EnviroCAD: A computer tool for analysis and evaluation of waste recovery, treatment and disposal processes

D.P. Petrides[a,*], K.G. Abeliotis[a], V. Aelion[a], Ed Venkat[b], S.K. Mallick[a]

[a]*Department of Chemical Engineering, Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, NJ 07102, USA*
[b]*Merck Research Laboratories, Merck and Co., Inc. P.O. Box 2000, RY 50D-201, Rahway, NJ 07065, USA*

Abstract

The successful design and evaluation of integrated material reclamation, waste treatment and disposal processes is a challenging task that can be facilitated by the use of computer-aided process design and simulation tools. EnviroCAD, an advanced computing environment of such a software tool, has been developed at the New Jersey Institute of Technology in collaboration with a number of industrial partners. EnviroCAD runs on personal computers and assists scientists and engineers to simulate efficiently and analyze new integrated environmental processes and improve the performance of existing ones. In short, it helps in process optimization from an environmental standpoint. An important feature of the program is its ability to carry out material balances on individual compounds and track the fate of hazardous chemicals (e.g., chlorinated organic solvents, heavy metals, etc.) in integrated environmental processes. EnviroCAD includes a wide variety of unit operation models, ranging from biological treatment units, to membrane filters for material reclamation, to ion exchangers for heavy metals removal, to incinerators for ultimate disposal, etc. This paper describes the architecture of EnviroCAD, its process modeling, economic evaluation, graphical user interface, and environmental assessment capabilities. An example demonstrates the use of EnviroCAD in an industrial environment.

1. Introduction

The variety of options in material reclamation, waste treatment, and waste disposal have rendered the design and evaluation of such technologies a challenging task. The requirement for tracking the fate of heavy metals and volatile organic compounds (VOCs) in integrated environmental processes has made necessary the use of rigorous

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* Corresponding author. Fax: (201) 596-8436. Telephone: (201) 596-3614.

process modeling that involves detailed material balances on individual chemical components.

The number of pollution control alternatives is large, with wide differences in performance and annualized capital and operating costs. Significant differences exist in the underlying science and the technology. For instance, destruction techniques may be based on oxidation (chemical, thermal or biological), hydrolysis and photolysis. Separation techniques for material reclamation and recycle may be based on distillation, stripping, absorption, adsorption, membrane separation, sedimentation, precipitation, flotation, etc. For each of these technologies a number of variations exist. For instance, biological treatment may be aerobic or anaerobic, using a single type or a consortium of microorganisms which are in suspension or immobilized, operated in batch or continuous mode, in well mixed or plug-flow reactors, etc. Often, combinations of various technologies are required to accomplish a certain environmental objective.

The question is, how can we select and design systems that would solve environmental problems in an efficient and cost-effective way?

Computer-aided process design tools have been used in the chemical process industries for over four decades to facilitate process analysis, evaluation and optimization with a good degree of success. Now that the cost and complexity of environmental processes has reached the complexity level of manufacturing processes, one would expect that similar benefits could be realized in the environmental arena if appropriate computer-aided process design tools became available.

Unfortunately, the modeling of environmental processes, particularly those of biological treatment, is a difficult problem because:

1. the matrices are complex, involving consortia of microorganisms, soluble and suspended organic and inorganic compounds possessing properties that are difficult to predict using thermodynamic and microtransport principles;

2. most previous modeling work on aeration basins and other biological treatment units has focused on kinetic studies based on lumped environmental stream properties (e.g., BOD5, COD, TOC) as opposed to biodegradability of individual chemicals present in a multicomponent mixture;

3. limited work has been done on modeling VOC volatilization from treatment units and predicting sorption of heavy metals and other pollutants on sludge;

4. limited work has been done on the prediction of the contribution of various chemicals to environmental stream properties (e.g., residual oxygen demand, effluent toxicity, etc.);

5. a number of compounds are present at very low concentrations requiring more accurate material balances that can predict trace contaminant levels.

The above limitations, at present, prevent the development of a tool that can accurately predict the performance of an integrated waste treatment system strictly based on first principles. Some experimental information and engineering judgment is currently required for process performance prediction and equipment sizing.

1.1. The process design loop

The design of environmental processes, similar to chemical manufacturing, can be subdivided into three main interrelated activities, namely synthesis, analysis, and evaluation (Fig. 1). Typically we (a) propose a process, (b) analyze it either by simulation or by experimental means, and (c) evaluate it based on whatever objectives we deem important. We then use the information generated during this design loop to modify the proposed process until a desired convergence is reached. The design process is terminated either because we arrive at a satisfactory process, or because we run into time or financial constraints.

