

***Life Cycle Inventory (LCI) Data –
Treatment Chemicals, Construction
Materials, Transportation, On-site
Equipment, and Other Processes for
Use in Spreadsheets for
Environmental Footprint Analysis
(SEFA)***



***Life Cycle Inventory (LCI) Data-Treatment
Chemicals, Construction Materials,
Transportation, On-site Equipment, and Other
Processes for Use in Spreadsheets for
Environmental Footprint Analysis (SEFA)***

Submitted Under
Approved QA ID #S-20578-QP-1-0

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Notice

The research has been subject to the Agency's review and has been approved for publication as a US EPA document. Use of the methods or data presented here does not constitute endorsement or recommendation for use. Mention of trade names or commercial products does not constitute endorsement or recommendation.

The appropriate citation for this report is:

Randall, P., Meyer, D., Ingwersen, W., Vineyard, D., Bergmann, M., Unger, S., and Gonzalez, M., 2016. *Life Cycle Inventory (LCI) Data- Treatment Chemicals, Construction Materials, Transportation, On-site Equipment, and Other Processes for Use in Spreadsheets for Environmental Footprint Analysis (SEFA)*. U.S. Environmental Protection Agency, Office of Research and Development, Cincinnati, OH. EPA Report #

Abstract

This report estimates environmental emission factors (EmF) for key chemicals, construction and treatment materials, transportation/on-site equipment, and other processes used at remediation sites. The basis for chemical, construction, and treatment material EmFs is life cycle inventory (LCI) data extracted from secondary data sources and compiled using the openLCA software package. The US EPA MOVES 2014 model was used to derive EmFs from combustion profiles for a number of transportation and on-site equipment processes. The EmFs were calculated for use in US EPA's Spreadsheets for Environmental Footprint Analysis (SEFA). EmFs are reported for cumulative energy demand (CED), global warming potential (GWP), criteria pollutants (e.g. NO_x, SO_x, and PM₁₀), hazardous air pollutants (HAPs), and water use.

Foreword

Congress charges the U.S. Environmental Protection Agency (EPA) with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet this mandate, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory (NRMRL) is the Agency's center for investigation of technological and management approaches for preventing and reducing risks from pollution that threaten human health and the environment. The focus of the Laboratory's research program is on methods and their cost-effectiveness for prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites, sediments, and ground water; prevention and control of indoor air pollution; and restoration of ecosystems. NRMRL collaborates with both public and private sector partners to foster technologies that reduce the cost of compliance and to anticipate emerging problems. NRMRL's research provides solutions to environmental problems by: developing and promoting technologies that protect and improve the environment; advancing scientific and engineering information to support regulatory and policy decisions; and providing the technical support and information transfer to ensure implementation of environmental regulations and strategies at the national, state, and community levels.

This publication has been produced as part of the Laboratory's strategic long-term research plan. It is published and made available by US EPA's Office of Research and Development to assist the user community and to link researchers with their clients.

**Cynthia Sonich-Mullin, Director
National Risk Management Research Laboratory**

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List of Abbreviations and Acronyms

AFCEE	U.S. Air Force Center for Engineering and the Environment
ARB	California Air Resources Board
ASTM	American Society for Testing and Materials
BMP	Best management practice
BOD	Biological Oxygen Demand
BSFC	MOVES output for fuel consumption
BTS	U.S. Department of Transportation's Bureau of Transportation Statistics
Btu	British thermal unit
CAH	chlorinated aliphatic hydrocarbons
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act of 1980
CED	Cumulative Energy Demand
CF	Characterization Factor
CFC	Chlorofluorocarbon
CH ₄	methane
cm	centimeter
CNG	compressed natural gas
CO ₂	carbon dioxide
CO ₂ e	carbon dioxide equivalents of global warming potential
COC	contaminant of concern
COD	chemical oxygen demand
CSTR	continuous stirred tank reactor
CtG	Cradle to gate
CVOC	chlorinated volatile organic compound
cy	cubic yards
DNAPL	dense non-aqueous phase liquid
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
EERE	U.S. DOE Office of Energy Efficiency and Renewable Energy
EIA	U.S. Energy Information Administration
EIPPCB	European Integrated Pollution Prevention and Control Bureau
ELCD	European Reference Life Cycle Database
EmF	emission factor
EPA	U.S. Environmental Protection Agency
ESTCP	Environmental Security Technology Certification Program
ET	evapotranspiration
ETSC	U.S EPA Engineering Technical Support Center
FBR	fluidized bed reactor
FHWA	Federal Highway Administration

FML	flexible membrane liner
FS	feasibility study
ft	feet
FU	functional unit
GAC	granular activated carbon
gal	gallon
GHG	greenhouse gas
GWP	global warming potential
gpm	gallons per minute
GR	green remediation
HAP	hazardous air pollutant as defined by the Clean Air Act
HDPE	high density polyethylene
hp	horsepower
HWI	hazardous waste incinerator
IMAA	International Mastic Asphalt Association
IPCC	Intergovernmental Panel on Climate Change
ISCO	in-situ chemical oxidation
ISO	International Organization for Standardization
ITRC	Interstate Technology & Regulatory Council
kg	kilogram
kW	kilowatt
kWh	kilowatt-hour
lbs	pounds
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LHD	light heavy duty engine
LPG	liquefied petroleum gas
LSD	low-sulfur diesel
MA	mastic asphalt
MCL	maximum contaminant level
MHD	medium heavy duty engine
MJ	mega joule
MMBtu	million British thermal units
MOVES	EPA's Motor Vehicle Emission Simulator
mpg	mile per gallon
mph	miles per hour
MT	metric ton(s)
MW	megawatt
MWh	megawatt-hour
NETL	U.S. DOE National Energy Technology Laboratory

N ₂ O	nitrous oxide
NO _x	nitrogen oxides (e.g., nitrogen dioxide)
NONROAD	a term used by regulators to classify engines in order to control their emissions
NPL	National Priorities List
NREL	U.S. DOE National Renewable Energy Laboratory
NRMRL	U.S. EPA National Risk Management Research Laboratory
O&M	operations and maintenance
OPC	ordinary Portland cement
ORD	U.S. EPA Office of Research and Development
OSRTI	U.S. EPA Office of Superfund Remediation and Technology Innovation
OSWER	U.S. EPA Office of Solid Waste and Emergency Response
PM ₁₀	particulate matter (particles 10 µm or less in diameter)
PM _{2.5}	particulate matter less than 2.5 µm in diameter
POTW	publicly owned treatment works
psi	pounds per square inch
PV	photovoltaic
PVC	polyvinyl chloride
RCRA	Resource Conservation and Recovery Act of 1976, as amended
RER	code used byecoinvent for Europe
RI	remedial investigation
RMC	ready mixed concrete
SEFA	Spreadsheets for Environmental Footprint Analysis
SO _x	sulfur oxides (e.g., sulfur dioxide)
S-PVC	polyvinyl chloride, suspension process
SQL	Structured Query Language
STD	U.S. EPA Sustainable Technology Division
THC	total gaseous hydrocarbons
Tonne	metric ton(s)
TRACI	Tool for the Reduction and Assessment of Chemicals and Other Environmental Impacts
TRI	EPA's Toxic Release Inventory
ULSD	ultra-low sulfur diesel
USACE	U.S. Army Corps of Engineers
USLCI	U.S. Life Cycle Inventory
VCM	vinyl chloride monomer
VOCs	volatile organic compounds
WPPA	wet-process phosphoric acid
wt	weight
yr	year

Acknowledgements

An EPA project team coordinated its efforts to produce this report. Personnel from EPA's Region IX (San Francisco, CA) and from the Life Cycle Assessment Research Center within the National Risk Management Research Laboratory (Cincinnati, OH) worked on this report. Our thanks and appreciation is extended to all these participants as well as the project team members:

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We appreciate the effort of peer reviewers who greatly improved the report: Briana Niblick (EPA, Cincinnati, OH) and Gurbakhash Bhander (EPA, Research Triangle Park, NC).

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1.0 Study Overview and Objectives

1.1 Introduction

For remedial activities, chemicals, construction and treatment materials, nonroad vehicles, on-site diesel generators and other equipment are used to improve environmental and public health conditions. Cleanup activities use energy, water, and natural resources and create an environmental footprint based on their life cycles. To minimize the environmental footprints of remediation sites, the U.S. Environmental Protection Agency (EPA) encourages “green remediation” practices that consider all environmental effects of remedy implementation and incorporate strategies to minimize them. The term green remediation is documented in a 2008 report entitled "Green Remediation: Incorporating Sustainable Environmental Practices into Remediation of Contaminated Sites" (USEPA, 2008b). The EPA defines “green remediation” as the practice of considering all the environmental effects of implementing a remedy, and incorporating options to minimize the environmental footprint of cleanup actions. This definition is a departure from the term “sustainable remediation” because green remediation focuses on the environmental aspect of a project, whereas sustainable remediation addresses environmental, social, and economic aspects of the cleanup activities actions (green remediation is sometimes used interchangeably with greener cleanups). Green remediation strategies may include a detailed analysis in which the remedy is closely examined and large contributions to the footprint are identified. Steps, therefore, may be taken to reduce the footprint while meeting regulatory requirements driving the cleanup (USEPA, 2012a).

In the last few years, the EPA has implemented several case studies which highlight the net environmental gains as well as the challenges to minimize environmental footprints in cleanup actions (ITRC (Interstate Technology & Regulatory Council), 2011; USEPA, 2008a, 2010a, 2010b, 2011, 2013a, 2013b, 2013c, 2014a; USEPA Region 7, 2015). Besides the EPA efforts, other federal and state cleanup programs (McDonough, Woodward et al., 2013) have begun to consider how remedial actions could lower their environmental footprint. In addition, there has been a substantial industry effort and a DOD effort to determine how green remediation should be defined and implemented. As of 2015, the following tools/spreadsheets are the most prominent for estimating the potential environmental burdens of remediation projects:

- Spreadsheets for Environmental Footprint Analysis (SEFA) – developed by EPA in 2012 (Version 1) updated in 2013 (Version 2) and most recently updated in August 2014 (Version 3).
- SiteWise – developed by Battelle, the Naval Facilities Engineering Command, and the U.S. Army Corps of Engineers (USACE) in 2010 (Version 1), 2012 (Version 2), and 2013 (Version 3).
- Sustainable Remediation Tool (SRT™) – developed by the U.S. Air Force Center for Engineering and the Environment (AFCEE) in 2009 (Version 1) and 2011 (Version 2) - Currently unavailable as of January 29, 2016.
- SimaPro® and GaBi®, two commercial life cycle assessment (LCA) tools with extensive databases.

The EPA developed the Spreadsheets for Environmental Footprint Analysis (SEFA) to estimate energy usage, greenhouse gas emissions, air pollutants, and hazardous air pollutants (HAPs). SEFA was originally developed for internal use by EPA staff and contractors. It was used in earlier formats within EPA, and was made publicly available in its current format in 2012 for the benefit of other users. It was last updated in August 2014. SEFA is based on life cycle thinking and designed to be compatible with EPA's report: "Greener Cleanups Methodology for Understanding and Reducing a Project's Environmental Footprint" (USEPA, 2012a). An overview of the general steps in performing an environmental footprint analyses is shown in Figure 1.

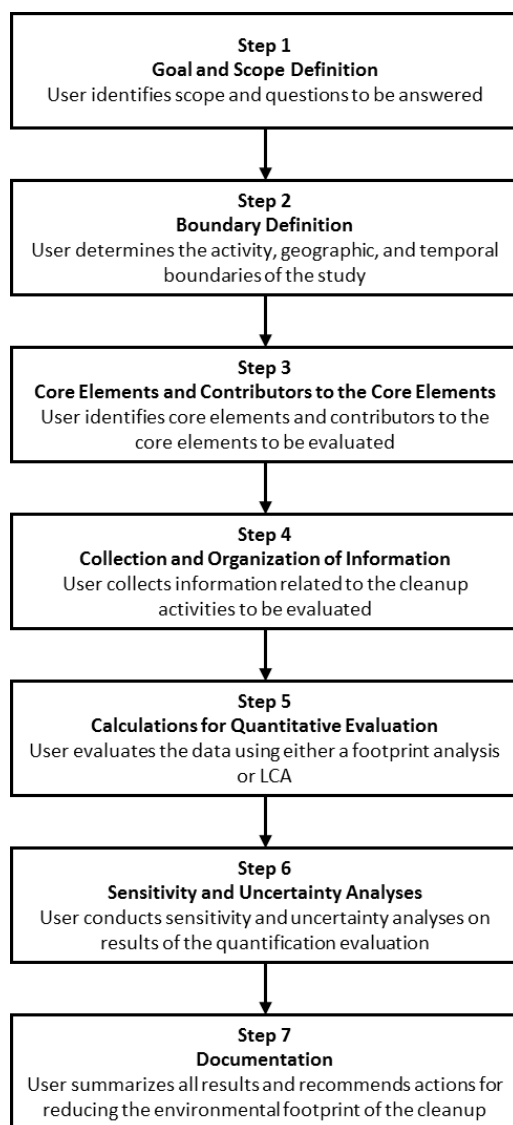


Figure 1. The steps of an environmental footprint analysis (ASTM 2013b)

Reducing a project's environmental footprint is based on life cycle thinking. EPA's 2006 document, "Life Cycle Assessment: Principles and Practice," provides an overview of life cycle assessment (LCA) and describes the general uses and major components of LCA. Life cycle assessment may be a cradle to grave, cradle to gate, or a gate to gate approach for assessing industrial systems and/or activities. Cradle to grave begins with the gathering of raw materials

from the earth to create the product and ends at the point when all materials are returned to the earth. LCA evaluates all stages of a product's life from the perspective that they are interdependent, meaning that one operation leads to the next. LCA enables the estimation of the cumulative environmental impacts resulting from all stages in the product life cycle, often including impacts not considered in more traditional analyses (e.g., raw material extraction, material transportation, ultimate product disposal, etc.). By including the impacts throughout the product life cycle, LCA provides a comprehensive view of the environmental aspects of the product or process and a more accurate picture of the true environmental trade-offs in product and process selection (USEPA, 2006).

At the core of the LCA process is the life cycle inventory (LCI). An LCI quantifies all energy and raw material requirements, atmospheric emissions, waterborne emissions, solid wastes, and other releases for the entire life cycle of a product, process, or activity. The level of accuracy and detail of the data collected will determine the accuracy and reliability of the subsequent impact assessment results. The inventory can be separated by life cycle stage, by media (air, water, and land), by specific processes, by materials, or any combination thereof.

EPA's 1993 document, "Life Cycle Assessment: Inventory Guidelines and Principles," and the 1995 document, "Guidelines for Assessing the Quality of Life Cycle Inventory Analysis," provide a framework for performing an inventory analysis and assessing the quality of the data used for an LCA (USEPA, 1993c, 1995b). In addition, ASTM's E2893 standard "Standard Guide for Greener Cleanups" provides more details on the steps required for a quantitative evaluation in identifying opportunities to reduce the environmental footprint of a selected remedy. Shown in Figure 1, steps may include: 1. Goal and Scope Definition; 2. Boundary Definition; 3. Core Elements and Contributors to the Core Elements; 4. Collection and Organization of Information; 5. Calculations for Quantitative Evaluation; 6. Sensitivity and Uncertainty Analyses; and 7. Documentation (ASTM, 2013b).

1.2 Study Objectives

The study objectives are as follows:

- Collect secondary data to model LCI for remediation chemicals, materials, and processes specified by US EPA's Region 9 Office.
- Develop life cycle inventories for the specified chemicals and materials using OpenLCA and the collected secondary data.
- Perform motor vehicle emissions simulations to model operation of vehicles and equipment associated with remediation sites.
- Develop life cycle inventories for the vehicles and equipment using OpenLCA and the emissions simulation data.
- Create and apply a footprint methodology in OpenLCA to quantify environmental emission factors (EmFs) for use in SEFA
- Document the methodology and calculations used to derive the reported material, chemical, and process EmFs.
- Document the methodology used to model use of vehicles and equipment.

1.3 Intended Audience

The primary intent of the report is to document and communicate the methodology used to derive the chemical, material, and process EmFs and support their use by EPA's Region 9 as input to SEFA. Once the EmFs are input into the SEFA method, it will assist federal, state, and local government officials, industry, EPA site contractors, and NGOs with evaluating and implementing activities to reduce the potential footprint of environmental cleanups. The EPA Region 9 Superfund and RCRA staff requested the information through EPA's Engineering Technical Support Center (ETSC). The Sustainable Technology Division (STD) within the National Risk Management Research Laboratory (NRMRL) performed this project. The underlying inventory models described in this report may be useful to LCA practitioners and anyone else working in the area of chemical and material sustainability. Chemical, material, and process LCIs developed from publically available secondary data are included in the report for transparency. Proprietary LCIs obtained from ecoinvent have been excluded in accordance with copyright laws and only the applicable ecoinvent process name is reported.

2.0 Material LCI Modeling and Emission Factor Results

2.1 Methodology

Although there are specific calculation procedures for performing LCI analysis by hand, these procedures can be made more efficient and automated by using computer software. In this study, the preferred method was to use open-source computer software coupled with a commercially available inventory database to promote consistency between material models. The LCA software selected for this study is OpenLCA version 1.4, as created and maintained by GreenDelta. The database selected for this study is the proprietary ecoinvent version 2.2 database developed by the Swiss Center for Life Cycle Inventories beginnings in the 1990s and containing over two thousand unit process inventories. Although the unit process LCIs in ecoinvent are proprietary, it is permissible to release system-level EmFs calculated for this project using ecoinvent data because the aggregated nature of the footprint categories at the system (i.e., cradle-to-gate) level sufficiently mask the copyrighted data. For some materials included in this study, either no unit process LCI existed in ecoinvent or more relevant and preferable data from other secondary sources was identified. Additional secondary data sources can include government data (e.g. EPA's Toxics Release Inventory (TRI)), industry reports, engineering estimates based on estimated parameters, Kirk-Othmer Encyclopedia of Chemical Technology, Ullmann's Encyclopedia of Industrial Chemistry, journal articles, and other computer databases (e.g. US LCI). When applicable, new LCIs were created for the materials in OpenLCA using the best available secondary data.

