An integrated approach to process waste minimization research

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Abstract

Waste minimization for industrial processes is evolving, with at least three generations of activity apparent. Initially, waste minimization programs focussed on good housekeeping practices, inventory control and minor changes in operating practices. This generation of waste minimization resulted in impressive reductions of waste, but the methods are rapidly reaching their limits. A second generation of waste minimization is underway. In this second generation, current technologies are being used to modify processes, reducing effluents. These retrofit operations employing current technologies will also reach their limits, however, and a third generation of waste minimization activity is inevitable. In this third generation, highly selective separation and reaction technologies, specifically designed for waste minimization applications, will be employed. Further, new methods for process synthesis will be developed which minimize effluents (maximizing mass efficiency), evolving in the same way as energy efficient process design methods. This paper will describe an integrated research effort aimed at addressing these third generation technological needs. The research results are demonstrated through case studies focussing on particular waste streams. The streams selected for research emphasis were chosen by examining and prioritizing the nationwide mass flow of pollutants. This quantitative, nationwide flow mapping of waste streams will also be presented, along with the prioritization scheme used to select targets for waste minimization research.

Introduction

As treatment and disposal methods for hazardous waste become increasingly expensive and as long term financial liabilities associated with waste disposal grow, generators of waste have become more conscious of the need to reduce or eliminate the wastes leaving their facilities. Programs to reduce or eliminate wastes at the source have gone under the heading of waste minimization, source reduction, pollution prevention and waste reduction. Just as there are many names for these activities, there have been numerous attempts to define them precisely. One of the more restrictive definitions of this area, which we choose to call waste minimization, has been given by the Office of Technology As-

sessment (OTA). The OTA defines waste minimization as in-plant processes that reduce, avoid or eliminate the generation of waste [1]. Using this as our operating definition of waste minimization, we will describe an integrated research program underway at the University of California at Los Angeles (UCLA), which addresses the key technical issues in this field.

In order to understand the nature of the technical roadblocks to waste minimization, one must understand how waste minimization is currently practiced. Initial efforts at waste minimization have been aimed at the most easily achieved targets. Good housekeeping practices, inventory control, and minor changes in operating practices have resulted in an impressive amount of waste reduction. This type of activity is rapidly approaching its limit, however, and a second generation of waste reduction is beginning to be implemented. In this second generation of waste reduction, industry uses current technology, most often separation technologies, to reduce emissions. A typical example, cited in the OTA report on waste minimization [1], is the use of carbon adsorption for solvent recovery and recycle. In this type of non-selective separation, the contaminants in the solvent are recycled along with the solvent. The next generation of improvements in pollution prevention, after simple separation and recycling operations, will require much more selective separation processes. Similarly, waste streams are often generated due to unwanted reaction byproducts in chemical synthesis. More selective reaction technologies have the potential to significantly reduce waste. Finally, many complex chemical operations are not fully realizing their waste minimization potential. Consider, as an example, the case of phenol and related compounds in refinery wastewaters. In wastewaters, phenol is a contaminant that can be very difficult to degrade, yet in many refinery streams phenol has value as an oxidation inhibitor and fuel stabilizer. If phenol can be exchanged between the proper streams, waste is reduced. A new generation of design methods will be required to indentify the extent to which such opportunities can be exploited.

