1,3-diol	1.96	1.96	1.96
29053930	2,4,7,9-Tetramethyldec-5-yne-4,7-diol	2.73	2.73	2.73
29053980	Other	2.00	1.40	2.60
	Other polyhydric alcohols	0.00	0.00	0.00
29054100	2-Ethyl-2-(hydroxymethyl)propane-1,3-diol (trimethylolpropane)	1.97	1.97	1.97
29054200	Pentaerythritol	1.62	1.62	1.62
29054300	Mannitol	1.45	1.45	1.45
290549	Other	0.00	0.00	0.00
29054910	Triols; tetrols (Furan)	2.59	2.59	2.59
	Other	0.00	0.00	0.00
	Esters of glycerol formed with acid-function compounds of heading No 2904	0.00	0.00	0.00
29054951	With sulphohalogenated derivatives	1.79	1.72	1.87
29054959	Other	1.79	1.72	1.87
29054990	Other	1.43	1.15	1.72
290560	Halogenated, sulphonated, nitrated or nitrosated derivatives of acyclic alcohols	0.00	0.00	0.00
29056020	Of monoalcohols	0.80	0.56	1.04
290560900	Of other alcohols	0.00	0.00	0.00
29056091	2,2-Bis(Bromomethyl)-1,3-Propanediol	0.84	0.84	0.84
29056099	Other	0.80	0.56	1.04
2906	Cyclic alcohols and their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
	Cyclanic, cyclenic or cycloterpenic	0.00	0.00	0.00
29061200	Cyclohexanol, methylcyclohexanols and dimethylcyclohexanols	2.70	2.64	2.75
	Cyclohexanol	2.64	2.64	2.64
	Methylcyclohexanols	2.70	2.70	2.70
	Dimethylcyclohexanols	2.75	2.75	2.75
	Aromatic	0.00	0.00	0.00
29062100	Benzylalcohol	2.85	2.85	2.85
29062910	Other aromatic dialcohols	2.80	1.96	3.64
29062990	Other	2.80	1.96	3.64
29071200	Cresols and their salts	2.85	2.28	3.42
	Cresol	0.00	0.00	0.00
29071300	Octylphenol, nonylphenol and their isomers; salts thereof	3.00	2.99	3.01
	Octylphenol	2.99	2.99	2.99
	Nonylphenol	3.01	3.01	3.01
29071400	Xylenols and their salts	2.89	2.31	3.46
	Xylenol (dimethyl phenol)	0.00	0.00	0.00
290715	Naphthols and their salts	0.00	0.00	0.00
29071510	1-Naphthol	3.06	2.44	3.67
29071590	Other	3.00	2.10	3.90
29071900 (1910+1990)	Other	3.00	2.10	3.90
	Polyphenols; phenol-alcohols	0.00	0.00	0.00
29072100	Resorcinol and its salts (resorcinol)	2.40	2.40	2.40
29072210	Hydroquinone (quinol) and its salts	2.40	1.68	3.12
29072290	Other	2.40	1.60	3.12
29072910 (2900)	Other dialcohols	2.40	1.92	2.88
29072990	Other dialcohols	2.40	1.92	2.88
29073000	Phenol alcohol (phenol)	2.81	2.81	2.81
2908	Halogenated, sulphonated, nitrated or nitrosated derivatives of phenols or phenol-alcohols	0.00	0.00	0.00
29081000	Derivatives containing only halogen substituents and their salts	2.00	1.40	2.60
29081010 and 29081090	Bromo derivatives with single halogene groups	2.00	1.40	2.60
29082000	Derivatives containing only sulpho groups, their salts and esters	2.00	1.40	2.60
29089000	Other	2.00	1.40	2.60
	IV. ETHERS, ALCOHOL PEROXIDES, ETHER PEROXIDES, KETONE PEROXIDES, EPOXIDES WITH A THREE-MEMBERED RING, ACETALS AND HEMIACETALS, AND THEIR HALOGENATED, SULPHONATED, NITRATED OR NITROSATED DERIVATIVES	0.00	0.00	0.00
29091100	Diethyl ether	2.38	2.38	2.38
29091900	Other	2.30	1.61	2.99
29092000	Cyclanic, cyclenic or cycloterpenic ethers and their halogenated, sulphonated, nitrated or nitrosated derivatives	2.30	1.61	2.99
290930	Aromatic ethers and their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
29093010	Diphenyl ether (diphenyl oxide)	3.11	3.11	3.11
	Brominated derivatives	0.50	0.35	0.65
29093031	Pentabromodiphenyl ether; 1,2,4,5-tetrabromo-3,6-bis(pentabromophenoxy)benzene	0.55	0.55	0.55
29093035	1,2-Bis(2,4,6-tribromophenoxy)ethane, for the manufacture of acrylonitrile-butadiene-styrene (ABS)	0.50	0.35	0.65
29093038 / 3039	Other	0.50	0.35	0.65
29093090	Other	1.00	0.70	1.30
29094100	2,2'-Oxydiethanol (diethylene glycol, diglycol)	1.66	1.66	1.66
29094200	Monomethyl ethers of ethylene glycol or of diethylene glycol	1.79	1.74	2.24
	Monomethyl ethers of ethylene glycol (ethanol)	1.74	1.74	1.74
	Monomethyl ether of diethylene glycol	1.83	1.83	1.83
29094300	Monobutyl ethers of ethylene glycol or of diethylene glycol	2.15	2.05	2.24
	Monobutyl ethers of ethylene glycol	2.24	2.24	2.24
	Monobutyl ethers of diethylene glycol	2.05	2.05	2.05
29094400	Other monoalkylethers of ethylene glycol or of diethylene glycol	1.83	1.47	2.20
29094910	Other	1.41	1.13	1.70
29094911	2-(2-Chloroethoxy)ethanol	1.41	1.41	1.41
29094919	Other	1.41	1.13	1.70
29094990	Other	1.41	1.13	1.70
290950	Ether-phenols, ether-alcohol-phenols and their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
29095010	Guaiacol and guaiacolsulphonates of potassium	1.74	1.74	1.74