This study examines cradle to gate (CtG) LCIs for the production of chemical and materials specified by US EPA's Region 9 Office. The LCIs developed in this study were constructed in accordance with ISO 14040 International standard documents on life cycle thinking (ISO, 1998, 2000, 2006a, 2006b) as well as the ASTM standard documents on greener and sustainable cleanups (ASTM, 2013a, 2013b). System boundaries for a CtG LCI include everything from the cradle (excavation of the raw materials and resources from the ground) to the end of the production process, or facility gate (Figure 2). For each material of interest, OpenLCA was used to model the

material life cycle and construct the corresponding CtG LCI. Such a dataset can involve numerous individual unit processes throughout the supply chain (e.g., the extraction of raw resources, various primary and secondary production processes, transportation, etc.) and account for all resource inputs and process outputs associated with a chemical or material. Resource inputs include raw materials and energy use, while process outputs include manufactured products and environmental emissions to land, air, and water. The cradle to gate LCI models stop at the gate of the production process and therefore, do not include downstream and/or onsite cleanup activities such as onsite construction, implementation, monitoring, and decommissioning. All flows to and from the environment are defined as elementary flows in LCA while flows between unit processes are termed technosphere flows. The inputs and outputs are expressed in terms of a reference flow, or functional unit, for the chemical or material of interest. The chemicals and materials selected by Region 9 for inclusion in this study are listed in Table 1.

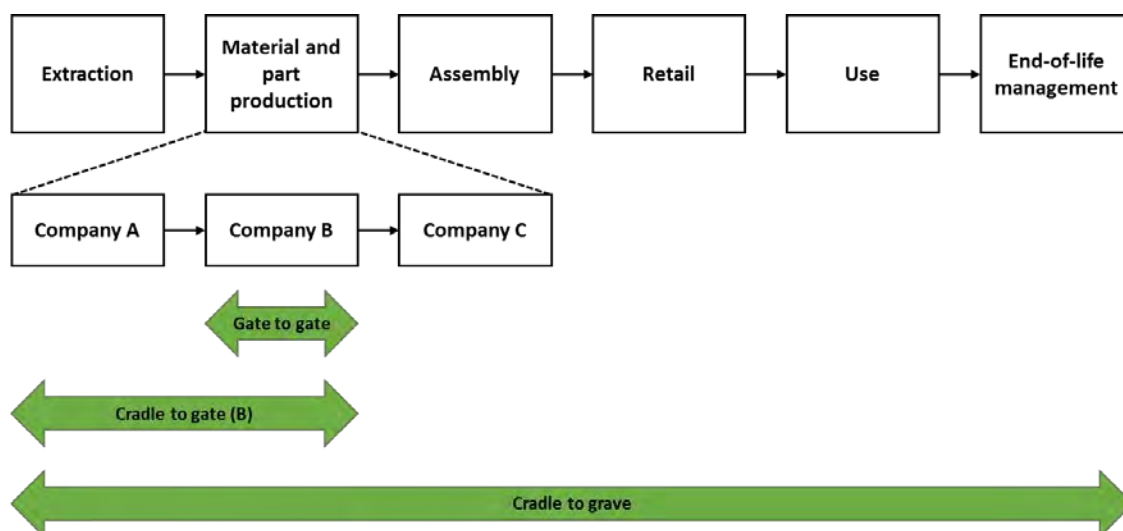


Figure 2. Cradle to grave, cradle to gate and gate to gate data sets as parts of the complete life cycle (EC 2011)

Table 1. Selected Chemicals and Materials for Emission Factor Development

Aluminum, Rolled Sheet	Lime, Hydrated, Packed	Primary Activated Carbon
Corn Ethanol, 95%	Mastic Asphalt	Ready Mixed Concrete
Corn Ethanol, 99.7%	Paving Asphalt	Regenerated Activated Carbon
Gravel/Sand Mix, 65% gravel	Petroleum Ethanol, 99.7%	Round Gravel
Hazardous Waste Incineration	Phosphoric Acid, 70% in water	Sand
High Density Polyethylene	Polyvinyl Chloride	Sodium Hydroxide, 50% in water
Hydrogen Peroxide, 50% in water	Portland Cement	
Iron (II) Sulfate, Hydrated	Potassium Permanganate	

Inventory analysis for this study involved the sorting and aggregation of relevant elementary flows into the environmental footprint categories considered in SEFA. These categories include Cumulative Energy Demand (CED, MMBtu); Global Warming Potential on a 100-year time frame (GWP, lb. CO₂ equivalents); the EPA criteria pollutants: nitrogen oxides (NO_x, lb.), sulfur dioxides (SO_x, lb.), particulate matter $\leq 10 \mu\text{m}$ (PM₁₀, lb.); hazardous air pollutants as defined by the EPA (HAPs, lb.) (USEPA, 2014b); and water use (gals). While the meanings of NO_x, SO_x, PM₁₀, and HAPs are straightforward, explanations of CED, GWP, and Water Use are presented

here for the benefit of the reader. The current list of HAPs as defined by US EPA is provided in Appendix 1.

The Cumulative Energy Demand (CED) of an activity represents the direct and indirect energy use in units of MJ throughout the life cycle, including the energy consumed during the extraction, manufacturing, and disposal of the raw and auxiliary materials. The total CED is composed of the fossil cumulative energy demand (i.e., from hard coal, lignite, peat, natural gas, and crude oil) and the CED of nuclear, biomass, water, wind, and solar energy in the life cycle. Typical upper heating values for the primary energy resources required in the CED calculations were used in the ecoinvent datasets (Huijbregts, Hellweg et al., 2010).

Global Warming Potential (GWP) is based on the commonly accepted carbon dioxide (CO₂) equivalency factors published in the IPCC (2007) report. GWP is calculated to express the global warming impacts of a given gas relative to a similar mass of CO₂. Similarly, GWP is calculated for a process by taking the masses of the gaseous emissions of the process multiplied by their respective GWPs and summed to arrive at the total GWP. The GWPs of various greenhouse gases are compared to determine which will cause the greatest integrated radiative forcing (i.e. energy absorbed) over the time horizon of interest (i.e. 100 years). Carbon dioxide, by definition, has a GWP of 1, regardless of the time period used, because it is the gas being used as the reference. Besides CO₂, other GWP gases include methane (CH₄) and nitrous oxide (N₂O). The complete list of species of gases and their GWPs values for time horizons of 20, 100 and 500 years are in table 2.14 of the IPCC 2007 report (Solomon, 2007).

Given the concerns regarding the depletion of water resources, the importance of tracking Water Use has grown significantly in recent years. For SEFA, this is performed by calculating the net freshwater use (water withdrawal – water discharge) for a system to determine the potential impact on water scarcity. Therefore, Water Use calculations in OpenLCA account for all elementary freshwater input and output flows to a chemical or material LCI from river, lake, and well water sources. In some cases, unspecified water sources were included in secondary data sources and were tracked.

The sorting and aggregation of the inventory into the appropriate footprint categories was performed in openLCA. Sorting and categorical aggregation for footprinting is analogous to impact assessment in LCA. However, footprinting differs from impact assessment because the characterization factors (CF) used to translate the elementary flow values to appropriate category values typically have a value of one and result in EmFs as opposed to impact scores. This leads to a simple summation of all like elementary flows (F) from the CtG LCI into an EmF for each desired footprint category:

$$EmF = \sum_{i=1}^m \sum_{j=1}^n F_{i,j} \times CF_j$$

where, i , denotes the unit process, m is the maximum number of unit process represented in the LCI, j is an individual flow that contributes to a footprint indicator, and n is the maximum number of flows included in the footprint indicator. For example, the HAPs value for the production of ethanol would be the summation of the masses of all HAP substances emitted from growing the

corn, transporting and processing it into ethanol, and distilling the ethanol to high purity. The exceptions to this approach are the categories of CED and GWP where inventory flows are converted to energy (MMBtu) and carbon dioxide equivalents (CO₂e), respectively. In these cases, the characterization factors have values other than one as defined in each methodology's documentation. Although CED is still a footprinting category because it makes no evaluation of the impact of energy demand, GWP does consider the potency of substances for inducing global warming when converting to carbon dioxide equivalents and is therefore more like an impact indicator.

The material emission factors developed for each of the footprint categories are intended for implementation in EPA's SEFA workbooks. For example, in-situ oxidants such as potassium permanganate or hydrogen peroxide may be used in a cleanup. The emission factors for the oxidants will be stored as default values in SEFA. A user for a site involving in-situ oxidation can then specify how much potassium permanganate or hydrogen peroxide is used as part of the site's remediation activities and the SEFA method will incorporate the material's production footprint (e.g., CED (MMBtu/lbs. of material produced) or GWP (lbs. of CO₂e per lb. of material produced)) into the life cycle environmental footprint for the remediation site.

As with any model of the real world, there is some uncertainty in the calculated EmFs. LCI quality issues have been broadly discussed since the 1990's (USEPA, 1995b). More recently, ecoinvent has discussed the basic structure of the database and data quality (Weidema, Bauer et al., 2013). The data quality is affected by certain variables such as the dependence on data from different countries, different unit operations, and different sources. At the LCI level, data uncertainty may be introduced due to data inaccuracy, data gaps, lack of representative inventory data, model uncertainty (i.e. static vs dynamic, linear vs non-linear modeling), spatial and temporal variability (USEPA, 2012b). Quantification of the uncertainty of the reported EmFs was not performed as part of this work based on the lack of ample data describing potential value distributions for the various data contained within the material LCIs.

Qualitatively, use of the reported EmFs for decision making should only be done with acknowledgement of the assumptions employed for this study, which may affect the accuracy and certainty of the factors. This study assumed that LCI datasets developed with ecoinvent data for chemical processes in Europe are transferable to the U.S. In general, the chemistry, mass balances, and energy balances are similar but there may be slight differences. For example, electricity grid mixes for Europe are different from the U.S., which may be significant to the calculated EmFs if electricity production is a dominant part of the material life cycle. Similarly, transportation modeling can differ between Europe and the U.S., both in terms of distance and mode of transport. Finally, waste management has not been included in the material LCIs because there are large data gaps for this part of the life cycle in life cycle inventory modeling in general, especially for waste processing in the United States.

It is important to note the EmFs reported for this study should not be confused with characterization factors for life cycle impact assessment. Except for GWP, they do not attempt to determine the fate and transport of the total emissions nor do they attempt to determine the risk to humans or the environment arising from these emissions. Similarly, they infer no judgments regarding the impacts of obtaining and using natural resources.

2.2 Corn Ethanol, (95% in H₂O or 99.7% Dehydrated)

2.2.1 Introduction

In general, ethanol or ethyl alcohol (CH₃CH₂OH) is an organic chemical with many applications (e.g. transportation, alcoholic beverages beer and spirits; solvent; raw material in chemical synthesis; fuel; environmental remediation). For environmental cleanups, ethanol is used for enhanced in-situ anaerobic bioremediation of groundwater. Enhanced in situ anaerobic bioremediation has emerged in recent years as a remediation strategy for chlorinated aliphatic hydrocarbons (CAHs) in groundwater. Advantages include complete mineralization of the contaminants in-situ with little impact on infrastructure and relatively low cost compared to more active engineered remedial systems (e.g., groundwater extraction, permeable reactive iron barriers, or chemical oxidation). Regulatory acceptance of enhanced anaerobic bioremediation has evolved over the last several years under various federal programs, including the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) and the Resource Conservation and Recovery Act (RCRA) (Leeson, Beevar et al., 2004)

Ethanol can be produced as a biofuel from sugars in sugar cane or sugar beet, or from starch hydrolyzed into sugars derived from crops such as maize, wheat or cassava (Worldwatch Institute, 2007). Most ethanol production in the US uses grains (i.e. corn or “maize”) as the feedstock. Production of corn-based ethanol has grown from less than 2 billion gallons in 1999 to over 14 billion gallons in 2014 (RFA, 2015).

Ecoinvent data indicate that 1 kg of 95% corn ethanol has a number of processes that are associated with varying quantities of kg CO₂ eq emitted. However, the production of corn outweighs these values, where corn production sequesters a greater value of kg CO₂ eq than the summed processes associated with varying quantities of kg CO₂ eq emitted.

2.2.2 LCI Modeling

- Functional unit: 1 kg of ethanol (either 95% or 99.7% after molecular sieve dehydration)
- System boundaries: The main processes for corn ethanol are the cultivation and production of corn and subsequent fermentation and distillation of ethanol as shown in Figure 3. An additional molecular sieve process is required after distillation if a 99.7 % dehydrated ethanol product is desired.

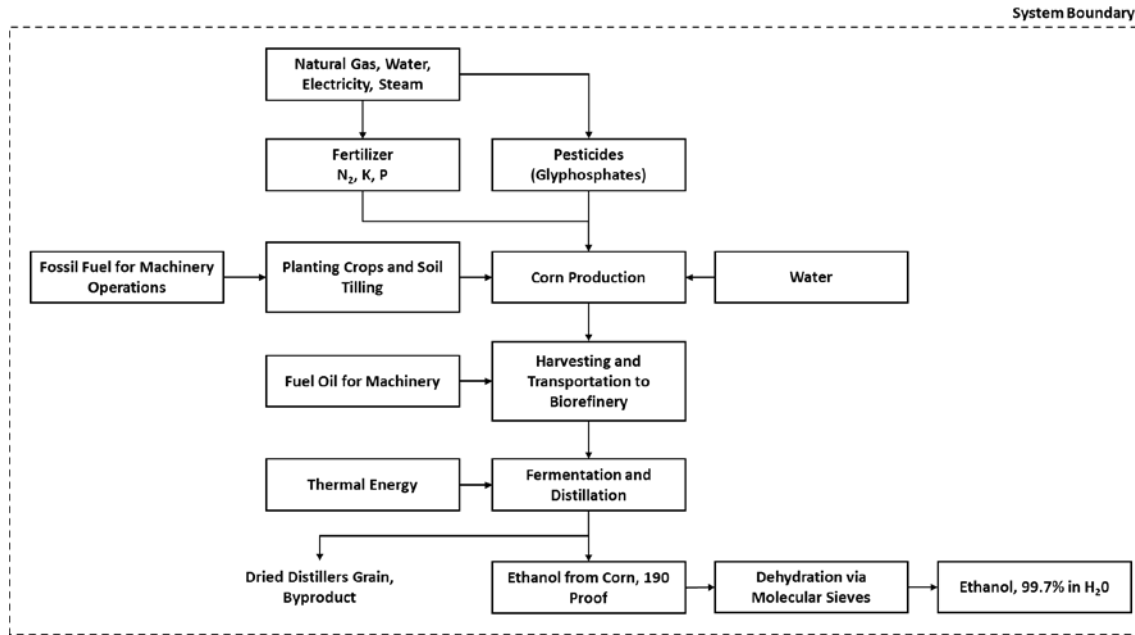


Figure 3. Production of 99.7% corn ethanol as presented by (Jungbluth, Chudacoff et al., 2007)

- Inventory data: “ethanol, 95% in H₂O, from corn, at distillery – US”; “ethanol, 99.7%, in H₂O, from biomass, at distillery – US”; ecoinvent v2.2; (Jungbluth, Chudacoff et al., 2007).

2.2.3 Emission Factors

- Unit conversion calculations were necessary to convert from SI units (OpenLCA results) to English units (SEFA factors). These calculations are shown here for 95% Corn Ethanol, but are the same for all chemicals and materials covered in this report. The only exception is ready mixed concrete because it is reported on a volume basis instead of mass.

Cumulative Energy Demand (CED)

$$\left(7.39 \times 10^1 \frac{MJ}{kg}\right) \times \left(9.48 \times 10^{-4} \frac{MMBtu}{MJ}\right) \times \left(\frac{1 kg}{2.2 lb}\right) = 3.18 \times 10^{-2} \frac{MMBtu}{lb}$$

Global Warming Potential (GWP 100)

$$\left(-1.99 \times 10^{-2} \frac{kg CO_2 eq}{kg}\right) \times \left(\frac{2.2 lb}{1 kg}\right) \times \left(\frac{1 kg}{2.2 lb}\right) = -1.99 \times 10^{-2} \frac{lb CO_2 eq}{lb}$$

Hazardous Air Pollutants (HAPs)

$$\left(8.46 \times 10^{-5} \frac{kg \text{ HAPs}}{kg}\right) \times \left(\frac{2.2 \text{ lb}}{1 \text{ kg}}\right) \times \left(\frac{1 \text{ kg}}{2.2 \text{ lb}}\right) = 8.46 \times 10^{-5} \frac{\text{HAPs}}{\text{lb}}$$

Nitrogen Oxides (NO_x)

$$\left(4.25 \times 10^{-3} \frac{kg \text{ NO}_x}{kg}\right) \times \left(\frac{2.2 \text{ lb}}{1 \text{ kg}}\right) \times \left(\frac{1 \text{ kg}}{2.2 \text{ lb}}\right) = 4.25 \times 10^{-3} \frac{\text{lb NO}_x}{\text{lb}}$$

Sulfur Oxides (SO_x)

$$\left(3.03 \times 10^{-3} \frac{kg \text{ SO}_x}{kg}\right) \times \left(\frac{2.2 \text{ lb}}{1 \text{ kg}}\right) \times \left(\frac{1 \text{ kg}}{2.2 \text{ lb}}\right) = 3.03 \times 10^{-3} \frac{\text{lb SO}_x}{\text{lb}}$$

Particulate Matter (PM₁₀)

$$\left(4.69 \times 10^{-4} \frac{kg \text{ PM}_{10}}{kg}\right) \times \left(\frac{2.2 \text{ lb}}{1 \text{ kg}}\right) \times \left(\frac{1 \text{ kg}}{2.2 \text{ lb}}\right) = 4.69 \times 10^{-4} \frac{\text{lb PM}_{10}}{\text{lb}}$$

Water Use

$$\left(3.60 \times 10^{-2} \frac{m^3 \text{ H}_2\text{O}}{kg}\right) \times \left(\frac{1000 \text{ L}}{1 \text{ m}^3}\right) \times \left(0.2642 \frac{\text{gal}}{\text{L}}\right) \times \left(\frac{1 \text{ kg}}{2.2 \text{ lb}}\right) = 4.32 \frac{\text{gal H}_2\text{O}}{\text{lb}}$$

- Emission Factor Calculation Results

Table 2. SEFA Emission Factors for Corn Ethanol

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM ₁₀ (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Corn Ethanol, 95%	3.18E-02	-1.99E-02	8.46E-05	4.25E-03	4.69E-04	3.03E-03	4.32E+00
Corn Ethanol, 99.7%	3.24E-02	5.91E-02	8.70E-05	4.31E-03	4.72E-04	3.10E-03	4.35E+00

2.3 Petroleum Ethanol, 99.7%

2.3.1 Introduction

As an alternative ethanol is produced from extracting crude oil and making ethylene. Ethylene can be produced from either crude oil or natural gas recovered from conventional wells or shale rock, but we have based this scenario on crude oil from conventional wells only. With ethylene from crude, the life cycle begins with the extraction of petroleum crude oil from conventional wells into crude oil storage tanks. From the crude oil storage tanks, the crude oil is transported (i.e. ocean freighter, pipelines) to the oil refinery where it is refined into naphtha. In the production of naphtha from crude oil, depending on the crude oil composition, the proportion of the individual fractions can vary greatly and can produce LPG, paraffinic naphtha, heavy naphtha, kerosene, diesel, and residual oil. Naphthas, which are the most important feedstock for ethylene production, are mixtures of hydrocarbons in the boiling range of 30–200 °C. Processing of light naphthas (boiling

range 30–90 °C), full range naphthas (30–200 °C) and special cuts (C₆–C₈ raffinates) as feedstock is typical for naphtha crackers (Hischier, 2007).