A critical issue in the development of waste minimization design methods, separation technologies and reaction technologies is the identification of target waste streams. There are tens of thousands of waste streams produced annually by large quantity generators that fall under the provisions of the Resource Conservation and Recovery Act (RCRA) [2]. Deciding which pollutants and which waste streams should be the focus of research activities is therefore a complex task. An overall mapping of RCRA regulated hazardous waste flows is given in Fig. 1. The data provided by this figure can serve as an overall guide to identifying target streams for waste minimization, however, the data must be examined carefully. Consider, for example, the waste flows reported for incineration. Incineration and cofiring of wastes (reuse as fuel) are used to manage 2–3 million metric tons of waste per year. Yet, incineration produces about 40 million metric tons per year of hazardous wastewater and ash residue. Any evaluation of the overall impact of incinerating a waste stream
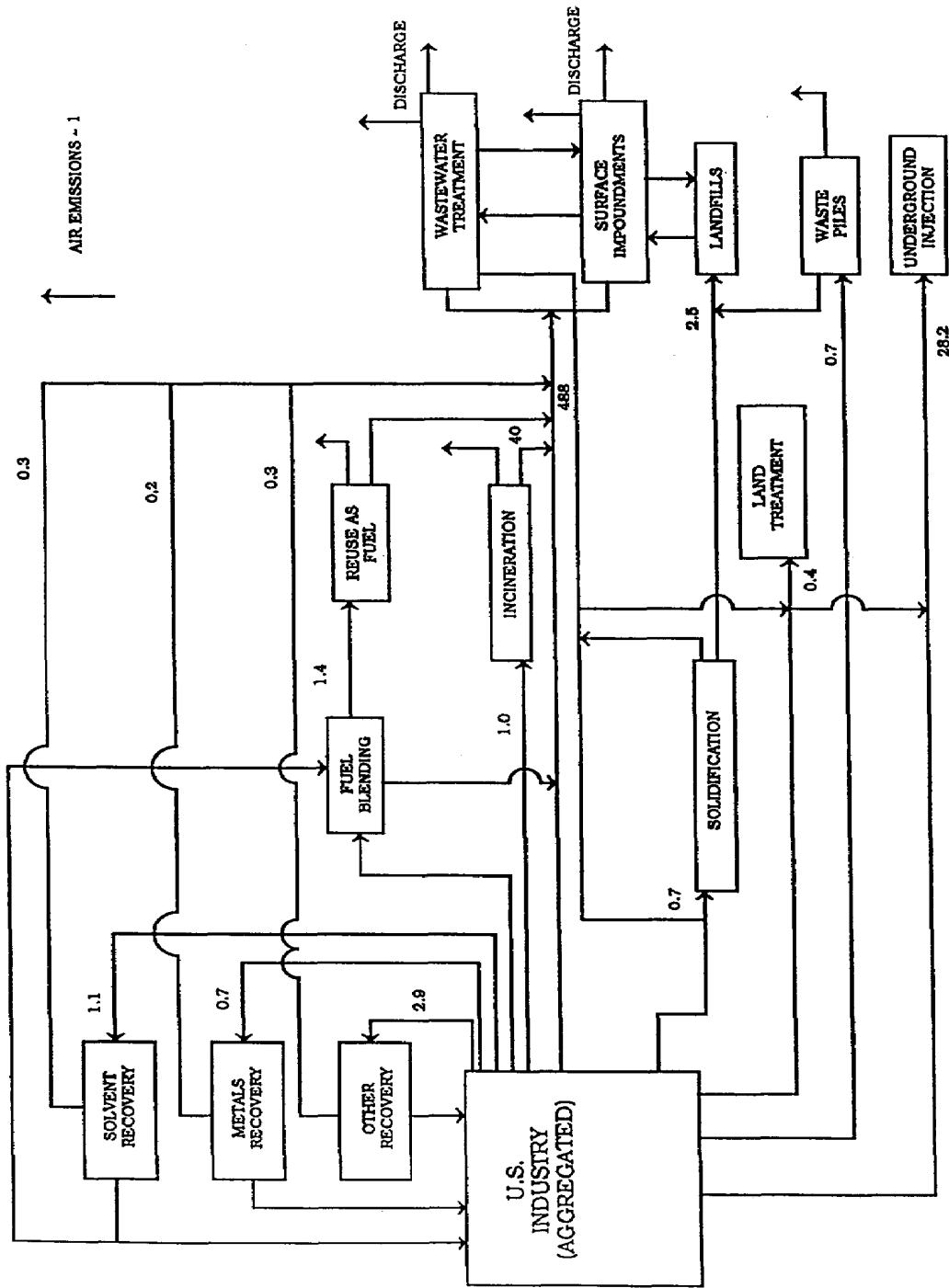
Fig. 1. Mass flows of hazardous wastes (data are for 1986 and are in millions of metric tons).

must also include these residual streams. Similar residual streams are generated by most treatment processes. Thus, determining which streams pose the greatest risk to the environment is complex, but it is essential if waste minimization efforts are to be properly directed. It should be noted that national rankings may not necessarily agree with the prioritization of waste streams for any one particular plant or industry. Nonetheless, global prioritization should be a helpful tool for a national program.

After the key pollutants and waste streams have been identified, the roadblock to waste minimization becomes designing new or modified processes which optimize the use of waste minimization and treatment technologies. The role of academic research in this process is to help develop new design methods, new reaction and separation technologies needed for the modified designs, and where appropriate, to participate with industry in case study development. Thus, and integrated approach to waste minimization research involves the following elements:

• identification of key pollutants and waste streams,
• development of design methodologies and process analysis methods for waste minimization, and
• development of selective reaction and separation technologies.

Programs in each of these phases of waste minimization research will be discussed in this paper. The development of substitutes for hazardous products and materials is also a key roadblock to waste minimization, but material and product substitution research problems are application specific. Generic research issues have yet to be identified. Thus, material and product substitution are difficult to address in a University environment. The UCLA waste minimization research team is focussing its efforts on developing a new generation of design procedures and a new generation of highly selective engineering unit operations. These efforts are being focussed on target waste streams identified as extreme environmental hazards.