Process design is almost always hierarchical. The most basic decisions, such as process chemistry, are addressed initially and more detailed issues, such as operability, energy integration and process scheduling, are considered at later stages. This is because high-level decisions have a profound impact on the overall structure of the process and it would be counter-productive to consider peripheral decisions at an early stage.

Process synthesis uses new as well as existing technologies to select process chemistry, solvents, reaction schemes, separation technologies, etc. Hierarchical synthesis methodologies have been discussed in detail [1, 2]. Synthesis methodologies adapted to address waste management appear elsewhere [3, 4]. The result of process synthesis is a flowsheet for continuous processes or a batch sheet for batch processes. This is the input to the analysis step. If the analysis is not done experimentally, then it becomes synonymous with process simulation. The results of process simulation usually include material and energy balances, capital and operating costs, and other measures of system performance.

1.2. The current state of waste treatment process simulation

A number of established process simulators are commercially available that address the manufacturing needs of the chemical process industries. Limited work has been done so far on the formulation and development of simulators that explicitly address environmental issues. Some of the commercially available software packages in this area are the following.

ENPRO [5] is a process simulator developed to address primarily the needs of the wastewater treatment industry. It includes models for primary and secondary treatment of wastewater, absorption, stripping and activated carbon adsorption. It supports two methods of stream specification: (i) compositional, and (ii) non-composi-
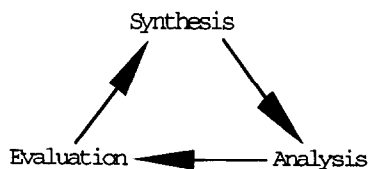

Fig. 1. Process design loop.

tional. In the compositional method, the user specifies the actual chemical composition of a feed stream as in traditional process simulators. In the non-compositional method, the environmental properties (e.g., BOD_5, COD, TOC, TKN) of a feed stream are entered by the user describing the whole stream rather than its components. A stream conversion utility is used to interchange the stream types. Currently, there is a limitation in ENPRO concerning which of the two stream types can be fed to a particular unit operation model. More specifically, biological treatment units only accept non-compositional streams. This limitation prevents the use of ENPRO for tracking the fate of individual chemicals of interest (e.g., heavy metals, volatile organics) in integrated wastewater treatment facilities. The current version of ENPRO also lacks economic evaluation capabilities.

The Environmental Simulation Program (ESP) is a set of modeling and simulation tools for environmental and other applications [6]. ESP includes models for biological treatment, clarification, neutralization, precipitation, crystallization, generic separation, absorption, stripping, flash distillation, incineration, and others. The main strength of ESP is in modeling reaction and equilibrium phenomena in aqueous systems involving molecular as well as ionic species. It does an excellent job, for instance, in modeling precipitation of heavy metals from an aqueous stream. It is equipped with a component physical property databank that includes data for nearly all the elements of the periodic table. Based on the molecular species present in an aqueous system, the program automatically generates all ionic species that may be present and develops a set of equilibrium reactions that describe the system. A limitation of the current version is its inability to handle multiple substrates in biological treatment reactors. Also, it lacks economic evaluation capabilities.

Researchers at the University of Illinois at Urbana-Champaign have developed a simulator for environmental processes that includes some economic evaluation and process optimization capabilities [7]. The emphasis of the tool is on wastewater treatment. It also does material balances based on lumped environmental properties, and, thus lacks the capability to track the fate of individual compounds.

The goal of this work was to formulate and develop a user friendly tool that can be used to analyze efficiently and evaluate integrated processes for material reclamation, waste treatment, and disposal. Particular emphasis was placed on the requirement to carry out material balances on individual components and predict the fate of hazardous chemicals (e.g., heavy metals, VOCs) in integrated environmental processes. This is particularly important for industrial wastes because the US Environmental Protection Agency (EPA) regulates the amount and concentration of discharged priority pollutants (various organic chemicals, heavy metals and ions). In the following section, an overview of EnviroCAD is provided.

2. Description of EnviroCAD

2.1. Scope and system architecture

EnviroCAD can be used to practice waste minimization by all waste generating industries. It takes as input data, the waste streams (gas, liquid or solid), that

a manufacturing plant generates and facilitates the efficient analysis and evaluation of alternatives for material reclamation, waste treatment, and disposal. The general structure of the software consists of the graphical user interface, the analytic component, and the economic evaluation component (Fig. 2).

