Environmental Life-Cycle Inventory of Detergent-Grade Surfactant Sourcing and Production

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Life-cycle inventories were compiled to characterize natural resource requirements and environmental emissions associated with the sourcing and production of selected, detergent-grade surfactants and surfactant feedstocks. Petrochemical surfactant types examined were linear alkylbenzene sulfonate, alcohol sulfate (AS), alcohol ethoxylate (AE) and alcohol ethoxylate sulfate (AES). Oleochemical surfactants derived from palm oil, palm kernel oil and inedible tallow were AS, AE, AES and (for palm oil and tallow) methyl ester sulfonate. It was determined that natural resource requirements were primarily related to the source of feedstock and secondarily to surfactant type. Likewise, the composition and mass of atmospheric, aqueous and solid emissions were principally determined by feedstock source. Energy requirements varied as a function of both feedstock and surfactant type. The inventories do not support fundamental shifts in surfactant usage or feedstock sourcing on the basis of environmental concerns, as no single surfactant or feedstock was identified as superior across all resource and emissions criteria examined. The data provide baselines for evaluating opportunities for resource optimization, pollution prevention and waste minimization within each production technology surveyed.

KEY WORDS: Detergent, environment, life-cycle, palm oil, petrochemical, surfactant, tallow.

Detergent-grade surfactants are produced from selected oleochemical and petrochemical feedstocks through globally integrated sequences of chemical processing (Table 1). Corporations specializing in distinct technology areas interact through international markets to produce surfactants for eventual formulation in consumer products. Sound longterm economic management strategies dictate that surfactant feedstocks and energy resources are efficiently used and that industrial operations, by-products and emissions are safe. In the face of increasing global pressures on natural resources and the environment, detailed understanding of the raw-material requirements, energy demands and emissions of an international chemical technology such as surfactant production is essential to meet the demands of sustainable development.

Life-cycle analysis can contribute uniquely to this understanding by providing a global perspective to resource usage and environmental emissions of surfactant production. Lifecycle analysis is an objective accounting procedure to systematically inventory and evaluate the environmental aspects of a product, package, system or process. Synonymous with "ecobalance" or "cradle-to-grave assessment," life-cycle analysis has been described as a three-component process (1). Initially in the life-cycle inventory (LCI), raw materials, energy and environmental emissions to air, land and water are quantified per unit volume or mass of the item studied. Objective procedures for accomplishing the final two components, the life-cycle impact and improvement analyses,

TABLE 1

Feedstock Conversions in Detergent-Grade Surfactant Production

Feedstock	First intermediate(s)	Second intermediate(s)	Surfactant
Palm and palm kernel oils	Fatty acid methyl esters	Alcohols	AS, AE, AES ^{a,b}
	Fatty acid methyl esters	(None)	MES^b
Animal fat (tallow)	Fatty acid methyl esters	Alcohols	AS, AE, $AES^{a,b}$
	Fatty acid methyl esters	(None)	MES^b
Natural gas	Ethylene and methanol	Olefins and alcohols	AS, AE, AES^a
Petroleum	Aromatics and paraffins	Alkylbenzene	Linear alkylbenzene sulfonate
	Ethylene	Olefins and alcohols	AS, AE, AES^a

 a Ethylene oxide for alcohol ethoxylate (AE) and alcohol ethoxylate sulfate (AES) sourced from natural gas or petroleum. AS, alcohol sulfate.

^bMethanol for fatty acid methylation sourced from natural gas. MES, methyl ester sulfonate.

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are not as well developed (1). Accordingly, the focus of this paper will be the LCI.

The Procter & Gamble Company commissioned Franklin Associates, Ltd. (FAL; Prairie Village, KS) to develop a series of LCI's characterizing the sourcing and production of selected petrochemical and oleochemical surfactants. The objective of these studies was to compile natural resource and emissions data representative of current, industry-wide practices used in the production of surfactants from petrochemical (*i.e.*, derived from petroleum and natural gas) and oleochemical feedstocks (*i.e.*, from palm and palm kernel oils and from animal fats).

A range of anionic and nonionic surfactants with unique performance characteristics were examined within each feedstock category. The compounds differ broadly in chemical structure and related physical properties critical to manufacturing efficient and well-performing detergent products. The surfactants also differ significantly in economic value and availability on global markets. It should not be inferred that the surfactants chosen for study are functionally interchangeable or available in volumes required to meet global market demands.

Life-cycle studies are not designed to provide detailed chemical fate and effects information sufficient to assess the environmental safety of the surfactants themselves or the emissions generated in their manufacture. Compound-specific data related to chemical fate, toxicity and environmental exposures of surfactants are available (2). It remains the responsibility of those public and private institutions involved in each stage of a surfactant's life-cycle (*i.e.*, raw material sourcing, manufacturing, transportation, consumer use and disposal) to ensure safe manufacturing and disposal practices.

With these considerations, broad application of these studies is possible. They can serve as quantitative baselines for chemical producers and manufacturers alike to assess environmental consequences of potential process changes. They can provide guidance in pollution prevention programs to identify waste reduction and resource conservation opportunities. They can inspire joint involvement of public and private institutions in initiatives to address issues of mutual concern, particularly those of global scale. These applications of LCI effectively complement environmental safety and pollution prevention programs within integrated environmental quality strategies.

METHODS

Methods for estimating raw materials, energy and emissions of the surfactants studied followed procedures developed by FAL (3). The production of each surfactant was initially defined as a sequence of discrete operations (e.g., petroleum or natural gas procurement, refinery operations) for which relevant process data were independently compiled. Process data (raw material/energy requirements, environmental emissions) were then integrated over the production sequence by proportionally weighting the material contributions of each operation to the production of 1000 kg finished surfactant. Energy and emissions calculations were based upon databases compiled by FAL and summarized in the study reports. Process data and key assumptions regarding each operation examined are summarized in the following section.

Study scope. Production sequences of the surfactants

studied included feedstock procurement and refining, intermediate processing, material transport and final processing prior to formulation in a detergent product. The feedstock procurement operations evaluated began with the acquisition of raw materials from the earth, *i.e.*, drilling and refining of petroleum and natural gas; oil palm agriculture; fertilizer manufacture and raising corn to support livestock. Energy and emissions estimates included those expended in the acquisition of energy sources ("precombustion" energy and emissions; (3)) and those directly consumed or generated in an operation ("combustion" energy and emissions).

Surfactant production sequences were evaluated through the delivery of finished surfactants to detergent manufacturing plants. Subsequent consumer use and disposal were not within the scope of this study. Following conventions of FAL (3), neither energy and emissions related to the manufacture of capital equipment (e.g., drilling rigs, boilers, etc.) were considered, nor energy and emissions associated with administrative and manual labor needs (e.g., driving to a work-site) were examined.

An industrial operation often generates multiple coproducts. Raw materials, energy and emissions were allocated among co-products on an output weight basis, regardless of the operation's purpose or the co-products' economic values (3). Co-products in this study were defined as materials resulting from the same operation having current and routine application for purposes other than surfactant production (e.g., wood ashes used as fertilizer, petroleum coke used in iron ore processing). Emissions were classified as material not subsequently used and which are routinely released to the environment following typical treatment and disposal practices.

Technical process data from private corporations were contributed by a minimum of three chemical producers for each surfactant type studied (see Acknowledgments) and were averaged by FAL. FAL maintained sole access to the primary data and confidentially calculated industry averages of raw materials, energy and emissions data. This ensured that the proprietary rights of the study's contributors would not be compromised.

Feedstocks and surfactants. Surfactants from three feedstock classes were examined: (i) petrochemical surfactants derived from fossil fuels (petroleum and natural gas); (ii) oleochemical surfactants derived from palm and palm kernel oils; and (iii) oleochemical surfactants derived from animal fats (inedible tallow from cattle and white grease from hogs) (Table 1). Petrochemical surfactants examined were linear alkyl(docecyl)benzene sulfonate (LAS); C12-15 alcohol sulfate (AS); C12-15 alcohol ethoxylate (AE) with an ethoxylate molar ratio (average number of ethylene oxide units contained within the surfactant molecule) of three; and C12-15 alcohol ethoxylate sulfate (AES) with the same alcohol derivation and ethoxylate ratio.