Research

Target waste streams

The selection of waste streams that can serve as focal points for technology development is a critical issue in the development of waste minimization research. The identification and prioritization of chemical wastes to be minimized is a four step process. These steps are:

(1) establish emission rates,
(2) estimate the partitioning and fate of the emissions in the ambient environment,
(3) calculate human exposure to the emission, and
(4) estimate a measure of risk associated with the exposures.
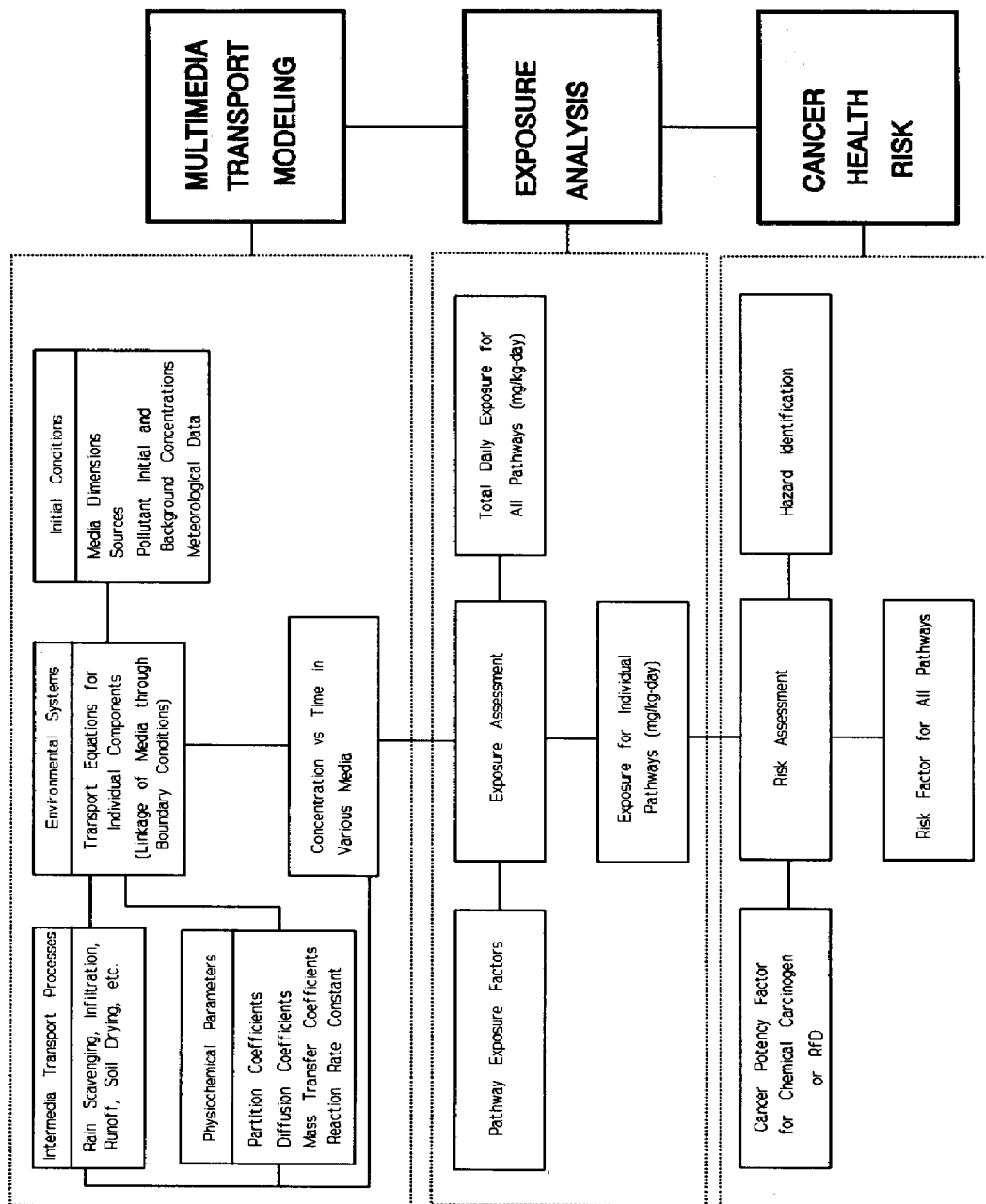
The interplay between these steps is shown in Fig. 2.

Fig. 2. Risk assessment methodology.

