

**"LIFE CYCLE ANALYSIS AND MATERIALS/
ENERGY FORECASTING MODELS"**

by

Robert U. AYRES*

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* Professor of Environmental Economics, Sandoz Chair in Management and the Environment at INSEAD, Boulevard de Constance, Fontainebleau 77305 Cedex, France.

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LIFE CYCLE ANALYSIS AND MATERIALS/ENERGY FORECASTING MODELS

**Robert U. Ayres
CMER, INSEAD
Fontainebleau, France**

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Abstract

Life Cycle Analysis (LCA) is an increasingly important tool for environmental policy, and even for industry. To choose the "greener" of two products or policies it is necessary to know the indirect as well as the direct contributions to environmental disturbance. Moreover, it is important to consider the future (downstream) fate of a product as well as its past, since every material product must eventually become a waste. Analysts are also increasingly interested in forecasting future materials/energy fluxes on regional and global scales, as a function of various economic growth and regulatory scenarios.

A tool that economists would naturally consider using for either of these purposes is the Leontief-type of Input-Output (I-O) model, which was explicitly developed to trace the indirect output requirements associated with final demand. However, I-O models have certain characteristics that limit their applicability for LCA. Process analysis avoids three characteristic problems of I-O, viz. (1) aggregation errors (2) inability to handle arbitrary combinations of co-product and co-input relationships and (3) inability to reflect nonlinearities and feedback loops. For these reasons LCA normally depends heavily on more detailed process analysis. However process analysis, at least as exemplified by many published LCA's, also suffers from excessive aggregation of "upstream" materials transformation processes, combined with unnecessary disaggregation of "downstream" processes, despite the fact that the latter typically contribute very little to emissions. Both LCA's and forecasting scenarios also suffer from similar data problems, largely arising from the persistent use of unpublished "confidential" data, directly or indirectly from industry sources, that is both internally inconsistent and unverifiable. The paper suggests that systematic use of materials balance conditions at the unit process and industry levels can overcome much of this difficulty. It concludes that a hybrid combination of process analysis and I-O analysis is the most promising approach.

Life-Cycle Analysis (LCA)

Life-cycle analysis is a relatively new methodology. The first detailed quantitative life-cycle analysis (comparing three alternative materials for beverage bottles, PVC, PE and glass) was demonstrated for the U.S. National Science Foundation in 1974 [Ayres *et al* 1974; Ayres & Cummings-Saxton 1975]. At the time, data and computational requirements were too great for widespread application. However, LCA is now becoming a popular tool for environmental analysis, and even for industry. The exact definition is the subject of some controversy, and has been the subject of several workshops [e.g. IMSA and IPRE 1990; SETAC 1991]. Recent usage distinguishes LCA and Eco-Profile Analysis [e.g. Lubkert *et al* 1991]. The former is taken to be the compilation of quantitative data on composite, direct and indirect materials/energy inputs and waste emissions, both in production and disposal of a product. The latter is taken to be the interpretation of these quantitative data for purposes of addressing policy questions.

Only with the help of a tool like LCA is it possible to make rational judgments on the relative environmental load of competing end-use products such as different kinds of packaging materials. The case for (or against) recycling in specific cases also depends on such analysis. A classic example was the groundwood (papier-maché) vs. polystyrene hamburger shells. This was decided by McDonald's in favor of the former, but apparently in response to a "green" campaign that had already prejudged the issue. It is not at all clear that, when manufacturing processes are considered, polystyrene causes more environmental harm than either virgin or recycled paper pulp. In a similar case, it has been estimated recently that, though polystyrene foam cups occupy more space in landfills than paper cups, the latter requires 36 times more electricity and 580 times more wastewater to manufacture [Hocking 1991]. In addition, when paper is buried in a landfill it eventually decays anaerobically, generating methane.

Another classic case is the unresolved competition between reusable cloth diapers and disposable paper diapers [Barber *et al* 1977, 1977a]. In this case, disposables create 90 times more solid waste (but only 2% of the total of municipal waste, whereas reusable cloth diapers generate 10 times as much water pollution (including detergents) and consume 3 times as much energy [N.Y. Times Feb 26 1991]. Another example is the unresolved competition between returnable and re-usable glass bottles, recyclable glass bottles, recyclable aluminum cans and various non-recyclable plastic containers [e.g. Franklin 1985; Lundholm & Sundstrom 1985, 1986; Boustead 1989; Sellers & Jere 1989; IMSA and IPRE 1990; Mekel & Huppel 1990; Habersatter & Widmer 1991; Lubkert *et al* 1991].

In none of the above cases has LCA offered a clear-cut answer. In part this arises from the difficulty of comparing eco-profiles with completely different characteristics. How is the analyst to choose between a theoretically biodegradable product manufactured by a dirty process and a non-biodegradable product whose manufacturing process is relatively clean? The choice could well depend on the mode of disposal, which is very much a policy question itself. Thus, if municipal waste is disposed of in a traditional open landfill, paper will eventually be consumed by decay bacteria, whereas polystyrene will not. However, if solid waste is to be stored indefinitely in modern airtight and waterproof landfills, or if it is incinerated for energy recovery, polystyrene should probably be preferred to paper on the

basis of a cleaner manufacturing process. Evidently, in many — perhaps most — cases LCA can only expose the tradeoffs. It cannot point unambiguously at the "best" technological choice.

But LCA suffers from another problem that is less obvious. A detailed critique of the above-cited studies (among others) would require a substantial effort. However, all the studies of which I am aware suffer from two generic deficiencies which make the results difficult to take seriously. The first, and least understood, of these problems is the persistent use in such studies of unpublished (and consequently unverifiable) but inconsistent primary data. The second problem is inappropriate aggregation. I discuss the general problem of methodology, first. I then discuss these two specific problems, in order.

The Scenario Forecasting Problem

The recent recognition that some environmental problems are inherently global in scope has resulted in increased interest in long range economic models to assist in policy formulation. The "global warming" problem, in particular, has spawned a number of model-based studies of alternative energy supply scenarios. There are two general approaches, the "general equilibrium" approach and the "dynamic I-O" approach.

Models in the general equilibrium tradition often combine a rather aggregated economic forecasting model combined with a very disaggregated energy supply sector that optimizes supply choices using linear programming techniques. Perhaps the first operational example was the Brookhaven Energy System Optimization Model (BESOM) [Cherniavsky 1974; Behling *et al* 1975]. Other examples include the ETA-Macro model developed at Stanford University and the Electric Power Research Institute (EPRI) [Manne 1977; Manne & Richels 1989, 1991], the more recent Brookhaven MARKAL model [Fishbone & Abilock 1981; Morris *et al* 1990], and the DOE Fossil 2 model [Bradley *et al* 1991].

Other studies are based on less detailed energy sector disaggregations. These include the Nordhaus-Yohe model [Nordhaus & Yohe 1983], the ERM model [Edmonds & Reilly 1985, 1991; Edmonds *et al* 1986], and the Wharton/DRI/EPA model [Shackleton *et al* 1992]. The general scheme of several of these models is similar to that employed by ERM. The model calculates GNP directly from exogenous assumptions about labor force and labor productivity. The energy sector is treated explicitly, with energy demand derived from exogenous determinants including population, GNP, end-use efficiency, energy prices and energy taxes/subsidies/tariffs. Energy supply is typically determined by a linear programming model, which optimizes the choice of fuel and conversion technology, for given levels of aggregate energy demand. The energy-GNP interaction is taken into account through demand price elasticities. The ERM is regional (9 regions). ERM and similar models have been used to estimate both future emissions and the cost of reducing such emissions.

Important recent examples of dynamic Computable General Equilibrium (CGE) models that have been applied to energy policy or environmental issues such as the climate warming question include Goulder [Goulder & Summers 1989; Goulder 1992] and Jorgenson and Wilcoxon [Jorgenson & Wilcoxon 1990, 1990a; Jorgenson *et al* 1992]. European examples

include studies by Conrad *et al* [Conrad & Henseler-Unger 1986; Conrad & Schroeder 1991], Stephan [Stephan 1989] and Bergman [Bergman 1991, 1993]. In principle, the CGE models are able to endogenize the energy-GNP feedback, taxes, and prices. However labor productivity, energy supply schedules and end-use efficiency assumptions continue to be exogenous. Abatement costs are also exogenous in most models. Jorgenson & Wilcoxon cover the whole range of environmental regulations, but with exogenous costs. Stephan's model introduces water pollution abatement cost functions for wastewater treatment. Bergman's deals with the economic effects of air pollution on the same basis.