The production of ethanol from ethylene is due to the catalytic hydration of ethylene to ethanol. In direct catalytic hydration, ethanol is produced by the vapor-phase reaction of ethylene and water over a catalyst impregnated with phosphoric acid. For more details on the direct catalytic hydration process, see (Sutter, 2007).

2.3.2 LCI Modeling

- Functional unit: 1 kg of petroleum-based ethanol, 99.7% (anhydrous)
- System boundaries: The main processes for petroleum ethanol are the refinement and processing of crude to produce ethylene (Figure 4), which is then hydrated to make ethanol (Figure 5).

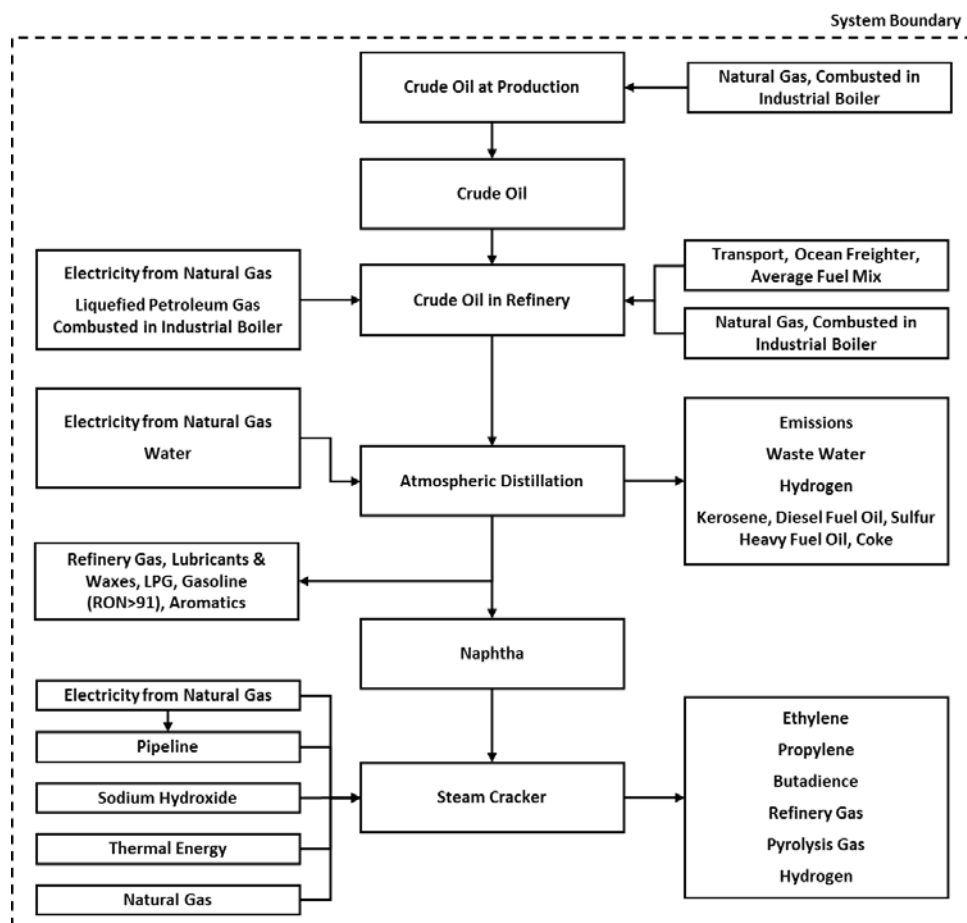


Figure 4. Production of ethylene as reported by (Ghanta, Fahey et al., 2014)

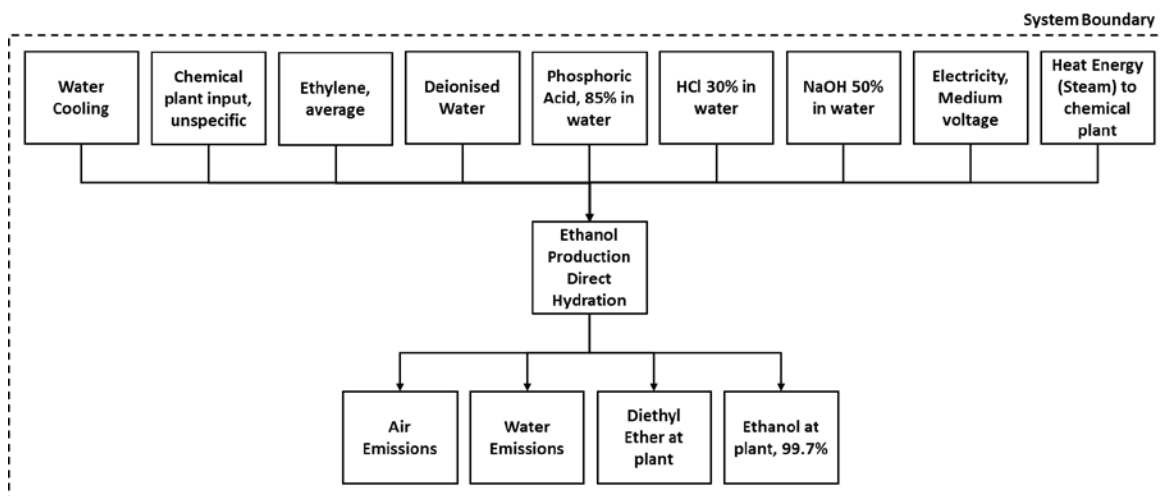


Figure 5. Production of anhydrous petroleum ethanol as reported by (Sutter, 2007)

- Inventory data: “ethanol from ethylene, at plant – RER”; ecoinvent v2.2; (Sutter, 2007).

2.3.3 Emission Factors

- Emission Factor Calculation Results

Table 3. SEFA Emission Factors for Petroleum Ethanol

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Petroleum Ethanol, 99.7%	2.05E-02	1.25E+00	5.89E-05	1.99E-03	2.77E-04	2.14E-03	4.16E+00

2.4 Potassium Permanganate (KMnO₄)

2.4.1 Introduction

Potassium permanganate (KMnO₄) is industrially very important and an indispensable oxidant. It is used principally as an oxidizing agent in the following applications: municipal water treatment, wastewater treatment, chemical manufacturing and processing, aquaculture (fish farming), metal processing, and air and gas purification. In addition, potassium permanganate is used as a decoloring and bleaching agent in the textile and tanning industries, as an oxidizer in the decontamination of radioactive wastes, as an aid in the flotation processes used in mining, and in cleaning printed circuit boards (Pisarczyk, 2005; Reidies, 2000; USEPA, 2015b; USITC, 2010). For environmental applications, a concentrated KMnO₄ solution (typically 1-5 % where it is its optimal solubility) is generated on-site using dry potassium permanganate.

World production capacity for potassium permanganate is estimated to be 43 000–51 000 tons/yr., although actual demand is less than 30 000 tons/yr.(Reidies, 2000). Carus Corporation was the only commercial producer of KMnO₄ in the US in 2009. KMnO₄ may be manufactured by a one-step electrolytic conversion of ferromanganese to permanganate, or by a two-step process involving the thermal oxidation of manganese (IV) dioxide to potassium manganate (VI), followed

by electrolytic oxidation to permanganate. Carus markets permanganates under various trade names (AQUOX[®], CAIROX[®], LIQUOX[®], ECONOX[®], CARUSOL[®] and RemOx[®]) (Carus Corporation, 2009). Three grades of KMnO₄ are produced (i.e. free-flowing, technical, pharmaceutical). The free-flowing grade is produced by adding an anti-caking agent to the technical grade, preventing the particles from sticking together when in contact with moisture. The pharmaceutical grade must be at least 99% KMnO₄ by weight and involves additional recrystallization to remove impurities or to meet customer specifications. The three grades of KMnO₄ are generally interchangeable in their various applications, except for pharmaceutical applications.

2.4.2 LCI Modeling

- Functional unit: 1 kg of KMnO₄
- System boundaries: The main processes for KMnO₄ are the mining and beneficiation of manganese ore, oxidation to manganese dioxide, and further oxidation to the final product (Figure 6).

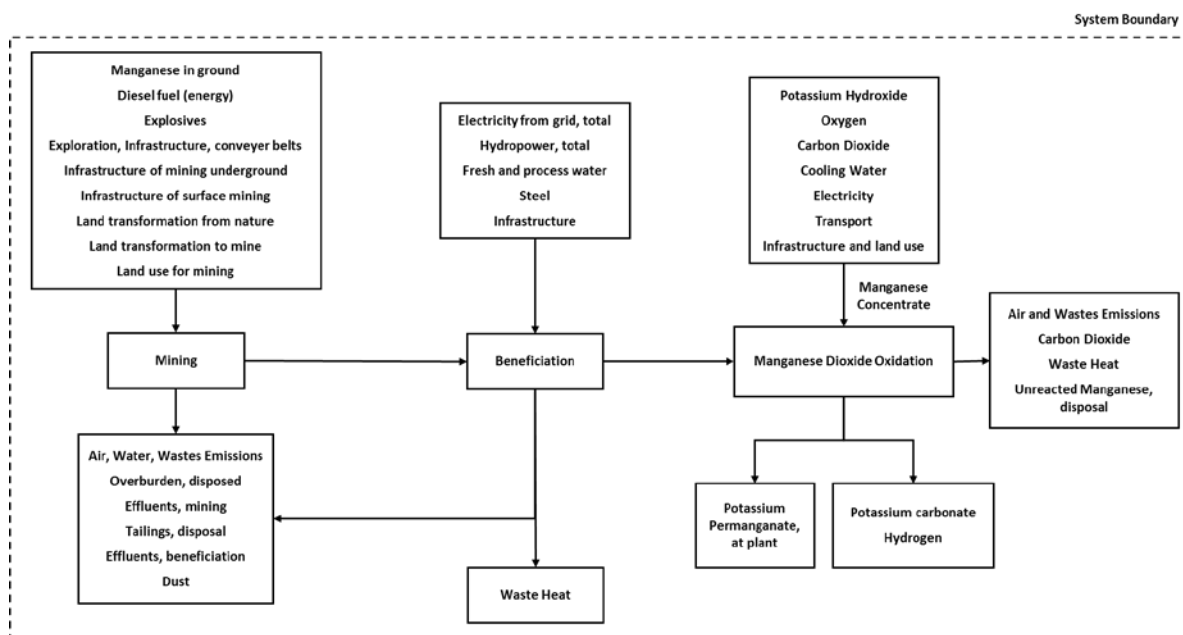


Figure 6. Production of KMnO₄ as reported by (Classen, Althaus et al., 2007)

- Inventory data: “potassium permanganate, at plant – RER”; ecoinvent v2.2; (Sutter, 2007).

2.4.3 Emission Factors

- Emission Factor Calculation Results

Table 4. SEFA Emission Factors for KMnO₄

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Potassium Permanganate	9.81E-03	1.16E+00	1.22E-04	2.34E-03	4.22E-04	3.20E-03	7.45E+00

2.5 Lime, Hydrated and Packed

2.5.1 Introduction

Hydrated lime refers to a dry calcium hydroxide powder produced from the calcination of limestone, a naturally occurring mineral that consists principally of calcium carbonate but may contain magnesium carbonate as a secondary component. Hydrated lime is widely used in aqueous systems as a low-cost alkaline chemical.

2.5.2 LCI Modeling

- Functional unit: 1 kg of hydrated lime, packed
- System boundaries: The main processes involved with the production of hydrated lime are limestone mining, crushing, washing, calcination, and milling as shown in Figure 7.

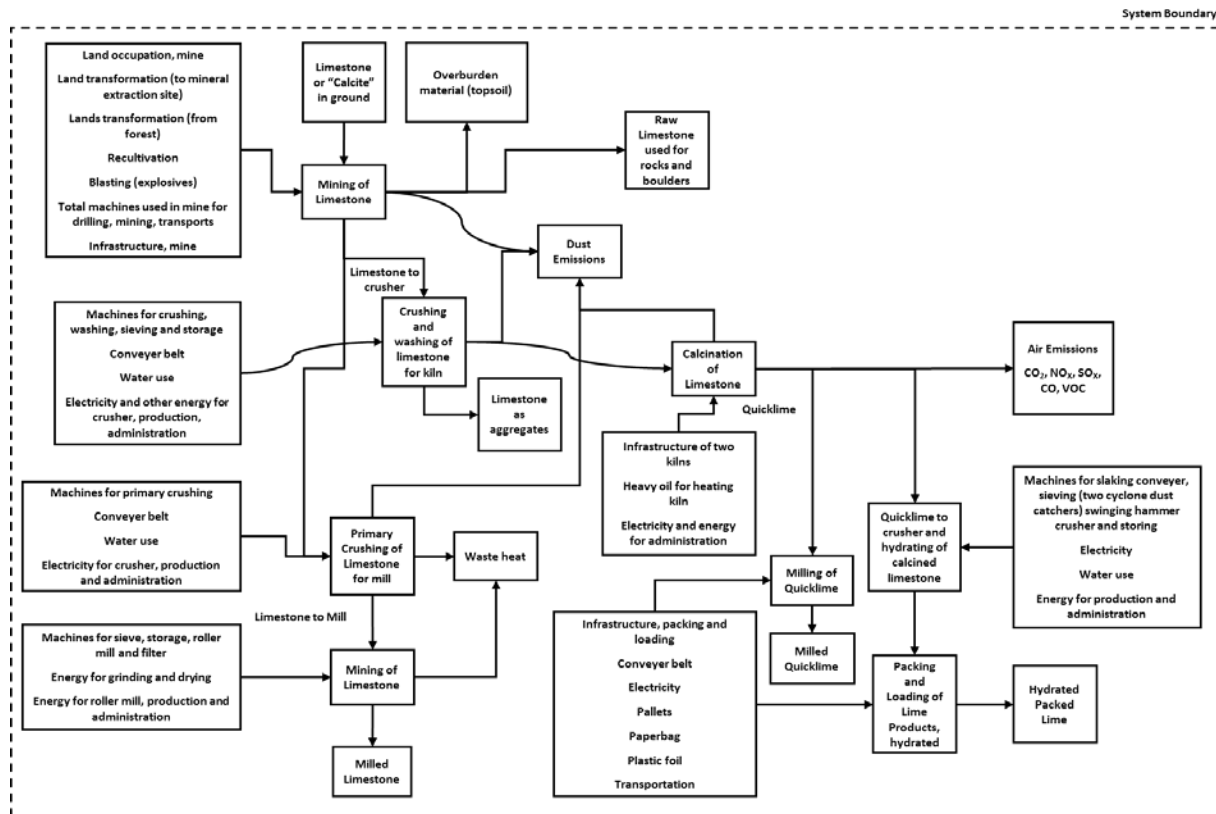


Figure 7. Production of hydrated lime as presented in (Kellenberger, Althaus et al., 2007)

- Inventory data: "lime, hydrated, packed, at plant – CH"; ecoinvent v2.2; (Kellenberger, Althaus et al., 2007).

2.5.3 Emission Factors

- Emission Factor Calculation Results

Table 5. SEFA Emission Factors for Hydrated Lime

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Lime, Hydrated, Packed	2.06E-03	7.62E-01	6.57E-06	5.13E-04	1.30E-04	3.58E-04	2.94E-01

2.6 Sodium Hydroxide (NaOH), 50% in Water

2.6.1 Introduction

Sodium hydroxide often referred to as caustic soda or just caustic, is a strong base. It is typically produced as a coproduct with chlorine through the electrolytic decomposition of sodium chloride solutions (brines). According to the Chlorine Institute, in 2010, the U.S. chlor-alkali industry produced 11.6 million short tons of chlorine and 12.2 million short tons of caustic soda (sodium hydroxide) (American Chemistry Council, 2015).

Three basic processes (diaphragm, mercury, and membrane) account for almost all total world chlorine capacity. Up to the end of the 20th century, the mercury cell technique dominated in Europe, while the diaphragm cell technique dominated in the United States and the membrane cell technique in Japan. Recently, new plants worldwide are based on the membrane cell technique. Generally, most producers operate their plants to make chlorine since it is hard to store and is used for derivatives like ethylene dichloride, phosgene, and epichlorohydrin. Caustic soda is generally sold on the merchant market and consumed in a myriad of uses (Linak & Inui, 2002). Due to customers' requirements, sodium hydroxide is produced commercially in two forms: as a 50 wt.-% solution (most common) and less frequently in the solid state as prills, flakes, or cast shapes.