2.2. User interface

EnviroCAD makes use of a graphical interface to enhance the human/computer communication and reduce the learning period, resulting in a tool that is simple to use and easy to learn, even for occasional users with limited process design and environmental background. The user builds a flowsheet by selecting equipment from the "Unit—Ops" menu and drawing the material streams that connect the units. All input–output information is provided/displayed through dialog windows. Fig. 3 shows how information about a flowsheet is displayed on the main window. Fig. 4 shows a typical input dialog window for initializing unit operation models. EnviroCAD also features on-line help.

2.3. Process analysis

The process simulation component of EnviroCAD assists the engineer to develop interactively and analyze integrated flowsheets for material reclamation, waste
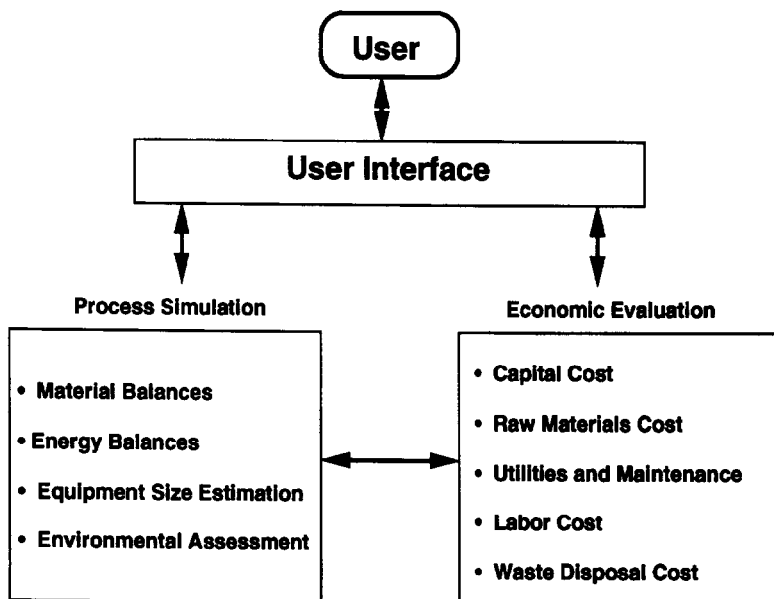

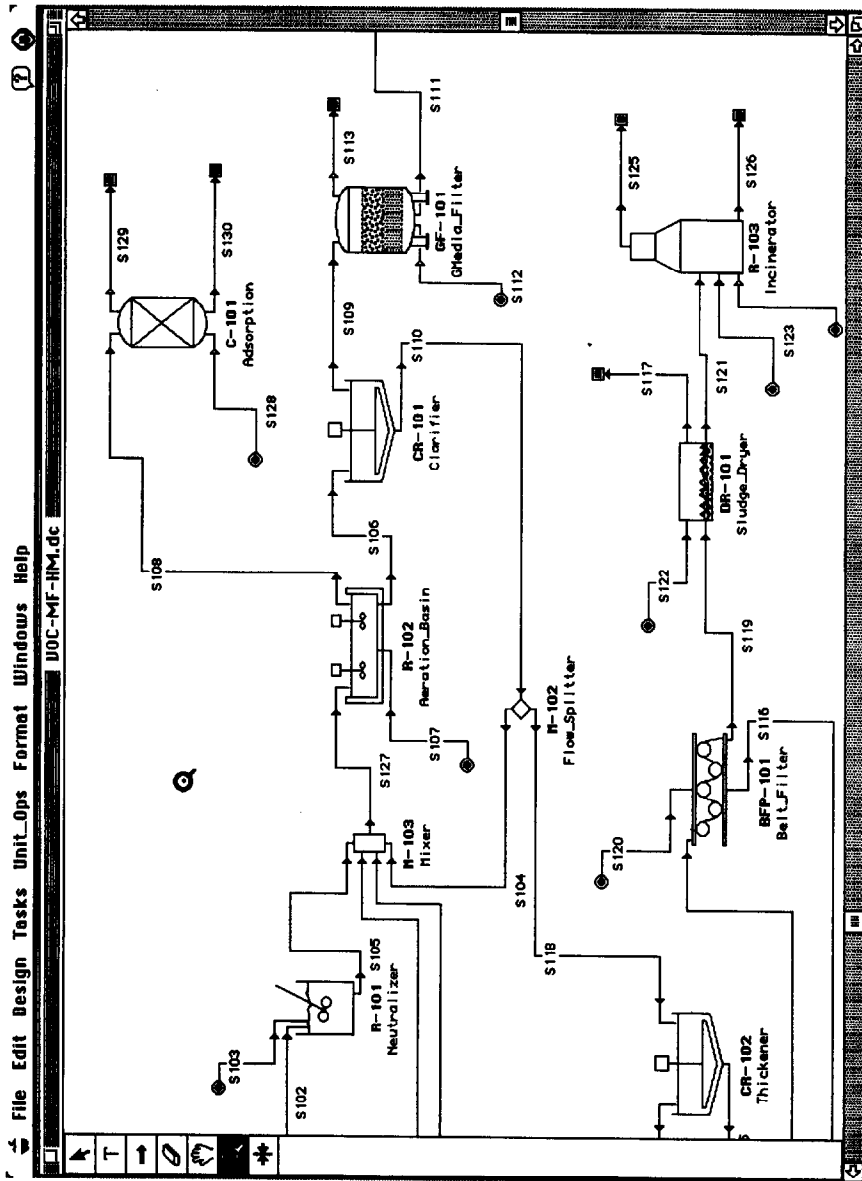Fig. 2. Schematic architecture of EnviroCAD.