The other approach to model-based regional long-range scenario building has been developed mostly by Wassily Leontief and his colleagues. The Leontief system approximates the economy as a set of N industrial activities and an equal number of products (or product categories), such that each activity sector requires inputs from the other sectors in strict proportion to the output X_i of the sector. (This strict proportionality, or fixed coefficient, assumption is what characterizes a Leontief model ¹). The number of sectors, N , can be extremely large, but most developing the I-O tables (mainly from Census data) is exceedingly expensive and time consuming. In practice, N is usually chosen to be between 80 and 150. In addition, fixed labor coefficients and energy coefficients can fairly easily be added, along with pollution or waste coefficients [Ayres & Kneese 1969; Leontief 1970].

In his Nobel Memorial Prize lecture, in December 1973, Leontief outlined a scheme for building a model of the world economy, at the regional level, for use as a guide to international economic development planning [Leontief 1974]. At that time the U.N. General Assembly formally endorsed New Economic World Order, which was a formal goal statement by the "Group of 76" developing countries at the Lima Conference. The U.N. financed Leontief's proposed model, which was completed in 1976 [Leontief *et al* 1977]. The "world" model was unique, in that it ran in reverse. Rather than projecting the consequences of current trends in a forward direction, it specified future targets (in terms of shares of world output by various regions and sectors) and calculated the required investment levels and other factors needed to achieve the Lima goal. More recently, the U.N. sponsored a major revision and improvement of the original study in preparation for the UNCED meeting in Rio [Duchin & Lange 1991]. Whereas the older I-O models were really static "balancing" models, driven by a set of exogenous assumptions with regard to labor force, productivity, and investment the more recent version is explicitly dynamic [Duchin & Szyld 1985].

While the CGE type of model is arguably feasible for purposes of energy supply/demand forecasting, for purposes of estimating economy-wide materials requirements and pollution emissions, an I-O approach is really unavoidable. Certainly, the I-O model is regarded as being more realistic in a technical (i.e. engineering) sense than aggregate production functions

¹ As a matter of interest, a similar type of model can be constructed assuming fixed output coefficients instead of fixed input coefficients. The latter type of model has the advantage that it need not be "square", but can accommodate a much larger number of outputs than sectors. The non-square Canadian industry-commodity model is of this type [Stats Can 1967].

². On the other hand, the traditional I-O approach is also inadequate for purposes of scenario-building for exactly the same reasons that prompted the building of elaborate linear-programming modules for the energy supply sector. It is much too aggregated to reflect the real technological possibilities in many sectors. Moreover, there is no provision in the I-O model for tradeoffs between inputs (labor & capital, capital & energy, etc). Nor can the Leontief model reflect scale effects of any kind. These weaknesses, together with the difficulty of keeping the coefficients up to date, limit its value for many purposes.

Does process analysis offer further improvements on I-O, apart from greater detail, over the Leontief scheme? The answer is clearly yes, for three reasons. They are: (1) avoidance of aggregation errors (2) flexibility with regard to the treatment of co-product and co-input relationships in arbitrary combinations, and (3) the ability to take into account non-linear relationships, especially internal feedback loops. Consider the three points in order.

First, a materials-process model avoids aggregation errors, which are inherent in Leontief-type models. To illustrate the problem, consider a fairly important industrial metal: cobalt. Cobalt is used, essentially, for two purposes: permanent magnets and so-called superalloys for gas turbines and jet engines used by the aircraft industry. In process analysis, these links would be perfectly straightforward, and the demand for cobalt would be correctly determined by the demand for magnets, and aircraft. However, in a Leontief model cobalt is aggregated with other ferrous metals, including manganese, chromium, nickel, and iron. Moreover, cobalt constitutes an insignificant fraction of the ferrous metals sector, whose demand is driven by the construction sector and the automotive sector.

In general, the I-O model is reasonable for determining the indirect demand for major commodities, such as electric power, fuels, paper, portland cement, or iron and steel. For similar reasons, the I-O model can predict, with reasonable accuracy, the aggregate waste emissions broadly associated with a single sector (like agriculture) or emissions of a generic nature, such as CO₂, SO₂, or NO_x from fuel combustion. On the other hand, aggregation errors make Leontief models highly inaccurate for estimating indirect demand for specialized commodities or products, or for predicting pollutant emissions associated with specialized subsectors (e.g. artichokes, oranges, grapes) or production or intermediate use of such commodities or products. Emissions of toxic heavy metals like mercury (associated with chlorine production), fluorides (associated with phosphate rock processing and aluminum smelting), dioxins (associated with chlorobenzene production) or nitrosamines (associated with production of alkyl amines) would be examples.

The second advantage of process analysis over I-O analysis is its ability to reflect a combination of co-input and co-product relationships. The Leontief type of I-O model assumes fixed input ratios (co-inputs), whether applicable or not, but it cannot handle fixed output ratios (co-products)³. No I-O model can deal with combinations of fixed and variable input and output relationships. As an example of co-inputs, coke and limestone are co-inputs

² For a detailed discussion of the use of I-O models for materials flow analysis, see [Ayres 1978, Chapter 4, especially 4.4]

³ The Canadian version of I-O has the same limitation in reverse.

of iron-smelting from virgin ore. Bauxite, cryolite, petroleum coke and electric power are co-inputs of aluminum production. Rubber, carbon black and zinc oxide are co-inputs of tire manufacturing. On the output side, chlorine and caustic soda are co-products; sulfur is increasingly a by-product of natural gas processing, petroleum refining and copper smelting; arsenic is a by-product of copper smelting, while cadmium is a by-product of zinc smelting. All of these combinations are produced in relatively fixed ratios.

Arsenic and cadmium illustrate another problem, too. Both are highly toxic in virtually all forms. However, most of the arsenic from copper ores mined in the U.S. is left behind in mine or smelter wastes, because of weak demand for the metal (and cheap imports). On the other hand, demand for cadmium for batteries is strong, so almost all cadmium is recovered and embodied in products. However, in this case, the products themselves typically end up in landfills. An I-O model cannot reflect these relationships.

The final advantage of process analysis is its ability to handle non-linearities, such as recycling loops and scale effects. The I-O model is inherently linear, whereas many real industrial processes are not. For instance, the need for coke by the steel industry is a function of the size of the electric minimill subsector, which depends on the availability of scrap metal for remelting. This, in turn, is largely a function of the demand for new cars. Similarly, increased demand for phosphate fertilizers (together with tighter emissions controls) is likely to increase the supply of by-product fluorine (as fluosilicic acid), thus displacing natural sources. This is partly a scale effect. Scale effects determine the ratio of capital equipment inputs to labor inputs, of course. But in some cases, the scale-dependant choice of technology also involves different choices of input materials, as in the case of fluorine. Thus, when nitrate fertilizer demand was small, most ammonia was a by-product of coke ovens. Now it is produced on an enormous scale from natural gas.

Problems of Life Cycle Analysis:

(I) Inconsistent, Unverifiable Data

As an illustration of the data problem, consider *Table 1*, taken from one of the most recent and detailed studies of packaging materials. It is trivial to verify that mass balance conditions are not satisfied. For instance, in the case of PVC the total of "used materials" input per kg is 1930.82 gm per kg of product, while products and by-products add up to 2174.47 gm. not including emissions. The inconsistency is not immediately obvious, since the input list is incomplete (atmospheric oxygen is omitted, for example, as are fuels) and the output list (not shown) omits major mass flows like carbon dioxide and water vapor. Nevertheless it is easy to see that the missing mass on the output side is greater than the missing mass on the input side. However, it is impossible to cross-check the calculations or reconcile the obvious discrepancy⁴. Such a table — presented without backup calculations or references — cannot be trusted. Nor can any LCA based on it.