2.6.2 LCI Modeling

- Functional unit: 1 kg of sodium hydroxide, 50% in H₂O
- System boundaries: The data set considers a production mix of sodium hydroxide with 23.5% produced by diaphragm cell, 55.1% produced by mercury cell, and 21.4% produced by membrane cell. As shown in Figure 8, the same basic flow of primary materials applies to all three pathways.

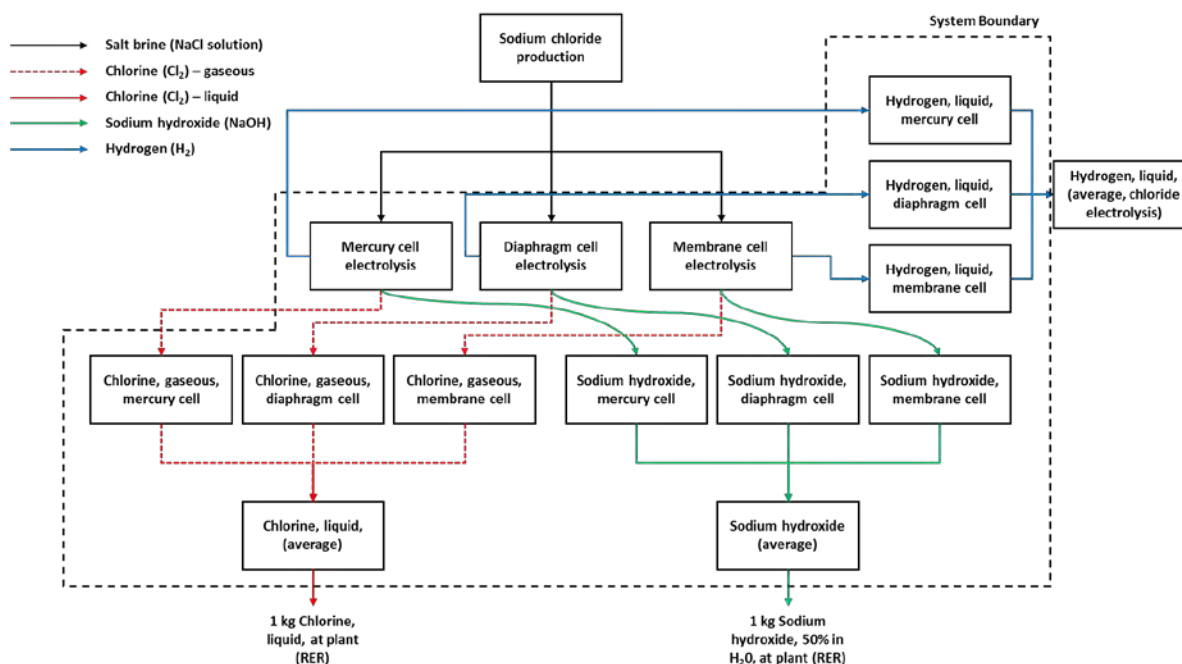


Figure 8. Production of average mix sodium hydroxide as shown in (Althaus, Chudacoff et al., 2007)

- Inventory data: “sodium hydroxide, 50% in H₂O, production mix, at plant – RER”; ecoinvent v2.2; (Althaus, Chudacoff et al., 2007).

2.6.3 Emission Factors

- Emission Factor Calculation Results

Table 6. SEFA Emission Factors for Sodium Hydroxide

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Sodium Hydroxide, 50% in water	9.77E-03	1.09E+00	1.29E-04	1.94E-03	4.03E-04	3.52E-03	1.39E+01

2.7 Hydrogen peroxide, 50% in Water

2.7.1 Introduction

Hydrogen peroxide is ubiquitous in the environment. In surface water, photochemical processes generally produce H₂O₂. In the atmosphere H₂O₂ is generated by photolysis of O₃ (Wayne, 1988) or aldehydes (Calvert & Stockwell, 1983). H₂O₂ is a weakly acidic, nearly colorless clear liquid that is miscible with water in all proportions. In addition, H₂O₂ is a strong oxidizing agent commercially available in aqueous solution over a wide range of concentrations. Aqueous H₂O₂ is sold in concentrations ranging from 3 to 86 wt. %, most often containing 35, 50, and 70 wt. %

H₂O₂ is used in various industrial and environmental applications. Due to its characteristics as a strong oxidizing agent, H₂O₂ is widely used as a bleaching agent in the paper and the textile industry. Further important uses are disinfection applications, hydrometallurgical processes, or wastewater treatment. In dilute solutions, H₂O₂ acts as a very efficient antiseptic. With regard to SEFA, H₂O₂ is used as an in-situ chemical oxidant for remediation. *In situ* chemical oxidation (ISCO), a form of advanced oxidation process is an environmental remediation technique used for soil and/or groundwater remediation to reduce the concentrations of targeted environmental contaminants to acceptable levels. ISCO is accomplished by injecting or otherwise introducing strong chemical oxidizers directly into the contaminated medium (soil or groundwater) to destroy chemical contaminants in place. It can be used to remediate a variety of organic compounds, including some that are resistant to natural degradation.

2.7.2 LCI Modeling

- Functional unit: 1 kg of hydrogen peroxide, in H₂O at plant
- System boundaries: The production of 50% hydrogen peroxide involves bubbling oxygen through anthracene as shown in Figure 9.

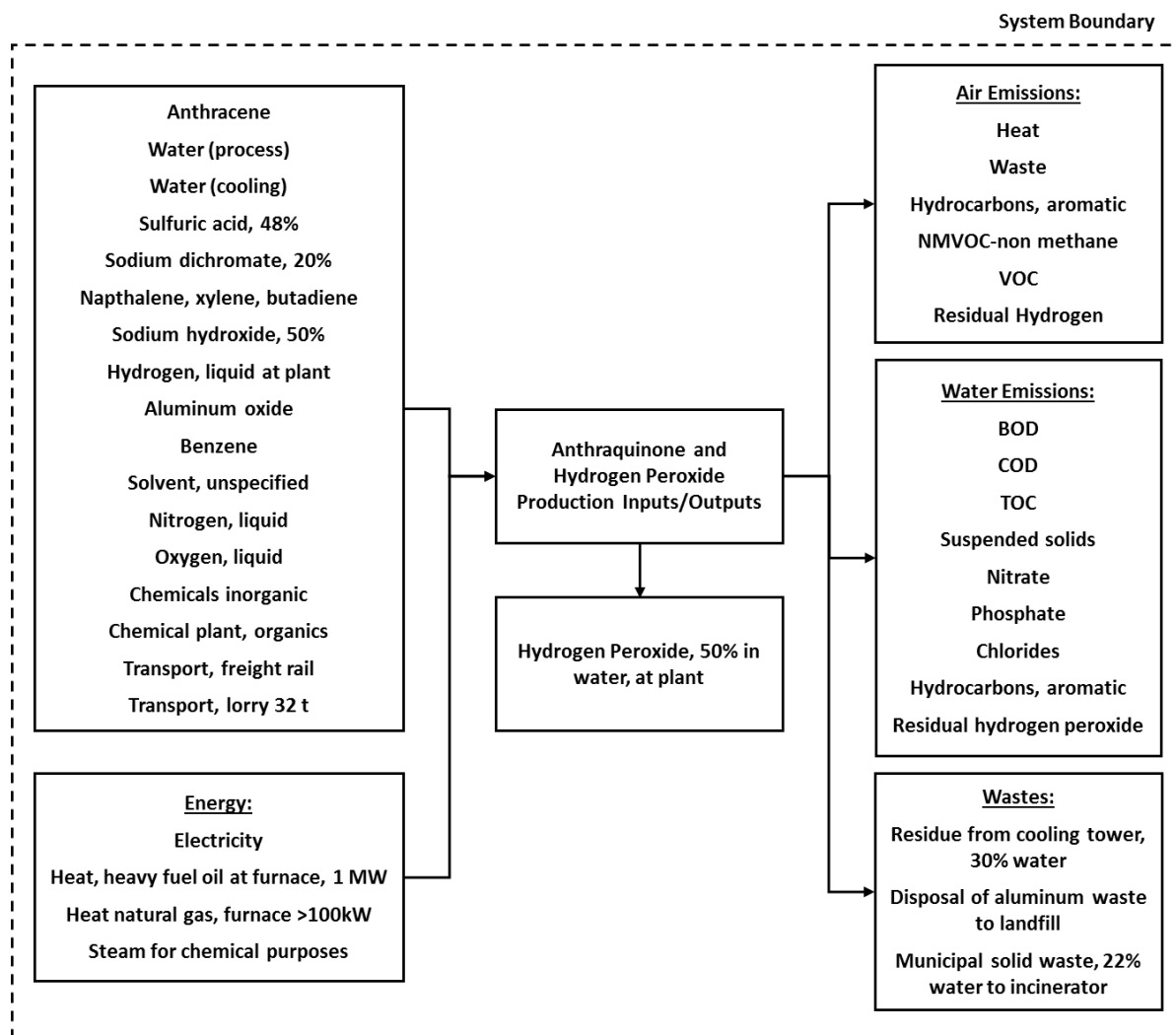


Figure 9. Production of hydrogen peroxide as shown in (Althaus, Chudacoff et al., 2007).

- Inventory data: “hydrogen peroxide, 50% in H₂O, at plant – RER”; ecoinvent 2.2; (Althaus, Chudacoff et al., 2007).

2.7.3 Emission Factors

- Emission Factor Calculation Results

Table 7. SEFA Emission Factors for Hydrogen Peroxide

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Hydrogen Peroxide, 50% in water	9.79E-03	1.19E+00	6.29E-05	1.42E-03	3.08E-04	2.40E-03	2.35E+01

2.8 Phosphoric Acid, 70% in Water

2.8.1 Introduction

Pure, anhydrous phosphoric acid, H_3PO_4 , is a colorless, crystalline compound that is readily soluble in water. After sulfuric acid, phosphoric acid is the most important mineral acid in terms of volume and value. This is mainly due to the enormous demand for wet phosphoric acid for further processing to fertilizers (Schrödter, Bettermann et al., 2000).

Phosphoric acid is produced by either a wet process or thermal process. The majority of phosphoric acid, approximately 96 %, is produced using the wet-process phosphoric acid (WPPA) method (USEPA, 1993a). The thermal process uses a high amount of energy and produces strong phosphoric acid liquid (of about 85 wt. % of H_3PO_4) which is required for high grade chemical production. Most of the WPPA produced world-wide is made with the dihydrate process (Althaus, Chudacoff et al., 2007; Gard, 2005; Schrödter, Bettermann et al., 2000; USEPA, 1993b).

Phosphoric acid plays a critical role in the restoration of environmental sites contaminated with heavy metals. Phosphoric acid forms insoluble complexes with metal ions typically found in contaminated soils, which occurs over a wide range of pH values and conditions. Once complexed, the metal ions are immobilized and are unable to leach out beyond the phosphoric acid-treated soil. Heavy metal contaminants that are capable of phosphoric acid immobilization include: lead, strontium, zinc, cadmium, iron, chromium, and selenium. The use of this technology has been successful at various industrial sites, including metal mining, waste, ammunition, scrap metal, paint, and battery industries.

2.8.2 LCI Modeling

- Functional unit: 1 kg of phosphoric acid, fertilizer grade, 70% in H_2O
- System boundaries: The production of phosphoric acid includes the mining and digestion of phosphate rock in sulfuric acid followed by filtration and concentration of the product (Althaus, Chudacoff et al., 2007).

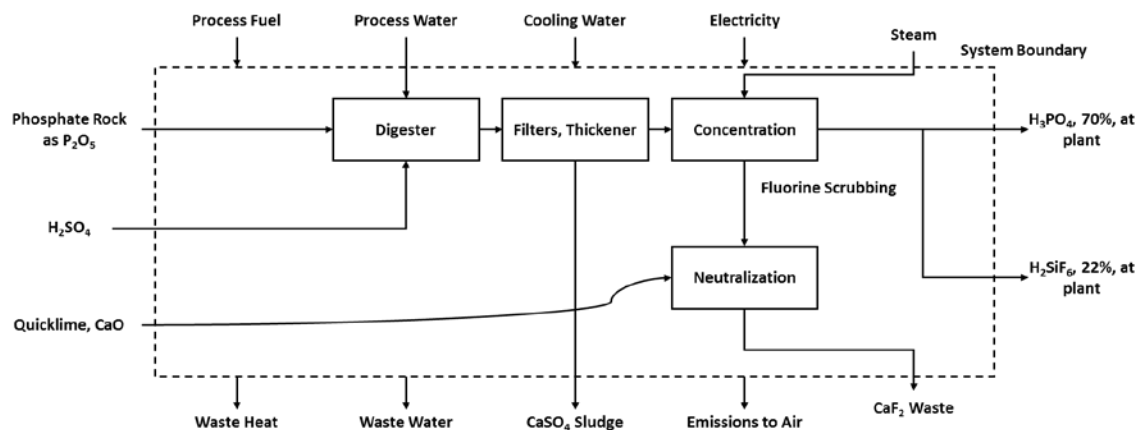


Figure 10. Production of phosphoric acid as shown in (Althaus, Chudacoff et al., 2007).

- Inventory data: “phosphoric acid, fertilizer grade, 70% in H₂O, at plant – US”; ecoinvent 2.2; (Althaus, Chudacoff et al., 2007).

2.8.3 Emission Factors

- Emission Factor Calculation Results

Table 8. SEFA Emission Factors for Phosphoric Acid

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Phosphoric Acid, 70% in water	6.70E-03	8.82E-01	1.63E-04	2.82E-03	1.71E-03	2.94E-02	1.61E+01

2.9 Iron (II) Sulfate, Hydrated

2.9.1 Introduction

Iron (II) sulfate heptahydrate, ferrous sulfate, FeSO₄ • 7H₂O, crystallizes from an aqueous iron solution as green, monoclinic crystals that are readily soluble in water (Stolzenberg, 2000; Wildermuth, Stark et al., 2000). Most iron (II) sulfate is a by-product of the steel industry. Prior to tinning, galvanizing, electroplating, or enameling, steel surfaces are dipped in sulfuric acid for cleaning (pickling). The resulting pickle liquor contains ca 15% iron (II) sulfate and 2–7% acid. Scrap iron is added to reduce the acid concentration to ca 0.03%. The solution is filtered, concentrated at 70 °C to a specific gravity of 1.4, and is allowed to cool to room temperature, which results in crystallization of the heptahydrate. Industry produces on the order of 10⁶ tons/yr. of the iron sulfate. Because supply exceeds demand, the pickling liquor presents a serious waste disposal problem. Iron(II) sulfate has a large variety of uses including iron oxide pigments and salts, fertilizer production, food and feed supplements, inks and dyes, reducing agents, polymerization catalysts, and water treatment. In water treatment, iron (II) sulfate is commonly used for municipal and industrial wastewater treatment as coagulants or flocculants, for odor control to minimize hydrogen sulfide release, for phosphorus removal, and as a sludge thickening, conditioning and dewatering agent.

2.9.2 LCI Modeling

- Functional unit: 1 lb. of Iron (II) sulfate heptahydrate
- System boundaries: The production of iron (II) sulfate heptahydrate involves the dissolution of iron scrap in dilute sulfuric acid (Figure 11).

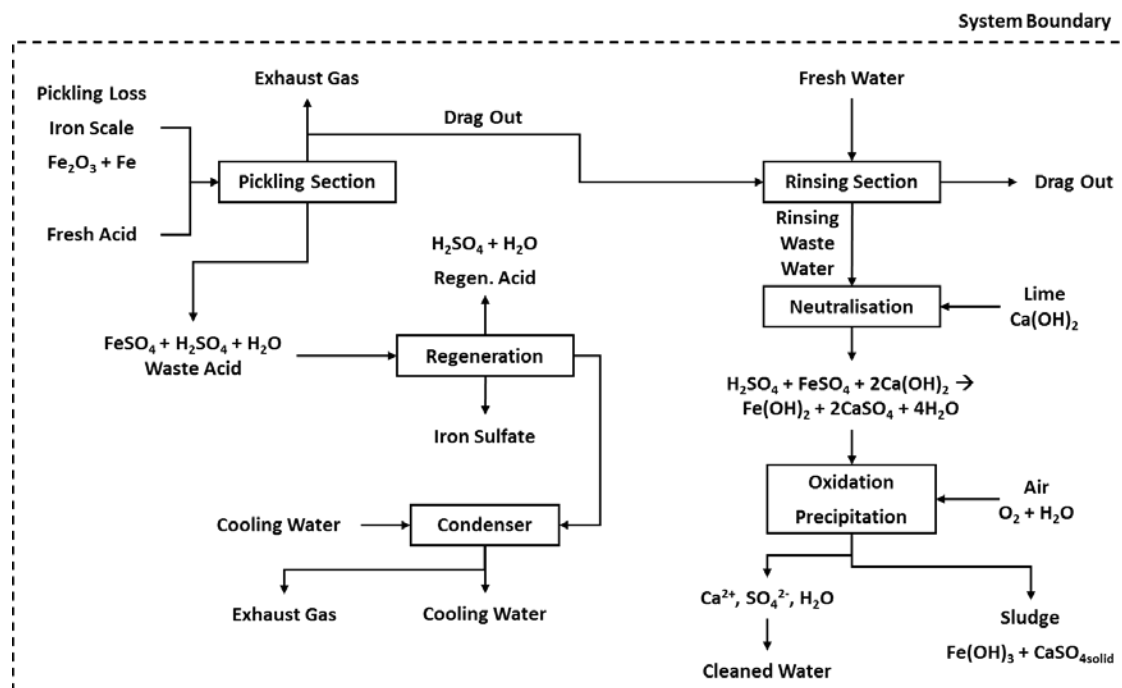


Figure 11. Production of iron (II) sulfate as shown in (EIPPCB, 2001).

- Inventory data: “iron sulphate, at plant - RER”; ecoinvent 2.2; (Jungbluth, Chudacoff et al., 2007).