TABLE 1

1987 California emissions reported through the Toxic Release Inventory (pounds/year)

Chemical	Fugitive gas emissions	Stack gas emissions	Direct releases to water	Underground injection	Land disposal	Release to publicly owned treatment works	Other off site releases	Total
High emission rate chemicals								
Methanol	533,649	1,320,428	10,304,201	0	250	2,599,625	1,437,877	16,196,030
1,1,1-Trichloroethane	9,523,254	9,650,084	202	0	15,238	33,404	3,219,619	22,441,801
Methyl ethyl ketone	1,605,158	3,260,919	250	0	2,763	31,812	4,563,321	9,464,223
Tetrachloroethylene	2,562,680	2,918,620	13	0	2,455	1,935	2,001,349	7,487,042
Acetone	2,999,148	2,517,874	87,250	0	37,044	356,320	6,838,919	12,836,555
Toluene	2,011,054	3,062,236	3,913	10,250	934,924	98,348	2,164,089	8,284,814
Freon-113	4,917,910	1,869,989	560	0	0	5,486	1,299,323	8,093,268
Xylene	1,188,619	1,841,712	4,691	1,700	1,171,490	135,275	3,486,063	7,829,550
n-Butyl alcohol	750,976	1,163,684	0	0	0	1,423	486,601	2,402,684
Styrene	704,247	1,449,545	101	0	900	38,126	456,500	2,649,419
Phenol	112,902	307,272	3,669	250	5,670	399,558	115,629	944,950
U.S. EPA priority chemicals								
Chloroform	107,860	464,304	180,000	0	430	400	24,501	777,495
Carbon tetrachloride	7,240	48,015	8	0	2,610	270	30,774	88,917
Benzene	188,192	156,073	889	640	6,592	87,693	23,775	463,854
Ethylene oxide	54,237	299,276	34,303	0	0	33,553	0	421,369
Trichloroethylene	45,585	36,521	0	0	0	423	27,653	110,182
Methylene chloride	1,820,628	4,073,308	261	750	0	56,310	637,086	6,588,343
1,3-Butadiene	4,950	2,610	250	0	250	0	400	8,460
Vinyl chloride	42	890	0	0	0	240	1	1,173
TOTALS	29,138,331	34,443,350	10,620,561	13,590	2,180,616	3,880,201	26,813,480	107,090,129

Data on emission rates have been made available through the U.S. Environmental Protection Agency (EPA) Toxic Release Inventory (TRI), released in the spring of 1989. This waste inventory provides the type of data shown in Table 1 [3], i.e., emission rates of individual chemicals to various environmental media. The emission rates are for large generators (i.e., organizations with ten or more employees which handle more than a threshold volume of listed chemicals). The TRI does not report the total composition of the waste stream. For example, release of a 100 lb (45.3 kg) aqueous mixture consisting of 1% (w/w) methanol and release of one pound of pure methanol are reported in the same way. Despite its shortcomings, the TRI is the only comprehensive data base on chemical emissions currently available.

A preliminary ranking of chemicals, and thus waste streams, can be obtained by examining the mass emission rates reported by the TRI. As an illustration, the top 10 chemicals, rated by mass released in California, are given in Table 1. Not all emission rates are equivalent, however. Stack emissions, fugitive emissions, and releases to surface waters are emitted directly to the environment. In contrast, pollutants released to Publicly Owned (Wastewater) Treatment Works (POTWs) and other treatments processes are treated to some extent before entering the environment. Future work must focus on developing emission factors associated with releases to treatment processes such as POTWs.

Given emission rates, such as those available through the Toxic Release Inventory, the next step in prioritizing waste streams for minimization research is to evaluate the transport and fate of the emissions. A subset of the stack and fugitive emission rates of Table 1 were used in a Spatial Multimedia Compart-
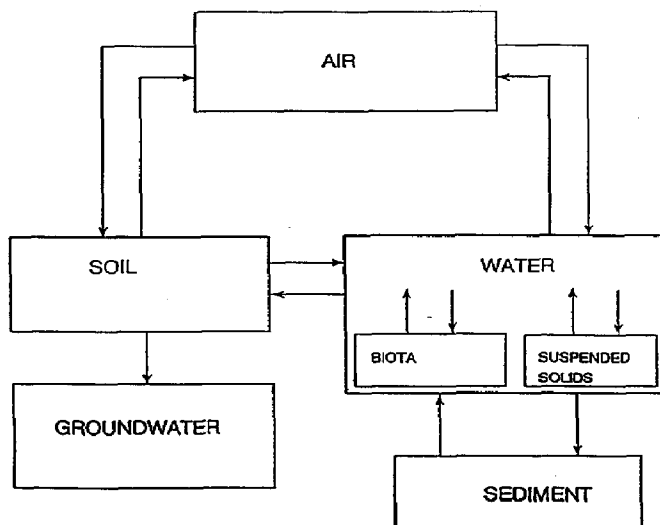

Fig. 3. Structure of the spatial multimedia compartmental model (Cohen [5]).

mental Model (SMCM) developed by the UCLA/EPA National Center for Intermedia Transport Research [4,5]. This model, shown conceptually in Fig. 3, estimates the concentrations of the pollutant in air, water, sediment, soil and biota compartments.

A detailed description of multimedia modeling is beyond the scope of this paper, however, it is important to review the various levels of multimedia models that can be applied to the problem of describing the environmental fate of hazardous substances. Existing multimedia models can be classified as uniform compartmental models and spatial multimedia models. Spatial multimedia models are designed to provide the spatial resolution of pollutant concentration-time profiles. However, most of the existing spatial multimedia models such as the UTM-TOX model (Unified Transport Model for Toxicant [6,7], the ALWAS model (Air, Land, Water Analysis System) [8], and TOX-SCREEN model [9] have been designed by using single-medium models that are linked in series. Spatial multimedia models require large amounts of data [10–12]. Due to their structure of linked single-medium modules, existing spatial multimedia models often neglect feedback transport loops. An alternative to spatial multimedia models are homogeneous compartmental models. Examples of compartmental models in which all compartments are assumed to be well mixed include site-generic equilibrium fugacity-type models [13–17], the ADL model [18], the kinetic-type model [19], and the GEOTOX model [20]. These early models require user's input of intermedia transport parameters and partition coefficients. These parameters were not calculated by these models. Moreover, the available compartmental multimedia models consider the multiphase soil matrix to be well mixed [10,11,13–16,18–22]. This latter simplification is physically unacceptable, and as Cohen and Ryan noted [23], even the simplest multimedia model should treat the soil and sediment as non-uniform compartments in which pollutant transport is described by a diffusion type equation with convection and chemical reactions [24–26]. Despite the above shortcomings, compartmental models are attractive because of their simplicity and modest requirements for input data.