⁴ Unfortunately, the example illustrated is by no means an isolated case.

Table 1: Ecobalances of plastics
source: [Habersatter & Widmer 1991]

Balance per kg plastics	Unit	HD-PE	LD-PE	PET	PP	PS	HI-PS	PVC
Used materials								
Petroleum	[g]	1964.21	1966.42	4014.37	1964.21	3493.89	3406.56	906.35
Hydrogen	[g]	1.88	1.88	23.52	1.88	6.48	6.20	0.87
Oxygen	[g]			527.00				
Rock salt	[g]							1016.43
NaOH	[g]			0.45				
By-products	[g]			-1303.85		-321.32	-301.55	-716.28
By-products with calor. value	[g]	-945.46	-950.70	-2103.20	-946.96	-2189.44	-2116.51	-458.19
Adjuvants, additives	[g]	9.00	3.78	0.06	1.30	35.05	35.11	7.17
Miscellaneous	[g]	5.00		20.07				
Energy carriers								
(excl. transp. + electr. prod.)								
Fuel gas	[dm3]	255.35	255.63	189.00	227.00	108.00	114.00	192.56
Residues with calorific value	[g]	418.49	418.96	652.00	381.43	407.00	406.00	193.11
Steam	[kg]	-3.29	-3.96	0.32	-1.45	2.11	2.23	0.89
Energy balance								
Energy from material input	[MJ]	44.36	43.74	35.10	43.66	40.93	41.37	17.24
Process energy	[MJ]	19.00	16.94	38.74	21.98	29.88	30.44	20.14
Auxiliary plants	[MJ]	0.17	0.19	0.60	0.35	0.21	0.24	0.67
Precombustion	[MJ]	-0.96	-1.15	0.15	-0.40	0.64	0.68	0.33
Total production								
Thermal energy	[MJ]	62.57	59.72	74.59	65.59	71.66	72.73	38.37
Electric energy	[kWh]	0.53	0.88	1.04	0.57	0.38	0.41	1.34
E eq as per UCPT 88	[MJ]	67.6	68.1	84.5	71.0	75.3	76.6	51.1
Disposal								
Credit WIP	[MJ]	-20.78	-20.78	-15.07	-21.12	-19.15	-19.20	-8.64
Transportation	[MJ]	0.04	0.04	0.04	0.04	0.04	0.04	0.04
Total production and Disposal	[MJ]	41.83	38.98	59.56	44.52	52.55	53.57	29.77
Disposal	[kWh]	0.53	0.88	1.04	0.57	0.38	0.41	1.34
E eq as per UCPT 88	[MJ]	46.9	47.3	69.5	50.0	56.2	57.5	42.5

It is likely that the inconsistent data comes from unpublished, "confidential" or "proprietary" industry sources. But the practice of disguising the source of such data obscures a more fundamental problem: namely the fact that process descriptions available from published sources are almost invariably *unbalanced*. One of the reasons for this is the universal tendency, in industry, to distinguish purchased feedstocks from fuels and energy inputs. The problem is that the former are quantified in mass terms (tonnages) while the latter are quantified in energy units (BTU or Joules). This is an accounting convention that has the sole advantage of providing a uniform way of tracking energy-use efficiency. But, for purposes of life cycle analysis it is unnecessary. Worse, it precludes the systematic use of materials balances for verification.⁵

A related problem is that chemical process data as published in standard encyclopedias [e.g. Faith, Keyes & Clark 1975; Kirk-Othmer 1985] are also usually unbalanced. This is also true of the data in Stanford Research Institute's Process Economics Program (PEP). In general, waste streams are simply neglected in these publications. Understandably, chemists in the past have been relatively uninterested in the detailed composition of process waste streams. Moreover, chemical engineering reference books tend to simplify process descriptions, since authors do not have access to proprietary company data on yields, catalysts and process conditions (temperatures, pressures, reaction times).

But past disinterest in process waste streams on the part of the chemists and chemical process designers is no excuse for total neglect of this problem in LCA where the whole point of the exercise is to account for wastes. In the first place, any LCA based on unbalanced process data cannot be credible. In the second place, there are ways of filling in the missing data, at least approximately. The laws of physics tell us that mass flows into and out of each process, in steady state, *must* balance. This must be true for both large units and small ones, for each nation, for each region, for each industry and each factory. It must also be true for each unit process, and the balance must apply to each chemical element.

At the national, industry, and factory levels accounting data can be extremely helpful. It is not always necessary to determine the quantity and composition of waste streams by direct measurement. In fact, it is often not possible to do so with any accuracy. However, a competent factory manager must know (or have the means of knowing) exactly what materials are purchased, and what products are sold. His process engineers must know exactly what inputs are required (including air and water) to produce each unit of salable product. Moreover, the laws of chemistry can tell him (and us) a good deal about the likely composition of process waste streams, based on approximately known reaction conditions. In fact, computer software embodying much of this knowledge has been available for several years. In fact, the use of materials-balance conditions is absolutely central to chemical process design [e.g. Rudd *et al* 1973, chapter 3]. However, this approach has not yet been applied except in rare instances to the problem of estimating process waste flows and compositions. This deficiency can only be rectified by the consistent use of *balanced* unit process input/output data.

⁵ For a detailed application to the nuclear industry, see [Avenhaus 1977; also Ayres 1978, p 117]