Surfactants derived from palm and palm kernel oils possess characteristic alkyl chainlengths of C16-18 and C12-14, respectively. Palm oil surfactants examined were C16-18 AS, AE with an ethoxylate molar ratio of 7.9, AES (same ethoxylate ratio) and methyl ester sulfonate (MES). Palm kernel oil surfactants were AS, AE with an ethoxylate ratio of 3, and the corresponding AES (same ethoxylate ratio). The origin of ethoxylated surfactants (AE and AES) was distinguished solely on the basis of the feedstock used to produce the alcohol, as petrochemical sourcing of ethylene oxide was assumed for all ethoxylated surfactants. The tallow surfactants studied were AS, AE, AES and MES, each of which was assumed to have the same alkyl chainlength as the palm oil surfactants.

Energy estimation procedures and assumptions. Consistent with FAL methodology (3), energy requirements for surfactant sourcing and production were distinguished among three categories: transportation energy, process energy and material resource energy. Calculations of fuel energies from alternative sources and energy required for fuel production and for material transport were based upon FAL databases. These were compiled and are updated largely from U.S. government sources. The same energy data and assumptions were applied to all feedstocks and surfactants examined.

Transportation energy was calculated as the energy required per metric ton-kilometer to transport raw materials, process intermediates and finished surfactants. Energy estimates considered efficiency of transport and fuel type. Representative shipment weights and distances were estimated from producer data, assuming final delivery to a manufacturing location in the midwestern U.S.

Process energy required for nontransport-related industrial operations (e.g., heating, cooling, mixing, pumping) included fuels combusted on-site for utility heating (*i.e.*, steam generation) and the consumption of electrical power generated off-site. Electrical power requirements for each operation were converted to average fuel volumes from U.S. utility industry data (3) and included losses during power transmission to processing sites.

Material resource energy was estimated as the energy equivalence of fossil fuel-derived feedstocks conventionally used as fuel sources. This energy calculation is a convention of FAL pertaining only to fossil fuel-derived feedstocks. It should not be confused with the thermodynamic energy content of the surfactants. Calculations were made by identifying fossil fuel-derived moieties of a surfactant molecule, determining volumes of fossil fuel(s) required for their syntheses and estimating their energy contents. In this study, material resource energy expenditures were estimated for petroleum and natural gas used to synthesize hydrocarbons in petrochemical surfactants, natural gas used to synthesize methanol for methyl esters derived from palm/palm kernel oils and tallow, and for natural gas and petroleum used in ethylene oxide production for ethoxylated surfactants (AE and AES).

Emissions estimation procedures and assumptions. Process and fuel-related emissions released to air, water and land from each operation were calculated by procedures of FAL (3) and totaled for this paper. Process emissions were those resulting directly from agricultural or industrial operations excluding energy usage. Fuel-related emissions included the procurement and consumption of fuels used as energy sources in both transportation and plant operations.

The composition of process emissions from each operation were characterized to the level of detail commensurate with the data received. Data were drawn from a variety of sources, including process and safety monitoring reports, regulatory audits and waste treatment process evaluations. Therefore, categories of emissions as surveyed by FAL reflect the format and constraints of the original datasets. Specific identification of compounds contained within a given emission or their environmental concentration was frequently not included in the original data sources.

Fuel-related emissions were calculated using FAL historical data bases on fuel combustion, categorized by the following: type of fuel (e.g., residual and distillate oils, coal, natural gas, gasoline, diesel fuel, biomass); means of combustion (e.g., utility and industrial boilers, internal combustion engines); mode of transport (e.g., diesel truck, rail, barge, ocean tanker, pipeline) and efficiency of treatment. Treatment practices assumed application of conventional emission control practices representative of U.S. and Malaysian conditions.

Process data and assumptions. Process data for production operations examined by FAL are summarized in Tables 2-4. Raw materials, energy and emissions were estimated independently for discrete operations and are expressed on the basis of 1000 kg output from each. Technical descriptions of the operations and key assumptions required in compiling the data are provided below.

(i) Petrochemical feedstock procurement and processing. Process data related to the procurement and processing of petroleum and natural gas for feedstocks and energy included the following operations: drilling, pumping and separation of crude oil from brine water, tank storage and transport by ocean tanker or pipeline (Table 2). Crude oil production was assumed to be acquired from 60% domestic (25% Alaska, 75% U.S. Gulf Coast) and 40% from Middle Eastern sources, with 25% of the natural gas being co-produced with crude oil. Losses of 35 kg crude oil and 10 kg natural gas per 1000 kg recovered were assessed to account for spills and valve leakage during procurement. Aqueous emissions were attributed to surface discharges of oiled brinewater from marine drilling platforms (4). Atmospheric emissions were primarily attributed to losses during transmission and unflared venting (5).

Refinery operations included distillation, desalting, hydro-treating and fractionation of crude oil into 67%paraffin and 33% aromatic (benzene) streams (Table 2). A net loss of 10 kg per 1000 kg refined oil was assumed. Data for thermal cracking of petrochemical feedstocks (*e.g.*, ethane, propane, naphtha) to produce ethylene assumed an average feedstock distribution of 75% ethane/propane from natural gas and 25% naptha from crude oil. Ethylene yields from the ethane, propane and naphtha feedstocks were assumed to be 80, 45 and 35% respectively (6).

Linear alkylbenzene sulfonate. Linear alkylbenzene (LAB) production from benzene and paraffin is diagrammed in Figure 1 (upper segment). Process data were weighted for two commercial processes according to typical U.S. production practices as determined by FAL. Use of 75% hydrogen fluoride and 25% aluminum chloride as catalysts was assumed. Feedstock volumes were assumed to be the same for both processes. Production of 1000 kg benzene was estimated to require 1105 kg naphtha. Data shown for the LAB alkylation reaction (Table 2) include the preparation of paraffin from refined oil and the transport of feedstocks to LAB production facilities.

Process data for LAB sulfonation (Table 2) were averaged as a composite of conventional processes using

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TABLE 2

Raw Materials, Energy and Emissions Process Data for Discrete Operations Involved in Petrochemical Surfactant Production

Operation	Raw materials (kg/1,000 kg)	Energy ^a (MJ/1,000 kg)	Atmospheric emissions ^b (kg/1,000 kg)	Aqueous emissions ^b (kg/1,000 kg)	Solid wastes (kg/1,000 kg)
1. Crude oil procurement	Crude oil: 1,035 Water: 600	MR: 46,571 P: 499 T: 1435	Hyd: 4.7	DSol: 12.7 Oil: 0.16	0.6
Petroleum refining	Crude oil: 1,010 Water: 7,761	P: 875	Part: 0.06 Hyd: 0.3 SOX: 0.2 Alde: 0.04 NH ₃ : 0.02	BOD: 0.01 COD: 0.07 TSS: 0.01 O&G: 0.004 Phen: 0.0001 NH ₃ : 0.001 Cr: 0.0002	3.5
2. Natural gas (NG) procurement	NG: 1,038 Water: 225	MR: 54,143 P: 928	Hyd: 18.4	DSol: 0.16 O&G: 0.004	_
NG retining	NG: 1,022 Water: 2,345	P: 1,954 T: 300	Hyd: 10 SOX: 1.7	_	_
3. Linear alkylbenzene sulfonate (LAS) production					
Benzene production	Naphtha: 1,105 Water: 1,560	P: 6669 T: 88	SOX: 3.4 Hyd: 3.1 Alde: 0.05 NH ₃ : 0.06 Part: 0.35	BOD: 0.04 COD: 0.12 O&G: 0.02 Phen: 0.01 SSol: 0.07 Sulf: 0.01	1.0
Alkylation	Benzene: 320 Kerosene: 716 Water: 12,518	P: 16,960 T: 641	Hyd: 1.5 NOX: 0.7 CO: 0.18 Part: 0.05 HF: 0.05 Orgs: 0.08	BOD: 0.29 COD: 1.08 Oil: 0.05 SSol: 0.45 F: 0.003 Cr: 0.0001	12.8
Salt mining	Salt mineral: 1,036 Water: 2,670	P: 1,377 T: 916	_	_	36.0
NaOH production	Salt: 790 Water: 2,086	P: 26,216 T: 351	Cl: 4.1	_	80.0
Sulfur mining	Water: 6,676	P: 7,182 T: 1,422	Part: 10	_	205.0
Linear alkylbenzene (LAB) sulfonation	LAB: 710 Sulfur: 115 NaOH: 204 Water: 709	P: 8,048	CO: 0.02 Hyd: 0.02 NOX: 0.07 Part: 0.01 SOX: 0.42	BOD: 0.04 COD: 1.00 SSol: 3.6 DSol: 2.2	0.1
4. Alcohol sulfate production					
Ethylene production	NG: 750 Petroleum: 250 Water: 10,006	P: 19,938	Hyd: 0.48 Part: 0.04 SOX: 0.00 NOX: 1.3 CO: 0.26	BOD: 0.02 TSS: 0.03	2.1
Aluminum production	Petroleum: 418 Coal: 22 Water: 205,287	P: 18,508 T: 23,623	Hyd: 4 Part: 51 NOX: 1.8 CO: 95 SOX: 16.3 Alde: 0.03 NH ₃ : 0.04 HF: 2.1	BOD: 1.5 COD: 17.6 F: 3.1 DSol: 0.35 Oil: 0.39 SSol: 18.7 Acid: 0.04 Met: 0.5 CN: 0.03 NH ₃ : 0.55	3,314.6
Hydrogen production	NG: 200 Water: 1,669	P: 824	Hyd: 0.13 NH ₃ : 0.03	NH ₃ : 0.008	0.025
Alcohol production	Ethylene: 978 NG: 31 Hydrogen: 10 Aluminum: 3 Water: 684	P: 18,181 T: 886	Hyd: 2.7 Part: 0.01 NOX: 1.0 CO: 0.57	BOD: 0.01 TSS: 0.06 TDS: 3.1 TOC: 0.35	9.9
	·				(continued)