Given the above considerations, the Spatial Multimedia Compartmental (SMCM) approach for modeling multimedia pollutant fate and transport has been developed to facilitate a rapid screening level prediction of the multimedia partitioning of organic chemicals in the environment. In this hybrid approach, the environment is taken to consist of uniform (air, water, biota, and suspended solids) and non-uniform (soil and sediment) compartments. Although air and water compartments are treated as being uniform, non-ideal mixing or corrected residence time is implemented in these compartments. The air and water compartments can also be subdivided in order to account for some degree of non-uniformity in these compartments. The hybrid approach provides greater resolution than the conventional uniform compartmental models. Yet, the SMCM approach results in models much less complex

than the existing spatial models. The uniform and non-uniform compartments are linked through the appropriate boundary conditions. For example, interfacial mass transport, infiltration, and deposition of pollutant are taken into account at the top boundary of the soil compartment, whereas chemical transport to groundwater is considered at the bottom boundary of the soil compartment.

The results of the above screening-level analysis, applied to TRI emission inventories, is illustrated for the three pollutants, trichloroethylene (TCE), phenol, and benzene. These three pollutants were chosen for presentation because they represent a wide range of water solubility, volatility and toxicity. The multimedia partitioning of these three pollutants in Southern California was determined using the SMCM model [27]. Steady state concentration estimates for the three pollutants are listed in Table 2. Calculation of human exposures [28], and relative human risk [29] shown in Table 3, imposes an additional reordering of the chemicals. Details of the calculations and a more complete prioritization of waste streams will be provided in future publications. For this overview we seek to illustrate that emission rates do not provide direct estimates of environmental concentrations, human exposure or risk. Thus, prioritization of pollutants for waste minimization activities must involve an evaluation of the chemical's properties, its eventual environmental fate and the risks associated with that fate.

Process design for waste minimization

Once the wastes to be eliminated have been identified, the design process for waste minimization can begin. The overall objective in the design is to arrive at the process configuration which results in the lowest generation of waste mass. This design problem is somewhat analogous to the design of energy efficient processes. During the late 1970's and early 1980's, design methods were developed for Heat Exchange Networks (HENs) that would minimize the energy lost be processes. The UCLA group has developed the concept of Mass Exchange Networks (MENs) [30]. A mass exchange network is a system of separators and mass transfer units that achieves, in a cost effective manner, minimal discharge of hazardous waste streams. The general MEN synthesis problem can be states as: Given a set of pollutant rich process streams and a set of pollutant lean streams, synthesize a network of mass exchange units that can transfer certain species from the rich streams to the lean streams at minimum venture cost. Conceptually, the MEN synthesis problem is shown in Fig. 4. The lean streams, flowing at rate L, enter the mass exchange network and are exposed to the rich streams, flowing at rate R. Mass is exchanged across units of cross-sectional area S in order to achieve final concentration y in the pollutant rich stream. The goal of the synthesis is to identify the set of exchangers and the configuration of streams that optimize the transfer. The characteristics of the optimal network of mass exchangers could be that it

TABLE 2

Predicted environmental compartment concentrations[a] in the south coast air quality management district

Environmental media	Trichloroethylene			Phenol			Benzene		
	Concentration (mol/m^3)	Concentration (other units)	Amount of chemical present in compartment (%)	Concentration (mol/m^3)	Concentration (other units)	Amount of chemical present in compartment (%)	Concentration (mol/m^3)	Concentration (other units)	Amount of chemical present in compartment (%)
Air	0.162×10^{-10}	0.396×10^{-3} ppb	95.6	0.179×10^{-10}	0.437×10^{-3} ppb	96.9	0.757×10^{-9}	0.0185 ppb	96.7
Water	0.420×10^{-10}	0.552×10^{-2} ng/l	0.02	0.765×10^{-8}	0.720×10^{0} ng/l	3.0	0.106×10^{-7}	0.828 ng/l	0.1
Soil	0.119×10^{-9}	0.104×10^{-1} ng/kg	4.4	0.800×10^{10}	0.502×10^{2} ng/kg	0.09	0.511×10^{-8}	0.266 ng/kg	3.2
Sediment	0.460×10^{-10}	0.403×10^{-2} ng/kg	2×10^{-4}	0.109×10^{-8}	0.685×10^{-1} ng/kg	2×10^{-3}	0.714×10^{-8}	0.372 ng/kg	8×10^{-4}
Biota	0.528×10^{-9}	0.694×10^{-1} ng/kg	1×10^{-7}	0.105×10^{-7}	0.992×10^{0} ng/kg	2×10^{-6}	0.684×10^{-7}	5.35 ng/kg	3×10^{-7}
Suspended solids	0.281×10^{-8}	0.246×10^{-1} ng/kg	6×10^{-7}	0.574×10^{-8}	0.360×10^{0} ng/kg	1×10^{-5}	0.367×10^{-7}	1.91 ng/kg	2×10^{-6}

[a]Predicted total amounts of TCE, phenol and benzene (mol) in the multimedia system at a simulation time of 2000 hour are 5.66×10^2, 6.16×10^2 and 2.62×10^4, respectively.