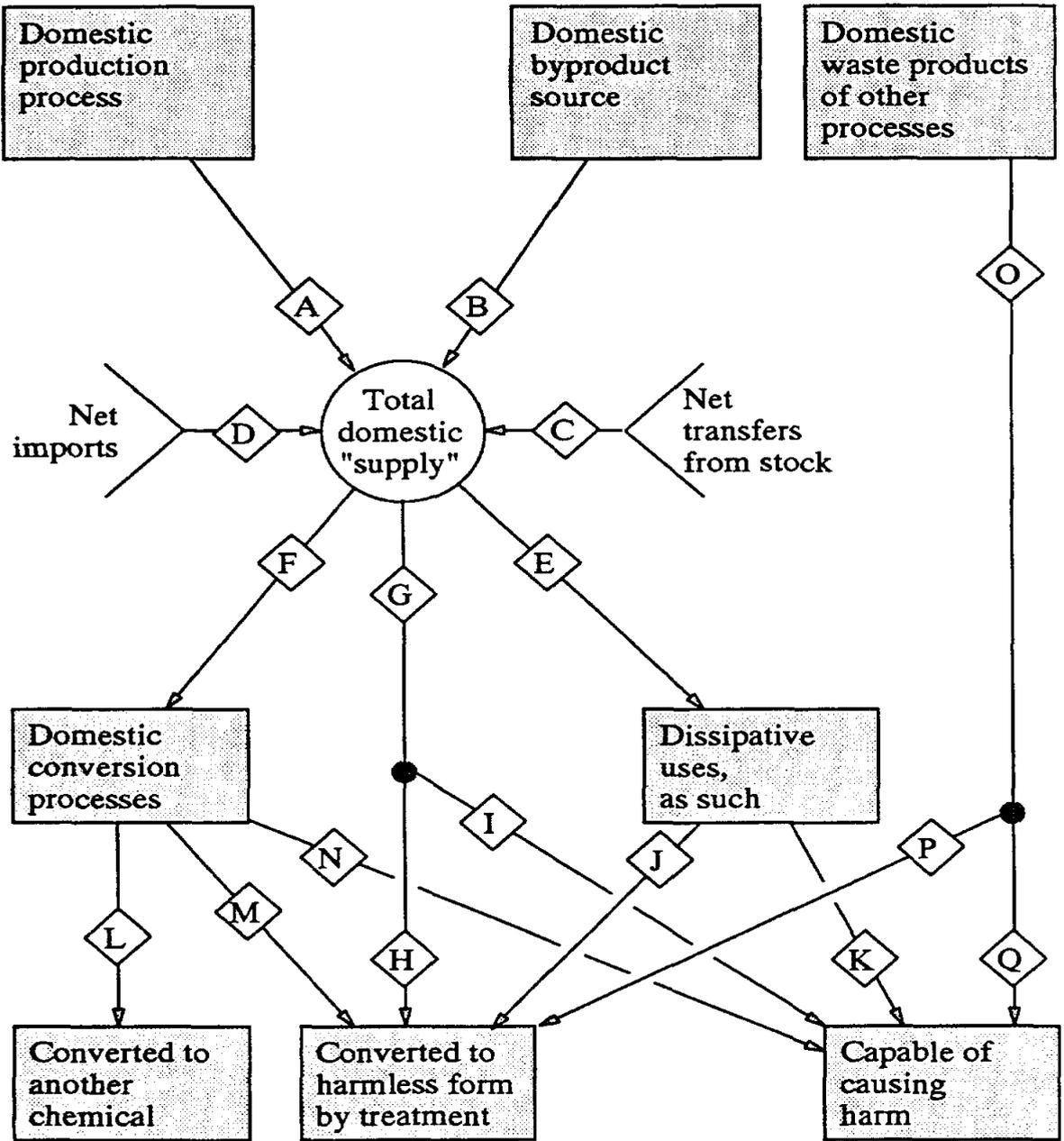


Figure 1: Materials Balance for a Chemical Product
source: author

The same logic applies at higher levels of aggregation. For example, *Figure 1* shows a schematic materials balance for a chemical product. There are 16 distinct mass flows, labelled A through Q. Mass flows A through F represent quantities for which economic statistics are normally available. These are, respectively, domestic (or local) production, by-products of other domestic production processes, net transfers from stock, net imports, dissipative uses and conversion uses. The last two add up to total domestic consumption; however the allocation between them requires some market data that may not be published. The 10 streams G through Q, represent other pathways for the chemical, as shown on the schematic. There are five steady-state materials balance conditions that can be used to reduce the number of unknowns. These are as follows:

1). $G = A + B + C + D - E - F$ (steady-state supply)

2). $F = L + M$

3). $G = H + I$

4). $E = J + K$

5). $O = P + Q$

This set of equations leaves 5 unknowns to be determined by means of process data, especially including treatment processes. As noted, G — aggregate wastes from the domestic (or local) production process can be computed most accurately by using accounting data. This is available to a plant manager, if not to outsiders. However, G can also be estimated from process simulation models that are generally available to chemical engineers, as mentioned above. Thus, there are external means of verification. Next, H represents wastes from the domestic production process that are treated on site by impoundment or conversion to a harmless form. This can be determined from the throughput of the treatment process (which must be known to the plant manager, and should also be available to the regulatory agency). An outsider with some knowledge of the process technology would also be able to make use of simulation models for verification purposes. Untreated emissions I would thus be the difference between G and H. (Direct measurement is a much less reliable means of determination).

Similarly, the amount of the chemical actually converted into other downstream products, L, can be estimated quite accurately by the on-site process engineer — or by computerized process models available to outsiders — from knowledge of the downstream conversion process yield. The unconverted fraction of inputs must then be treated (M) or discharged (N). Again, M can be estimated most accurately from the throughput of the treatment or disposal process in use in connection with the conversion process (if any), leaving N as the difference. The same logic applies to dissipative uses. In some cases, at least, it is possible to treat an effluent stream from a dissipative uses, such as solvents, used motor oil or detergents. The stream J accounts for such cases, while K is the untreated remainder. Finally, the same logic applies to the indirect flux O, of which some (P) may be treated, leaving an untreated remainder Q.

Again, direct measurement of emissions is potentially helpful as a means of verifying treatment efficiency process data, but that it cannot be relied upon as the exclusive means of determining aggregate waste flows, especially from dispersed consumption streams.

The foregoing scheme is applied to the estimation of aggregate waste streams at the U.S. national level, in subsequent papers.

Problems of Process Analysis:

(II) Inappropriate Aggregation/Disaggregation

The other generic problem of many LCA's based on process analysis is inappropriate aggregation. It must be acknowledged at the outset that there are practical limits to any process analysis. This understandable creates an incentive for aggregating individual processes into composite modules. For instance, it might make sense to consider all the alternative processes for producing a major industrial intermediate (e.g. chlorine, methanol or ethylene) as a single module. Similarly, one might do this for a finished material, like aluminum. The basic scheme for constructing such modules, along with some of the data requirements, is considered in more detail in the next section.

However, process analysts often aggregate processes by omission of "minor" inputs without any consistent justification. For example, consider *Figure 2* taken from the same LCA cited earlier. In this case a number of processes leading into primary aluminum smelting are aggregated into a much smaller number. The process inputs seem to consist of 27.5 kg of bauxite, 2.4 kg of an output of electrolysis of rock salt (actually sodium hydroxide, NaOH) and 0.5 kg of some output of calcination of limestone (lime, CaO). While the diagram is quite confusing, it appears that 30.4 kg of inputs flow into process K (aluminum fluoride manufacturing), producing 18 kg of product and leaving 12.4 kg of inputs unaccounted for.

It is interesting to compare *Figure 2* with *Figure 3*, which is about 15 years older (author; several sources). The first refers to Switzerland or central Europe c. 1990; the second refers to the U.S. c.1975. There are significant differences. For instance, *Figure 2* states that 430 kg of carbon anodes are used per metric ton of aluminum, while *Figure 3* allocates 510 kg of carbon anodes per tonne. Probably this reflects increasing efficiency in the electrolysis process. There are also modest differences in the process that converts bauxite to alumina (the Bayer process) probably reflecting different assumptions about the chemical composition of the bauxite feed. The big difference in the two diagrams (apart from the fact that *1* is unbalanced) has to do with the fluorine input to aluminum electrolysis. Aluminum reduction requires both synthetic cryolite ((3NaF)AlF₃) as the electrolyte and aluminum fluoride AlF₃. The latter is used for process makeup, due to fluorine losses (emissions) to the air at the anode.

Figure 2 apparently aggregates the production of the two different materials under the single label "aluminum fluoride". Taking them together, it shows only 18 kg per metric ton, compared to 70 kg in *Figure 3*. The sodium in the synthetic cryolite obviously comes from an input stream of sodium hydroxide, as correctly indicated both by *Figure 2* and *Figure 3*.

The aluminum in both chemicals is ultimately derived from bauxite, though *Figure 3* shows an intermediate stage, refined alumina. This difference may be accidental and is probably unimportant.

However, fluorine is the most dangerous pollutant in the aluminum reduction process, and the only reason for adding aluminum fluoride to the electrolytic bath is to replace this loss. If the figure of 18 kg shown in *Figure 2* does actually refer to both fluorides, then remarkable progress has been made in reducing fluorine emissions (hence usage) over the last 20 years. However *Figure 2* completely omits one critical input, namely hydrofluoric acid (or another precursor such as fluosilicic acid). This omission is so strange and pointless that it raises serious doubts about the rest of the analysis. Yet, the same study unnecessarily disaggregates the forming of aluminum foil from aluminum ingots into four distinct processes (casting, sawing, rolling, etc) despite the fact that only electric power is needed, with no other significant inputs or waste streams. There is simply no good reason to disaggregate these downstream processes, while lumping the upstream processes together so carelessly.

Another case of inappropriate aggregation is the tendency of some LCA's to lump mineral ore extraction and concentration into a single "black box" with virtually no detail. Yet the mining sector generates far more solid and liquid waste (and probably more hazardous waste) than any other sector, including the chemical industry. But these mining and processing wastes are not uniformly distributed across the sector any more than they are uniformly distributed across the landscape. The differences between iron mining or limestone quarrying, on the one hand, and copper mining (or, worse, platinum or uranium mining) make any such aggregation ludicrous. (Uranium mining involves more ore processing, worldwide, than iron mining). It is totally inappropriate to attribute refuse, hazardous wastes and pollution associated with an aggregated "mining" sector to individual metals or minerals on the basis of monetary values of the output. Allocation on the basis of tonnages would be even worse.

It is possible that mining and concentration of minerals tends to be neglected in many LCA's because the activity and the associated wastes occur primarily in remote locations, not in Europe. (The mining industry is still very important in North America, however). But, while mining and associated wastes may be generated far from major population centers, it is not appropriate to neglect them in the LCA. If there is a valid argument for giving such wastes less weight in a policy sense, that judgment should be made explicitly in the ecoprofile analysis.