Fig. 3. Main window of EnviroCAD.

Fig. 4. First input/output dialog window of the aeration basin model.

treatment, and waste disposal processes. Flowsheets consist of unit operations, material streams, and chemical components. A flowsheet in EnviroCAD can have any number of these objects.

Chemical components are used to describe flow and composition of material in streams. EnviroCAD distinguishes among conventional components, components that can be fully described with thermodynamic models, and non-conventional components, such as biomass, which cannot be satisfactorily modeled with currently available thermodynamic models. The program is linked to a database module that provides access to thermodynamic (molecular weight, boiling point, melting point, critical pressure and temperature, accentric factor, vapor pressure, Henry's law constant, octanol–water partition coefficient, density, specific heat, and particle size), environmental (contributions to COD, TOC, BOD_5/COD, TSS, aquatic toxicity, etc.) and regulatory properties (e.g., SARA Title III chemical, etc.) for around 300 chemicals. These properties are taken into account by the various unit operation models in the estimation of material balances and sizing of equipment. The environmental component properties are used to calculate environmental cumulative or lumped stream properties (BOD, COD, TSS, etc.) based on the composition of the stream.

Streams represent the flow of material from one unit operation to the next and are displayed as line segments on the computer screen. A stream object stores information about the flow rate of each component, the biomass/solution distribution of each component, the weight fraction of each component, the total mass flow rate, its name, and several stream properties (temperature, pressure, etc.). To account for material sorption on biomass, EnviroCAD keeps track of the fraction of each component associated with biomass and considers that information in the material balance calculations. For instance, if a filter press is used to dewater sludge, the model assumes

S110 Environmental Properties		
	mg/L	kg/day
TOC:	17588.447	11721.099
COD:	65575.859	43700.340
ThOD:	65593.562	43712.138
BODu:	60310.059	40191.163
BOD5:	55443.418	36947.991
TKN:	4098.001	2730.945
NH3: 100.0 % TKN Fraction	4098.001	2730.945
Nitrates-Nitrites:	0.000	0.000
Total Phosphorus (TP):	1529.676	1019.390
TSS:	40000.055	26656.395
VSS: 91.0 % TSS Fraction	36405.316	24260.829
DVSS: 80.0 % VSS Fraction	29117.377	19404.081
TDS:	128.887	85.892
VDS: 0.0 % TDS Fraction	0.000	0.000
DVDS: 0.0 % VDS Fraction	0.000	0.000

Previous   Cancel   OK

Fig. 5. Environmental stream properties calculated by EnviroCAD.

that the retention fraction of heavy metals sorbed onto biomass is equal to the retention fraction of biomass.

Environmental characterization of streams. Based on stream composition, EnviroCAD calculates and displays a number of environmental stream properties (Fig. 5). These properties apply to liquid waste streams and are indicators of environmental impact on the receiving water body. To estimate these properties, EnviroCAD either calculates or retrieves the appropriate contribution factors from the component database. More specifically, contribution factors for ThOD and TOC are calculated based on the elemental composition of the various chemicals while factors such as BODu/COD (that cannot be computed) come from experimental data retrieved from the database or provided by the user. Fig. 6 shows the multiplier values for some environmental properties for certain chemical compounds.