TABLE 3

Average dose rate and relative risk

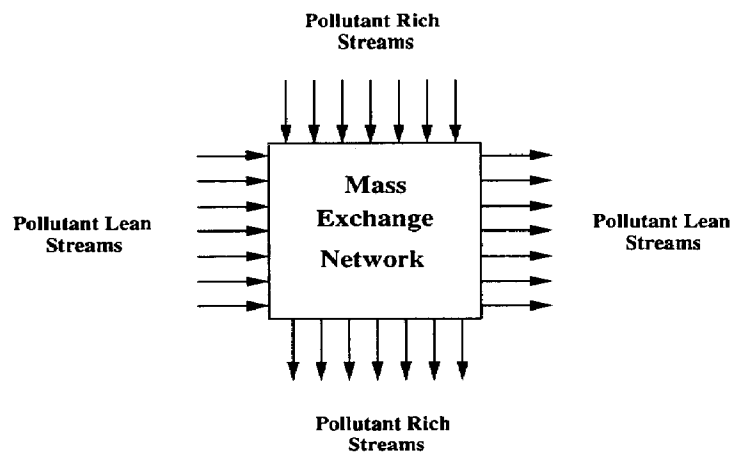| Chemical	Dose rate (mg/kg day)	Risk[a]
TCE	6.13×10^{-7}[b] (9.7×10^{-5})[c]	1[b] (1916)[c]
Phenol	6.55×10^{-7}	3.7×10^{5}[d]
Benzene	1.74×10^{-5} (8.18×10^{-4})	141 (6446)

[a]Relative lifetime risk non-dimensionalized with respect to TCE (TRI calculation).
[b]Based on TRI emissions.
[c]Based on non-TRI emissions.
[d]Hazard index for adult relative to reference dose.

Fig. 4. A mass exchange network contacting rich (R) and lean (L) streams.
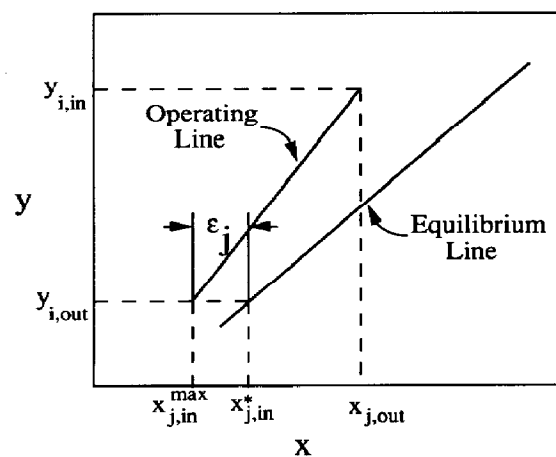
Fig. 5. Thermodynamic and driving force constraints on the mass exchange synthesis problem.

achieves the separation at minimum capital cost, minimum operating cost, or some combination of these two. A key feature of this approach is that it combines thermodynamic and driving force constraints into the optimization. Clearly, thermodynamic laws cannot be violated in designing networks and, in addition, some mass exchange units will require a minimum concentration driving force, ε, in order to transfer mass from rich to lean streams. This concept is shown in Fig. 5, which gives typical equilibrium and operating lines used in the analysis. These thermodynamic and operating constraints can result in a "pinch point", which defines the waste minimization potential of the mass exchange network. This concept is shown in Fig.6. In Fig. 6, three regions are shown. The integrated mass exchange is the fraction of the pollutant mass that can be transferred to the lean streams in the mass exchange network. The external MSA is the material that, due to equilibrium or operating constraints, cannot be transferred from the rich to the lean streams. Finally, the excess process MSA represents the unused capacity of the lean streams to take up pollutants. These three variables characterize the waste minimization potential of a process. For more details see El-Halwagi and Manousiouthakis [30].

As an example of the implementation of a MEN, consider refinery wastewaters. One of the waste components of interest in refinery wastewaters is phenol. Phenol can be found in water effluent from cracking units, desalter wash water and spent sweetening waters. In these streams, phenol is a waste component, however, in other refinery streams phenol can be a valuable additive. The goal of the MEN synthesis is to identify the optimal process configuration for transferring phenol between these streams.