Aggregation is clearly appropriate in some cases. Since electricity in one location is indistinguishable from electricity in another, and all the networks are interconnected, it is reasonable in most cases to assume that all electric power in a given country (or even the whole of Europe) is "average" in terms of its mode of production. Similarly, trucks or barges in one country are much like trucks or barges in another. Again, averages are probably appropriate. However, transportation cannot safely be aggregated beyond this level of detail, inasmuch as some modes of transportation — notably aircraft and light trucks — are far more polluting than others. Similarly, waste disposal techniques are hardly uniform from country to country, or from sector to sector. Distinctions must be made.

**Material flow chart of aluminium production
(Production of aluminium after the Bayer-process)**

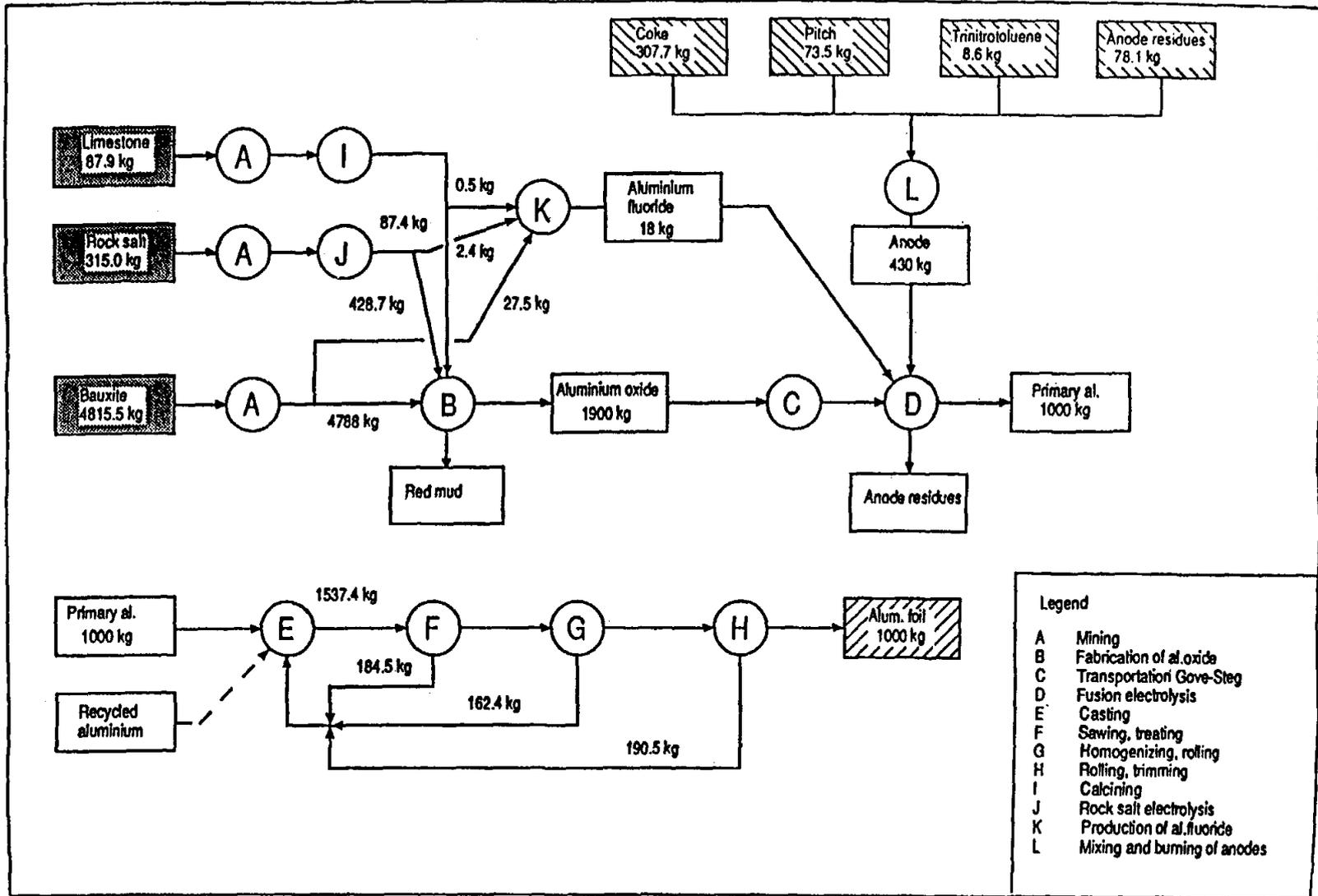


Figure 2: Material flow chart of aluminium production
Source: [Habersater & Widmer 1991]

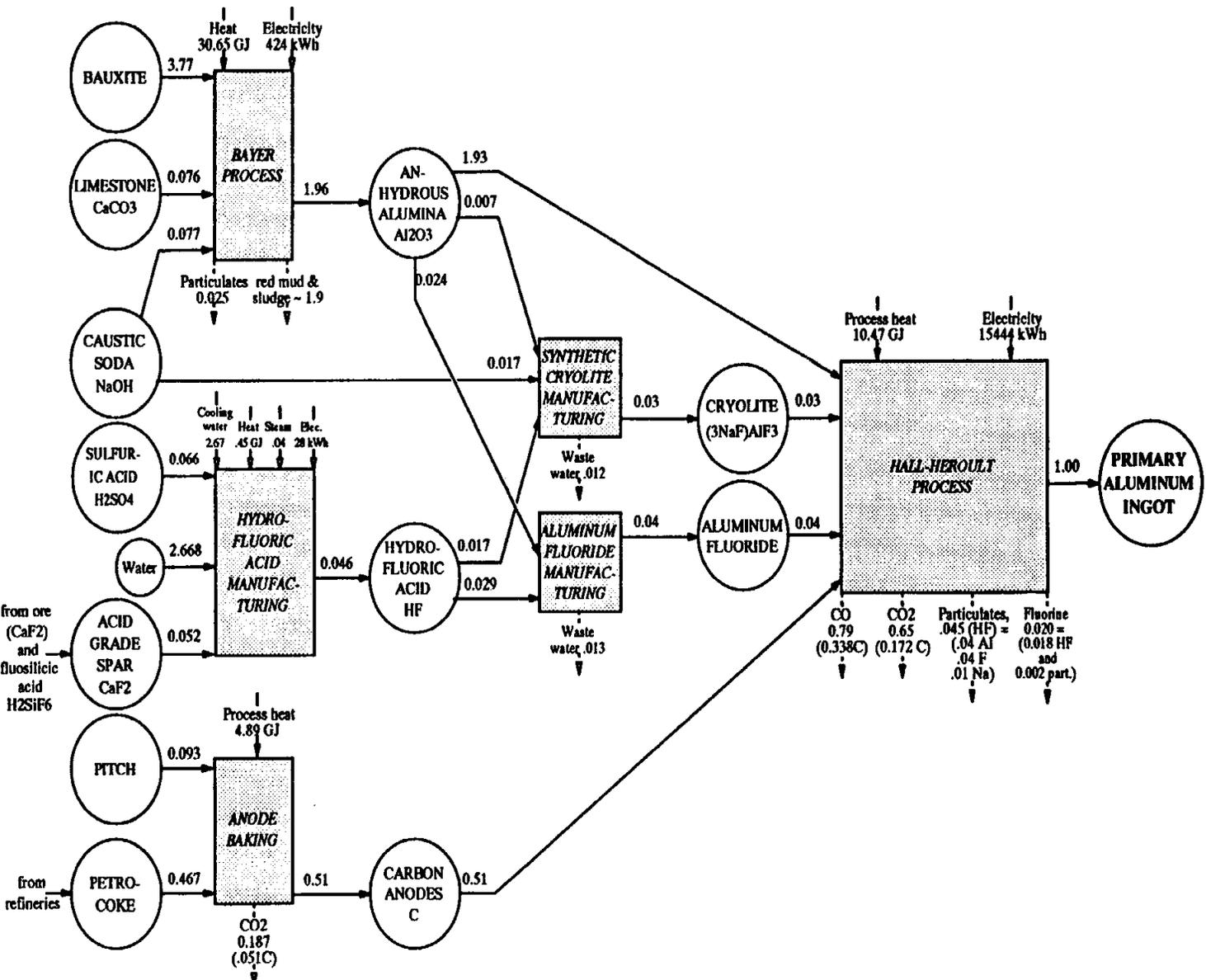


Figure 3: Aluminum Ingot Unit Process
Source: author

Indeed, for extraction, reduction, refining and transportation activities LCA's cannot be reliably based on the use of Input-Output tables of the Leontief type, because of the aggregation problem just noted (among others). To be sure, I-O data can play a minor role, e.g. in estimating the indirect energy requirements for various service sectors which are, themselves, indirect contributors to products. However, it is important to construct the direct process chains for all major materials (and fuels) as far back as raw materials extraction. This backward chain should also include (for instance) the actual modes and amounts of transportation required for each product, rather than proxies based on averages. On the other hand, for dealing with indirect contributions from service sectors, or from capital goods, I-O models are probably the only choice.