TABLE 2 (continued)

Operation	Raw materials (kg/1,000 kg)	Energy ^a (MJ/1,000 kg)	Atmospheric emissions ^b (kg/1,000 kg)	Aqueous emissions ^b (kg/1,000 kg)	Solid wastes (kg/1,000 kg)
Alcohol sulfation	Alcohol: 705 Sulfur: 108 NaOH: 100 Water: 1,552	P: 6,558 T: 1.004	Part: 0.02 SOX: 0.43	DSol: 8.1	1.1
5. Alcohol ethoxylate production Oxygen production	Water: 23,399	P: 3,714 T: 373	_		_
Ethylene oxide production	Ethylene: 810.9 Oxygen: 922.7 Water: 47,900	P: 8,660	Hyd: 7.2 Part: 0.003 SOX: 0.001 NOX: 0.24 CO: 0.04 VOC: 3.7	BOD: 1.6 COD: 2.7 SSol: 0.014 DSol: 0.11 Cr: 0.02 Acet: 0.05	12.1
Alcohol ethoxylation	Ethylene oxide: 387 Alcohol: 612	P: 2,057 T: 1,473	HYD: 0.04 NOX: 0.01 CO: 0.002 EO: 0.01	BOD: 1.03 SSol: 0.008 DSol: 0.034	4.9
6. Alcohol ethoxylate	Alcohol ethoxylate: 824	P 3.944	SOX 0.11	DSol: 10.2	4,3
sulfation	NaOH: 99 Sulfur: 75 Water: 1,702	T: 1,004			

^aEnergy key: P = process energy, T = transportation energy, MR = material resource energy.

^bEmissions key: Hyd = hydrocarbons, Part = particulates, SOX = sulfur oxides, Alde = aldehydes, NH_3 = ammonia, NOX = nitrogen oxides, CO = carbon monoxide, HF = hydrogen fluorides, Orgs = organics, Cl = chlorine, VOC = volatile organic carbons, EO = ethylene oxides, DSol = dissolved solids, BOD = biological oxygen demand, COD = chemical oxygen demand, TSS = total suspended solids, O&G = oil and grease, Phen = phenols and phenolics, Cr = chromium, SSol = suspended solids, Sulf = sulfides/sulfuric acid, F = fluorides, Met = metals, CN = cyanide, TDS = total dissolved solids, TOC = total organic carbon, Acet = acetaldehyde.

sulfur trioxide gas, sulfur trioxide liquid or oleum as the sulfonating agent. Production of 1000 kg LAS was estimated to require 710 kg LAB; other feedstock volumes can be calculated proportionally from Figure 1. Caustic soda (NaOH) and chlorine were assumed to be produced electrolytically from salt deposits mined by Frasch process solution methods. Sulfuric acid production data were based on the sulfur-combustion contact process and included sulfur-mining wastes.

Alcohol sulfate. Production of detergent-grade alcohols from refined oil and natural gas (Fig. 1, lower segment) was characterized by FAL based on conventional U.S. industrial processes (Alfol, Epal, Oxo and SHOP processes; (7)). Ethylene feedstocks were assumed to be 750 kg natural gas and 250 kg refined oil per 1000 kg alcohol (Table 2).

Process data for the sourcing and synthesis of aluminum catalysts used in alcohol production included: mining and refining of bauxite ore, alumina production by the Bayer process, mining and refining of limestone to produce NaOH, coke production for carbon electrodes and electrolytic reduction of alumina to elemental aluminum by smelting (Table 2). Hydrogen production data were based upon the condensation and cryogenic distillation of synthesis gas used in ammonia production.

Production of 1000 kg AS was estimated to require 705 kg alcohol; other feedstocks can be calculated proportionally (Fig. 1). Data related to sulfur mining and sulfuric acid production were those described for LAS. Alcohol sulfation by the falling film reactor process using sulfur trioxide was assumed for all alcohol feedstocks and chainlengths examined in this study (Table 2). Alcohol ethoxylate. Production of detergent-grade (C12-15, EO 3) AE incorporated AS process data for ethylene, alcohol, hydrogen and aluminum production (Table 2). Process data for oxygen were based upon the cryogenic fractionation of liquified air. Alcohol ethoxylation data were composited for batch and continuous processes assuming similar energy requirements and emissions for both.

Alcohol ethoxylate sulfate. Process data for petrochemical AES production were those described above for AE and (for sulfation) AS. Use of 824 kg AE per 1000 kg AES (other feedstocks can be calculated proportionally) was assumed.

(ii) Palm and palm kernel oil procurement and processing. Process data related to the procurement and processing of Malaysian palm/palm kernel oils included operations at oil palm plantations, palm extraction mills, kernel crushing plants and oil refineries (Table 3). Estimated annual yields of palm/palm kernel oil on plantations were 4535 and 635 kg/ha, respectively. Manual harvesting and vehicular (diesel truck) transport of fresh fruit bunches to mills were assumed. Residues from pruned and composted palm fronds (*i.e.*, in harvesting fruit bunches) and from felled and burned trees during replanting were designated as soil conditioners rather than solid emissions (8). Combustion gases from burned trees were treated as atmospheric emissions.

Co-products from fresh fruit bunch processing were allocated as: 21% crude palm oil (9); 6.5% palm kernels; 3.7% shell material and de-oiled fiber, used in road construction; and 0.5% bunch ash, used as soil conditioner (10,11). Combustion of de-oiled fiber and shell material