2.9.3 Emission Factors

- Emission Factor Calculation Results

Table 9. SEFA Emission Factors for Hydrated Iron (II) Sulfate

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Iron (II) Sulfate, Hydrated	1.47E-03	1.67E-01	2.30E-05	3.16E-04	1.03E-04	5.89E-04	7.44E-01

2.10 Asphalt, Mastic-type and Pavement Grade

2.10.1 Introduction

Bitumen is a generic class of amorphous, dark colored, cementitious substances, natural or manufactured, composed principally of high molecular mass hydrocarbons, soluble in carbon disulfide (ASTM, 2013c). Asphalt is defined as a cementitious material in which the predominating

constituents are bitumens. The terms bituminous and asphaltic then refer to materials that contain or are treated with bitumen or asphalt. Thus, some confusion exists, but in this report, asphalt and bitumen are used interchangeably.

Since the early 1900's most of the asphalts produced from the refining of petroleum have been used primarily in paving and roofing applications. Mastic asphalt has been used in some industrial applications. According to the International Mastic Asphalt Association(IMAA), mastic asphalt (MA) is a dense massmass composed on suitably graded mineral matter and/or sand, and /or limestone fine aggregate, and/or crushed limestone powderpowder and bitumen, which may contain additives (for example polymers, waxes). The mixture is designed to be of low void content. The binder content is so adjusted that the voids are completely filled and that even a slight excess of binder may occur. .

In environmental applications, asphalt can be used as a barrier material. Prior to the mid-1960s, asphalt barriers were primarily used to control water seepage from facilities such as impoundments and earth dams (Creegan & Monismith, 1996). For these applications, asphalt was applied as hot-sprayed asphalt membranes or as asphalt concrete for barrier layers. The petroleum shortage of the 1970's, along with the establishment of rules for hazardous and solid waste landfill designs, focused the industry toward composite liners consisting of geomembranes and compacted soil. However, in the mid-1980's, resurgence into the use of asphalt for waste isolation was initiated by the US Department of Energy (DOE) in their quest for very-long-term hydraulic barriers (1000+ years) for radioactive and mixed waste sites (Gee & Wing, 1993).

2.10.2 LCI Modeling – Mastic Asphalt

- Functional unit: 1 lb. of mastic asphalt
- System boundaries: The production of mastic involves the following inputs: bitumen, limestone powder, sand, infrastructure, and transport. Producing mastic outputs VOCs, benzopyrene, and waste heat (Figure 12).

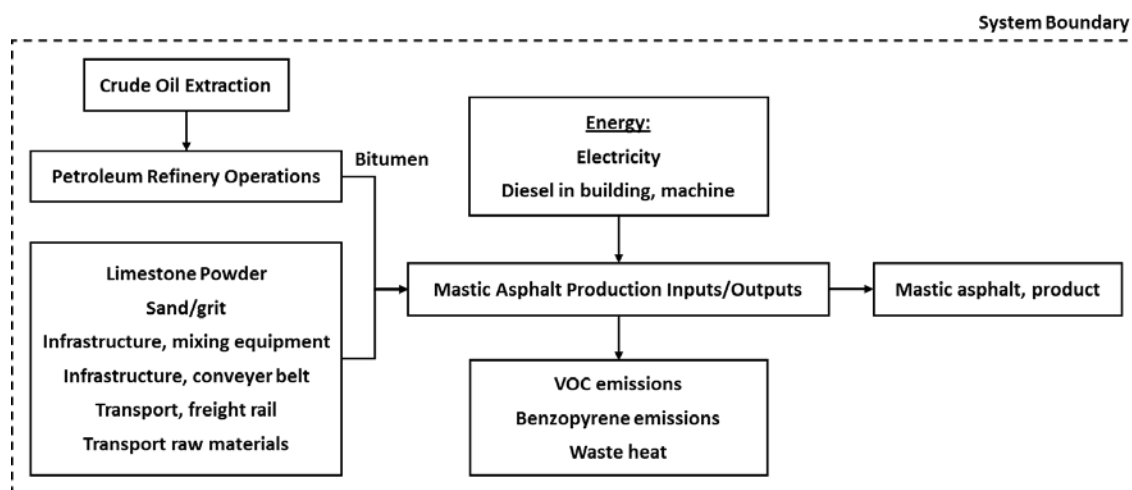


Figure 12. Production of mastic asphalt as shown in (Kellenberger, Althaus et al., 2007)

- Inventory data: “mastic asphalt, at plant - RER”; ecoinvent 2.2; (Kellenberger 2007); Process was modified by using the Eurobitume bitumen inventory in place of the ecoinvent bitumen inventory.

2.10.3 LCI Modeling – Pavement-grade Asphalt

- Functional unit: 1 lb. of pavement grade asphalt
- System boundaries: Producing pavement grade asphalt requires crude oil, which is transported, then refined and stored at a complex refinery (Figure 13).

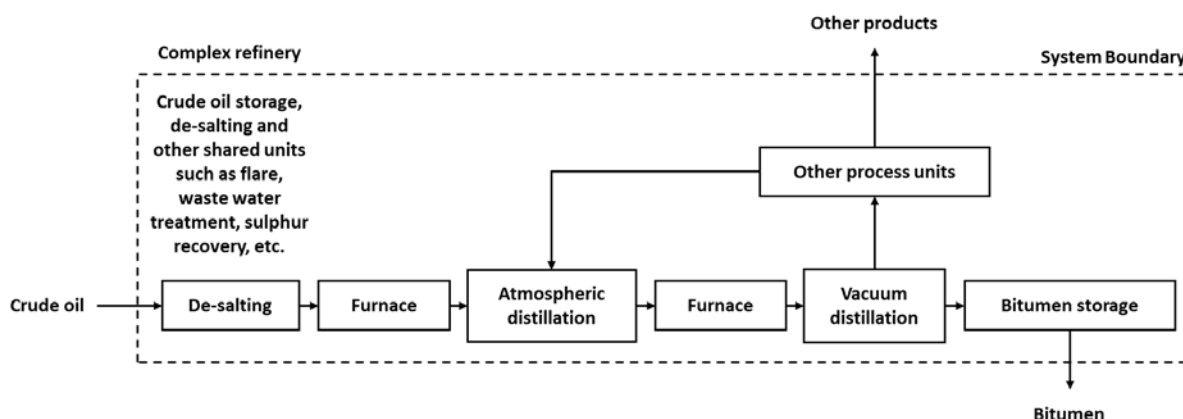


Figure 13. Bitumen production at a complex refinery as presented in (Eurobitume, 2012)

2.10.4 Emission Factors

- Emission Factor Calculation Results

Table 10. SEFA Emission Factors for Mastic and Paving-Grade Asphalt

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Mastic Asphalt	4.12E-02	8.50E-01	1.07E-03	2.71E-03	7.66E-04	7.98E-03	5.46E-01
Paving Asphalt	5.00E-01	8.58E+00	1.33E-02	2.99E-02	9.10E-03	9.69E-02	3.88E+00

2.11 Aluminum, Rolled Sheet

2.11.1 Introduction

Aluminum is the third most abundant element in the earth’s crust and is usually combined with silicon and oxygen in rock. When aluminum silicate minerals are subjected to tropical weathering, aluminum hydroxide may be formed. Rock that contains high concentrations of aluminum hydroxide minerals is called bauxite (Frank, Haupin et al., 2000; Sanders, 2012).

Although bauxite is, with rare exception, the starting material for the production of aluminum, the industry generally refers to metallurgical grade alumina, Al_2O_3 , extracted from bauxite by the Bayer Process, as the ore. It takes roughly 4 – 7 tons of bauxite to produce 2 tons of alumina, which again yield 1 ton of aluminum (Norsk Hydro, 2012). Aluminum is obtained by electrolysis of this purified ore. The production of aluminum in the US is forecasted to total 7.1 million metric tons in 2017 (The Freedonia Group, 2013). According to the USGS, world production in 2013 was 47.3 million metric tons (USGS, 2014).

Aluminum is a common piling material, where piling is a method of horizontal sealing to prevent the movement of groundwater. Aluminum pile enclosures minimize or eliminate the need for contaminant plume control by groundwater pumping and/or water treatment. Contaminants are prevented from moving off site, while site control activities (e.g., source removal, plume remediation) are carried out in the isolated subsurface environment inside the piled enclosure.

2.11.2 LCI Modeling

- Functional unit: 1 lb. of rolled aluminum
- System boundaries: Figure 14 is the system boundary for the extraction of bauxite to the production of primary Al ingots to Al sheets. Several processes lead to the production of primary aluminum, including bauxite mining, alumina extraction, production of other raw materials, and anode fabrication. Following primary aluminum production, the aluminum is sawed, scalped, rolled, and then heat treated. Once heat treated, the aluminum is finished, packaged, used, collected, sorted, and then recycled with associated metal losses.

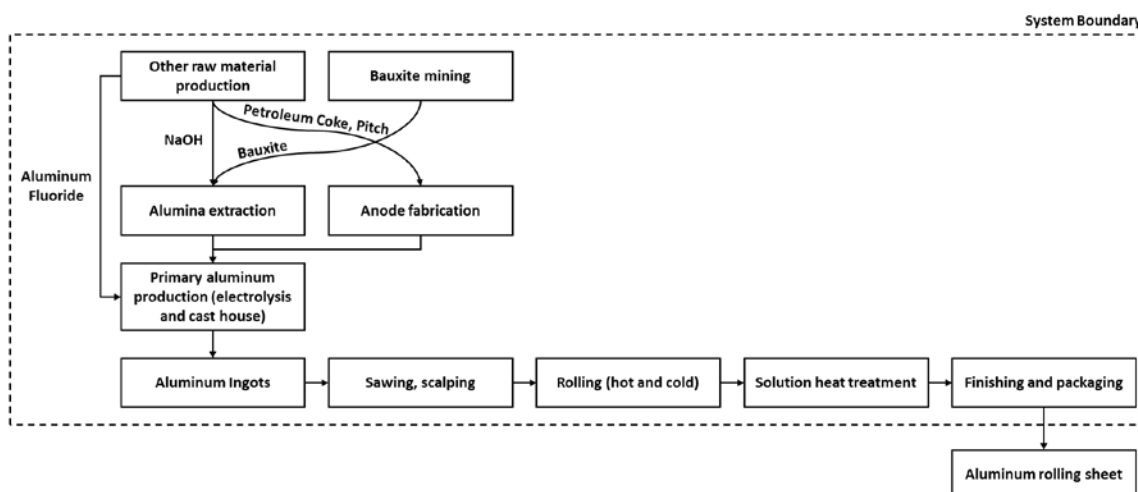


Figure 14. System Boundary-Production of Aluminum as adapted by (EAA, 2013) and (Classen, Althaus et al., 2007)

- Inventory data: “aluminum, primary, at plant - RER”; ecoinvent 2.2; (Althaus, Chudacoff et al., 2007); “anodizing, aluminum sheet - RER”; ecoinvent 2.2; (Classen, Althaus et al., 2007); “sheet rolling, aluminum - RER”; ecoinvent 2.2; (Werner, Althaus et al., 2007).

2.11.3 Emission Factors

- Emission Factor Calculation Results

Table 11. SEFA Emission Factors for Rolled Aluminum

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Aluminum, Rolled Sheet	6.33E-02	9.15E+00	1.02E-03	1.48E-02	8.80E-03	2.83E-02	2.78E+01

2.12 Granular Activated Carbon (GAC), Primary and Regenerated

2.12.1 Introduction

Granular activated carbon (GAC) is a carbonaceous material used to remove various contaminants through adsorption from either liquid or gas streams. The most common precursor materials for GAC are bituminous coal, lignite coal, coconut shells, and wood.

Commercial activated carbon production is a two-step process involving carbonization of a precursor material followed by activation. In the pyrolytic carbonization process, the temperature of the raw material is raised to the range of 500 to 800 °C in the absence of oxygen. Volatile organic matter of the raw material is thermally released, and the carbon atoms realign to form a crystalline structure. The carbonized product at this point in the process is heavily influenced by the raw materials used. For activated carbon products used in water treatment, a thermal or physical activation process follows in which the temperature of the carbonized product is increased to the range of 850 to 1,000 °C in the presence of an oxidizing agent, typically steam or carbon dioxide. Activation increases the pore sizes and creates a continuous pore structure, which increases the micropore volume (pore width < 2 nm) and the internal surface area where most of the adsorption occurs. The activation step can involve either a direct activation process in which the raw material is crushed and then activated, or in a reagglomeration process in which the raw material is crushed, reagglomerated, crushed again, and then activated.

Reactivation of spent activated carbon is the destruction of contaminants and the reactivation of useful carbon. Contaminants are desorbed and destroyed at high temperatures (typically exceeding 1500 °F) in a reactivation furnace. Furnaces can either be rotary kilns or multiple hearths, and can be heated by either natural gas, electricity, or fuel oil. Off-site carbon reactivation manufacturers reactivate anywhere from 5 to 60 tons of spent carbon on a daily basis. While larger-capacity furnaces are not typically cost-effective for a single hazardous waste site, smaller furnaces are more cost-effective for on-site use at a single site. Reactivation furnaces output reactivated carbon, air emissions, and some carbon fines. Reactivation furnaces do not produce organic wastes.

2.12.2 LCI Modeling

- Functional unit: 1 lb. of granular activated carbon (primary or regenerated)
- System boundaries: For primary GAC, the modeled process includes the extraction and conversion of coal using pyrolytic carbonization and thermal activation (Figure 15). Regenerated GAC includes the thermal desorption and reactivation of captured contaminants (Figure 16). Data describing emission profiles during regeneration could not be identified.

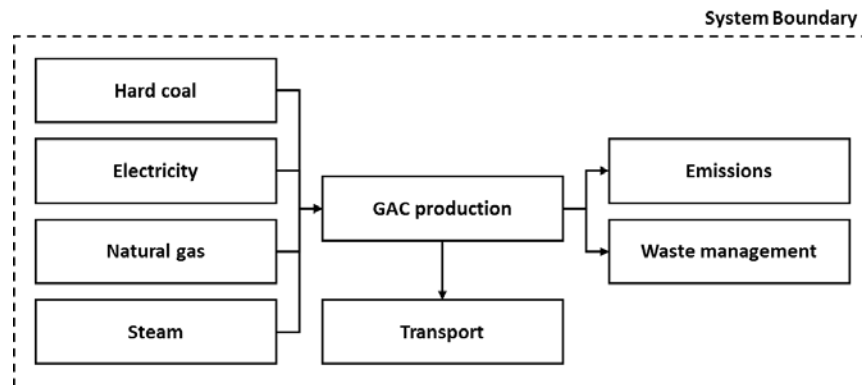


Figure 15. System boundary for primary GAC as adapted from (Gabarrell, Font et al., 2012)

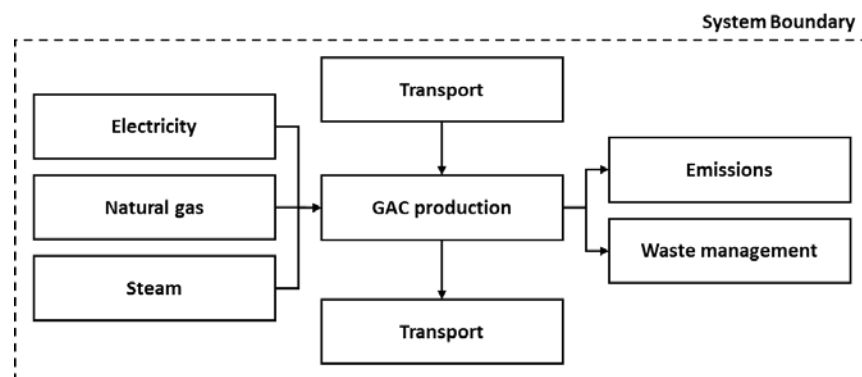


Figure 16. System boundary for regenerated GAC as adapted from (Gabarrell, Font et al., 2012)

The inventories from (USEPA, 2010a) and (He, 2012) were created separately in openLCA and analyzed using the footprint method. The resulting EmFs were arithmetically averaged to create the reported EmFs in Section 2.12.3.

2.12.3 Emission Factors

- Emission Factor Calculation Results

Table 12. SEFA Emission Factors for Primary and Regenerated Granular Activated Carbon

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO₂e/lb)	HAPs (lb/lb)	NO_x (lb/lb)	PM10 (lb/lb)	SO_x (lb/lb)	Water Use (gals/lb)
Primary Activated Carbon	3.56E-02	4.82E+00	6.57E-04	7.93E-02	9.87E-04	1.28E-01	1.53E+00
Regenerated Activated Carbon	8.73E-03	1.70E+00	6.71E-04	7.33E-03	8.86E-04	1.29E-02	1.20E+00

2.13 Portland Cement

2.13.1 Introduction

Portland cement is the most common type of cement used globally. It is the hydraulic binder in concrete and mortar. Portland cement is made by heating limestone (i.e., calcium carbonate) with other materials (e.g., clay) in a 1450 °C kiln. This process is known as calcination, where a molecule of CO₂ is liberated from the calcium carbonate to form calcium oxide, which is then mixed with the other materials to form calcium silicates and other cementitious compounds. The resulting hard substance, clinker, is then ground with gypsum into a powder to make ordinary Portland cement (OPC).

Cement is primarily used as a constituent of concrete, and concrete has a number of remediation site applications. The most common concrete application at remediation sites is in the form of buildings and foundations. Not limited to remediation sites, concrete is extensively used to form building walls, foundations, and other elements within a building.

2.13.2 LCI Modeling

- Functional unit: 1 lb. of Portland cement.
- System boundaries: The production of Portland includes rock quarrying and crushing; raw meal preparation through grinding and blending; calcination of rock and mix components to form clinker, and final grinding and bagging (Figure 17).