Future LCA's will have to use both I-O and process analysis judiciously. Where process analysis is used, the materials/energy balance principle is an indispensable tool for error detection and correction. The materials balance principle is discussed next.

Materials/Energy Balance Principle

The first law of thermodynamics — conservation of mass-energy — is applicable to every process and every process network. It is therefore applicable to every firm. This means, in words, that, over the life of the process-chain, the mass of inputs (including any unpriced materials from the environment) must exactly equal the mass of outputs, including wastes. For continuous process, this balance condition must hold for any arbitrary time period.⁶ The materials balance condition is much more powerful than it appears at first glance, since chemical elements do not transmute under normal terrestrial conditions. Taking this into account, the balance condition holds independently for each chemical element. Moreover, in many processes, non-reactive chemical components, such as process water and atmospheric nitrogen, can also be independently balanced. Thus half a dozen, or more, independent materials balance constraints may have to be satisfied for each steady-state process.⁷

Practitioners often attempt to separate energy carriers from "feedstocks". This is traditional among government and industry accountants and statisticians, but the distinction is somewhat arbitrary when applied to endothermic processes where the heat is produced by partial combustion yielding an intermediate — such as carbon monoxide — that participates chemically in the rest of the reaction. Major examples include ammonia synthesis and carbothermic smelting. It is both unnecessary and extremely confusing to insist on counting

⁶ The case of batch processes or continuous processes with time variability, requires more careful consideration. In general, however, the accounting rule holds: stock changes equal inputs minus outputs. When stock changes are zero, or can be neglected, inputs equal outputs.

⁷ These conditions can be very helpful in filling in missing data. For instance, chemical engineering textbooks [e.g. Faith, Keyes & Clark 1975], tend to provide "recipes" for standard chemical processes that specify inputs (per unit output) in some detail, but neglect to specify waste products. While a detailed chemical characterization of the wastes requires very complex model calculations (or direct measurements), one can derive some useful information about the elementary composition of the wastes.

feedstocks and fuels in separate categories in such cases. If energy carriers and combustion wastes are not counted in mass terms, no materials balance is possible. For this reason, among others, the materials balance principle is rarely applied in practice at the commodity or industrial levels, even though it is a standard tool in process design [e.g. Rudd *et al* 1973].

A point of some importance here is that, even if the balances are partly based on theory and not always on direct measurement, the additional conditions imposed by the balancing requirement leave far less room for uncertainty than an unbalanced process would do. In short, systematic use of materials balance conditions can increase the accuracy of empirical data by reducing error-bounds. Alternatively, the materials balance conditions can be used to "fill in" missing data. The following simple example illustrates this point. Ethyl chloride (C_2H_5Cl) is a chemical used in the manufacture of tetraethyl lead. One (obsolete) manufacturing process was to react ethylene (C_2H_2) directly with anhydrous hydrochloric acid (HCl) in the presence of an aluminum chloride catalyst. According to a standard source the reaction requires 488 kg of ethylene and 625 kg of hydrogen chloride to yield 1 metric ton (1000 kg) of ethyl chloride [Faith, Keyes & Clark 1975 p 371 *et seq.*].

The inputs add up to 1113 kg. Applying the materials balance principle, it seems that 113 kg of outputs are unaccounted for. But we can do better by comparing inputs and outputs one element at a time. Inputs of carbon, hydrogen and chlorine, in that order, were 417 kg, 87 kg and 607 kg. Subtracting outputs accounted for in the ethyl chloride product, we have unaccounted for outputs of 45 kg C, 58 kg Cl and 9 kg H. Presumably, the waste (or by-product) stream consists of a number of other compounds of these three elements. In actual fact, according to the same source, the major component of this waste stream should be ethylene dichloride ($C_2H_4Cl_2$). However, the mass ratio in the waste is 5:6.444:1, whereas the mass ratio in ethylene dichloride is about 6:30:1. In other words, the waste stream has either too little hydrogen, or much too much chlorine for this outcome.

One can test various other hypotheses, however. Suppose all the leftover chlorine (58 kg) is used up in making ethylene dichloride. Based on the chemical formula given above, it is easy to verify that this would use up a little less than 12 kg of C and 1 kg of H, leaving just over 33 kg of C and 8 kg of H. This combination of masses would work if all the carbon remained in the form of unreacted ethylene (38.5 kg) leaving 2.5 kg of hydrogen gas. Or, suppose all the chlorine were left in the form of unreacted hydrogen chloride? In this case 58 kg of chlorine would use up about 1.7 kg of H, leaving 45 kg of C and 7.3 kg of H. But, even if the carbon and hydrogen combined as methane (CH_4) the available hydrogen could only combine with 22 kg of carbon, leaving 23 kg uncombined (as carbon black?).

Neither of the above hypotheses seems likely, but that is not the point. Notice that all of these possible outcomes can be tested using materials balance information and simple chemical combinations alone, without even knowing the reaction conditions. No deep knowledge of chemistry was involved. Of course, there are many possible combinations of chemicals in the waste stream that would satisfy the materials balance conditions, but an even larger number of possibilities can be eliminated from consideration. Needless to say, far more detailed predictions of complex chemical reaction paths are possible today, and much of this knowledge has been programmed into software packages available even for desk-top

computers. In short, it is feasible to estimate the *molecular* composition of waste streams from the composition of process inputs and approximate knowledge of reaction conditions, notably temperatures, pressures and catalysts.

The energy conservation condition, in practice, is quite complex. Unit processes are of two kinds: *exothermic* (literally, "heat generating") and *endothermic* ("heat absorbing"). The combustion of hydrocarbons is an example of the former, though there are many others. The synthesis of ammonia and the reduction of iron ore to pig iron (mentioned previously) are both examples of the latter. The energy conservation condition states that the so-called "free energy" (or "available work") used in any endothermic process steps must either be supplied from exothermic processes or by external heat or electricity inputs.

The conversion of free energy (in the form of chemical energy) to heat in exothermic processes is usually quite efficient. However, the *availability* of the heat — its ability to perform useful work — depends on the temperature of the working fluid (i.e. combustion products). The second law of thermodynamics implies that there will be some entropy production, or reduction in availability, generally reflected by the non-infinite temperature of process heat. Actual entropy production in each case depends on specific details of the reaction chemistry and the process. Conversely, the conversion of heat to chemical energy in endothermic processes tends to be much less efficient. Entropy losses tend to be quite large in "real" processes, as compared to idealized processes.

It is tempting to interpret the free energy consumption per unit output of a unit process as an "energy coefficient". Given such a coefficient for each step in the process-chain, one can perform a "net energy" analysis of any product.⁸ However, the so-called "second-law efficiency" of an energy conversion process was introduced to give some of the early net energy studies a more rigorous theoretical basis [Ross *et al* 1975]. It is the ratio between the theoretical minimum free energy requirement for the transformation, and the actual free energy loss in the process. The numerator is simply the free (chemical) energy of the product(s). The denominator of this ratio is the difference between free (chemical) energy embodied in all of the inputs, including heat and electric power, and the free (chemical) energy embodied in the final products.