Raw Materials, Energy and Emissions Process Data for Discrete Operations Involved in Palm Oil/Palm Kernel Oil Derived Surfactant Production (does not include data for operations previously covered in Table 2)

	noration	Raw materials (kg/1 000 kg)	Energy ^{a} (M I/1 000 kg)	Atmospheric emissions ⁶ (kg/1 000 kg)	Aqueous emissions ^b (kg/1 000 kg)	Solid wastes (kg/1 000 kg
		(Kg/1,000 Kg/	(MO/1,000 Kg)	(Kg/1,000 Kg)	(Kg/1,000 Kg/	(Kg/1,000 Kg
1.	Fraim on Fresh fruit bunch (FFB) Harvesting	FFB: 1,000	T: 26	Part: 3.8 CO: 11.5 Hyd: 1.4 NOX: 0.4	-	-
	Crude palm oil Production/palm kernel production	FFB: 3,086 Water: 2,921	P 14,595 T: 34/54	Part: 5.4 SOX: 0.8 CO: 1.5 Hyd: 1.7 NOX: 4.1	BOD: 0.3 COD: 2.7 TSS: 8.4 SSol: 1.2 O&G: 0.08 TKN: 0.16	97.0
	Crude palm kernel oil production	Palm kernels: 2,700 Water: 2,921	P 1055 T: 36	-	SSol: 3.0	28.0
	Palm/palm kernel oil refining	Crude palm oil: 1,070 Water: 1,252	P: 12,098 T: 2,664	Hyd: 0.002	COD: 0.001	22.0
2.	Methyl ester sulfonate production					
	Methanol production	NG: 550 Water: 417	P: 45,078 T: 322	Hyd: 5.0	BOD: 0.06 SSol: 0.09	0.5
	Methyl ester	Palm oil: 1,010 NaOH: 3 Methanol: 104 Water: 125	P 6,580 T: 2,205	MeOH: 2.6	O&G: 0.1 TSS: 0.1 COD: 0.05 BOD: 0.02	_
	Methyl ester sulfonation	Methyl ester: 777 Sulfur: 115 Methanol: 89 NaOH: 174 Water: 242	P: 7,744	Part: 0.03 SOX: 2.2	DSol: 10.6	_
3.	Alcohol sulfate production					
	Alcohol production (palm oil/palm kernel oil)	Methyl ester: 1,001/992 Hydrogen: 22 Catalyst: 4 Water: 126	P 8,569 T: 1,411	Hyd: 6.3/7.7	O&G: 0.04 SSol: 0.06 COD: 0.04 BOD: 0.02	_
	Alcohol sulfation	Alcohol: 705 Sulfur: 108 NaOH: 100 Water: 1,552	P: 6,558 T: 1,004	Part: 0.02 SOX: 0.43	DSol: 8.1	1.1
4.	Alcohol ethoxylate production					
	Alcohol ethoxylation (palm oil/palm kernel oil)	Ethylene oxide: 578/387 Alcohol: 422/612	P 2,057 T: 1,473	Hyd: 0.04 NOX: 0.01 CO: 0.002 EO: 0.01	BOD: 1.03 SSol: 0.008 DSol: 0.04	4.9
5.	Alcohol ethoxylate sulfation (palm oil/palm kernel oil)	Alcohol ethoxylate: 858/824 NaOH: 56/99 Sulfur: 45/75 Water: 1,702/1,702	P: 3,944 T: 1,004	SOX: 0.11	DSol: 10.2	4.3

^aEnergy key: P = process energy, T = transportation energy, MR = material resource energy.

b Emissions key: Part = particulates, CO = carbon monoxide, Hyd = hydrocarbons, NOX = nitrogen oxides, SOX = sulur oxides, MeOH = methanol, EO = ethylene oxides, BOD = biological oxygen demand, COD = chemical oxygen demand, TSS = total suspended solids, SSol = suspended solids, O&G = oil and grease, TKN = total nitrogen, DSol = dissolved solids.

were estimated to provide 99% of total energy requirements for the mills. Emissions included atmospheric discharges from a mill's incinerator and boiler, aqueous emissions from treated effluents, and solid waste from unused boiler ash and sludge (12-15).

For palm kernel oil processing operations, an average distance of 100 km from the mill to the kernel crushing facility was assumed. Dried kernels comprising 6% of average fruit bunch weight were estimated to contain 45%crude palm kernel oil (16), extracted by mechanical pressing. Kernel fiber "cake" was treated as animal feed, and kernel shells were considered boiler fuel and base material for road construction.

Process data for palm/palm kernel oil refining operations

0	neration	Raw materials (kg/1.000 kg)	Energy ^a (MJ/1.000 kg)	Atmospheric emissions ^b (kg/1.000 kg)	Aqueous emissions ^b (kg/1.000 kg)	Solid wastes (kg/1.000 kg)
$\frac{1}{1}$	Bendered tallow production	((1,10,1,000 1.8)	(((19,1,000 19)
	Corn production	Seed: 2.0 Insecticides: 0.25 Herbicides: 0.50 Fertilizer: 29.3 Water: 67,595	P: 796 T: 746	Herb: 0.003 Pest: 0.001	Herb: 0.01 Pest: 0.01 N: 1.2 P: 0.27	_
	Fertilizer production	_	P: 7,262 T: 127	Part: 34.5 Hyd: 0.36 NH3: 0.36	BOD: 0.02 Oil: 0.02 COD: 0.08 SSol: 85.1 NH3: 0.02 P: 0.07	420.0
	Feedlot operations	Corn: 2,700 Feeder steer (hog): 700 Water: 14,020	P. 755 T: 335	NH3: 8.3 OS: 8.3		
	Production of raw materials for rendering	Steer: 1,050 Water: 11,683	P: 930	Part: 0.15 OS: 0.03	BOD: 0.2 SSol: 0.25 Gr 0.08 N: 0.12	5.0
	Tallow rendering	Tallow raw materials: 4,346 Water: 3,338	P 12,693 T: 183	_	_	10.0
2.	Methyl ester sulfonate production					
	Sulfuric acid production	Sulfur: 340 Water: 26,704	P 301 T: 176	P&AM: 1.7 SOX: 20.0	BOD: 0.2 SSol: 0.6 Acid: 7.0	3.5
	Methyl ester production	Tallow: 1,074 NaOH: 13 Sulfuric acid: 12 Methanol: 104 Water: 134	P 6,580 T: 732	MeOH: 2.6	O&G: 0.26 SSol: 0.26 COD: 0.11 BOD: 0.05	_
	Methyl ester sulfonation	Methyl ester: 777 Sulfur: 115 Methanol: 89 NaOH: 174 Water: 242	P. 7,744	Part: 0.03 SOX: 2.2	DSol: 10.6	
3.	Alcohol sulfate production					
	Alcohol production	Methyl ester: 1,001 Hydrogen: 22 Catalyst: 4 Water: 134	P 8,569 T: 1,411	Hyd: 6.3	O&G: 0.04 SSol: 0.06 COD: 0.04 BOD: 0.02	_
	Alcohol sulfation	Alcohol: 705 Sulfur: 108 NaOH: 100 Water: 1,552	P: 6,558 T: 1,004	Part: 0.02 SOX: 0.43	DSol: 8.1	1.1
4.	Alcohol ethoxylate production					
	Alcohol ethoxylate Production	Ethylene oxide: 578 Alcohol: 422	P 2,057 T: 1,473	Hyd: 0.04 NOX: 0.01 CO: 0.002 EO: 0.01	BOD: 1.03 SSol: 0.008 DSol: 0.04	4.9
5.	Alcohol ethoxylate sulfation	Alcohol ethoxylate: 858 NaOH: 56 Sulfur: 45 Water: 1,702	P 3,944 T: 1,004	SOX: 0.11	DSol: 10.2	4.3

Raw Materials, Energy and Emissions Process Data for Discrete Operations Involved in Tallow Sourced Surfactant Production (does not include data for operations previously covered in Tables 2 or 3)

 a Energy key: P = process energy, T = transportation energy, MR = material resource energy. b Emissions key: Herb = herbicide, Pest = insecticide, Part = particulates, Hyd = hydrocarbons, NH₃ = ammonia, OS = odorous sulfur, P&AM = particulates and acid mist, SOX = sulfur oxides, MeOH = methanol, NOX = nitrogen oxides, CO = carbon monoxide, EO = ethylene oxides, N = nitrogen, P = phosphorus, BOD = biological oxygen demand, SSol = suspended solids, Gr = grease, O&G = oil and grease, COD = chemcial oxygen demand, DSol = dissolved solids.



FIG. 1. Production of linear dodecyl alkylbenzene (LAB) and alcohol ethoxylate (C12-15AE3) from petroleum and natural gas. Mass requirements (kg) for each stage are expressed on the basis of 1000 kg LAB or alcohol ethoxylate produced.

(Table 3) were based on physical refining methods. Calculations were based on an average yield of 94% refined, bleached and deodorized oils from the crude oils (17). Aqueous emissions following advanced (secondary) wastewater treatment of refinery effluent were consistent with current practices at typical Malaysian refineries. A distance of 100 km from the mill to the refinery was the basis for transportation energy estimates.