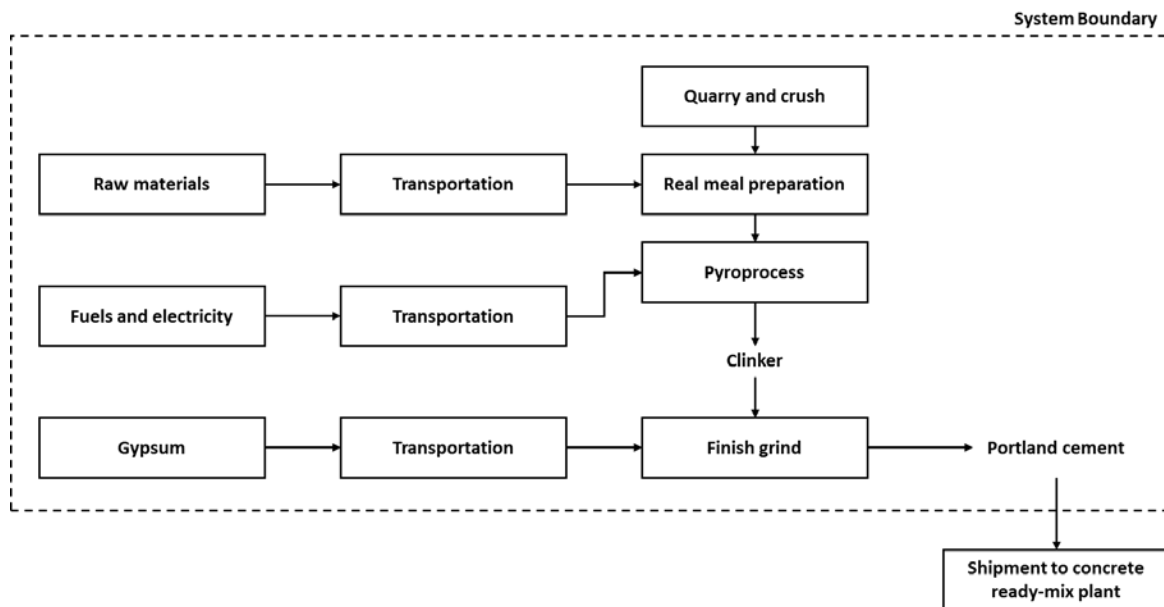


Figure 17. Production of Portland cement as reported by (Marceau, Nisbet et al., 2006)

2.13.3 Emission Factors

- Emission Factor Calculation Results

Table 13. SEFA Emission Factors for Portland cement

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Portland Cement	1.39E-02	1.34E+00	9.70E-04	6.54E-03	3.78E-03	1.04E-02	7.73E-01

2.14 Ready Mixed Concrete (20 MPa-3000psi)

2.14.1 Introduction

Concrete is a high-volume, low-cost building material produced by mixing cement, water, and aggregates. The use of concrete is nearly universal in modern construction, where it is an essential component of high rise buildings, pavement, bridges, dams, buildings, and other staples of the developed landscape. There are thousands of possible ready mixed concrete (RMC) products (a.k.a. mix designs, mixes, mixture compositions or mixtures), which ultimately balance the cost and performance of concrete for a wide variety of applications. There are many factors that can influence the way concrete is manufactured, designed, built, used, and recycled that ultimately affect the environmental footprint of concrete and the structures built with concrete. Several factors that can affect the environmental performance of concrete and concrete structures include: design

loads, structural efficiency, durability, constructability, energy efficiency, aesthetics, and concrete mixtures.

2.14.2 LCI Modeling

- Functional unit: 1 cubic foot of ready-mixed concrete
- System boundaries: The production of ready-mixed concrete includes the preparation of Portland cement (Section 2.13) and its mixing with aggregates and water to form concrete (Figure 18).

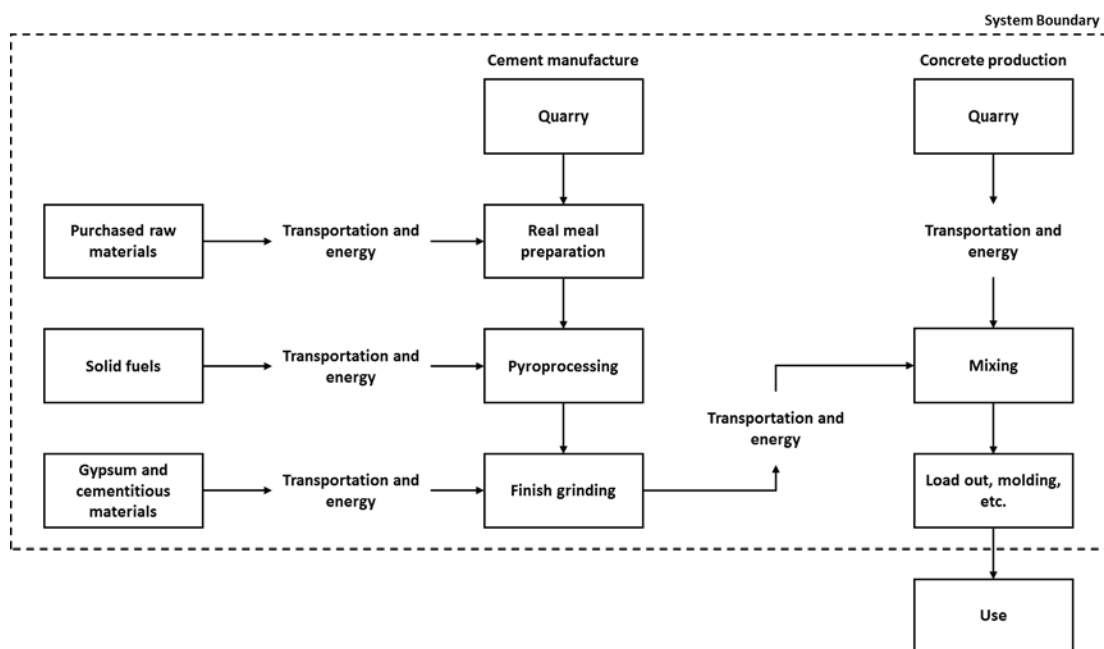


Figure 18. Production of ready mixed concrete as reported by (Nisbet, 2000)

2.14.3 Emission Factors

- Emission Factor Calculation Results

Table 14. SEFA Emission Factors for Ready Mixed Concrete

Chemical/Material	CED (MMBtu/ft ³)	GWP100 (lb CO ₂ e/ft ³)	HAPs (lb/ft ³)	NO _x (lb/ft ³)	PM10 (lb/ft ³)	SO _x (lb/ft ³)	Water Use (gals/ft ³)
Ready Mixed Concrete	2.17E-01	1.95E+01	1.41E-02	9.75E-02	5.70E-02	1.54E-01	3.32E+01

2.15 Gravel and Sand Mix, 65% Gravel

2.15.1 Introduction

Construction aggregates find use in a wide range of applications including road base and coverings, hydraulic concrete, asphaltic concrete, foundation fill, railroad ballast, roofing granules and snow

and ice control. The primary function for road base and subbase aggregates is to provide a solid, sturdy foundation for driving surfaces. A wide range of items (including natural aggregates and alternative, secondary, and recycled materials) comprises the segment and product specifications are generally less restrictive than other applications. Natural aggregates consist of crushed stone, sand, and gravel obtained from quarries. Natural aggregates are among the most abundant natural resources and a major basic raw material used by construction, agriculture, and industries employing complex chemical and metallurgical processes. Gravel and sand are used at remediation sites through several applications. Crushed stone (i.e., gravel) can be used in temporary roads at remediation sites. Temporary gravel roads provide periodic access points for remediation site employees, and are able to be removed and disposed once their useful lifetime is reached (USEPA, 1996). Gravel and sand are important constituents in geomembranes used as vertical barriers to prevent the spread of contaminated groundwater. A 1994 study by Burnette and Schmednecht focused on a geomembrane cutoff wall that encompassed a Great Lakes chemical plant, which consisted of layers of sand, gravel, and cobbles (Brunette & Schmednecht, 1994).

2.15.2 LCI Modeling

Note: Round gravel and sand are produced simultaneously in a quarry. As such, they are modeled as co-products of the same unit process in ecoinvent. The mixture here represents a typical blend for construction use and is modeled as 65% gravel 35% sand. The same process description and boundaries apply for the sand, gravel, and mixture processes. No allocation is applied to the ecoinvent process and both products receive identical impacts. Therefore, the emission factors reported in Table 15 apply to 1 lb. of sand by itself, 1 lb. of round gravel by itself, or 1 lb. of a gravel/sand mix as listed in the table. The consequence of this approach is that the impacts for the mixture are not a function of the composition.

- Functional unit: 1 lb. of a sand/gravel mix
- System boundaries: The system boundary for producing a gravel and sand mix includes processes related to the extraction of round gravel and sand (i.e., no crushed gravel) at a quarry, internal processes (i.e., transport, etc.), and infrastructure for the operation (i.e., machinery) (Figure 19).

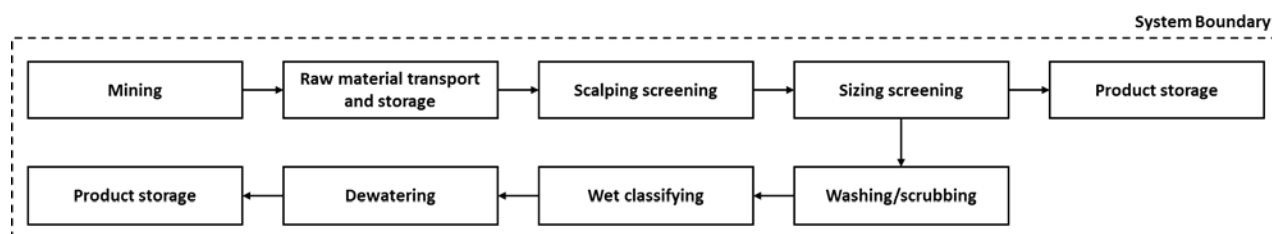


Figure 19. Typical production of sand and gravel as reported by (USEPA, 1995a)

- Inventory data: 0.65 lbs. of “gravel, round, at mine – CH”, ecoinvent 2.2, (Kellenberger, Althaus et al., 2007); 0.35 lbs. of “sand, at mine – CH”, ecoinvent 2.2, (Kellenberger, Althaus et al., 2007).

2.15.3 Emission Factors

- Emission Factor Calculation Results

Table 15. SEFA Emission Factors for a Gravel, Sand, or a Gravel/Sand Mix

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Gravel, Sand, or Gravel/Sand Mix	2.48E-05	2.40E-03	3.08E-07	1.80E-05	2.61E-06	4.52E-06	1.71E-01

2.16 High Density Polyethylene (HDPE)

2.16.1 Introduction

Because of this versatility, HDPE is one of the most popular plastics in use today, with a projected global market of almost \$70 billion by 2019 (Plastic News, 2013). HDPE resin is used in many applications, including industrial wrappings and films, crates, boxes, caps and closures, bottles and containers for food products, cosmetics, pharmaceuticals, household and industrial chemicals, toys, fuel tanks and other automotive parts, and pipes for gas and water distribution.

HDPE can be used as panels constituting vertical barrier systems in order to remediate polluted groundwater systems. For example, a 1997 case study focused on using HDPE panels as a remediation technique for a waterway seeping dense non-aqueous phase liquids (DNAPLs). The study found that advantages of using HDPE vertical barrier systems include: flexibility, low permeability rates (e.g., 2.7×10^{-13} cm/s), resistant to a variety of chemicals, long service life, quick installation, and low economic costs (Burson, Baker et al., 1997). HDPE has been shown to be a suitable flexible membrane liner (FML) at landfill sites. HDPE geomembranes are extremely resistant to leachates, which is a primary factor influencing the use of HDPE in FMLs (Eithe & Koerner, 1997).

HDPE is a polyolefin produced from the polymerization of ethylene. The polymer properties can be controlled and varied by adding co-monomers such as butene or hexene to the blend. The manufacturing of HDPE starts with applying heat to petroleum (i.e., cracking), which produces ethylene gas. Under controlled conditions the ethylene gas molecules link together to form long chains (or polymers), thus producing polyethylene. The reaction occurs in a large loop reactor with the mixture being constantly stirred. Upon opening a valve, the product is released with the solvent evaporated leaving the polymer and catalyst. Water vapor and nitrogen are then reacted with the polymer to cease catalytic activity. Residues of the catalyst, which are typically titanium (IV) and aluminum oxides, remain mixed in the polymer. The HDPE powder produced from the reactor is then separated from the diluent or solvent (if used) and is extruded and cut up into granules.

2.16.2 LCI Modeling

- Functional unit: 1 lb. of high density polyethylene, granulate type
- System boundaries: The production of HDPE includes the upstream extraction and processing of crude oil to make ethylene; the blending of ethylene with co-monomers, solvents, and

additives; catalyzed polymerization of the mixture to form HDPE; and finishing producing HDPE resin (Figure 20). The impacts of the downstream processing of HDPE resin to form product(s) used at remediation sites is assumed to be negligible compared to the included processes.

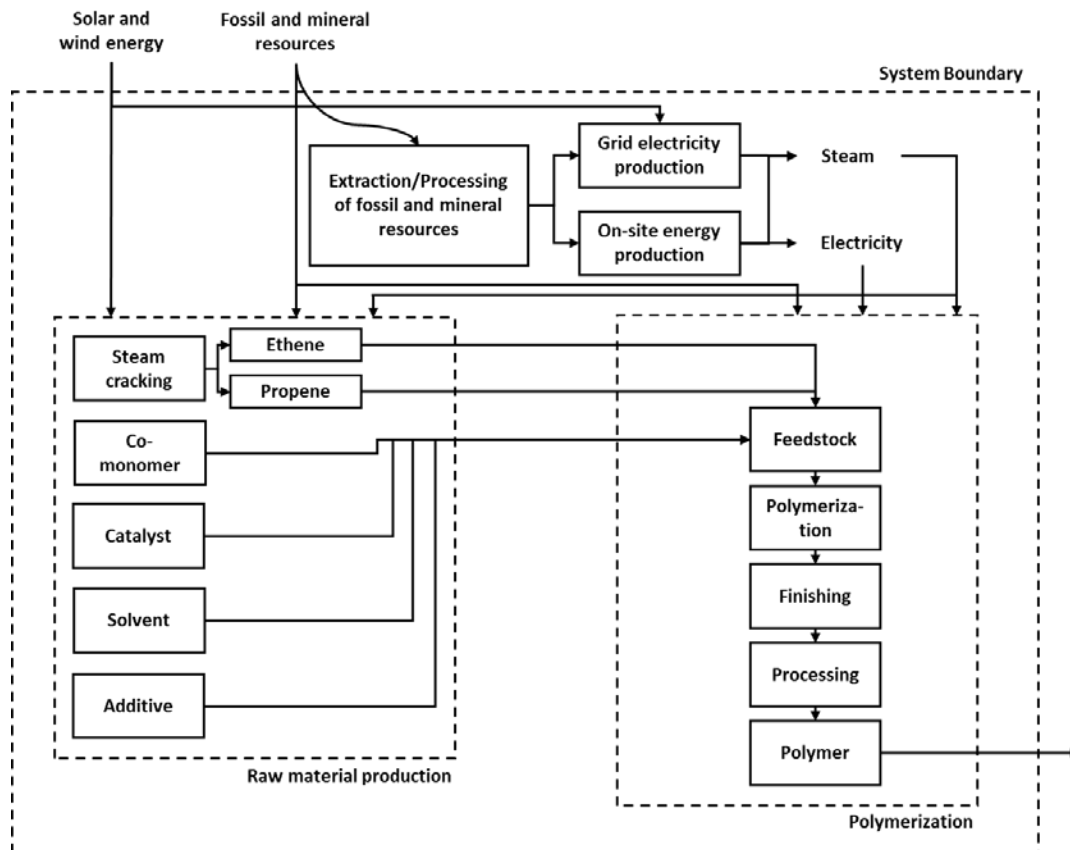


Figure 20. Production of High Density Polyethylene as reported by (PlasticsEurope, 2014)

- Inventory data: “polyethylene, HDPE, granulate, at plant- RER”; ecoinvent 2.2; (Hischier, 2007).

2.16.3 Emission Factors

- Emission Factor Calculation Results

Table 16. SEFA Emission Factors for High Density Polyethylene

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
High Density Polyethylene	3.32E-02	1.94E+00	6.41E-05	3.25E-03	4.39E-04	4.09E-03	3.88E+00

2.17 Polyvinyl Chloride (PVC)

2.17.1 Introduction

Polyvinyl chloride (PVC) is, by volume, the third-largest thermoplastic that is manufactured in the world. PVC is a key product of the chemical industry and, along with polypropylene and polyethylene, one of the most widely produced plastics. PVC use is highly dependent on the construction market, as about 70% of its world consumption is for pipe, fittings, siding, windows, fencing, electrical and other applications. At remediation sites, PVC is used for well casings, piping, cutoff walls, geomembranes, liners, and cap (USEPA, 2012a).

There are three main processes used for the commercial production of PVC: Suspension (providing 80% of world production), emulsion (12%) and mass, called bulk (8%) (Fischer, Schmitt et al., 2014). The first step of suspension PVC manufacturing is feeding vinyl chloride monomer (VCM) into a polymerization reactor with water and suspending agents. High-speed agitation forms small droplets of VCM, which are then introduced to a catalyst. PVC is then obtained by way of the catalyst, pressure, and temperatures ranging from 40 to 60°C. The slurry discharged from the polymerization reactor is then stripped of un-reacted VCM, and then dried by centrifugation. The result is PVC in the form of white powder, or resin. Emulsion polymerization is a far less common technology to manufacture PVC. Emulsion polymerization produces finer resin grades with much smaller particles, which are required by certain applications. Emulsion polymerization takes place in pressurized vessels under the influence of heat and catalysts. Polymerization occurs within the dispersed VCM droplets and with an initiator highly soluble in VCM, (that is not water). The product is then transferred to a blow-down vessel, where the unreacted monomer is extracted, recovered, and recycled back to the polymerization reactor. The polymer particles are then dried.

2.17.2 LCI Modeling

- Functional unit: 1 lb. of polyvinyl chloride
- System boundaries: Typical production of PVC includes the upstream production of ethylene from crude oil and chlorine from brine and rock salt; the chlorination of ethylene to yield vinyl chloride; the polymerization of vinyl chloride to make PVC resin; and the transport of the resin to a regional storehouse for distribution and downstream use (Figure 21). As with HDPE, the further processing of resin to products for use onsite during remediation is assumed negligible.