Appendix A

Table A7 (cont.): Chemicals included in the additional trade module of NEAT

	Guaiacol (methoxyphenol)	2.48	2.48	2.48
29095090	Other	2.48	1.99	2.98
29096000	Alcohol peroxides, ether peroxides, ketone peroxides and their halogenated, sulphonated, nitrated or nitrosated derivatives	2.00	1.40	2.60
29103000	1-Chloro-2,3-epoxypropane (epichlorohydrin)	1.43	1.43	1.43
29109000	Other epoxides, epoxyalcohols, epoxyphenols and epoxyethers, with a three-membered ring, and their halogenated, sulphonated, nitrated or nitrosated derivatives	1.40	0.98	1.82
29110000	Acetals and hemiacetals, whether or not with other oxygen function, and their halogenated, sulphonated, nitrated or nitrosated derivatives	2.24	1.79	2.68
	Acetal (1,1-diethoxyethane)	2.24	2.24	2.24
	Hemiacetal	2.24	1.79	2.68
	Aldehydes, whether or not with other oxygen function; cyclic polymers of aldehydes; paraformaldehyde	0.00	0.00	0.00
29121200	Ethanal (acetaldehyde)	2.00	2.00	2.00
29121300	Butanal (butyraldehyde, normal isomer)	2.44	2.44	2.44
29121900	Other Acyclic aldehydes without other oxygen function	2.61	2.69	2.93
29122100	Benzaldehyde	2.91	2.91	2.91
29122900	Other Cyclic aldehydes without other oxygen function	2.91	2.32	3.49
29123000	Aldehyde-alcohols	2.50	1.75	3.25
	Aldehyde-ethers, aldehyde-phenols and aldehydes with other oxygen function	0.00	0.00	0.00
29124100	Vaniline	2.32	2.32	2.32
29124200	Ethylvanillin (3-ethoxy-4-hydroxybenzaldehyde)	2.39	2.39	2.39
29124900	Other	2.30	1.61	2.99
29125000	Cyclic polymers of aldehydes	2.30	1.61	2.99
29126000	Paraformaldehyde	1.31	1.31	1.31
29130000	Halogene-, sulfo-, nitro- en nitrosoderivatives of 2912	1.75	1.23	2.28
29141200	Butanone (methyl ethyl ketone)	2.44	2.44	2.44
29141300	4-Methylpentan-2-one (methyl isobutyl ketone)	2.64	2.64	2.64
291419	Other	2.70	2.16	3.24
29141910	5-Methylhexan-2-one	2.70	2.70	2.70
29141990	Other Acyclic ketones without other oxygen function	2.70	2.16	3.24
29142100	Kamfer	2.69	2.69	2.69
29142300	Ionones and methylionones	2.98	2.98	2.98
	Ionones	2.98	2.98	2.98
	methylionones (irone)	2.99	2.99	2.99
29142900	Other Cyclanic, cyclenic or cyclocloterpene ketones without other oxygen function	2.80	1.96	2.55
29143100	Phenylacetone (phenylpropan-2-one)	2.96	2.96	2.96
29143900	Other Aromatic ketones without other oxygen function	2.80	1.96	2.55
29144010	4-Hydroxy-4-methylpentan-2-one (diacetone alcohol)	2.49	2.49	2.49
29144090	Other Ketone-alcohols and ketone-aldehydes	2.80	1.96	2.55
29145000	Ketone-phenols and ketones with other oxygen function	2.80	1.96	2.55
29146100	Antraquinone	2.96	2.96	2.96
29146900	Other Quinones	2.80	1.96	2.55
29146910	1,4-Naphthoquinone	2.78	2.78	2.78
29146990	Other	2.60	1.96	2.55
	Halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
29147010	4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (musk ketone)	2.10	2.10	2.10
29147090	Other	2.00	1.40	2.60
29151100	Formic acid	0.96	0.96	0.96
29151200	Salts of formic acid	0.61	0.77	0.86
29151300	Esters of formic acid	1.34	1.24	1.43
29152200	Sodium acetate	0.85	0.85	0.85
29152300	Cobalt acetate	0.88	0.88	0.88
29152400	Acetic anhydride	1.73	1.73	1.73
29152900	Other Acetic acid and its salts	1.25	1.17	1.32
	Acetic acid	1.47	1.47	1.47
29153100	Ethyl acetate	2.00	2.00	2.00
29153200	Vinyl acetate	2.05	2.05	2.05
29153300	n-Butyl acetate	2.28	2.28	2.28
29153400	Isobutyl acetate	2.28	2.28	2.28
29153500	2-Ethoxyethyl acetate	2.00	2.00	2.00
29153910	Propyl acetate and isopropyl acetate	2.16	2.16	2.16
29153930	Methyl acetate, pentyl acetate (amyl acetate), isopentyl acetate (isoamyl acetate) and glycerol acetates	2.04	1.64	2.37
	Methylacetaat	1.78	1.78	1.78
	Pentylacetate (amylacetate)	2.37	2.37	2.37
	isopentylacetate (isoamylacetate)	2.37	2.37	2.37
	Glycerolacetate	1.64	1.64	1.64
29153950	p-Tolyl acetate, phenylpropyl acetates, benzyl acetate, rhodiny acetate, santalyl acetate and the acetates of phenylethane-1,2-diol	2.45	1.68	3.12
	p-Tolyl acetate (cresyl acetate)	2.64	2.64	2.64
	Phenylpropyl acetate	2.40	1.68	3.12
	Benzylacetate	2.64	2.64	2.64
	Rhodinyl acetate	2.40	1.68	3.12
	Santalyl acetate	2.40	1.68	3.12
	Phenylethane 1,2-diol acetate	2.24	2.24	2.24
29153990	Other	2.40	1.68	3.12
29154000	Mono-, di- or trichloroacetic acids, their salts and esters	0.62	0.74	1.12
	Chloroacetic acid	0.93	0.93	0.93
	Dichloroacetic acid	0.68	0.68	0.68
	Trichloroacetic acid	0.54	0.54	0.54
29155000	Propionic acid, its salts and esters	1.96	1.43	2.14
	Propionic acid	1.78	1.78	1.78
29156010	Butanoic acids and their salts and esters	2.20	1.60	2.40
	Butanoic acids	2.00	2.00	2.00
29156011	1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate	2.00	1.40	2.60
29156019	Other	2.00	1.40	2.60
29156090	Pentanoic acids and their salts and esters	2.24	1.80	2.69
29159020	Chloroformates	0.60	0.56	1.04
29159080	--Others	2.00	1.40	2.60
29161110	Acrylic acid	1.83	1.83	1.83
29161190	Salts of acrylic acid	1.56	1.47	1.65
29161210	Methyl acrylate	2.05	2.05	2.05
29161220	Ethyl acrylate	2.20	2.20	2.20
29161290	Other Esters of acrylic acid	2.35	2.25	2.46
29161300	Methacrylic acid and its salts (methacrylic acid)	1.84	1.64	1.84

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Table A7 (cont.): Chemicals included in the additional trade module of NEAT

29161410	Methyl methacrylate	2.20	2.20	2.20
29161490	Other Esters of methacrylic acid	2.53	2.42	2.64
29161930	Hexa-2,4-dienoic acid (sorbic acid)	2.36	2.36	2.36
2916194n	Citronic acid	2.05	2.05	2.05
29161980	Other	2.00	1.40	2.60
29162000	Cyclanic, cyclenic or cycloterpenic monocarboxylic acids, their anhydrides, halides, peroxides, peroxyacids and their derivatives	2.00	1.40	2.60
29163100	Benzoic acid, its salts and esters	2.52	2.02	3.03
	Benzoic acid (benzocorboxylic acid)	2.52	2.52	2.52
291632	Benzoyl peroxide and benzoyl chloride	0.00	0.00	0.00
29163210	Benzoyl peroxide	2.55	2.55	2.55
29163290	Benzoyl chloride	2.19	2.19	2.19
29163400	Phenylacetic acid and its salts	2.33	2.07	2.33
	phenylacetic acid (benzene acetic acid)	2.59	2.59	2.59
29163500	Esters of phenylacetic acid	2.98	2.85	3.11
29163900	Other aromatic monocarboxylic acids, their anhydrides, halides, peroxides, peroxyacids and their derivatives	2.00	1.40	2.60
29171100	Oxalic acid, its salts and esters	0.70	0.56	0.84
29171210	Adipic acid and its salts	1.67	1.45	1.63
29171290	Esters of adipic acid	2.08	1.99	2.17
29171300	Azelaic acid, sebacic acid, their salts and esters	2.27	1.69	2.53
	azelaic acid	2.11	2.11	2.11
29171310	Sebacic acid	2.18	2.18	2.18
29171390	Other Azelaic acid, sebacic acid, their salts and esters	2.00	1.40	2.60
29171400	Maleic anhydride (2,5-Furandione)	1.80	1.80	1.80
29171910	Malonic acid, its salts and esters	1.86	1.47	2.20
	Malonic Acid (methanedicarboxylic acid)	1.63	1.63	1.63
	Malonic ester (ethyl malonate, diethyl malonate)	1.93	1.93	1.93
29171990	Other	1.80	1.26	2.34
29172000	Cyclanic, cyclenic or cycloterpenic polycarboxylic acids, their anhydrides, halides, peroxides, peroxyacids and their derivatives	2.00	1.40	2.60
	Aromatic polycarboxylic acids, their anhydrides, halides, peroxides, peroxyacids and their derivatives ³	0.00	0.00	0.00
29173100	Dibutyl orthophthalates (Dibutyl phthalate (DBP))	2.48	2.48	2.48
29173200	Diocetyl orthophthalates (di(2-ethylhexyl) phthalate (DOP))	2.71	2.71	2.71
29173400	Other esters of orthophthalic acid	2.85	2.73	2.98
291739	Other	0.00	0.00	0.00
29173910	Brominated derivatives	0.50	0.35	0.65
29173911	Ester or anhydride of tetrabromophthalic acid	0.58	0.55	0.60
29173919	Other	0.50	0.35	0.65
29173930	Other	0.00	0.00	0.00
	Benzene-1,2,4-tricarboxylic acid	1.89	1.89	1.89
	Isophthaloyl dichloride	2.10	2.10	2.10
29173940	Isophthaloyl dichloride, containing by weight 0.8 % or less of terephthaloyl dichloride	2.10	2.10	2.10
29173950	Naphthalene-1,4,5,8-tetracarboxylic acid	1.62	1.62	1.62
29173960	Tetrachlorophthalic anhydride	1.23	1.23	1.23
29173970	Sodium 3,5-bis(methoxycarbonyl)benzenesulphonate	0.70	0.49	0.91
29173980	Other	1.50	1.05	1.95
2918	Carboxylic acids with additional oxygen function and their anhydrides, halides, peroxides and peroxyacids; their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
	Carboxylic acids with alcohol function but without other oxygen function, their anhydrides, halides, peroxides, peroxyacids and their derivatives	0.00	0.00	0.00
29181700	Phenylglycolic acid	2.32	2.32	2.32
291819	Other	1.60	1.12	2.08
29181930+29181910	Cholic acid, 3-alpha,12-alpha-dihydroxy-5-beta-cholan-24-oic acid (deoxycholic acid), their salts and esters	2.61	2.53	2.69
	Cholic acid	2.53	2.53	2.53
29181940	Deoxycholic acid (desoxycholic acid)	2.69	2.69	2.69
29181990+29181980+29181990	2,2-Bis(hydroxymethyl)propionic acid (dimethylol propionic acid)	1.64	1.64	1.64
	Other	1.60	1.12	2.08
	Carboxylic acids with phenol function but without other oxygen function, their anhydrides, halides, peroxides, peroxyacids and their derivatives	0.00	0.00	0.00
29182100	Salicylic acid and its salts (salicylic acid, ortho-hydroxybenzoic acid)	2.01	1.79	2.01
29182200	O-Acetylsalicylic acid, its salts and esters (aspirin, ortho-acetoxybenzoic acid)	2.13	1.54	2.64
291823	Other esters of salicylic acid and their salts	2.30	1.61	2.99
29182310	Methyl salicylate and phenyl salicylate (salol)	2.63	2.59	2.67
	Methyl salicylate (gaultharia oil; wintergreen oil; betula oil; sweet birch oil)	2.59	2.59	2.59
	phenyl salicylate (salol)	2.67	2.67	2.67
29182390	Other	2.50	1.75	3.25
291829	Other	0.00	0.00	0.00
29182910	Sulphosalicylic acids, hydroxynaphthoic acids; their salts and esters	2.00	1.40	2.60
	Sulphosalicylic acids	1.21	1.21	1.21
	hydroxynaphthoic acids (3-hydroxy-2-naphthoic acid, beta-hydroxy naphthoic acid, 3-naphthol-2-carboxylic acid, beta-oxy-naphthoic acid)	2.57	2.57	2.57
29182930	4-Hydroxybenzoic acid, its salts and esters (meta hydroxybenzoic acid)	2.10	2.00	2.20
29182950	Gallic acid, its salts and esters (3,4,5-trihydroxybenzoic acid)	2.10	2.00	2.20
29182990	Other	2.00	1.40	2.60
29183000	Carboxylic acids with aldehyde or ketone function but without other oxygen function, their anhydrides, halides, peroxides, peroxyacids and their derivatives	2.00	1.40	2.60
291890	Other	1.50	1.05	1.95
29189010	2,6-Dimethoxybenzoic acid	2.18	2.18	2.18
29189020	Dicamba (ISO) (3,6-dichloro-ortho-anisic acid (2-methoxy-3, 6-dichlorobenzoic acid))	1.59	1.59	1.59
29189030	Sodium phenoxacetate	1.50	1.05	1.95
29189090	Other	1.50	1.05	1.95
	VIII. ESTERS OF INORGANIC ACIDS OF NON-METALS AND THEIR SALTS, AND THEIR HALOGENATED, SULPHONATED, NITRATED OR NITROSATED DERIVATIVES	0.00	0.00	0.00
291900	Phosphoric esters and their salts, including lactophosphates; their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
29190010	Tributyl phosphates, triphenyl phosphate, tritoyl phosphates, trixylyl phosphates, and tris(2-chloroethyl) phosphate	2.03	1.23	2.60
	Tributyl phosphates	1.98	1.98	1.98
	Triphenyl phosphate	2.43	2.43	2.43
	Tritoyl phosphates	2.51	2.51	2.51
	Trixylyl phosphates	2.00	1.40	2.60
	Tris(2-chloroethyl) phosphate	1.23	1.23	1.23
29190090	Other	2.00	1.40	2.60