A simplified version of this mass exchange problem is shown in Fig. 7. In this case study three phenol rich streams (R) and three phenol lean streams (L) were considered —Rich streams: R_1–water from the cracking unit, R_2– spent sweetening agent, and R_3–washing water to the desalter; lean streams: L_1–light gas oil, L_2–activated carbon, and L_3–crude oil.
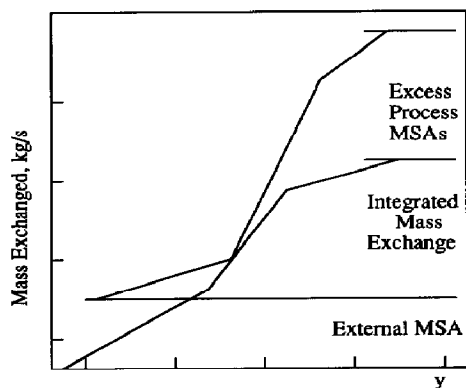

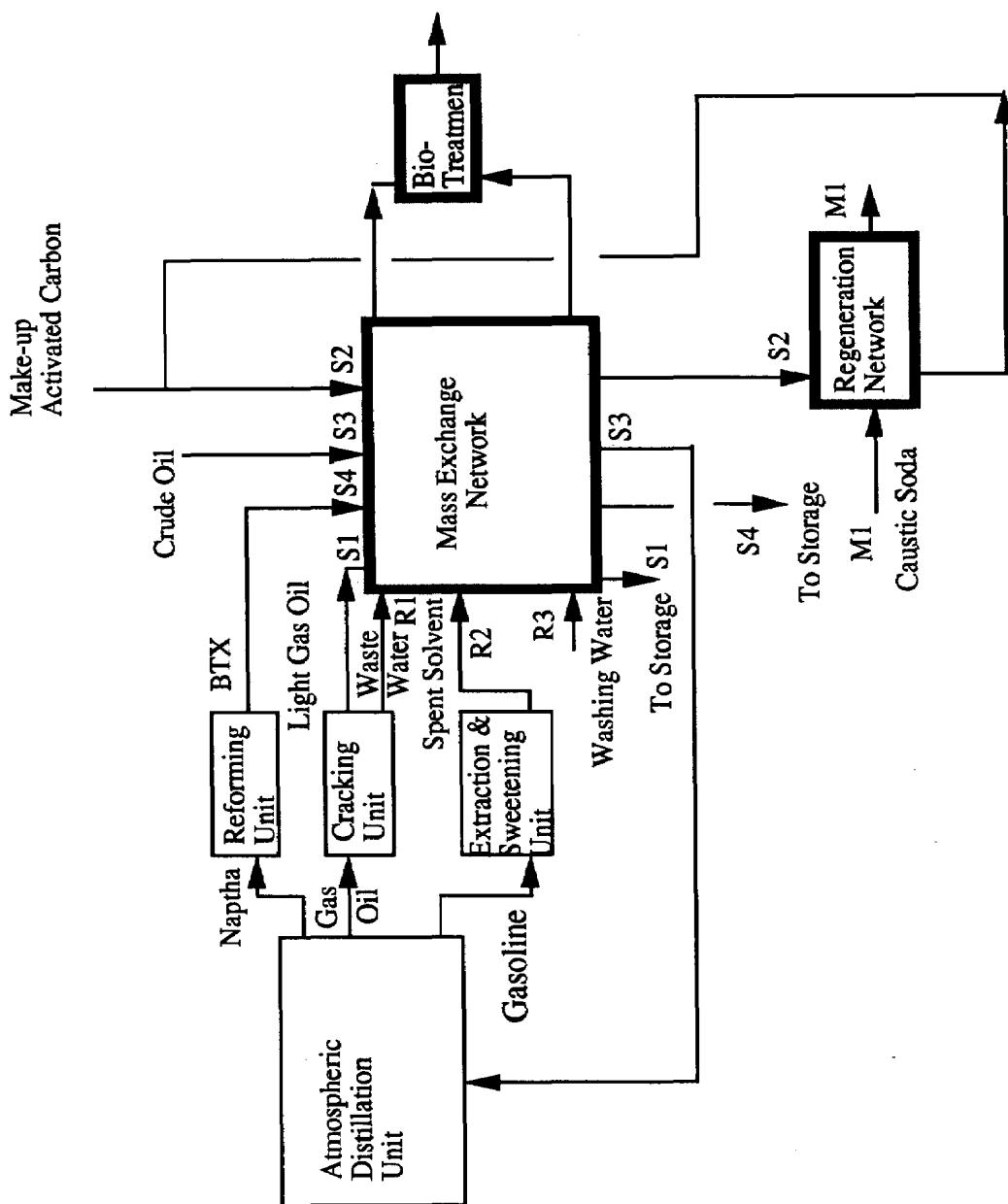Fig. 6. Estimates of waste minimization potential.

Fig. 7. A mass exchange network problem.

By using linear programming and mixed-integer non-linear programming formulations, the optimal network is obtained. This optimal network recovers 96.7% of the phenol present in the rich streams. Details of other MEN case studies can be found in El-Halwagi and Manousiouthakis [30].