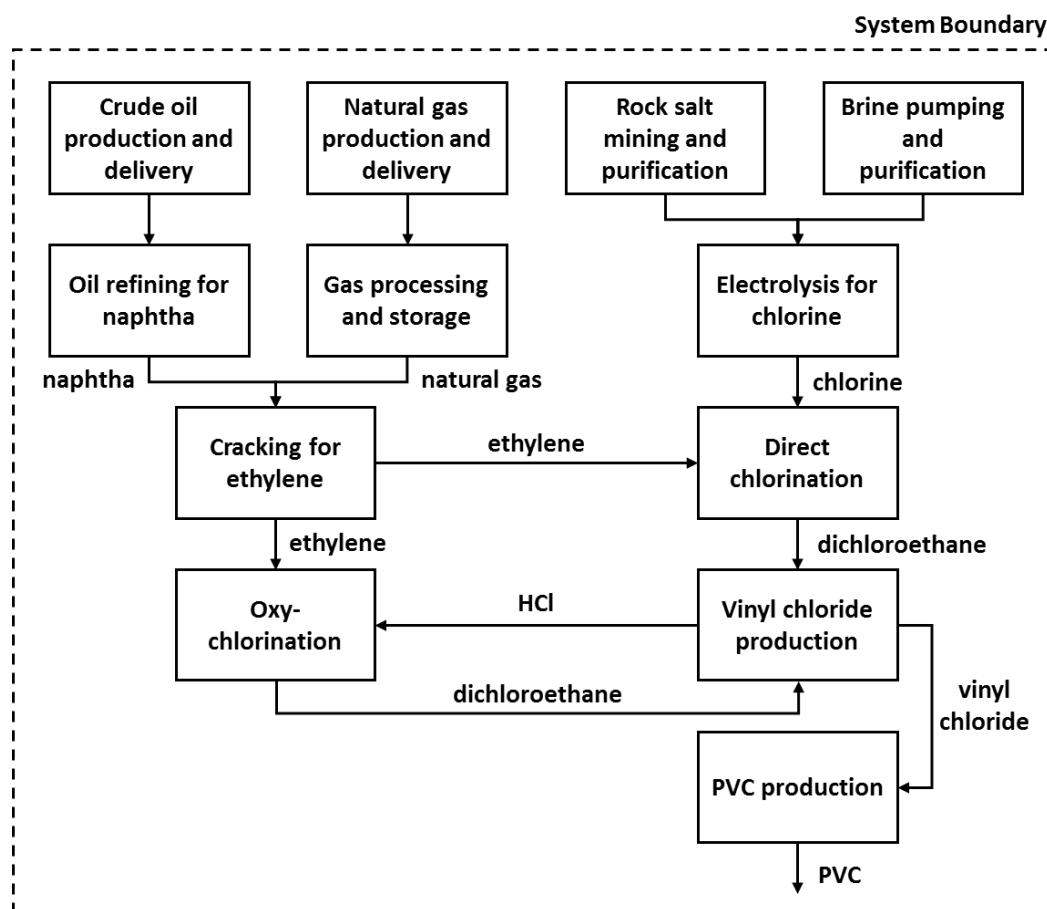


Figure 21. Flow Diagram for the Cradle to Gate Production of PVC as reported by (Hischier, 2007)

- Inventory data: “polyvinylchloride, at regional storehouse - RER”, ecoinvent 2.2, (Hischier, 2007); The cited process assumes 87% resin production from the suspension method and 13% from the emulsion method.

2.17.3 Emission Factors

- Emission Factor Calculation Results

Table 17. SEFA Emission Factors for Polyvinyl Chloride

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Polyvinyl Chloride	2.62E-02	2.02E+00	3.75E-04	4.00E-03	3.72E-04	2.74E-03	5.79E+01

2.18 Hazardous Waste Incineration

2.18.1 Introduction

The global hazardous waste management market reached \$23.8 billion in 2013 and \$25.9 billion in 2014 and will continue to grow steadily and reach \$33.9 billion by the end of 2019 (BCC Research, 2015). Over the last five years, the quantities of hazardous waste generated in North America varied between a low of 150.0 million metric tons and a high of 170.0 million metric tons in 2012. Hazardous waste is expected to increase consistently in the years to come mainly due to increasing industrial productivity.

Incineration is the most commonly used method for thermal treatment of organic liquids, and solids and sludge contaminated with toxic organics. During incineration, high temperatures between 871°C and 1204°C (1600°F and 2200°F) are used to combust (in the presence of oxygen) the organic constituents in hazardous wastes. Incinerators are usually classified by the type of combustion unit, with rotary kiln, liquid injection, fluidized bed, and infrared units being those most commonly used for hazardous wastes. Existing industrial boilers and kilns, especially cement kilns, are sometimes used for thermal treatment of hazardous wastes.

2.18.2 LCI Modeling

- Functional unit: 1 lb. of incinerated hazardous waste
- System boundaries: Hazardous waste incineration involves the following steps: (1) hazardous waste processing (which includes screening, size reduction, and waste mixing); (2) combustion; (3) air pollution control (measurement to collect or treat products of incomplete combustion, particulate emissions, and acid gases); and (4) solids removal and disposal (Figure 22).

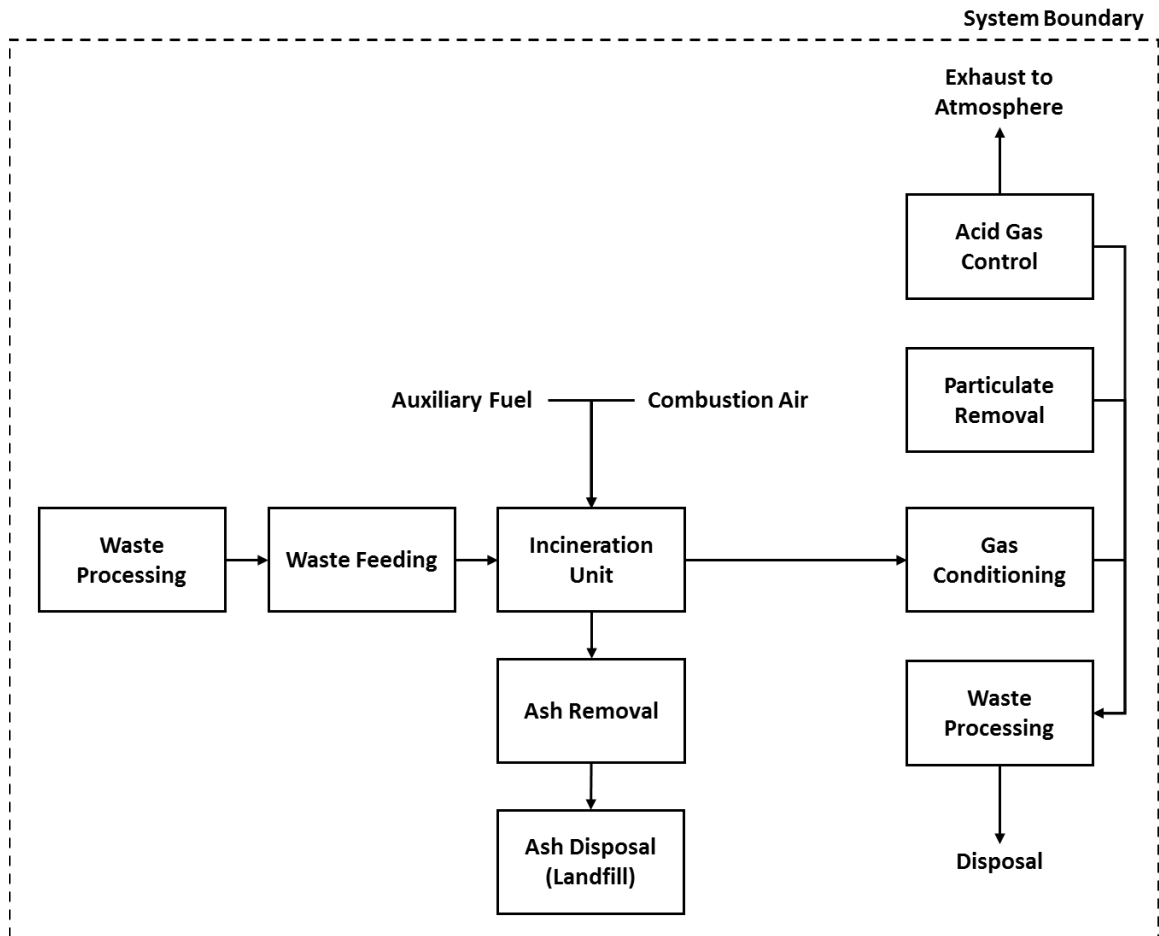


Figure 22. Simplified Diagram of Hazardous Waste Incineration as reported by (BCC Research, 2015)

- Inventory data: “disposal, hazardous waste, 25% water, to hazardous waste incineration – CH”, ecoinvent 2.2, (Doka, 2009).

2.18.3 Emission Factors

- Emission Factor Calculation Results

Table 18. SEFA Emission Factors for Hazardous Waste Incineration

Chemical/Material	CED (MMBtu/lb)	GWP100 (lb CO ₂ e/lb)	HAPs (lb/lb)	NO _x (lb/lb)	PM10 (lb/lb)	SO _x (lb/lb)	Water Use (gals/lb)
Hazardous Waste Incineration	6.09E-03	2.43E+00	8.70E-05	1.60E-03	2.09E-04	1.67E-03	3.77E+00

2.19 SEFA Material Emission Factor Update Summary

Table 19. A Summary of Emission Factors Derived for the SEFA Material Update

Chemical/Material/Process	Unit	Energy Used MMBtu	GHGs Emitted lb CO2e	HAPs Emitted lb	NOx Emitted lb	PM10 Emitted lb	SOx Emitted lb	Water Used gals	Source(s)
Aluminum, Rolled Sheet	lb	6.33E-02	9.15E+00	1.02E-03	1.48E-02	8.80E-03	2.83E-02	2.78E+01	(Classen, Althaus et al. 2009)
Asphalt, mastic	lb	4.12E-02	8.50E-01	1.07E-03	2.71E-03	7.66E-04	7.98E-03	5.46E-01	(Jungbluth, Chudacoff et al. 2007)
Asphalt, paving-grade	lb	5.00E-01	8.58E+00	1.33E-02	2.99E-02	9.10E-03	9.69E-02	3.88E+00	(Jungbluth, Chudacoff et al. 2007)
Ethanol, Corn, 95%	lb	3.18E-02	-1.99E-02	8.46E-05	4.25E-03	4.69E-04	3.03E-03	4.32E+00	(Kellenberger, Althaus et al. 2007)
Ethanol, Corn, 99.7%	lb	3.24E-02	5.91E-02	8.70E-05	4.31E-03	4.72E-04	3.10E-03	4.35E+00	(Doka 2009)
Ethanol, Petroleum, 99.7%	lb	2.05E-02	1.25E+00	5.89E-05	1.99E-03	2.77E-04	2.14E-03	4.16E+00	(Hischier 2007; PlasticsEurope 2014)
Granular activated carbon, primary	lb	3.56E-02	4.82E+00	6.57E-04	7.93E-02	9.87E-04	1.28E-01	1.53E+00	(USEPA 2010)
Granular activated carbon, regenerated	lb	8.73E-03	1.70E+00	6.71E-04	7.33E-03	8.86E-04	1.29E-02	1.20E+00	(USEPA 2010; He 2012)
Gravel/Sand Mix, 65% Gravel	lb	2.48E-05	2.40E-03	3.08E-07	1.80E-05	2.61E-06	4.52E-06	1.71E-01	(Kellenberger, Althaus et al. 2007)
Hazardous Waste Incineration	lb	6.09E-03	2.43E+00	8.70E-05	1.60E-03	2.09E-04	1.67E-03	3.77E+00	(Kellenberger, Althaus et al. 2007)
High Density Polyethylene	lb	3.32E-02	1.94E+00	6.41E-05	3.25E-03	4.39E-04	4.09E-03	3.88E+00	(Eurobitume 2012; Athena 2005)
Hydrogen Peroxide, 50% in H2O	lb	9.79E-03	1.19E+00	6.29E-05	1.42E-03	3.08E-04	2.40E-03	2.35E+01	(Sutter 2007)
Iron (II) Sulfate	lb	1.47E-03	1.67E-01	2.30E-05	3.16E-04	1.03E-04	5.89E-04	7.44E-01	(Althaus, Chudacoff et al. 2007)
Lime, Hydrated, Packed	lb	2.06E-03	7.62E-01	6.57E-06	5.13E-04	1.30E-04	3.58E-04	2.94E-01	(Hischier 2007; PlasticsEurope 2015)
Phosphoric Acid, 70% in H2O	lb	6.70E-03	8.82E-01	1.63E-04	2.82E-03	1.71E-03	2.94E-02	1.61E+01	(Marceau, Nisbet et al. 2006)
Polyvinyl Chloride	lb	2.62E-02	2.02E+00	3.75E-04	4.00E-03	3.72E-04	2.74E-03	5.79E+01	(Classen, Althaus et al. 2009)
Portland cement, US average	lb	1.39E-02	1.34E+00	9.70E-04	6.54E-03	3.78E-03	1.04E-02	7.73E-01	(Bhargava and Sirabian 2013; He 2012; USEPA 2010)
Potassium Permanganate	lb	9.81E-03	1.16E+00	1.22E-04	2.34E-03	4.22E-04	3.20E-03	7.45E+00	(Marceau, Nisbet et al. 2006)
Ready-mixed concrete, 20 MPa	ft3	2.17E-01	1.95E+01	1.41E-02	9.75E-02	5.70E-02	1.54E-01	3.32E+01	(Bhargava and Sirabian 2013; He 2012; USEPA 2010)
Round Gravel	lb	2.48E-05	2.40E-03	3.08E-07	1.80E-05	2.61E-06	4.52E-06	1.71E-01	(Kellenberger, Althaus et al. 2007)
Sand	lb	2.48E-05	2.40E-03	3.08E-07	1.80E-05	2.61E-06	4.52E-06	1.71E-01	(Kellenberger, Althaus et al. 2007)
Sodium Hydroxide, 50% in H2O	lb	9.77E-03	1.09E+00	1.29E-04	1.94E-03	4.03E-04	3.52E-03	1.39E+01	(Althaus, Chudacoff et al. 2007)

3.0 Transportation and Onsite Equipment

3.1 Methodology

Emissions and activity factors were created by developing life cycle models that combined data from a variety of sources. Emission factors are in the form of emissions or energy use per gallon fuel consumed. The activity factors are used to relate fuel consumption to equipment or vehicle activity, and are in the form of activity per gallon fuel (e.g., hp-hr./gallon for on-site equipment). The designation of equipment and vehicle classes for which factors are provided was specified by the SEFA project team in Region 9 and OSWER.

The overall workflow for the calculation of the emission and activity factors is summarized in Figure 23. The details are described in the following sections.

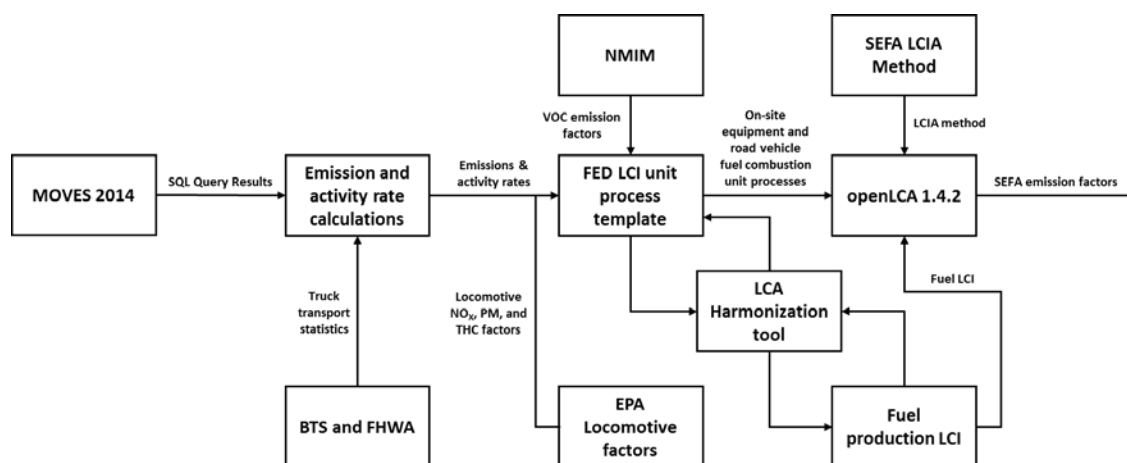


Figure 23. Workflow for SEFA emission and activity factor calculations.

3.1.1 Fuel Production and Distribution Data

A petroleum refinery and distribution model developed within EPA ORD's National Risk Management Research Laboratory and described in a peer-reviewed manuscript (Sengupta, Hawkins et al., 2015) was used as the primary source of data for developing emissions factors for conventional diesel, gasoline, and liquefied petroleum gas (LPG), which are all petroleum refinery co-products. This model includes a unique petroleum refinery process model based on national average emissions data. Original US data for distribution to a storage terminal and final dispensing station are included. These data are supplemented by upstream processes from the USLCI (NREL, 2008) for crude oil extraction and processes for other materials and infrastructure from the Ecoinvent 2.2 (Weidema & Hischier, 2012) databases. Electricity used at the refinery is based on another NRMRL LCI model described in Ingwersen et al (Ingwersen, Gausman et al., 2016). For compressed natural gas (CNG) fuels, which are not sourced from petroleum, we used USLCI natural gas processes to describe natural gas production and refining and estimated electricity consumption required to compress the gas. CNG compression energy was assumed to be 2% of the inherent energy content of the fuel and electricity was assumed to be the energy source (Sinor, 1992). The CNG and LPG processes do not include transportation processes between the manufacturer and the point-of-sale, but based on analysis of petroleum life cycles these stages are not expected to play a

significant role in life cycle emissions (Vineyard & Ingwersen, 2015), so the expected effects on results are negligible.