In other words, EnviroCAD carries out material balances on individual components and estimates the lumped environmental stream properties (e.g., BOD, TSS, etc.) based on stream composition. This is an important feature that enables the user to track the fate of individual hazardous chemicals in integrated pollution control processes. This is also important for predicting emissions of volatile organic compounds (VOCs) from treatment facilities (e.g., activated sludge, API separators and junction boxes).

A *unit operation* object is represented on the computer screen with a picture. For each unit operation, there is a model that describes its performance. An EnviroCAD model refers to the collection of subroutines used to model the unit operation and, in effect, defines the calculation of outlet stream variables from inlet stream(s) information. The primary function of a unit operation model is to carry out the material and

Component Name	TOC (g C/g)	COD (g O2/g)	ThOD (g O2/g)	BODu/COD (g/g)	BOD5/BODu (g/g)	
Toluene	0.90000	3.10	3.10000	0.81	0.353	⬆
Trichloroet...	0.18250	0.55	0.55000	0.20	0.200	
Acetone	0.60000	2.00	2.20000	0.89	0.455	
Tetrahydro...	0.66000	2.44	2.44000	0.85	0.600	
H3PO4	0.00000	0.00	0.00000	0.00	0.000	▪
Ca(OH)2	0.00000	0.00	0.00000	0.00	0.000	
Ca3(PO4)2	0.00000	0.00	0.00000	0.00	0.000	⬇

Biomass

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Fig. 6. Component multipliers for environmental stream properties.

energy balances around a process step and estimate outlet stream variables given inlet stream variables and engineering specifications. The user provides engineering information during initialization of unit operations through unit-specific dialog windows. For most of the engineering variables there are default values which can be used during a first pass until better values become available. Material balances in EnviroCAD are estimated in a sequential modular approach. The various unit operations of a flowsheet are sequenced according to their calculation order. Every unit operation model estimates the composition and flowrate of its outlet streams given its inlet streams and some unit-specific engineering information. If recycle streams are included in the flowsheet, the unit operations that are part of the recycle loop are solved iteratively until the flowsheet calculations converge.

Table 1 shows the list of unit operation models that are available in the current version of the program. In some cases, mathematical models have been combined with heuristic algorithms developed by experts in the field. The aeration basin model is a representative example.

To predict the fate of a chemical entering an aeration basin, the current version of EnviroCAD is equipped with a heuristic algorithm developed by Merck and Co. [8]. Fig. 7 illustrates some elements of the algorithm. Properties such as volatility (expressed by Henry's law constant), solubility in water, octanol–water partition coefficient, BOD/COD ratio, etc., are used to estimate the fraction of a substance that biodegrades, the fraction that volatilizes, and the fraction that is sorbed on biomass. These initial fractions are then adjusted to reconcile the overall material balances around an aeration basin with those predicted by the kinetic model. Three kinetic models for the aeration basin are currently available: (i) a Monod type, (ii) a Haldane type with substrate inhibition, and (iii) one that assumes first-order kinetics.

Table 1
List of unit operation models that are available in the current version

Mechanical separators	*Phase separators*
Plate and frame filter	Batch distillation
Membrane microfilter	Continuous distillation
Membrane ultrafilter	Condensation
Gas membrane filter	Flash distillation
Reverse osmosis filter	Evaporation
Rotary vacuum filter	Drying
Basket filter centrifuge	Extraction
Decanter centrifuge	Steam stripping
Clarifier	Air stripping
Thickener	Wet scrubbing
Flotation/flocculation unit	Decantation
Oil separator	
Granular media filter	*General reactors*
Belt filter	Stoichiometric reactor
Baghouse filter	Well mixed reactor
	Plug flow reactor
Biological treatment	Neutralizer
Aeration basin	
Aerobic bioreactor	*Adsorption separators*
Anoxic bioreactor	Activated carbon column
Anaerobic bioreactor	Ion exchange
Trickling filter	
	Sterilization
General unit operations	Continous heat sterilization
Liquid and slurry pump	Batch heat sterilization
Compressor	Chemical sterilization
Shell and tube heat exchanger	
Plate and frame heat exchanger	*Other models*
Spiral heat exchanger	Flaring
General mixer	Liquid injection incineration
Flow splitter	Fluid-bed incineration
Component splitter	Rotary kiln incineration
Storage tanks	Wet oxidation
Blending tanks	Electrostatic precipitation
Equalizer	

2.4. Economic evaluation

For an integrated waste treatment process, EnviroCAD calculates the purchase cost of equipment, the fixed capital investment, the annual operating cost, and carries out a thorough economic evaluation. Equipment cost is estimated as a function of equipment capacity, materials of construction, and certain design characteristics. A number of equipment vendor and literature sources have been used to derive the correlations for equipment purchase cost estimation [9–12].