The MEN synthesis represents a method for optimizing the configuration of separation units. It may be possible to develop similar design procedures that optimize reactor configurations or reaction pathways.

Selective separation processes

Process design and analysis methods can identify targets of opportunity for waste minimization. Some of these opportunities can be exploited using conventional technologies; exploiting other opportunities may require novel new unit operations. At the UCLA Research Center, the overall objective of the separations groups is to develop membranes and adsorbents that are selective and can withstand the interferences and severe conditions encountered in waste minimization applications. Work is underway in developing selective polymer adsorbents, ceramic ultrafilters, biomimetic membranes and hybrid membranes.

The objective of the research program in polymer adsorbents is to develop an approach to tailor-making a new class of selective, high capacity adsorbents, which can be easily regenerated, for the reclamation of organics from process and effluent waste streams. Novel polymer-silica resins, synthesized via graft polymerization, have been developed and evaluated as potential adsorbents for the selective removal of organic contaminants from aqueous systems [31]. These resins consist of an inorganic support with surface polymer chains that are terminally anchored by a patented graft polymerization process. Mechanical stability is therefore imparted by the solid while a large surface area for adsorption is provided by the swellable polymeric phase. The results from this program have demonstrated that terminally anchored polymer chains can be used for removing organic solutes from aqueous systems.

A second project in the UCLA program on separation methods is focussing on the development of biomimetic membranes. In this project, lipids are harvested from organisms able to grow at temperatures up to 105°C, pHs less than 1.0 or greater than 10.0 and high metal and salt concentrations. These harvested biological materials are then made into planar membranes or vesicles. The challenge associated with synthesizing these membranes that mimic biological functions (biomimetic membranes) are great. It is difficult to grow the organisms since conventional fermentation technology is unable to withstand the extreme culturing conditions, and the ultrathin membrane materials must be stabilized to allow practical application. Yet, the unique potential of these separation materials make this research program worth its risk. The membranes that could result from this work would exhibit high selectivity (sepa-

ration factors $> 10^3$), high metal sorbing capability (binding constants up to 10^{50}) and high flux rates due to ultrathin (5 nm) separation layers.

The materials synthesized as selective adsorbents and biomimetic membranes could both benefit from a supporting structure. For the selective adsorbents this supporting structure is currently non-porous silica, however, the UCLA group is currently conducting research to determine if ceramic ultrafilters can be used as support materials. The ceramic ultrafilters are synthesized using a sol–gel technique and can be engineered to have narrow pore size distributions with mean diameters ranging from 20 Å to 2000 Å. In addition, they are able to withstand extreme operating conditions. Two types of ceramic ultrafilters have been synthesized, a monolithic type and a supported membrane type. In the monolithic material, the pores can be coated with materials such as polymer adsorbents or biologically derived lipids. In the case of the selective membranes, *in situ* graft polymerization may allow almost complete pore filling. The supported membrane ceramic ultrafilters should be useful for immobilizing thin films, such as biomimetic membranes while at the same time screening large particles or molecules that could foul the supported membrane.

Selective reaction technologies

Development of more selective chemical synthesis pathways could lead to dramatic waste reduction. Alternatively, waste streams could react to form recyclable products, thereby reducing waste. Currently, our efforts at UCLA are focussed on the latter approach. In particular, we are examining catalytic hydrodehalogenation as a recycling process.

Halogenated organics are among the most significant and widespread toxic materials in the environment. They are also very difficult to destroy by incineration, therefore new technologies must be developed for recycling or destroying these materials. A process for recycling chlorinated organics that has been under development at UCLA is catalytic hydrodechlorination (HDC). Catalytic HDC has potential applications in recycling agricultural chemical wastes, in PCB and PCP remediation and in oil recycling. All of these applications involve hydrogenating a carbon–chlorine bond. Our work on the chemistry of this process is described elsewhere [32,33].

Conclusions

In this paper we have described an integrated research program for pollution prevention that has as its three primary elements:
- identification of target streams,
- development of design objectives and process synthesis methodologies for waste minimization, and
- development of new unit operations for waste minimization.

These three elements form more than just a research strategy. They can be viewed as a basic framework for the design of clean technologies.

Identification of target streams is a crucial first step in the waste minimization process. Because capital resources are limited, it is important to focus minimization activities on waste streams that are extreme environmental hazards. Even if capital resources were unlimited, it is thermodynamically infeasible to completely eliminate all waste streams. Choosing which streams to eliminate requires that a prioritization methodology be set.

Once objectives for waste minimization have been set, it is possible to design a process which optimizes this objective, i.e. it is possible to identify a process configuration which minimizes a specific waste leaving the plant. Process synthesis for waste minimization can identify targets of opportunity for waste minimization. Some of these opportunities can be exploited using conventional technologies; exploiting other opportunities may require novel new unit operations. Thus, a sequential approach to pollution prevention must involve target stream identification, process synthesis and the development of appropriate unit operations.

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