3.1.2 MOVES Model Runs for On-site Equipment and Transport Data

Data for creating the on-site equipment and transportation data were derived primarily from the Motor Vehicle Emission Simulator model (USEPA, 2014c), a model constructed and maintained by the United States Environmental Protection Agency's Office of Transportation and Air Quality. MOVES runs were performed to gather data on projected emissions for the average fleet performance for 2015, both in onroad and nonroad (on-site) applications. A MOVES RunSpec was set up to specify application type (onroad/nonroad), vehicle class (vehicle weight and fuel type) for onroad or engine specifications (equipment category, fuel type, horsepower, number of strokes) for nonroad, calculation type (inventory/emission rate), geographic scale, time scale, source use, data aggregation options (see Supporting Data). The onroad runs were all set to aggregate emissions quantities annually on a national scale for the year 2015. Nonroad runs in MOVES 2014 are based on the incorporation of a limited version of the EPA NONROAD 2008 model that only calculates emissions on a per day basis. For onroad, personal transport vehicles were captured in one run, which included all passenger cars and passenger trucks using gasoline or diesel fuel. Light commercial trucks were in a separate run, but were used to represent the LHD and MHD diesel pickup trucks used for personal transport. Additionally, there were runs for heavy duty trucks (combination, and single-units trucks). The nonroad emissions were generated using a single MOVES NONROAD run for typical equipment in the Construction and Industrial categories.

The output tables for MOVES simulations were generated as MySQL databases, from which the specific data desired was extracted using MySQL queries. The MOVES output contained emission data described with a series of identification codes for such things as pollutant type, equipment classification, day of the week, and month of the year. As part of the querying process, identification coding data from a run output table were used to extract corresponding descriptors from the default MOVES2014 input tables so that a custom output table could be created that displayed quantities and names instead of ID numbers. The output of the queries were saved as CSV files and imported into a spreadsheet where they were further processed and aggregated.

Given the nonroad runs generated emissions in terms of a typical weekday or weekend within each month of the year, annual emission quantities were obtained by first calculating the emissions for an average day within a month by multiplying the weekday value by 5/7 and the weekend value by 2/7 and summing the two values together. Each average daily value for a month was then multiplied by the number of days reported for that month in the MOVES NONROAD input tables to obtain the average monthly emissions. Finally, the average monthly emissions were summed across a year to obtain the annual emission rate. This method was based on instructions from the EPA MOVES team (E.E. Glover, personal communication, September 2, 2015).

For the returned nonroad results generated by MOVES, an additional carbon (C) mass balance check and filtering of records was performed after it was noted that C balance was not preserved in all cases. The fuel C content is reported in the MOVES database for each fuel type. It was assumed the total C in the emissions was made up of >99% from CO₂ and CO. Thus, the total C contained in CO₂ and CO should sum approximately to the fuel C (mass balance constraint). Based on this assumption, the total mass of carbon in the emissions per kg of fuel consumed was calculated for the various horsepower ranges and compared to the C in the fuels based using the following equations.

$$C \text{ Mass Balance} = \frac{C_{emissions} / \text{Fuel Ratio}}{C_{expected} / \text{Fuel Ratio}} \quad [1]$$

$$C_{emissions} = \frac{[CO_2] \times \left(\frac{12 \text{ kg C}}{44 \text{ kg CO}_2} \right) + [CO] \times \left(\frac{12 \text{ kg C}}{28 \text{ kg CO}} \right)}{[BSFC]} = \frac{\text{kg C}}{\text{kg Fuel}} \quad [2]$$

$$C_{expected} = \text{carbonContent} \left(\frac{\text{kg C}}{\text{MJ of Fuel Energy}} \right) \times \text{energyContent} \left(\frac{\text{MJ of Fuel Energy}}{\text{kg Fuel}} \right) = \frac{\text{kg C}}{\text{kg Fuel}} \quad [3]$$

where, BSFC is the MOVES output for fuel consumption in kg.

The C mass balance ratio was found to deviate >20% from the expected value of one for a number of equipment classes. Due to these discrepancies, only the equipment classes that met mass balance criteria were factored into the calculation of emission and activity factors reported here. For diesel, 4-stroke gasoline, and compressed natural gas engines, the only equipment classes with C mass balance within 5% of the expected values were used. For 2-stroke gasoline engines, this had to be expanded to values within 10% to capture any equipment, and for liquefied petroleum gas equipment it was expanded to values within 15%. A weighted average by hp-hr. was then performed for the average emission and activity factors for each equipment class.

3.1.3 Additional Calculations for On-site Equipment and On-road Vehicles

MOVES reports total PM_{2.5} and PM₁₀. Since PM₁₀ emission quantities include particles ≤ 2.5 μm (PM_{2.5}), the quantity of just PM₁₀ was included in the PM factors developed to avoid double counting.

For nonroad processes, only nine emissions are reported by MOVES, and these do not include the specific volatile organic compounds (VOCs), some of which are EPA hazardous air pollutants. The Total Gaseous Hydrocarbons (THC) reported in MOVES was used to calculate the emission factors for specific volatile organic compounds (VOCs) using specific VOC/THC factors (e.g., xylene/THC) from the National Mobile Emissions Model (USEPA, 2015a).

Locomotive emissions factors for PM, THC, and NO_x were derived from a 2009 EPA report “Emission factors for locomotive engines” (USEPA, 2009). Factors for other emissions including CO₂, SO₂, and HAP were adapted from the emission factors developed for the largest diesel engine class (>1200 hp) in the nonroad model.

The truck activity factors in ton-miles cargo transported/gallon were estimated from national statistics and the MOVES fuel economy values as described below.

The Bureau of Transportation Statistics reported total truck ton-miles and fuel consumption for 2011, but these statistics were not provided specifically for combination trucks (class 8) and single-unit trucks (class 6-7). Combination truck and single-unit truck ton-mile/gal factors were then estimated as proportional to the gross weights (tons carried plus vehicle weights) and total miles traveled that were reported from an earlier date (2002). The following equations were used to make these calculations:

$$CT_{tmg} = pST_{tmg} \quad [4]$$

$$T_{tmg} = CT_{gtmg} + ST_{gtmg} \quad [5]$$

$$CT_{gtmg} = \frac{CT_{gt} * CT_{vmt}}{CT_{gal}} \quad [6]$$

$$ST_{gtmg} = \frac{ST_{gt} * ST_{vmt}}{ST_{gal}} \quad [7]$$

CT_{tmg} = Combination truck ton-mile/gallon
 ST_{tmg} = Single unit truck ton-mile/gallon
 p = Combination truck gross ton-mile/gallon/short ton-mile gallon
 T_{tmg} = Total truck ton-miles/gallon.
 CT_{gtmg} = Combination truck gross ton-mile/gallon
 ST_{gtmg} = Single unit truck gross ton-mile/gallon
 CT_{gt} = Combination truck gross tons
 ST_{gt} = Single unit truck gross tons
 CT_{vvt} = Combination truck vehicle miles traveled
 ST_{vmt} = Single unit truck vehicle miles traveled
 CT_{gal} = Combination truck gallons consumed
 ST_{gal} = Single unit truck gallons consumed

T_{tmg} was provided by the combination of BTS (ton-miles) and FHWA(gallons) (BTS, 2015; FHWA, 2015). Gross weights and vehicle miles traveled for the two trucks types were provided for combination and short trucks by the BTS (BTS, 2015). The same sources provided the ton-mile/gallon ratio for freight, but no breakdown of into subtypes was necessary.

3.2 Modeling in the Federal LCI Data Template and openLCA

Data from the above sources were compiled into life cycle inventory (LCI) unit processes using the current EPA version of the Federal LCI unit process template. All chemical emission names, categories and units were

harmonized using the Beta 1 version of the LCA Harmonization Tool (Ingwersen, Transue et al.). The Excel® to OLCA program was then used to import the unit processes into an openLCA 1.4.2 database. Models were compiled and managed in the open-source life cycle assessment software OpenLCA 1.4.2 (GreenDelta, 2015). An openLCA “product system” was made from each unit process model. The product systems were further imported into their respective openLCA “Projects” from which results were calculated by creating project reports. Report results were copied into the final master dataset spreadsheet file.

3.3 Emission Factor Results for Vehicles and Equipment

3.3.1 Dataset File

The full dataset is available upon request in the file “Fuel, Equipment and Transport Emission and Activity Factors for SEFA.xlsx.” The resulting factors are summarized in Section 1.1.

3.3.2 Supporting Data

The following files are available as supporting data to the dataset and are available upon request. These include:

File name	Description
SEFAfuelquiptransportfactors.zolca	openLCA database
SEFAfuelquiptransportfactors_templates.zip	The Federal LCI unit process templates
SEFAfuelquiptransportfactors_MOVESrunspecs.zip	MOVES 2014 run file
SEFAfuelquiptransportfactors_MOVESsqlresults.zip	SQL queries for MOVES output databases
SEFAfuelquiptransportfactors_supportingExcel.zip	Results of SQL queries and emissions data processing for Fed LCI template incorporation

3.4 SEFA Vehicle and Equipment Emission Factory Summary

Table 20. Summary of SEFA Emission Factors for Vehicle and Equipment Operations

Item or Activity			Emission Factors						Activity Factors	
			Energy	GHG	NOx	SOx	PM	HAPs	Factor	Value
			Used	Emitted	Emitted	Emitted	Emitted	Emitted		
	Fuel	Unit	MMBtu	lbs CO2e	lbs	lbs	lbs	lbs		
Fuels upstream¹, except where noted										
Fuel production and distribution to retail	Diesel	gal	0.156	3.02	0.0051	0.0062	0.0017	0.0011	NA	
Fuel production and distribution to retail	Gasoline	gal	0.157	2.80	0.0046	0.0050	0.0015	0.0010	NA	
Fuel production and distribution to retail	Liquefied Petroleum Gas	gal	0.088	1.47	0.0016	0.0024	0.0007	0.0003	NA	
Fuel production and distribution to retail	Compressed Natural Gas ²	ccf	19.983	343.92	0.4732	2.1651	0.1846	0.2895	NA	
On-site equipment use³										
equipment operation, < 25 hp	Diesel	gal	NA	22.20	0.170	0.00015	0.016	0.00004	hp-hr./gal	16.4
equipment operation, > 25 hp and < 75 hp	Diesel	gal	NA	22.22	0.143	0.00014	0.013	0.00004	hp-hr./gal	16.3
equipment operation, > 75 hp and < 750 hp	Diesel	gal	NA	22.24	0.101	0.00013	0.009	0.00004	hp-hr./gal	18.2
equipment operation, > 750 hp and < 1200 hp	Diesel	gal	NA	22.24	0.157	0.00013	0.006	0.00004	hp-hr./gal	18.8
equipment operation, > 1200 hp	Diesel	gal	NA	22.24	0.141	0.00013	0.006	0.00004	hp-hr./gal	18.8
equipment operation, < 25 hp	Gasoline	gal	NA	17.48	0.037	0.00025	0.165	0.00008	hp-hr./gal	0.0002
equipment operation, > 25 hp and < 75 hp	Gasoline	gal	NA	19.93	0.032	0.00029	0.002	0.00009	hp-hr./gal	12.9
equipment operation, > 75 hp and < 750 hp	Gasoline	gal	NA	19.93	0.032	0.00029	0.002	0.00009	hp-hr./gal	12.9
equipment operation, > 25 hp and < 75 hp	Liquefied Petroleum Gas	gal	NA	12.69	0.021	0.00013	0.001	0	hp-hr./gal	10.4
equipment operation, > 75 hp and < 750 hp	Liquefied Petroleum Gas	gal	NA	12.69	0.021	0.00013	0.001	0	hp-hr./gal	10.4

			Emission Factors						Activity Factors	
			Energy Used	GHG Emitted	NOx Emitted	SOx Emitted	PM Emitted	HAPs Emitted	Factor	Value
Item or Activity	Fuel	Unit	MMBtu	lbs CO2e	lbs	lbs	lbs	lbs		
equipment operation, > 25 hp and < 75 hp	Compressed Natural Gas	ccf	NA	1953.25	16.153	0.02299	0.281	0	hp-hr./ccf	2031.0
equipment operation, > 75 hp and < 750 hp	Compressed Natural Gas	ccf	NA	1962.42	15.912	0.02310	0.274	0	hp-hr./ccf	2031.0

Personal Transport³										
passenger car, gasoline	Gasoline	gal	NA	19.77	0.027	0.00036	0.003	0.00670	miles/gal	25.0
passenger car, diesel	Diesel	gal	NA	22.57	0.015	0.00020	0.003	0.00252	miles/gal	28.4
passenger car, fleet average	Gasoline/diesel mix	gal	NA	19.79	0.027	0.00036	0.003	0.00668	miles/gal	25.0
passenger truck, gasoline	Gasoline	gal	NA	19.79	0.035	0.00036	0.003	0.00661	miles/gal	18.9
passenger truck, diesel	Diesel	gal	NA	22.54	0.055	0.00020	0.006	0.00244	miles/gal	15.1
passenger truck, fleet average	gasoline/diesel mix	gal	NA	19.85	0.036	0.00036	0.003	0.00655	miles/gal	18.8
work truck, LHD and MHD	Diesel	gal	NA	22.55	0.062	0.00020	0.008	0.00277	miles/gal	15.7
Transport of Goods and Services^{3, except where noted}										
combination truck	Diesel	gal	NA	22.53	0.122	0.00020	0.011	0.00205	ton-mile/gal	65.2 ^{4,5}
single-unit truck	Diesel	gal	NA	22.52	0.088	0.00020	0.012	0.00196	ton-mile/gal	31.0 ^{4,5}
freight train	Diesel	gal	NA	25.26	0.307 ⁶	0.00634	0.009 ⁶	0.00444 ⁶	ton-mile/gal	465.1 ^{4,5}

Notes. LHD = Light-heavy duty; MHD = Medium-heavy duty; NA = not applicable.

The number of decimal places presented is for presentation purposes but the precise number of significant figures could not be determined due to the use of numerous data sources where these were not reported.

Sources: (1) Sengupta et al. 2014 (2) NREL 2008 (3) USEPA 2014c (4) BTS 2015 (5) FHWA 2015 (6) EPA 2009

4.0 Conclusions

The material and chemical emission factors developed in this report provide a reasonable estimate for conducting site-based environmental footprint analyses that account for upstream emissions. The EmFs were derived from currently available life cycle inventory datasets developed for commercial databases, industry trade associations, and scholarly publications. The advantage of such sources is they provide datasets that have undergone more review to increase their reliability. Although the datasets are suitable for current use, future work should focus on replacing EmFs based on European datasets with data more consistent with US conditions. This may include the need to include global datasets to reflect importation of materials.

The vehicle and equipment emission factors constitute a significant contribution to improving the performance of SEFA. For the first time, numerous vehicle and equipment options have been modeled using a consistent approach based on emission profile simulations using US EPA's MOVES model. The approach presented in this report is easily reproducible and will make future updates to the factors much more feasible and manageable. The resulting EmFs provide adequate coverage for most vehicle and equipment options associated with remediation sites. Further enhancement of SEFA based on these factors can be made during future updates to the workbooks by increasing the number of factors maintained and aggregating vehicles and equipment at finer resolutions. Uncertainty related to engine power could be reduced by further refining the horsepower category ranges and/or associated cutoff values.

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6.0 Appendix 1 - Hazardous Air Pollutants included in openLCA

1,1,1-trichloroethane	chlorobenzene	naphthalene
1,1,2,2-tetrachloroethane	chloroethene	nickel (II)
1,1,2-trichloroethane	chloroform	nickel and nickel compounds
1,2,4-trichlorobenzene	chromium (III)	nitrobenzene
1,2-dichloroethane	chromium (VI)	o-anisidine
1,2-dichloropropane	chromium and chromium compounds	o-cresol
1,4-dichlorobenzene	cobalt (II)	o-toluidine
1,4-dioxane	cobalt and cobalt compounds	o-xylene
2,4,5-trichlorophenol	cobalt-60	PAH, polycyclic aromatic hydrocarbons
2,4,6-trichlorophenol	cresol	PCB-1
2,4-dinitrophenol	cumene	PCB-155
2,4-dinitrotoluene	cyanide and cyanide compounds	PCB-77 (3,3',4,4'-tetrachlorobiphenyl)
2-chloro-1-phenylethanone	dibenzofuran	p-cresol
3,3'-dimethoxybenzidine	dibutylphthalate	pentachlorophenol
4-aminobiphenyl	dichlorobenzene	phenol
4-methyl-2-pentanone	dichloromethane	phosphine
4-nitrophenol	diethanolamine	phosphorus
acetaldehyde	dimethyl formamide	plutonium-238
acetamide	dimethyl sulfate	plutonium-alpha
acetonitrile	dimethylphthalate	polychlorinated biphenyls
acetophenone	dioxins (as 2,3,7,8-tetrachlorodibenzo-p-dioxin)	propanal
acrolein	dioxins and furans, unspecified	propylene oxide
acrylic acid	epichlorohydrin	p-xylene
acrylonitrile	ethyl acrylate	radium-226
aniline	ethylbenzene	radium-228
antimony (III)	ethylene glycol	radon-220
antimony and antimony compounds	ethylene oxide	radon-222
arsenic (V)	formaldehyde	selenium
arsenic (III)	hexachlorobenzene	selenium (IV)
arsenic and arsenic compounds	hexachloroethane	styrene
arsine	hexane	t-butyl methyl ether
asbestos	hydrazine	tetrachloroethene
benzene	hydrogen chloride	tetrachloromethane
benzidine	hydrogen fluoride	thorium-228
benzyl chloride	hydroquinone	thorium-230
beryllium	iodine-129	thorium-232
beryllium (II)	iodine-131	thorium-234
biphenyl	iodine-133	toluene
bis(2-chloroethyl)ether	iodine-135	trichloroethene
bromoform	lead (II)	triethyl amine
bromomethane	lead and lead compounds	trifluralin
butadiene	manganese and manganese compounds	uranium
cadmium	mercury (II)	uranium-234
cadmium (II)	mercury and mercury compounds	uranium-235
carbon disulfide	methanol	uranium-238
catechol	methyl methacrylate	uranium-alpha
cesium-137	methylhydrazine	vinyl acetate
chlorine	monochloroethane	xylene
chloroacetic acid	m-xylene	

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