The fixed capital investment is calculated based on the total purchase cost of equipment using multipliers which the users can modify [13]. The annual operating cost includes cost of process chemicals and consumables, labor, utilities, equipment
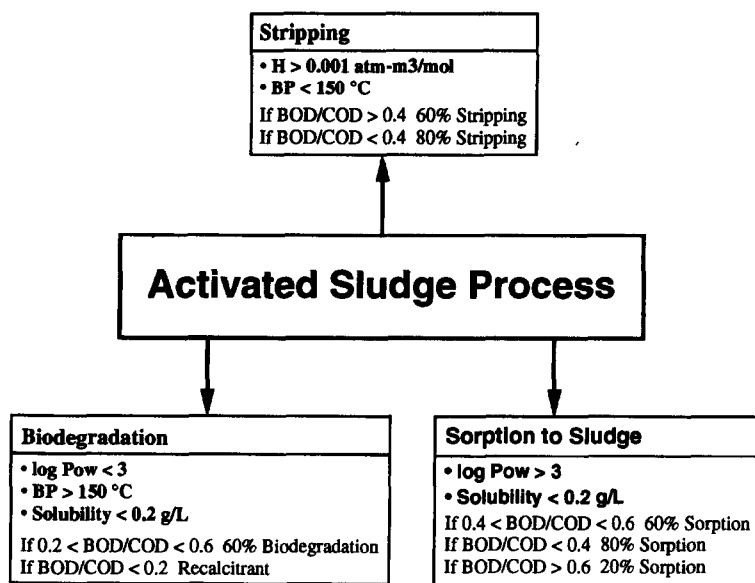
Fig. 7. Heuristic algorithm for predicting initial extents of biodegradation, stripping and sorption in the activated sludge process (Adapted from Ref. [8]).

depreciation, equipment maintenance, and disposal of waste that cannot be eliminated. The results of the economic evaluation have a maximum error of ± 30%, which is acceptable for preliminary design and evaluation of alternatives.

2.5. Computer implementation

EnviroCAD runs on personal computers and is written in C++ (Symantec on the Apple Macintosh [14] and Microsoft Visual on IBM compatibles [15]) taking advantage of object-oriented programming. C++ classes were extensively used to represent unit operations, material streams, chemical components and other objects. An illustrative example that demonstrates how EnviroCAD can be used in practice follows.