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Table A7 (cont.): Chemicals included in the additional trade module of NEAT

2920	Esters of other inorganic acids of non-metals (excluding esters of hydrogen halides) and their salts; their halogenated, sulphonated, nitrated or nitrosated derivatives	0.00	0.00	0.00
29201000	Thiophosphoric esters (phosphorothioates) and their salts; their halogenated, sulphonated, nitrated or nitrosated derivatives	1.00	0.70	1.30
292090	Other	0.00	0.00	0.00
29209010	Sulphuric esters and carbonic esters and their salts, and their halogenated, sulphonated, nitrated or nitrosated derivatives	1.00	0.70	1.30
29209020	Dimethyl phosphonate (dimethyl phosphite)	0.80	0.80	0.80
29209030	Trimethyl phosphite (trimethoxyphosphine)	1.06	1.06	1.06
29209040	Triethyl phosphite	1.59	1.59	1.59
29209050	Diethyl phosphonate (diethyl hydrogenphosphite) (diethyl phosphite)	1.28	1.28	1.28
29209065	Other products	1.00	0.70	1.30
	IX. NITROGEN-FUNCTION COMPOUNDS	0.00	0.00	0.00
29211110	Methylamine, di- or trimethylamine	1.87	0.99	1.57
	Methylamine	1.42	1.42	1.42
	Dimethylamine	1.96	1.96	1.96
	Trimethylamine	2.24	2.24	2.24
29211190	Salts	1.96	1.56	2.35
29211200	Diethylamine and its salts	2.09	1.69	2.17
	Diethylamine	2.41	2.41	2.41
29211910	Triethylamine and its salts	2.27	1.83	2.35
	Triethylamine	2.61	2.61	2.61
29211930	Isopropylamine and its salts (isopropylamine, 2-aminopropane)	2.01	1.57	2.24
29211940	1,1,3,3-Tetramethylbutylamine (tert-octylamine)	2.81	2.81	2.81
29211980	Other	2.00	1.40	2.60
29211990	Other	2.00	1.40	2.60
29212100	Ethylenediamine and its salts (ethylenediamine, 1,2-diaminoethane)	1.32	1.03	1.47
29212200	Hexamethylenediamine and its salts (hexamethylenediamine, 1,6-diaminohexane, 1,6-hexanediamine)	2.05	1.59	2.28
29212900	Other	2.00	1.40	2.60
29213010	Cyclohexylamine and cyclohexyldimethylamine, and their salts	2.45	1.94	2.77
	Cyclohexylamine (hexahydroaniline; aminocyclohexane)	2.40	1.87	2.67
	Cyclohexyldimethylamine	2.49	1.94	2.77
29213090	Other amino compounds of cycloalkanes, cycloalkenes of cycloalkenes and their derivatives	2.00	1.40	2.60
29213091	Cyclohex-1,3-ylenediamine (1,3-diaminocyclohexane)	2.32	2.32	2.32
29213099	Other Cyclic, cyclic or cycloterpene mono- or polyamines, and their derivatives; salts thereof	2.00	1.40	2.60
29214210	Halogenated, sulphonated, nitrated and nitrosated derivatives and their salts of Aniline derivatives and their salts	2.80	1.96	3.64
29214290	Other Aniline derivatives and their salts	2.80	1.96	3.64
29214300+29214310+29214390	Toluidines and their derivatives; salts thereof	2.62	2.32	2.62
29214400	Diphenylamine and its derivatives; salts thereof (diphenylamine, N-phenylaniline)	2.61	2.50	2.81
29214500	1-Naphthylamine (alpha-naphthylamine), 2-naphthylamine (beta-naphthylamine) and their derivatives; salts thereof	2.77	2.15	3.08
	1-Naphthylamine (alpha-naphthylamine)	2.77	2.15	3.08
	2-naphthylamine (beta-naphthylamine)	2.77	2.15	3.08
29214910	Xylidines and their derivatives; salts thereof (xylidine, dimethylbenzenamine)	2.62	2.33	2.91
29214990	Other	3.00	2.10	3.90
29215110	o-, m-, p-Phenylenediamine, diaminotoluenes and their halogenated, sulphonated, nitrated and nitrosated derivatives; salts thereof	2.24	1.71	2.52
	o-, m-, p-Phenylenediamine	2.20	1.71	2.44
	Diaminotoluene	2.27	1.77	2.52
29215111	m-Phenylenediamine, of a purity by weight of 99 % or more and containing: -1 % or less by weight of water, -200 mg/kg or less of o-phenylenediamine and -450 mg/kg or less of p-phenylenediamine	2.44	2.44	2.44
29215119	Other	2.40	1.68	3.12
29215190	Other	2.40	1.68	3.12
29215900	Other	2.40	1.68	3.12
29215910	m-Phenylenebis(methylamine)	2.40	1.60	3.12
29215920	2,2'-Dichloro-4,4'-methylenedianiline	1.65	1.65	1.65
29215930	4,4'-Bi-o-toluidine	2.91	2.91	2.91
29215940	1,6-Naphthylenediamine (naphthalenediamine, diaminonaphthalene)	2.78	2.78	2.78
29215990	Other	2.40	1.68	3.12
	Oxygen-function amino-compounds	0.00	0.00	0.00
	Amino-alcohols, other than those containing more than one kind of oxygen function, their ethers and esters; salts thereof	0.00	0.00	0.00
29221100	Monoethanolamine and its salts (MEA, ethanolamine, colamine, 2-aminoethanol, 2-hydroxyethylethylamine)	1.96	1.96	1.96
29221200	Diethanolamine and its salts (DEA, di(2-hydroxyethyl)-amine)	2.41	2.41	2.41
292213	Triethanolamine and its salts	2.61	2.61	2.61
29221310	Triethanolamine (TEA, tri(2-hydroxyethyl)amine)	2.61	2.61	2.61
29221390	Salts of triethanolamine	2.22	2.09	2.35
292219	Other	0.00	0.00	0.00
29221910	N-Ethyldiethanolamine (ethyldiethanolamine)	1.98	1.98	1.98
29221920	2,2'-Methyliminodiethanol (N-methyldiethanolamine)	1.85	1.85	1.85
29221990	Other	1.80	1.26	2.34
	Amino-naphthols and other amino-phenols, other than those containing more than one kind of oxygen function, their ethers and esters; salts thereof	0.00	0.00	0.00
29222100	Aminohydroxynaphthalenesulphonic acids and their salts	1.84	1.84	1.84
29222200	Anisidines, dianisidines, phenetidines, and their salts	2.28	1.75	2.57
	Anisidines	2.25	1.75	2.50
	dianisidines	2.27	1.77	2.52
	phenetidines	2.31	1.80	2.57
29222900	Other	2.00	1.40	2.60
29223000	Amino-aldehydes, amino-ketones and amino-quinones, other than those containing more than one kind of oxygen function; salts thereof	2.00	1.40	2.60
	Amino-acids, other than those containing more than one kind of oxygen function, and their esters; salts thereof	0.00	0.00	0.00
29224100	Lysine and its esters; salts thereof (lysine)	1.45	1.45	1.63
29224200+29224210+29224290	Glutamic acid and its salts (glutamic acid, alpha-aminoglutaric acid; 2-aminopentanedioic acid)	1.20	1.20	1.35
29224300	Anthrnic acid and its salts (ortho-aminobenzoic acid, anthranilic acid)	1.80	1.80	2.02
292249	Other	0.00	0.00	0.00
29224910	Glycine (aminoacetic acid)	1.17	1.17	1.17
29224920	Beta-Alanine (3-aminopropanoic acid; beta-aminopropionic acid)	1.48	1.48	1.48
29224970+29224980	Other	1.20	0.84	1.56
29225000	Aminofenolalcohols, aminofenolacids and other aminocompounds with acid groups	2.00	1.40	2.60
	Carboxamide-function compounds; amide-function compounds of carbonic acid	0.00	0.00	0.00