(iii) Palm/palm kernel oil surfactant production: Methyl ester sulfonate. Process data for co-production of methyl

esters and glycerine by transesterification of palm/palm kernel oils are summarized in Table 3 and Figure 2 (upper segment preceding alcohol synthesis). Operations examined included the production of methanol for sodium methylate catalysts and of sodium hydroxide from salt. Methanol production data were based upon the low-pressure reforming process and included de-sulfurization of petrochemical feedstocks, catalytic separation and distillation.

Alcohol sulfate, alcohol ethoxylate and alcohol ethoxylate sulfate. Ethoxylate molar ratios of AE and AES derived from palm and palm kernel oils were 7.9 and 3, respectively. Production of detergent alcohols by hydrogenation of palm/palm kernel methyl esters was composited for fixed-bed and suspended copper catalytic processes. Alcohol ethoxylation and the sulfation of alcohols and alcohol ethoxylates were based on the process data described for petrochemical surfactants (Table 2).

(iv) Tallow procurement and processing. Animal fat feedstocks used in surfactant production (tallow from cattle, white grease from hogs) were identified as co-products of the beef and pork industries. Energy and emissions estimated for cattle and hog production were equivalent per 1000 kg packed meat. Tallow procurement operations evaluated by FAL included the manufacture of fertilizers used to grow corn, agricultural practices to produce corn and corn silage as livestock feed, livestock feedlot operations, slaughtering and fat rendering (Table 4; Fig. 3, upper left segment).

Process data for raising corn included land preparation and fertilizer application, planting, irrigation, pesticide/ herbicide application, harvesting and transport of corn to feedlots. Application of a mixed-nutrient fertilizer formulation containing phosphorus, nitrogen, potassium and lime was assumed. Atmospheric emissions were primarily related to fertilizer manufacture, and aqueous emissions were the result of agricultural runoff. No solid waste from agricultural activities was assumed, as unused biomass is typically land-applied or used to produce silage.



FIG. 2. Production of alcohol ethoxylate (C16-18AE7.9) from palm oil, petroleum and natural gas. Mass requirements (kg) for each stage are expressed on the basis of 1000 kg alcohol ethoxylate produced.



FIG. 3. Production of alcohol ethoxylate (C16-18AE7.9) from inedible tallow, petroleum and natural gas. Mass requirements (kg) for each stage are expressed on the basis of 1000 kg alcohol ethoxylate produced.

Tallow yields were calculated for a steer with an average weight of 318 kg upon arrival at the feedlot. Steer weight gain was estimated to be 1.4 kg per day for 130 d at the feedlot, requiring a total of 1225 kg ground corn concentrates and 635 kg roughage. Energy requirements included feedlot equipment operation (e.g., feed elevators) and transportation of livestock to the slaughterhouse. Feedlot wastes were assumed to be land-applied and were not included as aqueous or solid emissions. Gaseous emissions from the animals and their wastes, however, were listed as atmospheric emissions.

Slaughterhouse and rendering operations included sacrificing animals, carcass trimming/cooling and the preparation of inedible tallow. Co-products from livestock were allocated as; 60% carcass for meat products; 25% inedible tissues, 25% of which was inedible tallow; 5% edible fat; 6% blood for use in pharmaceuticals and animal feeds; 2% bone and 2% hide. Inedible tallow was thus assumed to comprise 6% of the total weight of a steer (500 kg). Energy requirements included operation of continuous rendering equipment, conveyors and refrigerated storage areas. Aqueous and atmospheric wastes from slaughtering and rendering are typically treated with meat-packing wastes and were calculated assuming on-site wastewater treatment. Solid wastes consisted of bleaching clays used to filter tallow.

Tallow surfactant production: methyl ester sulfonate. Production of detergent-grade methyl esters from inedible tallow required evaluation of the following operations: refining to collect free fatty acids as co-products, esterification via methanolysis to produce methyl esters and glycerine; methyl ester washing, drying and distillation; and glycerine refining to collect and recycle methanol for esterification. Process data for salt mining, sodium hydroxide production, natural gas production and refining, methanol production and ester sulfation were those described for palm oil MES (Table 3). Alcohol sulfate, alcohol ethoxylate and alcohol ethoxylate sulfate. Energy and emissions datesets and assumptions for alcohol production, ethoxylation and sulfation were those used in producing respective surfactants from palm oil alcohols of similar alkyl chainlength and ethoxylate molar ratio (7.9). Production of 1000 kg AES was estimated to require 858 kg AE; other feedstock volumes can be calculated proportionally from data in Figure 3 and Table 4.

Surfactant life-cycle profiles: (i) Feedstock requirements. To facilitate evaluation of natural resource requirements for surfactant production, organic raw materials were distinguished as primary and secondary feedstocks (Table 5). Primary feedstocks were defined as hydrocarbons derived from fossil fuels, palm/palm kernel oils or tallow, and which are incorporated into the base structure (alcohol, methyl ester or alkylbenzene) of each surfactant. Secondary organic feedstocks were fossil fuel-derived hydrocarbons (methanol, ethylene) used in fatty acid methylation and in alcohol ethoxylation. Primary and secondary feedstocks for the petrochemical surfactants are, by definition, derived from fossil fuels and were thus combined. From this analysis the petrochemical contributions to the organic structures of oleochemical surfactants (more accurately termed composites of oleochemical and petrochemical hydrocarbons) are readily apparent.

Feedstock mass requirements shown in Table 5 were characteristic of each surfactant type and were largely independent of feedstock origin. Differences in alkyl chainlength and in levels of ethoxylation among the surfactants studied were not evident in the estimated feedstock requirements. Total feedstock requirements (primary and secondary) generally increased in order of: alcohol sulfates (715, 706, 700 and 705 kg for petrochemical, palm, palm kernel and tallow AS, respectively); LAS (759 kg); MES (850 kg for palm and tallow); and AES (771, 772, 758, 765 kg). Alcohol ethoxylates had a higher apparent mass re-

	Organic raw materials ^a		Inorganic raw materials			Energy requirements		
Surfactant class	Primary feedstock	Secondary feedstock	Salt	Sulfur	Water	Process	Transport	Raw material
Petrochemical								
AS	715		79	108	13	39	2	38
AE	612	323			40	39	3	50
AES	337	434	78	75	36	39	3	41
LAS	759		182	115	12	29	2	35
Palm oil								
AS	650	56	81	108	6	39	6	3
AE	388	511			49	37	5	26
AES	333	439	45	45	44	38	5	23
MES	714	136	158	115	7	41	4	8
Palm kernel oil								
AS	644	56	81	108	8	40	6	3
AE	558	362	_		35	40	6	19
AES	460	298	80	75	32	40	6	16
Tallow								
AS	653	52	86	110	618	43	10	3
AE	390	501	_		415	40	7	27
AES	335	430	47	46	358	40	7	23
MES	718	132	163	118	686	46	9	7

Major Raw Material and Energy Requirements for Surfactant Production (results expressed as kg raw materials or GJ energy per 1000 kg of each surfactant)

^aPrimary feedstocks (petroleum/natural gas, refined palm/palm kernel oils, rendered animal fat) are incorporated into alcohol (for AS, AE, AES), alkylbenzene (for LAS) or methyl ester (for ME). Secondary feedstocks (petroleum and natural gas) are required for methylation of fatty acids (for AS, AE, AES) and for alcohol ethoxylation (for AE and AES). Abbreviations: AS, alcohol sulfate; AE, alcohol ethoxylate; AES, alcohol ethoxylate sulfate; LAS, linear alkylbenzene sulfonate; ME, methyl ester; MES, methyl ester sulfonate.

quirement (891 and 931 kg for tallow and petrochemical AE) in this analysis due to the lack of anionic end-group, resulting in a higher organic weight basis than other surfactant types examined.

Major inorganic raw material requirements estimated by FAL were salt, sulfur and water (Table 5). Like the organic feedstocks, salt required for caustic production and sulfur required for sulfation or sulfonation were primarily dependent upon surfactant type (*i.e.*, the presence of sulfate/sulfonate end-groups). Nonionic AE surfactants had no significant requirement for either salt or sulfur. Among anionic surfactants, production of MES and LAS required greater volumes of both than that of AS or AES.