Table 2: Second Law Energy Efficiency in Process Industries

	1968 ^(a)	1988 ^(b)
Integrated iron & steel manufacturing	22.6%	25%
Petroleum refining	9.1%	12%
Primary aluminum	13.3%	15%
Cement production	10.1%	<12%

(a) [Gyftopoulos *et al* 1974]

(b) [Ayres 1991]

⁸ Net energy analysis introduced as a formal methodology in the early 1970's [e.g. Odum 1971; Hannon 1972; Berry 1972]. At first, rather broad claims were made for its usefulness as an evaluation tool, but the methodology was attacked by many economists [e.g. Huettner 1976].

It must be noted that second-law energy efficiencies of most real industrial processes tend to be fairly low, due to the practical limitations of the equipment used in the unit operations. Examples are shown in *Table 2*. Because of this, energy-balance conditions cannot be used to yield rigorous conclusions about the economic feasibility of future processes, or future versions of present ones. Energy coefficients for real industrial processes, or industrial sectors, merely reflect the present state of technology, not its future potential.

Unit Processes and Process Chains

The notion of a "unit process", consisting of a set of "unit operations" was apparently introduced into chemical engineering practice by Arthur D. Little, founder of the well-known consulting firm. Unit operations are physical changes, such as heating, cooling, evaporation, condensation, compression, evacuation, transport, etc. carried out by specialized pieces of equipment. A unit process, by contrast, generally involves a chemical transformation. It is characterized by a set of inputs and outputs, including one unit mass of a main product or several co-products, plus minor by-products and waste products. The main product, co-products and by-products are accounted for and exchangeable in markets. They have market prices. This is also true of most inputs, although some inputs (such as air, water, or sunshine) may be available at no cost. To be sure, this description is applicable to a very wide range of situations, including plants, firms and whole industries. However, a unit process is the *simplest* subunit that transforms one set of market commodities (inputs) into another set of marketable commodities (outputs). Thus a unit process is actually a fundamental economic entity, in the sense that it cannot be further subdivided into unit processes, but only into unit operations (e.g. grinding, compression, distillation or crystallization).

A firm can be defined as an economic entity that produces and sells goods or services in a market. To do so, it must buy raw or intermediate materials and add value to them. To do this it must purchase labor. It must also buy (or make) capital goods. Clearly, some firms are able to create salable services from labor alone or add value to materials without transforming them chemically. However, many products do involve chemical transformation. These products are outputs of unit processes. Primary producers, therefore, must be based on at least one unit process. (Hereafter, the qualifier "unit" will normally be omitted, except where it is essential for clarity). In general, producers can be regarded as process-chains or process networks. Indeed, the process-chain or network of such a firm constitutes its core technology.

A unit process-chain (or tree) is simply a sequence of unit processes that successively transform primary materials into a unit quantity of some finished material. See, for example *Figure 4*. A more complex example is shown in *Figure 5* which exhibits a network of processes leading to polyvinyl chloride (PVC) and polyethylene (PE) [Ayres 1978 *Figure 5.4* p 155]. The output of one process becomes the input for the next. A list of the processes signified by numbered boxes in *Figure 5* is given in *Table 3*. It is not necessary that input and/or output commodities actually be exchanged in a marketplace at each step in the chain; it is enough that markets exist in which they could be exchanged *in principle*. (Actually, some chemical intermediates, such as carbon monoxide are essentially never bought or sold, but are invariably manufactured on-site as needed. This is because they are bulky, low in value, and

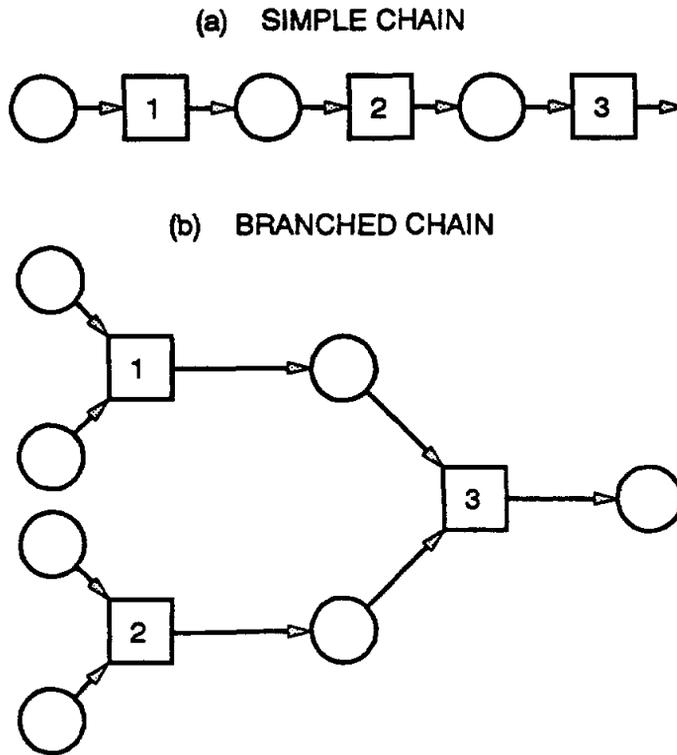


Figure 4: Unit Process Chains

inconvenient to store and transport. However, it is clear that carbon monoxide *could be* a marketable commodity if demand increased; the same is true of some other low value materials, such as calcium sulfate and ferrous sulfate).

Continuous processes can be described adequately, for many purposes, as vectors of inputs and outputs, including energy carriers (fuels, electricity, process steam) and wastes. Alternative processes can be easily compared. The schematic version of a process matrix is shown in *Table 4* while an illustration corresponding to *Figure 5* is given in *Table 5*.

A composite process is a process chain or set of chains (or networks) converting raw materials into some generic category of finished materials, such as PVC, carbon steel or paper products. The example of primary aluminum was shown in *Figures 2, 3*. A composite process may either be described in terms of total outputs and inputs (as in *Figure 2*), or in unit form i.e. in terms of inputs per unit output (as in *Figure 3*). For a composite process, the output may be a weighted mix of related commodities produced by the same family of processes. In addition to unit process data, it is necessary to have data on the actual "mix" of unit processes in use at a given time and in a given country or even for the whole world. A composite process is therefore a detailed characterization of an industry, in process terms, for a given region and year.