Appendix A

Table A7 (cont.): Chemicals included in the additional trade module of NEAT

29241000	Acyclic amides (including acyclic carbamates) and their derivatives; salts thereof	2.00	1.40	2.60
	Cyclic amides (including cyclic carbamates) and their derivatives; salts thereof	0.00	0.00	0.00
292421	Ureines and their derivatives; salts thereof	2.50	1.75	3.25
29242110	Isoproturon (ISO)	2.56	2.56	2.56
29242190	Other	2.50	1.75	3.25
29242200	Acetamidobenzoic acid	2.21	2.21	2.21
292429	Other	2.50	1.75	3.25
29242910	Lidocaine (INN) (alpha-diethylaminoaceto-2,6-xylidide)	2.63	2.63	2.63
29242930	Paracetamol (INN) (acetaminophen)	2.33	2.33	2.33
29242990	Other	2.50	1.75	3.25
	Carboxyimide-function compounds (including saccharin and its salts) and imine-function compounds	0.00	0.00	0.00
	Imides and their derivatives; salts thereof	0.00	0.00	0.00
29251100	Saccharin and its salts (saccharin, ortho-benzosulfimide, gluside; benzoysulfonic imide)	1.67	1.67	1.67
292519	Other	0.00	0.00	0.00
29251910	3,3',4,4',5,5',6,6'-Octabromo-N,N'-ethylenedipthalimide	0.50	0.35	0.65
29251930	N,N'-ethylenebis(4,5-dibromohexahydro-3,6-methanophthalimide)	0.50	0.35	0.65
29251980	Other	1.00	0.70	1.30
29252000	Imines and their derivatives; salts thereof	1.00	0.70	1.30
2926	Nitrile-function compounds	0.00	0.00	0.00
29262000	1-Cyanoguanidine (dicyandiamide)	1.05	1.05	1.05
292690	Other	2.00	1.40	2.60
29269020+29269010	Isophthalonitrile (1,3-dicyanobenzene)	2.75	2.75	2.75
29269099+29269080+29269090	Other	2.00	1.40	2.60
29270000	Diazo-, azo- or azoxy-compounds	1.00	0.70	1.30
2928	Organic derivatives of hydrazine or of hydroxylamine	1.00	0.70	1.30
29280010	N,N-Bis(2-methoxyethyl)hydroxylamine	1.50	1.05	1.95
29280090	Other	1.00	0.70	1.30
2929	Compounds with other nitrogen function	0.00	0.00	0.00
292910	Isocyanates	0.00	0.00	0.00
29291010	Methylphenylene diisocyanates (toluene diisocyanates, TDI, meta-tolylene diisocyanate)	2.28	2.28	2.28
29291090	Other	2.20	1.54	2.86
29299000	Other	2.20	1.54	2.86
	X. ORGANO-INORGANIC COMPOUNDS, HETEROCYCLIC COMPOUNDS, NUCLEIC ACIDS AND THEIR SALTS, AND SULPHONAMIDES	0.00	0.00	0.00
2930	Organo-sulphur compounds	0.00	0.00	0.00
29301000	Dithiocarbonates (xanthates)	1.50	1.05	1.95
29302000	Thiocarbonates and dithiocarbonates	1.50	1.05	1.95
29303000	Thiuram mono-, di- or tetrasulphides	1.50	1.05	1.95
293040	Methionine (INN)	1.50	1.05	1.95
29304010	Methionine (INN) (1-amino-4-(methylthio)butyric acid)	1.63	1.63	1.63
29304090	Other	1.50	1.05	1.95
29309020	Thiodiglycol (INN) (2,2'-thiodiethanol; thiodiethylene glycol; beta-bis-hydroxy-ethyl sulfide; dihydroxyethyl sulfide)	1.66	1.66	1.66
29309030	DL-2-hydroxy-4-(methylthio)butyric acid	1.47	1.47	1.47
29309040	2,2'-Thiodiethylbis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]	1.40	0.98	1.82
29309050	Mixture of isomers consisting of 4-methyl-2,6-bis(methylthio)-m-phenylenediamine and 2-methyl-4,6-bis(methylthio)-m-phenylenediamine	1.40	0.98	1.82
29309070+29309095	Other	1.40	0.98	1.82
2931	Other organo-inorganic compounds	0.00	0.00	0.00
29310010	Dimethyl methylphosphonate	1.06	1.06	1.06
29310020	Methylphosphonyl difluoride (methylphosphonic difluoride)	0.38	0.38	0.38
29310030	Methylphosphonyl dichloride (methylphosphonic dichloride)	0.30	0.30	0.30
29310050+29310085+29310095	Other	0.50	0.35	0.65
2932	Heterocyclic compounds with oxygen hetero-atom(s) only	0.00	0.00	0.00
	Compounds containing an unfused furan ring (whether or not hydrogenated) in the structure	0.00	0.00	0.00
29321100	Tetrahydrofuran (THF)	2.44	2.44	2.44
29321300	Furfuryl alcohol and tetrahydrofurfuryl alcohol	2.20	2.16	2.24
	Furfuryl alcohol	2.24	2.24	2.24
	tetrahydrofurfuryl alcohol	2.16	2.16	2.16
29321900	Other	2.20	1.54	2.86
	Lactones	0.00	0.00	0.00
29322100	Coumarin, methylcoumarins and ethylcoumarins	2.63	2.42	2.75
	Coumarin (curamin; benzopyrone; tonka bean comphor)	2.71	2.71	2.71
	methylcoumarins	2.75	2.75	2.75
	ethylcoumarin-3-carboxylate	2.42	2.42	2.42
293229	Other lactones	2.50	1.75	3.25
29322910	Phenolphthalein	2.77	2.77	2.77
29322920	1-Hydroxy-4-[1-(4-hydroxy-3-methoxycarbonyl-1-naphthyl)-3-oxo-1H, 3H-benzo[de]isochromen-1-yl]-6-octadecyloxy-2-naphthoic acid	2.00	1.40	2.60
29322930	3-Chloro-6'-cyclohexylaminospiro[isobenzofuran-1(3H), 9'-xanthen]-3-one	2.00	1.40	2.60
29322940	6'-(N-Ethyl-p-toluidino)-2'-methylspiro[isobenzofuran-1(3H), 9'-xanthen]-3-one	2.00	1.40	2.60
29322950	Methyl-6-docosyloxy-1-hydroxy-4-[1-(4-hydroxy-3-methyl-1-phenanthryl)-3-oxo-1H, 3H-naphtho[1,8-cd]pyran-1-yl]naphthalene-2-carboxylate	2.00	1.40	2.60
29322980+29322990	Other	2.00	1.40	2.60
29329200	1-(1,3-Benzodioxol-5-yl)propan-2-one	2.50	1.75	3.25
293299	Other	0.00	0.00	0.00
29329910	Benzofuran (coumarone)	2.98	2.98	2.98
29329950	Epoxides with a four-membered ring	2.80	1.96	3.64
29329970	Other cyclic acetals and internal hemiacetals, whether or not with other oxygen functions, and their halogenated, sulphonated, nitrated or nitrosated derivatives	2.80	1.96	3.64
29329980+29329930+29329990	Other	2.50	1.75	3.25
	Heterocyclic compounds with nitrogen hetero-atom(s) only	0.00	0.00	0.00
	Compounds containing an unfused pyrazole ring (whether or not hydrogenated) in the structure	0.00	0.00	0.00
293311	Phenazone (antipyrin) and its derivatives (phenazone, 2,3-dimethyl-1-phenyl-3-pyrazolin-5-one)	2.67	2.32	2.83
29331110	Propyphenazone (INN)	2.68	2.68	2.68
29331190	Other	2.60	1.82	3.38
293319	Other	0.00	0.00	0.00
29331910	Phenylbutazone (INN) (4-n-butyl-1,2-diphenyl-3,5-pyrazolidinedione)	2.71	2.71	2.71
29331990	Other	2.60	1.82	3.38
	Compounds containing an unfused imidazole ring (whether or not hydrogenated) in the structure	0.00	0.00	0.00
29332100	Hydantoin and its derivatives (hydantoin, glycolylurea)	1.00	1.00	1.00
293329	Other	0.00	0.00	0.00
29332910	Naphazoline hydrochloride (INN) and naphazoline nitrate (INN); phenolamine (INN); tolazoline hydrochloride (INN)	2.48	1.75	3.25
	Naphazoline hydrochloride	2.50	2.50	2.50