3. Process analysis and economic evaluation of an industrial wastewater treatment plant

This example focuses on the retrofit design of an industrial wastewater treatment plant that services a manufacturing facility located overseas. Fig. 8 shows the flowsheet of the current facility.
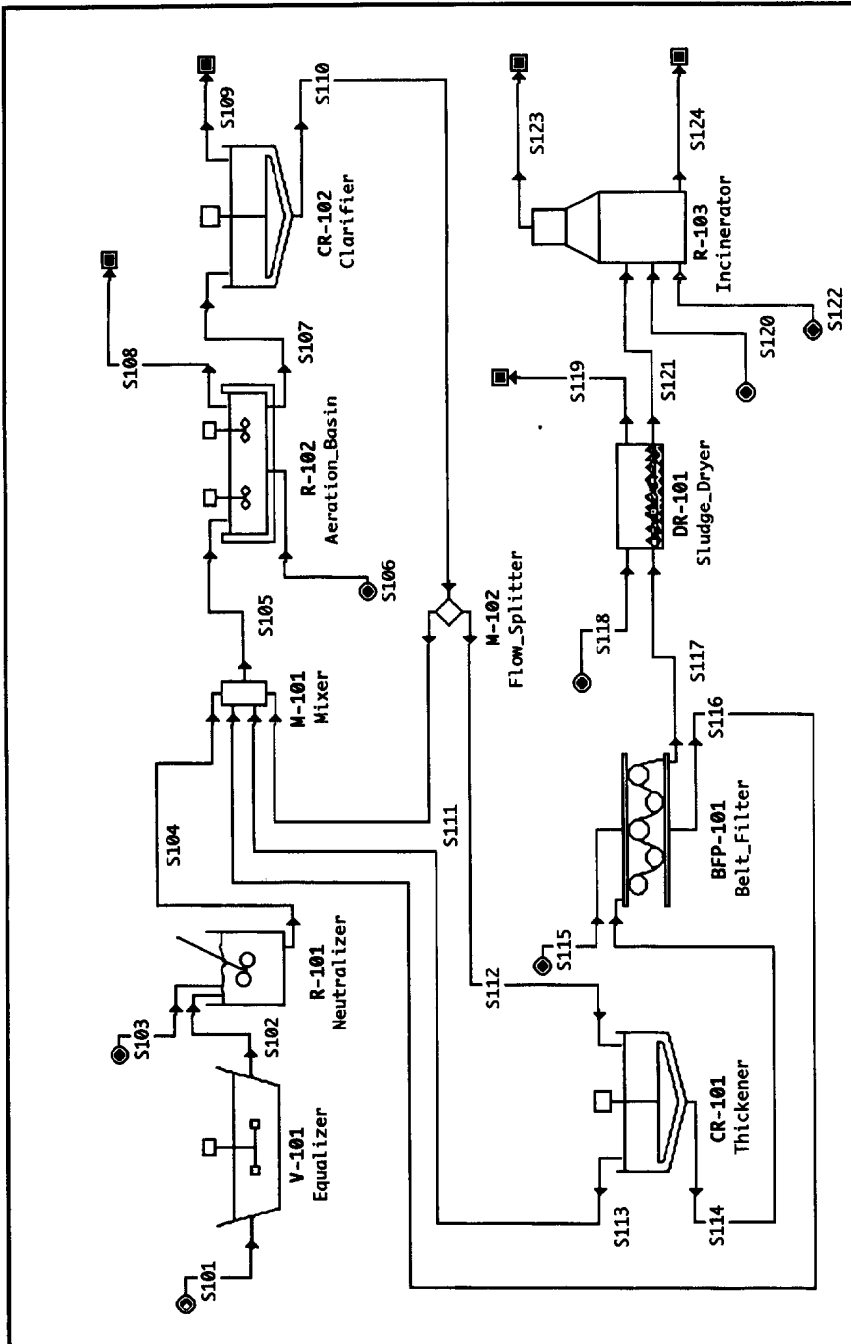
Fig. 8. Industrial wastewater treatment plant – base case.

3.1. Process description

During primary treatment, the flow rates and concentrations of the inlet streams are equalized in a large capacity tank (V-101) and the pH adjusted to near neutral in a neutralizer (R-101). The secondary treatment includes an aeration basin (R-102) for the biological oxidation of organic materials and a clarifier (CR-101) for the removal of sludge and carried-over solids. The aeration basin operates at an average hydraulic residence time of 6 h, an average sludge residence time of 12 days, and a minimum dissolved oxygen concentration of 2 mg/l. A fraction of the sludge (30%) is recycled to maintain a biomass concentration in the aeration basin of 3500 mg/l. The excess sludge (S112) is sent to the sludge treatment section. The sludge is thickened in a thickener (CR-102) to a solids concentration of 2% w/w, dewatered in a belt filter press (BFP-101) to a solids concentration of 12% w/w, and dried in a sludge dryer (DR-101) to a final solids concentration of around 30% w/w. The dried sludge is burned autothermally in an incinerator (R-103). The incinerator operates at 30% excess air and the flue gas sensible heat is used to preheat the sludge inlet stream. The final exit flue gas temperature is 250°C.