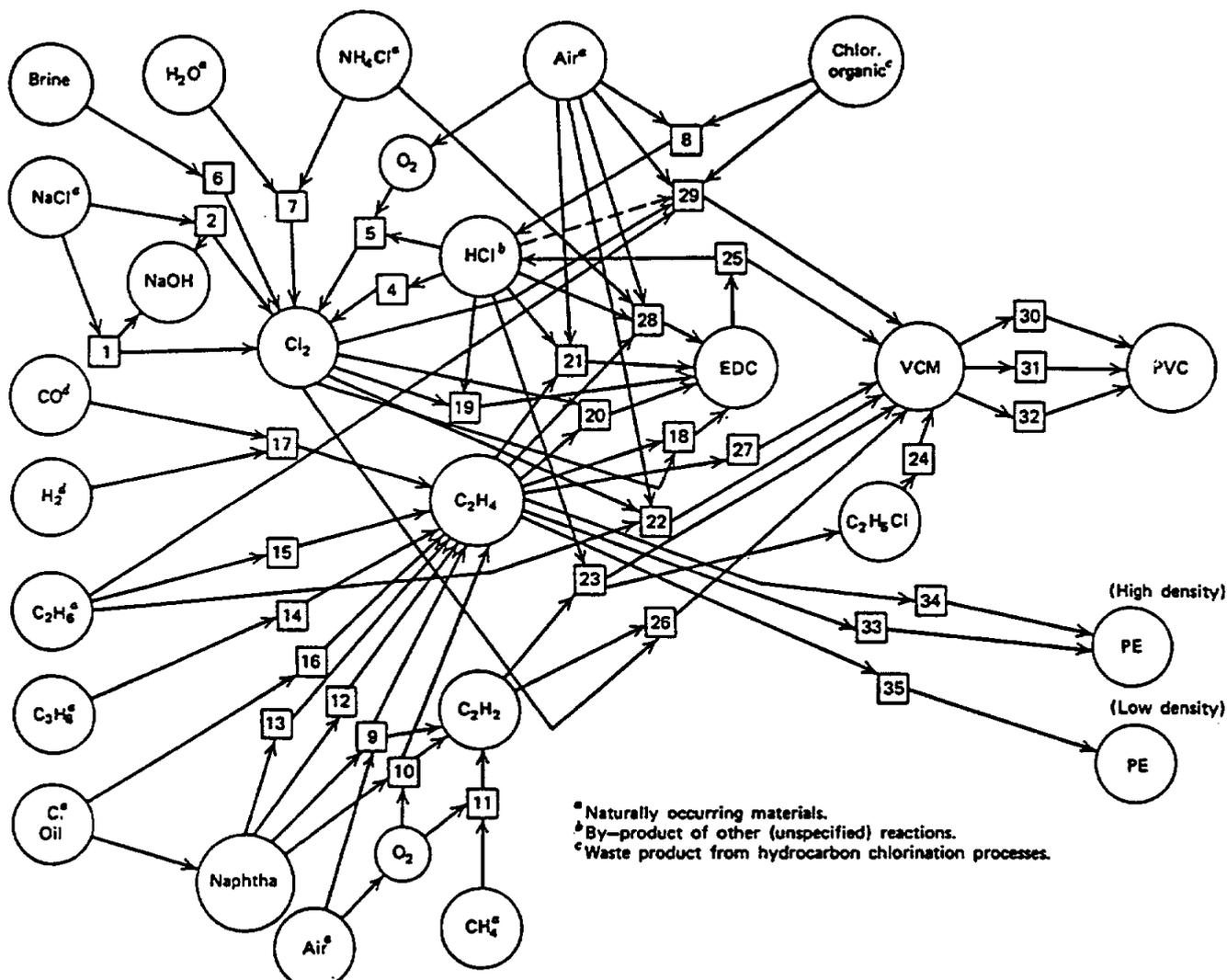


Figure 5: A Network Leading To Polyvinyl Chloride (PVC) and Polyethylene (PE)
source: [Ayres 1978]

Summary of Conclusions

In summary, the methods and models underlying both many published LCA's and many scenario-building efforts are inadequate to their stated purposes. The problems of LCA's are (1) failure to publish underlying process data attributable to credible sources, (2) failure to impose materials balance conditions (often because of unnecessary and confusing attempts to distinguish energy carriers from feedstocks) and (3) inappropriate aggregation. In the case of LCA's there is a tendency to aggregate "upstream" sectors too much, especially in mining and transportation, while disaggregating the manufacturing process beyond any need. The problems of scenario-building based on CGE's or I-O models are two-fold. One is the tendency to assume that an "optimal" path is the one that will be followed. The second is, again, the problem of aggregation errors.

As regards the unrealistic assumption of perpetual Pareto-optimality, upon which some economic forecasting models depend, one can only plead for common sense. The economic system is not in Pareto equilibrium now. It probably never has been. It probably never will be. Feasible scenarios need not be "optimal paths" in this sense.

To cure (or, at least, abate) the data-related problems it is suggested that it would be helpful to build a data base of *composite processes* (comparable to the example in *Figure 3*) for a number — between 20 and 50 — of major *finished* materials (e.g. carbon steel sheet, stainless steel sheet, aluminum sheet, glass, cement, paper, synthetic polymers). This, in turn, requires an underlying data base of about 500 chemical and metallurgical *unit-process* descriptions is needed, specifying unit inputs (including energy and process water) and outputs, including waste streams. Each composite process and each unit process should be explicitly balanced, with respect to every chemical element, to within a specified accuracy. Both data-bases should be updated at least every five years and published. The unit process data, together with market share data for constructing the composite processes, should be collected directly from industry as part of the Census of Manufactures.

Firm's concerns about revealing proprietary data can and should be met in two ways. First, proprietary process conditions (e.g. temperature and pressure) and catalysts can be kept confidential, provided the operator is able to guarantee that no emissions of hazardous or toxic chemicals are generated, or that any such emissions are below acceptable standards. Second, proprietary interests can be further protected by averaging⁹ over all establishments using the process. This should be done at the national level when more than three firms use the same process. However, the averaging could also be extended to the EEC region as a whole in cases where *any* of the member countries have three or fewer competing firms using a given process.

⁹ The average should, of course, be weighted by the level of output of each producer.

Table 3: Processes for PVC & PE

1. EDC via ethylene oxychlorination (liquid)	18. Cl_2 via salt electrolysis — mercury cell
2. EDC via ethylene chlorination (gas)	19. Cl_2 via salt electrolysis — diaphragm cell
3. EDC via ethylene oxychlorination (gas)	20. Cl_2 via HCL electrolysis
4. EDC via NH_4Cl oxychlorination	21. Cl_2 via HCL oxidation using $CuCl_2$ catalyst
5. Ethylchloride from ethane/ethylene	22. Cl_2 via HCL oxidation using HNO_3 catalyst
6. VCM from ethylchloride	23. Cl_2 via brine electrolysis & carbonation
7. VCM from EDC pyrolysis	24. Cl_2 via NH_4Cl oxidation — modified Solvay process
8. VCM from concentrated acetylene chlorination	25. Hcl from chlorinated HC waste
9. VCM from acetylene/ethylene chlorination	26. Acetylene/ethylene via Wulff process (naphtha feed)
10. VCM from ethane oxychlorination (transcat)	27. Acetylene from naphtha by partial oxidation
11. VCM from chlorinated HC waste	28. Ethylene from methane by partial oxidation
12. PVC from VCM — suspension polymerization	29. Ethylene from light naphtha
13. PVC from VCM — emulsion polymerization	30. Ethylene from full range naphtha
14. PVC from VCM — bulk process	31. Ethylene from propane
15. HDPE using metal oxide catalyst	32. Ethylene from ethane
16. HDPE using Ziegler catalyst	33. Ethylene via autothermic cracking
17. LDPE via tubular reactor	34. Ethylene synthesis from CO/H_2
	35. EDC via ethylene chlorination (liquid)

Source: [Ayres 1978: Table 5.7, p. 156]

Table 4: Typical Industry Process Matrix

	<i>Processes</i>			
	Z_1	Z_2	Z_3	Z_4
Inputs	$-q_{11}$ $-q_{21}$ $-q_{31}$	$-q_{12}$	$-q_{13}$.
Outputs	$+q_{41}$ $+q_{51}$ $+q_{61}$ $+q_{71}$ $+q_{81}$.	.	.

$\sum_{i=1}^8 q_{ij} = 0$ by conservation of mass, where q_{ij} is the weight of material i participating in process j .

Source: [Ayres 1978: Table 5.6, p. 154]

**Table 5: Materials/Energy Input-Output Vectors for Two Processes
Actually in Use (normalized to 1 unit of PVC output)**

<i>Material</i>	<i>1,2-Dichlorethane (EDC) Processes</i>	
	<i>Process 20 Product 31</i>	<i>Process 21 Product 31</i>
Utilities		
Power in kilowatt hours	0.01203	0.01406
Steam in pounds	1.14533	0
Cooling water in gallons	1.61261	3.89057
Energy intensiveness in 1000 Btu	—	-0.17432
Primary raw material		
Water	0.31103	0
Oxygen from air	0	0.10349
Hydrogen chloride	0	0.45018
Secondary raw materials, catalysts		
Sodium hydroxide	0.00229	0
Products		
Chlorine	0.73893	0
Ethylene	0.30745	0.16730
1,2-Dichlorethane (EDC)	-1.02295	-0.55082
By-products		
None		
Air pollutants		
Carbon monoxide	0	-0.00069
Ethane	0	-0.00033
Ethylene	-0.00007	-0.00153
Vinyl chloride monomer (VCM)	-0.00124	-0.00480
1,2-Dichlorethane (EDC)	-0.00173	0
Water pollutants		
Water	-0.34151	-0.00123
Sodium hydroxide	-0.00100	-0.00055
1,2-Dichlorethane (EDC)	-0.00493	-0.00109
Tetrachloroethane	-0.00418	
Contaminants		
Water	-0.04751	-0.10854
1,2-Dichlorethane (EDC)	0	-0.00081
Dichlorethylenes	0	-0.00452
Chloral	-0.00477	0

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