Appendix A

Table A7 (cont.): Chemicals included in the additional trade module of NEAT

	Naphazoline nitrate (INN)	2.50	1.75	3.25
	Phentolamine (INN)	2.66	2.66	2.66
	Tolazoline hydrochloride (INN)	2.24	2.24	2.24
29332990	Other	2.50	1.75	3.25
	Compounds containing an unfused pyridine ring (whether or not hydrogenated) in the structure	0.00	0.00	0.00
29333100	Pyridine and its salts	2.61	2.32	2.32
	Pyridine	2.90	2.90	2.90
29333200	Piperidine and its salts	2.33	2.07	2.07
	Piperidine (hexahydropyridine, pentamethyleneamine)	2.59	2.59	2.59
293339	Other	1.20	0.84	1.56
29333910	Iproniazid (INN); ketobemidone hydrochloride (INN); pyridostigmine bromide (INN)	2.02	1.06	1.64
	Iproniazid (INN)	2.21	2.21	2.21
	ketobemidone hydrochloride (INN)	2.34	2.34	2.34
	pyridostigmine bromide (INN)	1.52	1.52	1.52
29333920	2,3,5,6-Tetrachloropyridine	1.01	1.01	1.01
29333925	3,6-Dichloropyridine-2-carboxylic acid (clopyralid)	1.38	1.38	1.38
29333935	2-Hydroxyethylammonium-3,6-dichloropyridine-2-carboxylate	1.00	0.70	1.30
29333940	2-Butoxyethyl(3,5,6-trichloro-2-pyridyloxy)acetate	1.00	0.70	1.30
29333945	3,5-Dichloro-2,4,6-trifluoropyridine	1.23	1.23	1.23
29333950	Fluoroxypyr (ISO), methyl ester	1.21	1.21	1.21
29333955	4-Methylpyridine (gamma-picoline, 4-picoline)	2.84	2.84	2.84
29333995+29333980	Other	1.20	0.84	1.56
293340	Compounds with or without hydrogenated chinoliation or isochinoliation, not further condensed	0.00	0.00	0.00
29334010	Halogen derivatives of quinoline; quinolinecarboxylic acid derivatives	2.03	2.03	2.29
	quinolinecarboxylic acid	2.54	2.54	2.54
29334030	Dextromethorphan (INN) and its salts	2.59	2.25	2.92
	Dextromethorphan hydrobromide	2.25	2.25	2.25
29334090	Other	2.50	1.75	3.25
	Compounds containing a pyrimidine ring (whether or not hydrogenated) or piperazine ring in the structure	0.00	0.00	0.00
293351	Malonylurea (barbituric acid) and its salts	0.59	1.00	1.00
	Barbituric acid (pyrimidinetrione, 2,4,6-tri-oxohexahydro pyrimidine)	1.19	1.19	1.19
29335120+29335110	Phenobarbital (INN), barbital (INN), and their salts	2.09	1.91	2.28
	Phenobarbital (INN) (phenylbarbital, phenylethylmalonylurea; 5-ethyl-5-phenylbarbituric acid)	2.28	2.28	2.28
	Barbital (INN) (diethylmalonylurea; diethylbarbituric acid; "Veronal")	1.91	1.91	1.91
29335190+29335130	Other	2.00	1.40	2.60
293359	Other	0.00	0.00	0.00
29335910	Diazinon (ISO) (generic name of an insecticide, O,O-diethyl O-(2-isopropyl-4-methyl-6-pyrimidinyl)phosphorothioate)	1.74	1.74	1.74
29335920	1,4-Diazabicyclo[2.2.2]octane (triethylenediamine)	2.36	2.36	2.36
29335970+29335980	Other	2.00	1.40	2.60
	Compounds containing an unfused triazine ring (whether or not hydrogenated) in the structure	0.00	0.00	0.00
29336100	Meleamine	1.03	1.03	1.03
29336910	Atrazine (ISO); propazine (ISO); simazine (ISO); hexahydro-1,3,5-trinitro-1,3,5-triazine (hexogen, trimethylenetrinitramine)	1.37	0.59	1.73
	Atrazine (ISO) (generic name for 2-chloro-4-ethylamino-6-isopropylamino-s-triazine)	1.63	1.63	1.63
	propazine (ISO) (generic name for 2-chloro-4,6-bis(isopropylamino)-s-triazine)	1.73	1.73	1.73
	simazine (ISO) (generic name for 2-chloro-4,6-bis(ethylamino)-s-triazine)	1.53	1.53	1.53
	hexahydro-1,3,5-trinitro-1,3,5-triazine (cyclonite, hexogen, trimethylenetrinitramine)	0.59	0.59	0.59
29336920	Methenamine (INN) (hexamethylenetetramine)	1.89	1.89	1.89
29336930	2,6-Di-tert-butyl-4-[4,6-bis(octylthio)-1,3,5-triazine-2-ylamino]phenol	1.00	0.70	1.30
29336980+29336990	Other	1.00	0.70	1.30
	Lactams	0.00	0.00	0.00
29337900	Other lactams	2.34	1.64	3.04
29339010	Benzimidazole-2-thiol (mercaptobenzimidazole)	2.61	2.61	2.61
29339020	Indole, 3-methylindole (skatole), 6-allyl-6,7-dihydro-5H-dibenz[c,e]azepine (azapetine), phenindamine (INN) and their salts; imipramine hydrochloride (INN)	2.97	2.64	3.20
	Indole	3.01	3.01	3.01
	3-methylindole (skatole)	3.02	3.02	3.02
	phenindamine (INN)	3.20	3.20	3.20
	imipramine hydrochloride (INN)	2.64	2.64	2.64
29339050	Monoazepines	2.50	1.75	3.25
29339060	Diazepines	2.50	1.75	3.25
29339065	2,4-Di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol	2.40	2.40	2.40
29339095+29339080+29339040	Other	2.50	1.75	3.25

Appendix B

Appendix B: Assumptions for Calculating Non-energy Use and Related CO₂ Emissions with NEAT

Table B1: NEAT assumptions on the division between ODU and NODU product application

Product	Consumption	NODU [%]	ODU [%]	Minimum Release	Maximum Release
				ODU [%]	ODU [%]
<i>Basic Chemicals</i>					
Acetylene	Total ¹⁾	50	50	10	70
Ammonia	Process ²⁾	-	-	-	-
Benzene	Other ³⁾	50	50	20	70
Bitumen	Total	100	0	0	0
Butadiene	Other	100	0	0	20
Other C4	Other	84	16	5	50
Carbon black	Total	100	0	0	0
CO source	Other ⁴⁾	-	-	-	-
Ethylene	Other	5	95	85	100
Lubricants	Total	74	26	9	50
Methanol	Other	50	50	30	70
Petroleum coke	Total	0	100	100	100
Pitch	Total	0	100	100	100
Creosote oil	Other	100	0	0	0
Naphthalene	Total	50	50	20	70
Other tar products	Total	100	0	0	0
Propylene	Other	37	63	50	75
Toluene	Other	17	83	70	97
Waxes, paraffins	Total	0	100	40	100
Xylenes	Other	0	100	30	100
o-xylene	Other	0	100	30	100
m-xylene	Total	0	100	30	100
p-xylene	Other	0	100	30	100
<i>Intermediates</i>					
Acetaldehyde	Other	35	65	35	75
Acetic acid	Other	35	65	35	75
Acetone	Other	60	40	45	65
Acrylic acid	Other	100	0	0	5
Acrylonitrile	Other	100	0	0	10
Adipic acid	Other	100	0	0	5
Adiponitrile	Other	100	0	0	0
Aniline	Other	80	20	5	25
Bisphenol A	Other	100	0	0	0
Butanol	Total	19	81	70	90
Caprolactam	Other	100	0	0	0
Cumene	Other	100	0	0	5
Cyclohexane	Other	20	80	60	100
Cyclohexanone	Other	5	95	90	100
Dimethylterephthalate	Other	100	0	0	0
Ethanol	Total	0	100	70	100
Ethylbenzene	Other	100	0	0	70
Ethylenedichloride	Other	0	100	100	100
Ethylene glycol	Other	0	100	70	100

Appendix B

Table B1 (cont.): NEAT assumptions on the division between ODU and NODU product application