Water requirements estimated independently for each operation (Tables 2-4) are summed in Table 5. Differences in water usage were primarily related to irrigation needs in producing primary feedstocks and, to a lesser extent, to process chemistry. The high water requirements of tallow-derived surfactants were attributed to the conventional, water-intensive agricultural operations in the U.S. to feed livestock in beef production. Irrigation requirements would be significantly reduced for livestock grazed on pasture, albeit with effects upon tallow yields. Oil palm agricultural methods used in tropical climates with high annual rainfall were assessed as having no irrigation requirements. Thus, palm/palm kernel surfactants had net water requirements comparable to petrochemical surfactants.

Major operations requiring water for petrochemical surfactant production include petroleum and natural gas refining, olefins (ethylene) production, sulfur mining and sulfation/sulfonation. For LAS, approximately 70% (8.9 cu m per 1000 kg surfactant) of the net water requirement is consumed in the alkylation reaction. For palm/palm kernal surfactants, water usage was principally related to milling, oil extraction and refining operations, requiring a total of 4.7 cu m water per 1000 kg palm oil-derived AS.

Sulfation and sulfonation processes (including sulfur mining) required approximately 2.2 cu m water per 1000 kg surfactant for the production of the anionic surfactants studied (LAS, AS, MES and AES). Higher water requirements of the ethoxylated surfactants (AE and AES) relative to AS and MES were attributed to the production of oxygen and ethylene oxide. For 1000 kg palm oilderived AE, these operations consumed 12.5 and 27.7 cu m water respectively.

(ii) Energy requirements. Energy requirements for surfactant production sequences are summarized in Table 5, calculated by summing energy requirements for all operations (Tables 2-4) involved in the production of 1000 kg surfactant. By the raw material energy convention of FAL, fossil fuels used as primary or secondary feedstocks (Table 5) were also represented as a material resource energy requirement. (For example, 715 kg primary feedstock required in petrochemical AS production represented 39 GJ material resource energy.) Oleochemical feedstocks were not assigned raw material energy requirements because they are not widely used as conventional fuels. (The use of palm oil as vehicular fuel has been demonstrated only on a limited scale to date.)

By this approach, raw material energies were higher for petrochemical surfactants (35-50 GJ per 1000 kg, Table 5) than respective surfactants derived from palm/palm kernel oils (3-26 GJ) or tallow (3-27, GJ). Among the surfactant types examined, AS and MES required the least raw material energy. AE surfactants required the greatest due to petrochemical sourcing of ethylene oxide. Material resource energy of the AE and AES surfactants is directly proportional to the degree of ethoxylation required for a particular performance or function. While inherent energies (*i.e.*, heats of combustion) of all of the surfactants could be calculated thermodynamically, it is recognized that practical recovery of this energy is not feasible for any detergent-grade surfactant.

Consistent with the trend observed in feedstock requirements, differences in total process energy requirements (Table 5) were more closely related to surfactant type than feedstock derivation. Potential differences in process energy requirements due to differences in chainlength or ethoxylation were not detected in this study. LAS required less process energy (29 GJ) than the alcohol sulfates (39-43 GJ), AE's (37-40 GJ), AES's (38-40 GJ) or MES (41-46 GJ). The lower net process energy of LAS relative to surfactants derived from petrochemical alcohols (sequentially constructed from short-chain olefins) reflects the reduced chemical processing requirements of longer-chain (paraffin and benzene) hydrocarbons acquired directly from fossil fuel refining.

Transportation energy requirements were less than process energy requirements for all surfactants evaluated (Table 5). Transportation energies were < 8% of process energy requirements for petrochemical surfactants, < 16% for palm/palm kernel surfactants, and < 25% for tallow surfactants. Higher transportation energies for oleochemical surfactants were attributed to vehicular transport of fertilizer, corn and livestock for tallow surfactants (Table 4), and transport of fresh fruit bunches and crude oils for palm/palm kernel oil surfactants (Table 3). In contrast, large-volume transport of petroleum and natural gas feedstocks by tankers and pipeline resulted in greater efficiency and lower energy requirements.

(iii) *Emissions*. Emissions generated by discrete operations in the surfactant production sequences (Tables 2-4) were normalized to 1000 kg surfactant and summarized by emission category in Table 6. This summary is intended to illustrate general trends and should not be assumed to indicate equivalence of hazard or priority for remediation among the emissions. Environmental risks associated with the emissions cannot be gauged from mass loading data alone, as the information necessary to assess environmental exposure concentrations are not conveyed.

Characteristic emissions were identified for surfactants from each primary feedstock in one or more emission categories surveyed. Primary feedstock source principally determined the composition and distribution of emissions among atmospheric, aqueous and land-applied emission categories, particularly for surfactant types requiring less secondary feedstock (AS, MES, LAS).

Distributions of atmospheric and aqueous emissions among the petrochemical surfactants were consistent with the physical states of the primary feedstocks, with relatively higher atmospheric emissions and lower aqueous emissions associated with natural gas. The emissions profile for LAS was distinct among petrochemical surfactants due to its primary sourcing from petroleum (Table 6). For LAS, principal atmospheric emissions were hydrocarbons, particulates and sulfur oxides resulting from crude oil procurement and refining (Table 2). Dissolved solids in brine water discharged during oil production were the primary aqueous emission. Solid wastes were relatively low, derived chiefly from sulfur mining and sodium hydroxide production. For petrochemical AS, AE and AES, higher levels of atmospheric emissions (e.g., nitrogen oxides, hydrocarbons, carbon monoxide) and lower levels of aqueous emissions (oil, suspended solids) were observed. Natural gas production operations contributed approximately 65-70% of total atmospheric emissions for these surfactants. Approximately 60% of the aqueous emissions for AS and AES resulted from dissolved solids generated during sulfation. Ethylene oxide production and alcohol ethoxylation represented 34 and 14% of the respective aqueous emissions for AE and AES; the difference was attributed to higher total aqueous emissions of AES due to sulfation.

In general, land-applied (solid) emissions for surfactants sourced from petrochemical feedstocks were lower than comparable surfactants sourced from palm/palm kernel oils or tallow. Solid emissions of petrochemical AS, AE and AES were 120, 76 and 116 kg per 1000 kg surfactant, vs. 162-204 kg, 111-157 kg and 134-180 kg for respective oleochemical surfactants. This was attributed to the more highly-reduced oxidation state and decreased processing requirements of raw fossil fuel feedstocks (petroleum, natural gas) relative to those of unrefined oleochemical feedstock sources (fresh fruit bunches, live stock). The latter require extensive extraction and processing to prepare unrefined oils with the same approximate feedstock utility as fossil fuels drawn from subsurface geologic deposits.

Emissions for palm/palm kernel surfactants similarly had characteristics common to the primary feedstock source. The majority of atmospheric emissions (53-81%) including particulates, nitrogen oxides, hydrocarbons, sulfur oxides and carbon monoxide (Table 6) were generated through combustion of plant material at oil palm plantations, mills and kernel crushing facilities. Approximately 22-50% of aqueous emissions, chiefly dissolved and suspended solids, also resulted from these operations. While most plant material was used as soil conditioner either directly or through land application, accumulation of sludge from wastewater treatment contributed significantly to solid emissions estimates. Emissions of palm kernel surfactants in each media were slightly greater than those of respective palm oil surfactants due to the additional processing required in kernel extraction. As observed for petrochemical surfactants, aqueous (dissolved solids) and land-applied emissions were greater for AS and AES than for AE due to sulfation requirements. In contrast, atmospheric emissions of the AE's were higher due to ethylene oxide and ethoxylation operations.

Emissions profiles of tallow surfactants were dominated by fertilizer manufacturing, corn agriculture and livestock feedlot operations. Principal atmospheric emissions were odorous sulfur and ammonia from feedlot operations. Chief aqueous emissions were dissolved and suspended solids from fertilizer manufacturing and labile organics (biological oxygen demand (BOD)) and suspended solids from feedlots. Aqueous runoff of phosphorus and nitrogen resulting from fertilizer runoff were characteristic of tallow surfactants. Solid emissions were primarily contributed from fertilizer manufacturing and (for anionic surfactants) sulfur mining.