Product	Consumption	NODU [%]	ODU [%]	Minimum Release	Maximum Release
				ODU [%]	ODU [%]
Ethylene oxide	Other	29	71	65	95
Formaldehyde	Other	0	100	70	100
Hexamethylenediamine	Other	100	0	0	0
MTBE	Total ⁴⁾	-	-	-	-
Octanol	Total	50	50	10	90
Orthophthalate	Other	100	0	0	50
Phenol	Other	0	100	70	100
Phthalic anhydride PSA	Other	0	100	30	100
Polyether-Polyols	Other	100	0	0	50
i-Propanol	Other	7	93	80	100
Propylene oxide	Other	0	100	100	100
Styrene	Other	100	0	0	0
Terephthalic acid TPA	Other	100	0	0	0
TDI	Other	100	0	0	0
Urea	Other	0	100	0	100
Vinylchloride monomer VCM	Other	20	80	30	100
Final Products					
ABS	Total	100	0	0	0
BR	Total	100	0	0	0
EPDM	Total	100	0	0	0
Epoxy resin	Total	100	0	0	0
Melamineformaldehyde resin	Total	100	0	0	0
Phenolic resin	Total	100	0	0	0
Polyacetals	Total	100	0	0	0
Polyacrylates	Total	100	0	0	0
Polyacrylonitrile	Total	100	0	0	0
Polyamide 6,66	Total	100	0	0	0
Polycarbonate	Total	100	0	0	0
Polyethylene PE	Total	100	0	0	0
Polyethyleneterephthalate PET	Total	100	0	0	0
Polypropylene PP	Total	100	0	0	0
Polystyrene PS	Total	100	0	0	0
Polyurethane PUR	Total	100	0	0	0
Polyvinylacetate	Total	100	0	0	0
Polyvinylchloride PVC	Total	100	0	0	0
SAN	Total	100	0	0	0
Saturated polyester	Total	100	0	0	0
SBR	Total	100	0	0	0
Unsat. polyester/alkyd resin	Total	100	0	0	0
Urea formaldehyde resin UF	Total	100	0	0	0

¹⁾ Products labeled as 'Total' are not consumed for the production of other NEAT products.

²⁾ Ammonia is labeled as 'Process' because it does not contain Carbon itself. However, its production requires input of fossil feedstock and leads therefore to CO₂ emissions, which are dealt with in NEAT as industrial process emissions.

³⁾ Products labeled as 'Other' are consumed for the production of other NEAT intermediates or final products.

⁴⁾ CO is completely used as carbon source for the production of other chemicals.

⁵⁾ MTBE is used as additive in the fuels. The emissions are thus taken into account as CO₂ emissions from fossil fuel combustion.

Appendix B

Table B2: Process specific carbon losses (Neelis et al., 2005b)

Product	Specific Feedstock Consumption* in t/t product		Specific Loss in t CO ₂ /t product	Fuel Grade Byproducts in t CO ₂ /t product	Total Specific Loss** in t CO ₂ /t CO ₂ equivalents of product
Phenol	Cumene	1.35	0	0.28	0.10
	Toluene	1.20	1.17	0	0.42
Propylene oxide	Propylene	0.88	0.33	0	0.15
	Propylene	0.90	0	0	0.00
	Isobutene	2.35	0.97	0.31	0.56
	Propylene	0.74	0.06	0	0.03
	Ethylbenzene	2.52	0.62		0.27
Caprolactam	Cyclohexane	1.03	0.88	0	0.38
	Phenol	0.92	0.25	0	0.11
Phthalic anhydride	o-Xylol	0.92	0.60	0	0.25
	Naphthalene	0.92	0.78	0	0.33
Adiponitrile	Acrylonitrile	1.13	0.54	0	0.24
	Adipic acid	1.48	0.40	0	0.18
	Butadiene	0.63	0.76	0	0.33
	HCN	0.60	0	0	0.00
Acrylonitrile	Propylene	1.06	0.71	0	0.29
Adipic Acid	Cyclohexane	0.75	0.55	0	0.30
Ethylene oxide	Ethylene	0.78	0.45	0	0.23
Toluene Diisocyanate (TDI)	Toluene	0.67	0	0	0.00
	CO	0.43	0.44	0.18	0.27
Bisphenol-A	Phenol	0.88	0	0	0.00
	Acetone	0.29	0.37	0	0.13
	Toluene	0.04	0	0	0.00
Dimethylterephthalate	p-Xylene	0.63	0.27	0	0.12
	Methanol	0.38	0.07	0	0.03
Polyamide-6	Caprolactam	1.11	0.26	0	0.11
Isopropanol	Propylene	0.78	0.25	0	0.11
Polycarbonate	Bisphenol-A	0.90	0	0	0.00
	CO	0.23	0.19	0	0.07
Diethylphthalate	2-Ethylhexanol	0.73	0	0	0.00
	PA	0.38	0.17	0	0.06
Terephthalic acid	p-Xylene	0.66	0.07	0	0.03
	Acetic acid	0.05	0.07	0	0.03
MDI	Aniline	0.76	0	0	0.00
	Formaldehyde	0.14	0.07	0	0.02
	CO	0.26	0.07	0	0.02
Formaldehyde	Methanol	1.15	0.12	0	0.08
Acetaldehyde	Ethylene	0.67	0.11	0	0.06
Acetic acid	Acetaldehyde	0.76	0.06	0	0.04
	Methanol	0.54	0.05	0	0.04
	CO	0.53	0.05	0	0.03
n-Butanol	Propylene	0.66	0.07	0.05	0.05
	CO	0.44	0.02	0.02	0.02

* only feedstock and by-products containing fossil carbon are listed here

** including fuel grade by-products

Appendix B

Table B2 (cont.): Process specific carbon losses (based on Neelis et al., 2005b)

Product	Specific Feedstock Consumption* in t/t product		Specific Loss in t CO ₂ /t product	Fuel Grade Byproducts in t CO ₂ /t product	Total Specific Loss** in t CO ₂ /t CO ₂ equivalents product
Vinylchloride	Ethylene	0.47	0.07	0	0.05
Aniline	Benzene	1.35	0.06	0	0.02
Ethylene glycol	Ethylene oxide	0.83	0.05	0	0.04
Styrene	Ethylbenzene	1.07	0.05	0	0.01
Polyvinylchloride	Vinylchloride	1.03	0.04	0	0.04
PET	Ethylene glycol	0.33	0.03	0	0.01
	TPA	0.87	0	0	0.00
Cumene	Propylene	0.35	0.02	0	0.00
	Benzene	0.66	0.01	0	0.00
Polystyrene	Styrene	1.01	0.03	0	0.01
Aceton	Isopropanol	1.05	0.03	0	0.01
Polyethylene	Ethylene	1.01	0.03	0	0.01
Polyetherpolyols	Glycerol	0.03	0	0	0.00
	Propylene oxid	1.00	0.02	0	0.01
Urea	Ammonia	0.57	0	0	0.00
	Carbon dioxide	0.75	0.02	0	0.03
Cyclohexane	Benzene	0.93	0.02	0	0.01
Polypropylene	Propylene	1.01	0.02	0	0.01
Ethylbenzene	Bezene	0.74	0	0	0.00
	Ethylene	0.27	0.01	0	0.00

*) only feedstock and by-products containing fossil carbon are listed here

***) including fuel grade by-products

Appendix B

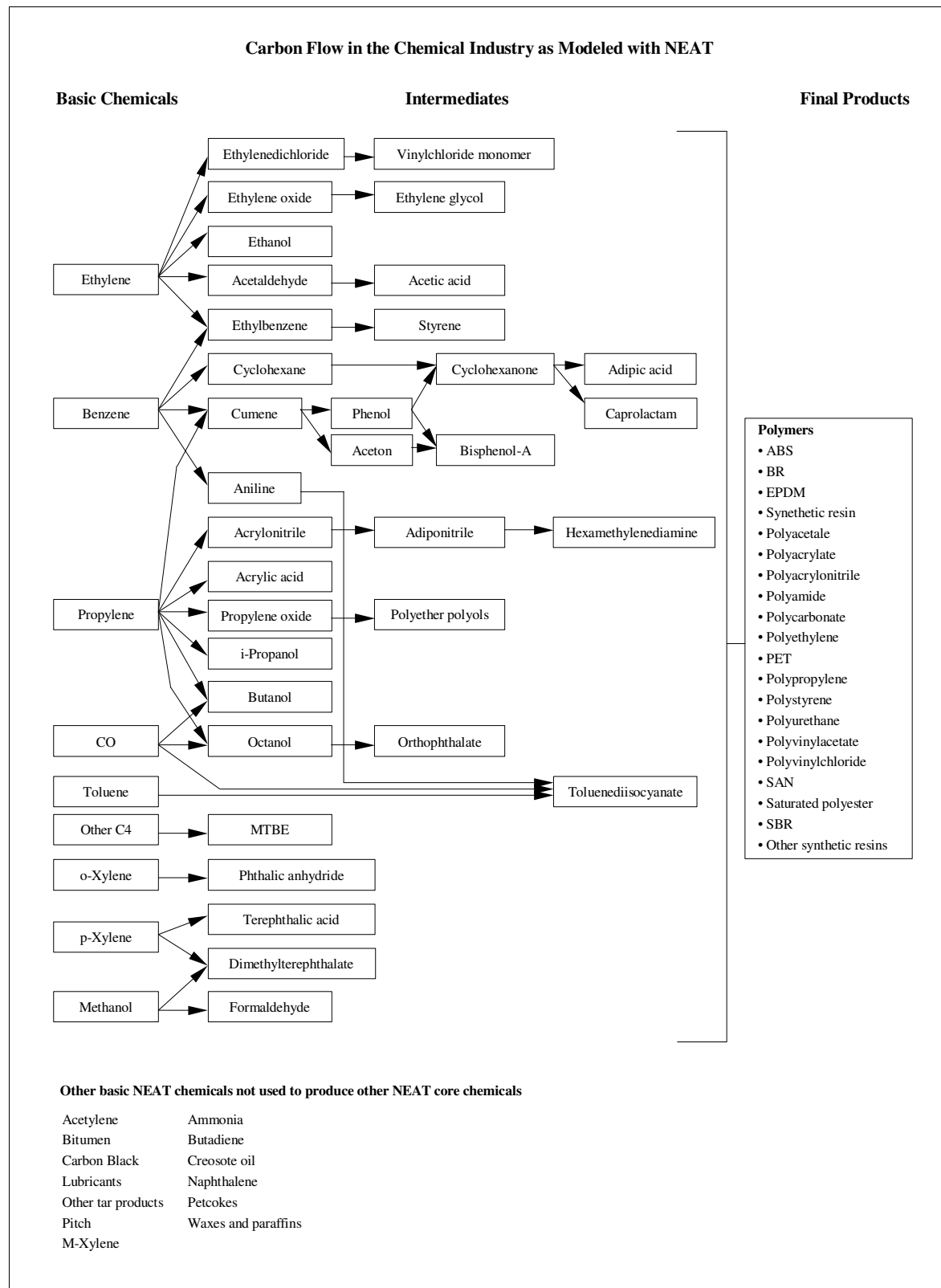
Table B3: Comparison of lubricants and bitumen as stated by different sources (Destatis, IPCC-RA, and the mineral oil statistics 'Mineralölstatistik')

Year		1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
Lubricants	Consumption (DESTATIS)* in Mt CO ₂	4.55	4.48	4.44	4.08	3.72	4.95	4.89	4.57	4.56	5.44	4.70	3.58	3.92	4.20
	Consumption (IPCC-RA) in Mt CO ₂	4.51	3.57	3.36	3.38	3.50	3.24	3.30	3.05	3.18	3.32	-	-	-	-
	Absolute deviation in Mt CO ₂	0.04	0.91	1.08	0.71	0.22	1.71	1.59	1.53	1.38	2.12	-	-	-	-
	Relative deviation in %	1	25	32	21	6	53	48	50	44	64	-	-	-	-
	Consumption (DESTATIS) in Mt	1.45	1.42	1.41	1.30	1.18	1.57	1.55	1.46	1.45	1.73	1.49	1.14	1.25	1.34
	Consumption ('Mineralölstatistik')* in Mt	1.14	1.23	1.19	1.13	1.15	1.17	1.13	1.17	1.15	1.16	1.12	1.06	1.08	1.07
	Absolute deviation in Mt	0.30	0.20	0.23	0.17	0.03	0.40	0.43	0.29	0.30	0.57	0.37	0.08	0.17	0.27
	Relative deviation in %	27	16	19	15	3	35	38	25	27	49	33	8	16	25
Bitumen	Consumption (DESTATIS) in Mt CO ₂	8.37	9.60	9.69	10.94	12.54	11.56	11.50	12.17	11.17	12.12	11.77	11.19	9.84	9.97
	Consumption (IPCC-RA) in Mt CO ₂	10.09	10.86	11.59	10.69	12.63	11.35	10.42	10.58	10.44	11.23	-	-	-	-
	Absolute deviation in Mt CO ₂	-1.72	-1.25	-1.90	0.25	-0.09	0.21	1.07	1.59	0.73	0.89	-	-	-	-
	Relative deviation in %	-17	-12	-16	2	-1	2	10	15	7	8	-	-	-	-
	Consumption (DESTATIS) in Mt	2.66	3.06	3.08	3.48	3.99	3.68	3.66	3.87	3.55	3.86	2.76	3.56	3.13	3.17
	Consumption ('Mineralölstatistik') in Mt	2.62	3.35	3.69	3.39	3.93	3.58	3.40	3.51	3.38	3.62	3.25	3.14	2.98	2.84
	Absolute deviation in Mt	0.04	-0.29	-0.60	0.09	0.06	0.10	0.26	0.36	0.17	0.23	-0.49	0.43	0.15	0.33
	Relative deviation in %	2	-9	-16	3	1	3	8	10	5	6	-15	14	5	12
<i>Total Deviation (DESTATIS-IPCC-RA) in Mt CO₂</i>		<i>-1.68</i>	<i>-0.35</i>	<i>-0.82</i>	<i>0.96</i>	<i>0.13</i>	<i>1.92</i>	<i>2.66</i>	<i>3.12</i>	<i>2.11</i>	<i>3.01</i>	-	-	-	-
<i>Total Deviation (DESTATIS-'Mineralölstatistik') in Mt</i>		<i>0.35</i>	<i>-0.10</i>	<i>-0.38</i>	<i>0.26</i>	<i>0.09</i>	<i>0.51</i>	<i>0.69</i>	<i>0.65</i>	<i>0.48</i>	<i>0.80</i>	<i>-0.12</i>	<i>0.51</i>	<i>0.32</i>	<i>0.60</i>

* Data as given in the lines named 'Mineralölstatistik' are derived from the official mineral oil statistics of Germany as published by BAFA (1990-2003)

Appendix B

Figure B1: Overview of carbon flow in the German chemical industry as modeled with NEAT



Appendix C: NEAT-SIMP - A simplified approach for calculating non-energy use and related CO₂ emissions

We give a short introduction to the simplified version of the detailed NEAT model (NEAT-SIMP) in Appendix C, where we also list all data requirements for NEAT-SIMP. The detailed NEAT model consists of several modules for calculating total and fuel specific non-energy use, the amount of carbon stored, and subsequently CO₂ emissions resulting from product use and industrial processes. In NEAT-SIMP, we estimate non-energy use as the sum of three components (gray fields in Figure C1),

- (i) consumption of refinery products⁴⁰,
- (ii) feedstock requirements for steam cracking and for the production of other chemicals (i.e., ammonia, methanol, and carbon black), and
- (iii) electrode and other solid carbon consumption for the production of non-ferrous metals and ferroalloys.

In NEAT-SIMP, we principally follow the definition of non-energy use as applied in the German Energy Balances, thereby including also the parts of oil and coal input into industrial processes and steam crackers, which are used for fuel purposes but excluding backflows from steam crackers to refineries and the parts of natural gas used for fuel purposes. We however, allow the model user to adapt NEAT-SIMP calculations based on changing system boundaries of non-energy use.

We distinguish industrial processes, product use and wastewater treatment as the two principle source categories for CO₂ emissions resulting from the non-energy use of fossil fuels. Estimating *industrial process emissions* with the detailed NEAT model is relatively simple and requires only a limited amount of data. **The spreadsheet model used in NEAT for calculating industrial process emissions is therefore also applied in NEAT-SIMP.**

Calculating *product use emissions* with the detailed NEAT model requires extensive amounts of production and trade data due to the detailed material flow and mass balance approach chosen. In NEAT-SIMP we avoid this highly disaggregated analysis by calculating CO₂ emissions based on a *bottom-up* approach.

For calculating product use emissions with the *bottom-up* approach, we differentiate four principle sources, i.e., the consumption of pesticides, lubricants, solvents, and waxes and paraffins. Emissions from pesticide and lubricant consumption are calculated based on activity data (available from national production statistics) and emission factors as given in Table C1.

⁴⁰ We use here the consumption and not the production of refinery products for calculating non-energy use because official energy statistics already account for trade of refinery products. The total consumption of refinery products for non-energy purposes is approximated in NEAT-SIMP by adding up the consumption of bitumen, lubricants, paraffins, and refinery-aromatics.

Appendix C

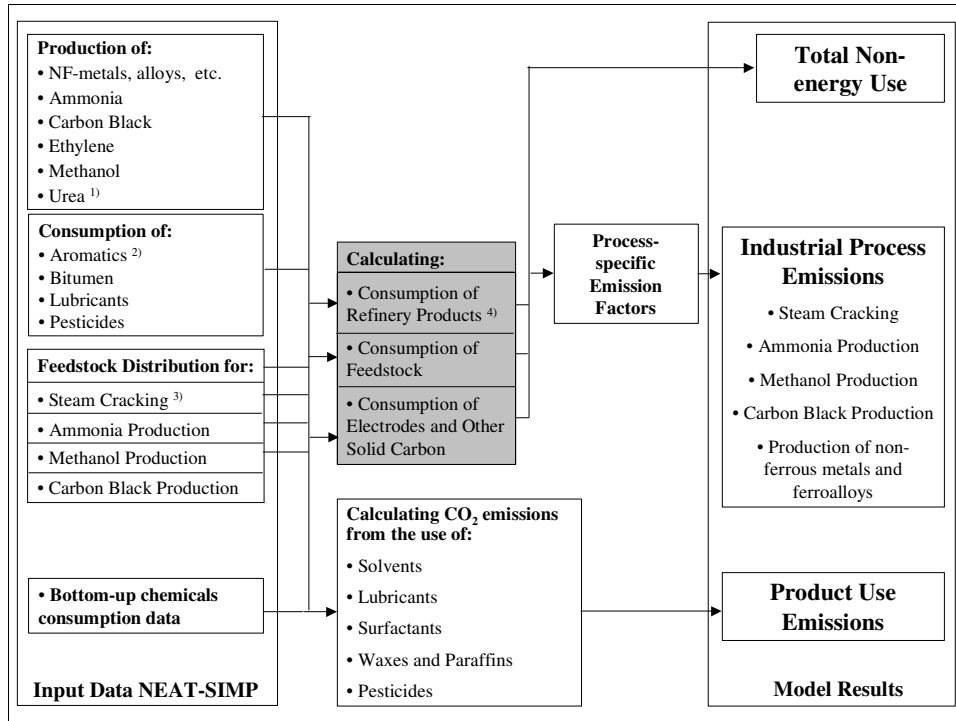


Figure C1: The NEAT-SIMP approach for modeling non-energy use and related CO₂ emissions

- 1) Urea is produced from ammonia and CO₂, with the CO₂ originating from ammonia production itself.
- 2) We include here only refinery aromatics. The feedstock requirements for aromatics produced in steam crackers are already accounted for under steam cracking.
- 3) The absolute feedstock requirements for steam cracking are estimated in NEAT-SIMP based on ethylene production. The process and feedstock specific energy requirements are derived from the detailed NEAT model.
- 4) In NEAT-SIMP, the total production of refinery products for non-energy purposes is approximated by the production of bitumen, lubricants, paraffins, and refinery-aromatics.