Net Life-Cycle Emissons Associated with Surfactant Sourcing and Production (results expressed as kg emission generated per 1000 kg surfactant)^a

		Petroche	mical			Pa	lm oil	
	LAS	AS	AE	AES	AS	AE	AES	MES
Atmospheric emissions								
Particulates	3.9	4.0	2.2	3.6	15.3	9.0	9.0	17.0
Nitrogen oxides	8.0	11.6	12.2	12.6	14.3	12.9	13.5	13.4
Hydrocarbons	12.8	29.8	39.2	34.1	21.0	33.2	30.1	18.6
Sulfur oxides	12.0	12.1	9.4	11.3	12.6	8.5	10.8	16.5
Carbon monoxide	2.5	4.1	4.1	4.6	28.4	17.9	16.7	30.0
Aldehydes	0.086	0.055	0.059	0.073	0.12	0.56	0.52	0.095
Odorous sulfur	0.015	—	0.004	—		_	_	
Ammonia	0.034	0.008	0.005	0.009	0.014	0.010	0.012	0.013
Hydrogen fluoride	0.036	0.004	0.004	0.003	-	-	_	_
Lead	$4.2 \text{E} \cdot 05$	3.5E-05	2.8E-05	4.1E-05	1.0E-04	6.3E-05	7.1E-05	9.9E-05
Chlorine	0.84	0.41	_	0.41	0.42	0.005	0.23	0.73
Unidentified	0.11	0.077	0.093	0.11	0.13	0.12	0.13	0.096
Aqueous emissions								
Fluorides	0.002	0.006	0.006	0.005	_	_		
Dissolved solids	12.3	13.2	5.6	15.2	14.9	5.3	15.6	17.6
BOD	0.26	0.028	1.7	1.4	0.23	2.1	1.8	0.25
Phenol	0.002	1.7E-05	2.3E-05	1.9E-05	_	8.6E-06	1.0E-05	_
Sulfides	0.003		_		_	_	_	
Oil	0.16	0.050	0.065	0.054	0.15	0.12	0.11	0.14
COD	0.85	0.047	1.1	0.90	1.8	2.7	2.3	2.0
Suspended solids	3.9	0.10	0.11	0.092	0.9	0.57	0.49	1.0
Acid	1.3	1.1	0.80	0.95	2.0	1.3	1.3	2.3
Metal ions	0.14	0.15	0.11	0.14	0 106	0.081	0.11	0.14
Cvanide	-	6 4E-05	5.9E-05	4.8E-05			_	
Chromium	2 1E-04	3 2E-05	0.008	0.064		0.012	0.010	
Ammonia	0.001	0.001	1 4E-03	0.001	1 2E-04	1 8E-04	1 9E-04	
Nitrogen	0.001	0.001	1.41 00	0.001	0.10	0.062	0.054	0.11
Phosphome	_	_			0.10	0.002	0.004	0.11
Unidentified	0.97	0.60	0.55	0.54	0.30	0.20	0.32	0.91
L and applied omissions	0.27	0.00	0.00	0.04	0.50	0.29	0.52	0.51
Mass (kg)	194	190	76.0	116.9	162.0	111 /	133.8	109 7
Waluma (m ³)	0.15	0.15	10.0	0.15	102.0	0.14	0.17	192.1
volume (m)	0.15	0.15	0.05	0.15	0.20	0.14	0.11	0.24
		Dalas lasaral	-11			T-1 -		
		Faim kernei					AEG	MEG
	AS	AE	AES		A5	AE	AES	MES
Atmospheric emissions							~ ~	
Particulates	15.3	12.1	11.7		12.9	8.0	8.1	15.3
Nitrogen oxides	14.6	14.4	14.4		19.6	17.7	17.3	21.7
Hydrocarbons	22.2	32.4	28.4		22.1	34.8	31.4	21.3
Sulfur oxides	13.0	9.3	11.1		12.2	10.9	12.1	19.7
Carbon monoxide	29.5	25.6	22.3		11.2	8.6	8.4	12.4
Aldehydes	0.12	0.83	0.70		0.28	0.19	0.19	0.29
Odorous sulfur	—	-	—		24.7	14.7	12.7	27.1
Ammonia	0.014	0.013	0.012		24.7	14.8	12.7	27.1
Hydrogen fluoride	—	-	_		-	-	-	-
Lead	1.0E-04	8.3E-05	8.1E-05		1.5E-04	1.1E-04	1.0E-04	1.7E-04
Chlorine	0.42	0.008	0.41		0.44	0.017	0.24	0.75
Unidentified	0.13	0.14	0.14		0.41	0.31	0.29	0.44
Aqueous emissions								
Fluorides		_	-		_			—
Dissolved solids	15.2	7.1	16.3		11.9	4.3	14.1	14.6
BOD	0.24	1.9	1.6		0.63	2.4	2.0	0.68
Phenol	_	7.9E-06	6.5E-06			1.2E-05	1.0E-05	_
Sulfides	—	_	_		_	_		
Oil	0.16	0.16	0.13		0.45	0.30	2.26	0.46
COD	1.9	2.7	2.2		0.13	1.6	1.4	0.11
Suspended solids	29	2.5	21		20.8	12.5	10.7	22.8
Acid	2.0	16	16		11	0.88	0.97	1 6
Motal ions	2.0 0.11	1.0 0.070	1.0		0.11	0.00	0.31	1.0
Cuanida	0.11	0.078	0.11		0.11	0.11	0.14	0.20
Chromium		0.009	0.000		_	0.019	0.010	
Ammonia	19504	0.008	17504		0.01	0.012	0.010	
Ammonia	1.26-04	2.1E-V4	1.112-04		0.01	0.003	0.003	0.01

^aAbbreviations: See Tables 4 and 5.

Nitrogen

Phosphorus

Unidentified

Mass (kg) Volume (m³)

Land-applied emissions

0.11

0.31

0.23

186.2

0.095

0.29

0.19

153.1

0.078

0.32

0.22

179.8

9.7

2.2

0.50

0.26

204.2

0.071

5.8

1.7

138.8

0.17

5.0

1.1

157.2

0.46

0.20

10.7

2.4

267.4

0.64

0.33

DISCUSSION

Conventional life-cycle analysis procedures were used in developing distinct natural resource and emission profiles for various surfactant types and feedstocks. The key strengths of the LCI approach, its broad scope and flexibility, provided overviews of surfactant sourcing and production sequences without constraints of international borders, private business concerns, or environmental heterogeneity. Its principal limitations are the converse of its strengths: a lack of specificity and an inviolate dependence upon the underlying assumptions. These must be carefully weighed in interpreting the data.

Given these strengths and limitations, LCI can be viewed as one tool complementing more traditional environmental management procedures. Complete evaluation of the environmental impacts of a chemical or nonchemical stress requires consideration of other datasets, such as those compiled in chemical risk assessments and pollution prevention programs for industrial plant sites and non-point-source emissions. While valuable in its own right, life-cycle analysis should not be misconstrued as a panacea for holistic environmental management of commercial chemicals and industrial operations.

Geographic relevance. The study was designed to characterize representative U.S. conditions by employing FAL's energy sourcing and transportation databases drawn from U.S. governmental sources. Broader application to other geographic areas is possible for several reasons, provided that the same production processes and waste treatment technologies are applicable. First, the majority of feedstocks used internationally in surfactant production have common origins (*i.e.*, petroleum from the Middle East, palm/palm kernel oil from Malaysia). (An exception is the inedible tallow feedstock, as the U.S. produces almost half 3.2 million metric tons (MT) of the world's production of tallow and grease (6.6 MT), and exports more than that produced by any other country (18)).

A second factor is that surfactant production technologies like those described here are used in many industrialized regions worldwide. Finally, energy and emissions associated with feedstock transport were generally small relative to industrial process requirements. Thus, the surfactant life-cycle profiles developed here are relevant to other geographic regions except where significant differences exist in energy sourcing (*i.e.*, from nonfossil fuel sources) and production technology.

Technical considerations in ranking feedstock quality. Interpretations of LCI's aimed at rating and ranking the environmental quality of consumer products within particular market categories (e.g., "ecoseals") have engendered a good deal of public debate and controversy. Such broad characterizations here with regard to scaling the environmental quality of various surfactant types and sourcing options are inappropriate. The surfactant types examined are not readily interchangeable detergent ingredients. Differences in their physical properties and economic availability dictate the selection of surfactants for particular detergent formulations. Also, the study demonstrates the great diversity of systems, operations and emissions involved in surfactant production from different feedstocks. Aggregation of dissimilar data and comparisons among nonequivalent systems in life-cycle studies have been criticized as lacking a sound technical basis (1).