Table C1: NEAT-SIMP emission factors for the consumption of pesticides and lubricants

	MEAN emission factor in kg CO ₂ / kg	MIN emission factor in kg CO ₂ / kg	MAX emission factor in kg CO ₂ / kg
Pesticides	0.89	0.37	1.65
	assuming a carbon content of 35% and an oxidation rate of 70%	assuming a carbon content of 25% and an oxidation rate of 40%	assuming a carbon content of 45% and an oxidation rate of 100%.
Lubricants	0.82	0.28	1.57
	Assuming a carbon content of 86% and an oxidation rate of 26%	assuming a carbon content of 86% and an oxidation rate of 9%	assuming a carbon content of 86% and an oxidation rate of 50%.

Emissions resulting from the consumption of solvents, and waxes and paraffins are calculated based activity data and emission factors as given in NEAT-SIMP.

Fossil emissions resulting from wastewater treatment are calculated based on domestic surfactant consumption.

The basic data requirements for NEAT-SIMP are given in Table C2.

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Table C2: Principle data requirements for applying NEAT-SIMP to Germany

Production Data for:	Imports of:	Export of:	Data Source:
Ammonia	-	-	Destatis, Fachserie 4, Reihe 3.1 (Production im produzierenden Gewerbe);
Aromatics	-	-	
Bitumen	Bitumen	Bitumen	
Carbon black	-	-	
Ethylene	-	-	
Lubricants	Lubricants	Lubricants	Destatis, Fachserie 7, Reihe 2 (Aussenhandel nach Waren und Laendern)
Methanol	-	-	
Urea	-	-	
Additional data:			
Feedstock distribution steam cracker			VCI, contact person Dr. Rothermel
Feedstock distribution ammonia production			VCI, ammonia producers
Feedstock distribution methanol production			VCI, methanol producers

For calculating product use emissions, emissions from carbon use for non-ferrous metals, ferroalloys and inorganics production as well as fossil emissions from wastewater treatment, additional data are required as model input. The data requirements are listed in Table C3 and Table C4. Principle source for these data are the official production and trade statistics from Destatis, which can be supplemented by information from producer organizations.

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Table C3: Data requirements for detailed calculation of emissions from non-ferrous metals and ferroalloy production

Product	Production Code	Trade Code
Primary aluminium	27.42.11.30 (+.53)	not required
Electric steel (EAF steel)	not specified	not required
White phosphorus	24.13.11.60	not required
Titanium dioxide	24.12.11.50	not required
Ferrosilicon	27.35.20.13	not required
Calcium carbide	included under 24.13.54.50	not required
Silicon	24.13.11.53 (+.55)	not required
Ferromanganese by EAF	27.35.11.00 and 27.10.12.00	not required
Ferrosilicon	27.35.20.13	not required
Ferromanganese		
- Blast Furnace	27.35.11.00 and 27.10.12.00	not required
- Electric Arc Furnace *)		
Silicon manganese	not specified	not required
Ferrochromium	27.10.08.000	not required
Ferrochromium-silicon	27.35.20.23	not required
Chromium	27.45.30.55	not required
Primary Lead		not required
- ISA smelting process	27.43.11.30 (+.50 +.90)	not required
- QSL plant **)		not required
Secondary Lead		
-Battery recovery without desulphurisation	included under 27.43.11.30 (+.50 +.90)	not required
-Battery recovery with desulphurisation		
- Whole battery recovery plant		
Magnesium		
-Chlorination of magnesia and mangesite	27.45.30.25	not required
-MagCan process		
Nickel	27.45.12.30 (+.50)	not required
Silicon	24.13.11.5	not required
Silicon carbide	included under 24.13.54.50	not required
Tin	27.43.13.30 (+.50)	not required
Zinc by Imperial smelting process		
Zinc by Waelz kiln process	27.43.12.30	not required
Zinc (eletrolytical)		
Calcium carbide	included under 24.13.54.50	not required

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Table C4: Data requirements for calculating emissions from product use and wastewater treatment based on detailed bottom-up data analysis

	Production code	Trade code
Wastewater treatment		
Surfactants consumption (without soaps)		
-anionic	2451.20.200	3402.11.10 (+.90)
-cationic	2451.20.300	3402.12.00
-non-ionic	2451.20.500	3402.13.00
-others	2451.20.900	3402.19.00
Product use		
Insecticides		
-based on chlor-hydrocarbons	2420.11.300	3808.10.20
-based on carbamates	2420.11.400	3808.10.30
-based on organo-phosphates	2420.11.500	
-based on pyrethroides	2420.11.600	3808.10.10
-based on mineral oils	2420.11.700	
-others	2420.11.900	3808.10.90
Fungicides		
-based on dithiocarbamates	2420.15.530	3808.20.30
-based on benzimidazoles	2420.15.550	3808.20.40
-based on diazolen und triazolen	2420.15.560	3808.20.50
-based on diazines or morpholines	2420.15.570	3808.20.60
-others	2420.15.590	3808.20.80
Herbizides		
-based on hormones with phenoxy-groups	2420.12.200	3808.30.11
-based on triazines	2420.12.300	3808.30.13
-based on acetamides	2420.12.400	3808.30.15
-based on carbamates	2420.12.500	3808.30.17
-based on dinitroanilines	2420.12.600	3808.30.21
-based on urea and others	2420.12.700	3808.30.23
-others	2420.12.900	3808.30.27
-germination suppressors	2420.13.500	3808.30.30
-other growth inhibitors	2420.13.700	3808.30.90
-others (rodentizides)	2420.15.730 (+.750 +.790)	3808.90.10 (.90)
Waxes and wax and paraffin cont. products		
Care products	2451.43.350 (+.370)	3405.10.00
	2451.43.550(+.570)	3405.20.00
	2451.43.750 (+.770 +.790)	3405.30.00
	2451.43.830	3405.90.10
	2451.43.890	3405.90.90
	50% of 2451.44.000	50% of 3405.40.00
Candles	3663.75.000	3406.00.11 (+.19 +.90)
other Waxes	2466.42.350	50% of 3407.00.00

Appendix C

Table C4 (cont.): Data requirements for calculating emissions from product use and wastewater treatment based on detailed bottom-up data analysis

Product	Production code	Trade code
Cosmetics, Personal Hygiene products, etc.		
lip sticks and others	2452.12.500 (+.700)	3304.20.00
hand care products and others	2452.13.031	3304.30.00
nail care products and others	2452.13.035	
foot care products	2452.13.050	
cremes and others	2452.15.030	
cremes, body lotions, and others	2452.15.050	
sun protection	2452.15.070	
other	2452.15.090	
hair cremes	2452.17.050	
Pure Vaseline and Paraffins		
Vaseline and Paraffins	2320.31.000	2712.10.10 (+.90) 2712.20.10 (+.90) 2712.90.11 (+.19 +.31 +.33 +.39 +.91 +.99)
Solvents		
	Data from Theloke et al. (2000) and Jepsen et al. (2004)	
Lubricants, Hydraulic oils etc.		
Lubricants, Hydraulic oils etc.	2320.18.300 (+.501 +.502 +.503 +.504 +.505 +.506 +.507 +.508	2710.19.71 (+.75 +.81 +.83 +.85 +.87 +.91 +.93 +.99)

Based on the data requirements stated in Table C4, it is possible to calculate fossil emissions from wastewater treatment and product use based on the consumption of:

- surfactants
- pesticides
- waxes and paraffins
- solvents
- lubricants

It is important to note that in both Table C4 and the provided NEAT-SIMP it is assumed that emissions from solvent use can be calculated based on the studies of Theloke et al. (2000) and Jepsen et al. (2004). Attention should be furthermore paid to emissions resulting from surfactants (as the status of these emissions, i.e., either as *product use* emissions or *waste* emissions is not always clear). We included this source category, however, under the treatment of wastewaters. It is therefore important to avoid double counting and either report surfactant use emissions under the source category '*product use*' or '*waste*' treatment in the National GHG inventory.