Like other environmental or economic accounting techniques, life-cycle analysis has its limitations. No single study can fully address the complexity of potential environmental issues and economic considerations associated with basic commodities. Global environmental and economic concerns such as renewability, global climate, deforestation and species extinction are immensely complex. Implications of feedstock sourcing toward these concerns cannot be reduced to simple quantitative comparisons by LCI procedures alone. For oleochemical and petrochemical feedstocks alike, benefits in one direction (e.g., renewability) are offset by liabilities in another (intensive land-use requirements). Evaluations within, rather than across, surfactant types and feedstock sourcing strategies are more effective in identifying opportunities for improvement.

Thus, these life-cycle data do not support fundamental shifts in worldwide surfactant usage of feedstock sourcing on the basis of environmental concerns. The studies provide no justification that any single surfactant type or feedstock source—petrochemical or oleochemical—is environmentally superior. None of the feedstocks demonstrated superior attributes across the entire range of natural resource and emissions criteria evaluated. Emissions from each discrete operation in feedstock procurement carry the potential for environmental impact, a potential that cannot be assessed from mass loading data alone. In each case, feedstock selection and use require expert evaluation of environmental risks and responsible management to maintain acceptable safety margins.

Surfactant feedstocks as co-products. The feedstocks evaluated are inextricably linked to larger and more basic industries than surfactant production, and these relationships are clearly reflected in their LCI profiles. Petrochemicals are co-products of the vast energy industry. Palm oil, palm kernel oil and inedible tallow are co-products of several food industries. By providing alternative markets for basic commodities, surfactant feedstocks can help to promote economic stability and resource conservation through more efficient management of surpluses. However, issues pertaining to the primary industries from which the feedstocks are drawn impinge upon the surfactant profiles as well.

This is best highlighted by the inedible tallow feedstock, characterized as having relatively high emissions and resource requirements stemming from basic agricultural operations. These "liabilities" cannot be viewed in isolation of the function of the primary industry. The U.S. beef and pork industries clearly represent the primary economic reason for livestock production. Like the use of tallow in candlemaking prior to the invention of the light bulb, oleochemical uses of inedible tallow represent an efficient use of a low-value co-product from an existing industry.

However, due to the conventional practice of weighting co-product requirements on a sheer mass basis, any economic efficiencies gained by using inedible tallow feedstock (*e.g.*, conservation of more highly valued feedstocks; diversion of surpluses from waste disposal) are not reflected in the LCI profile. As a result, the profile of a co-product industry such as tallow surfactant production parallels that of the primary industry: intensive landuse requirements, gaseous emissions from feedlots, and aqueous runoff of fertilizer and pesticides. Surfactant sourcing decisions based solely on these LCI findings might suffer from an incomplete or overly narrow economic assessment.

Similarly, palm and palm kernel oils are commodities shared with basic food industries in southeastern Asia and India. Approximately 90% of worldwide palm/palm kernel oils production, estimated at 12 MT in 1990 (19), are used in the preparation of foods (20). The use of these oils as feedstocks for detergent (21) and personal care product ingredients (22), plastics additives (23) and lubricating oils (24) may serve to stabilize the economics of the basic industry.

Nevertheless, environmental concerns associated with oleochemical feedstocks from tropical geographies are reflected in the life-cycle profiles of palm/palm kernel oil surfactants. Concerns about tropical rain forest depletion, potential climatic effects and species extinction stem primarily from the land-use requirements of oleochemical crops. Emissions of oleochemical-producing agricultural operations are less often voiced as a public concern, although mass loadings in certain emission categories in this study were significant.

The petrochemical surfactants are a third example of how more basic co-products, in this case fossil fuels used in energy production, can influence the LCI profile. Petrochemical feedstocks penetrate most major industries. The availability of numerous markets for petrochemicals has resulted in efficient processing and use of essentially all hydrocarbon fractions, such that relatively little waste is generated on a per unit basis. The use of fossil fuels as organic feedstocks is conceivably a more efficient and favorable option than their direct combustion to produce energy.

Concerns related to fossil fuels are both economic (e.g., exhaustibility; impact on international politics) as well as environmental (e.g., hazards of transport; impacts of combustion upon regional and global climates). Atmospheric emissions of combustion and depleting supplies of fossil fuels are clearly emerging as international priorities. In presenting both emissions and energy data in the LCI, the petrochemical life-cycle profiles contain elements of both areas of concern but do not clearly distinguish the impacts of either.

Surfactant feedstocks and raw material consumption. Data from the Chemical Economics Handbook (25) add perspective to the economic concern over fossil fuel depletion. Estimated 1990 consumption of raw materials for LAB, detergent alcohols and linear olefins in the U.S. (26), western Europe (1989 and 1990 data (27)) and Japan (28) totaled approximately 2.2 billion kg. In contrast, worldwide production of crude oil was estimated at 55.7 million barrels per day (1987 data), or 2.64×10^{14} kg/yr assuming 0.13 MT per barrel (29). Total world production of natural gas was estimated at 66.9 trillion cu ft/yr (1986 data), or 2.65×10^{12} kg/yr assuming 0.0396 kg per cu ft (30). Total crude oil and natural gas production therefore totaled 5.29×10^{12} kg/yr.

From this it is estimated that raw materials for LAB, detergent alcohols and linear olefins require approximately 0.042% of total crude oil and natural gas annual production. Fossil fuel requirements (*i.e.*, raw material energy) of these major surfactant precursors are small compared to global fossil fuel consumption levels. Thus, major international shifts in surfactant feedstock sourcing would appear to have little impact upon fossil fuel consumption rates, even if oleochemical feedstock sourcing, chemical processing and formulation were feasible. Effective resource conservation measures for fossil fuels are imperative, but must focus on major end-uses (*i.e.*, combustion to produce energy) which represent the bulk of the consumption.

Dramatic shifts in feedstock sourcing could have major environmental implications. The raw material requirement of 2.2 billion kg/yr would require some 500,000 ha $(5,000 \text{ km}^2)$ of oil plam plantations, assuming the yield of 4,535 kg palm oil/ha/yr stated previously. Of course, feedstocks are not readily interchangeable, and such a shift is not anticipated. However, it is clear that the scale of land-use required to support major conversions from petrochemicals to oleochemicals would not be trivial.

Beyond the life-cycle inventory. It has been proposed that "impact analysis" and "improvement analysis" are additional but less well-developed components of the lifecycle assessment process (1). Current research is advancing the scientific understanding needed to aggregate LCI datasets into sound mechanistic categories (e.g., ozonedepleting compounds), but proposed LCI applications to environmental risk assessments have yet to be validated. Nevertheless, the field of life-cycle analysis is rapidly developing in the U.S. and Europe. (An informative newsletter is published through the SETAC Foundation, 1010 North 12th Avenue, Pensacola, FL 32501.)

Significant opportunities for improvements in resource conservation and emission reduction are possible from LCI inventory data (1). Emerging oleochemical industries may offer the greatest opportunities through the introduction of advanced technology in agriculture, chemical and environmental engineering. Coordination among local governments and businesses as well as multinational corporations will be essential. For petrochemical technologies such as surfactant production, further improvements may be more challenging due to the already advanced state of current technology, but are equally important. Multinational corporations can play a major role by instituting equivalent standards of environmental quality across all global operations and by incorporating life-cycle considerations and criteria into technology advancement and product development decisions.

The comprehensive natural resource and emissions data embodied in this study can facilitate international coordination and implementation of effective environmental management policies. Already communication among private firms and governmental agencies worldwide has been enhanced through recognition of the interdependent raw material, energy and emissions associated with global surfactant production sequences. The ultimate value of the analyses will be realized through the implementation of meaningful waste reduction and resource conservation initiatives through the next decade and beyond.

Copies of the surfactant study reports by Franklin Associates, Inc., upon which this paper is based, are available by writing: The Procter & Gamble Company, U.S. Soap Sector P&RS, Ivorydale Technical Center, Cincinnati, OH 45217.

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