Table 2 shows the composition and flow rate of the feed stream (S101) to the treatment facility. This is a rather small treatment facility with an average throughput

Table 2
Average composition of entering wastestream

Component	Flow rate (kg/h)	ppm
Water	787 000.00	976 152
Biomass	100.00	124
Ammonia	10.00	12
Oxygen	5.00	6
Benzene	45.00	56
Acetonitrile	70.00	87
Chloroform	35.00	43
Ethylbenzene	25.00	31
Methylene chloride	20.00	25
Toluene	25.00	31
Trichloroethylene	20.00	25
Acetone	25.00	31
Tetrahydrofuran	20.00	25
Phosphoric acid	50.00	62
Methanol	45.00	56
Ethanol	35.00	43
Methylethylketone	30.00	37
Butyl acetate	25.00	31
Proteins	30.00	37
Fats	90.00	110
Carbohydrates	70.00	87
Heavy metals	2.54	3

Table 3
Overall plant performance based on environmental stream properties (kg/d)

Environmental stream property	Influent (S101)	Effluent	
		Water (S109)	Sludge (S121)
Total organic carbon (TOC)	9123	615	3857
Chemical oxygen demand (COD)	30968	2152	14385
Biochemical oxygen demand (BOD)			
Ultimate	27037	1829	13233
5-day	19626	1447	12174
Total Kjeldahl nitrogen	1416	100	901
Total phosphorus	427	14	528
Total suspended solids (TSS)	6900	659	9754
Heavy metals	61	7	54

of 5 MGD. The feed stream to this plant includes a number of regulated chemicals (e.g., benzene, chloroform, methylene chloride, trichloroethylene, heavy metals, etc.).

A key question concerning the environmental engineer is the fate of each of these chemicals in the treatment facility. Water-soluble and easily biodegradable substances will be oxidized in the aeration basin by bacteria and other microorganisms and converted into CO_2 and H_2O. A fraction of recalcitrant and non-biodegradable compounds with low water solubility will be sorbed on biomass and follow its path through the treatment plant. Finally, a fraction of volatile compounds will be stripped off in the aeration basin and end up in the atmosphere, contributing to VOC emissions.

Table 3 shows the overall performance of the plant based on removal of TOC, COD, BOD$_u$, BOD$_5$, TSS, etc., based on the simulation results which were in good agreement with actual plant data. The performance of this plant is quite good, removing around 95% of BOD and 90% of TSS. Note that approximately 88.5% of heavy metals associate with sludge classifying it as hazardous waste. Such sludge often cannot be land-filled, so it is incinerated and the resulting ash (that contains most of the heavy metals) undergoes stabilization treatment.

This plant, however, performs rather poorly as far as emissions of VOCs and heavy metals release are concerned. Table 4 presents the composition of the combined gas streams exiting the equalizer, the neutralizer and the aeration basin. For simplicity in the calculations, it was assumed that all gases exit the aeration basin (stream S108). A total of approximately 90.85 kg/h or 2180 kg/d of VOCs are emitted from this facility. If this plant were located in the USA, it would be considered a major source of VOCs according to the 1990 Clean Air Act Amendments [16, 17].

To comply with the current limit of 25 t/y, application of Reasonably Available Control Technology (RACT) would be required to reduce the amount. Such technologies include wet scrubbing (packed or mist towers), adsorption (based on activated carbon or zeolites), membrane filtration in combination with condensation [18], thermal destruction, and biodegradation (biofilter or bioscrubber).

Table 4
Aeration basin gas outlet (stream S108)

Component	Flow rate (kg/h)
Ammonia	1.20
Benzene	22.55
Chlorobenzene	8.83
Chloroform	30.10
Ethylbenzene	4.00
Methylene chloride	2.36
Toluene	1.53
Trichloroethylene	17.78
Acetone	0.45
Tetrahydrofuran	2.05
VOCs Total	90.85

Table 5
Clarifier effluent (stream S109)

Component	Flow rate (kg/h)	ppm
Biomass	9.78	12.47
Benzene	2.06	2.63
Acetonitrile	2.49	3.18
Chloroform	4.59	5.85
Ethylbenzene	1.58	2.02
Methylene chloride	0.52	0.66
Toluene	1.04	1.33
Trichloroethylene	1.56	1.99
Acetone	0.98	1.25
Tetrahydrofuran	2.27	2.90
Calcium hydroxide	6.22	7.92
Calcium phosphate	1.13	0.15
Methanol	1.74	2.21
Ethanol	1.35	1.72
Methylethylketone	2.32	2.96
Butyl acetate	1.94	2.47
Proteins	2.61	3.33
Fats	7.84	9.99
Carbohydrates	6.10	7.77
Heavy metals	0.29	0.37

Table 5 presents the final effluent of the clarifier (stream S109). The heavy metals concentration of 0.37 ppm in the effluent stream is above the US EPA limit (which is in the ppb range). Heavy metals, if present at high concentrations, can be removed efficiently by precipitation [19]. For dilute streams on the other hand, ion exchange is usually more effective and economical.
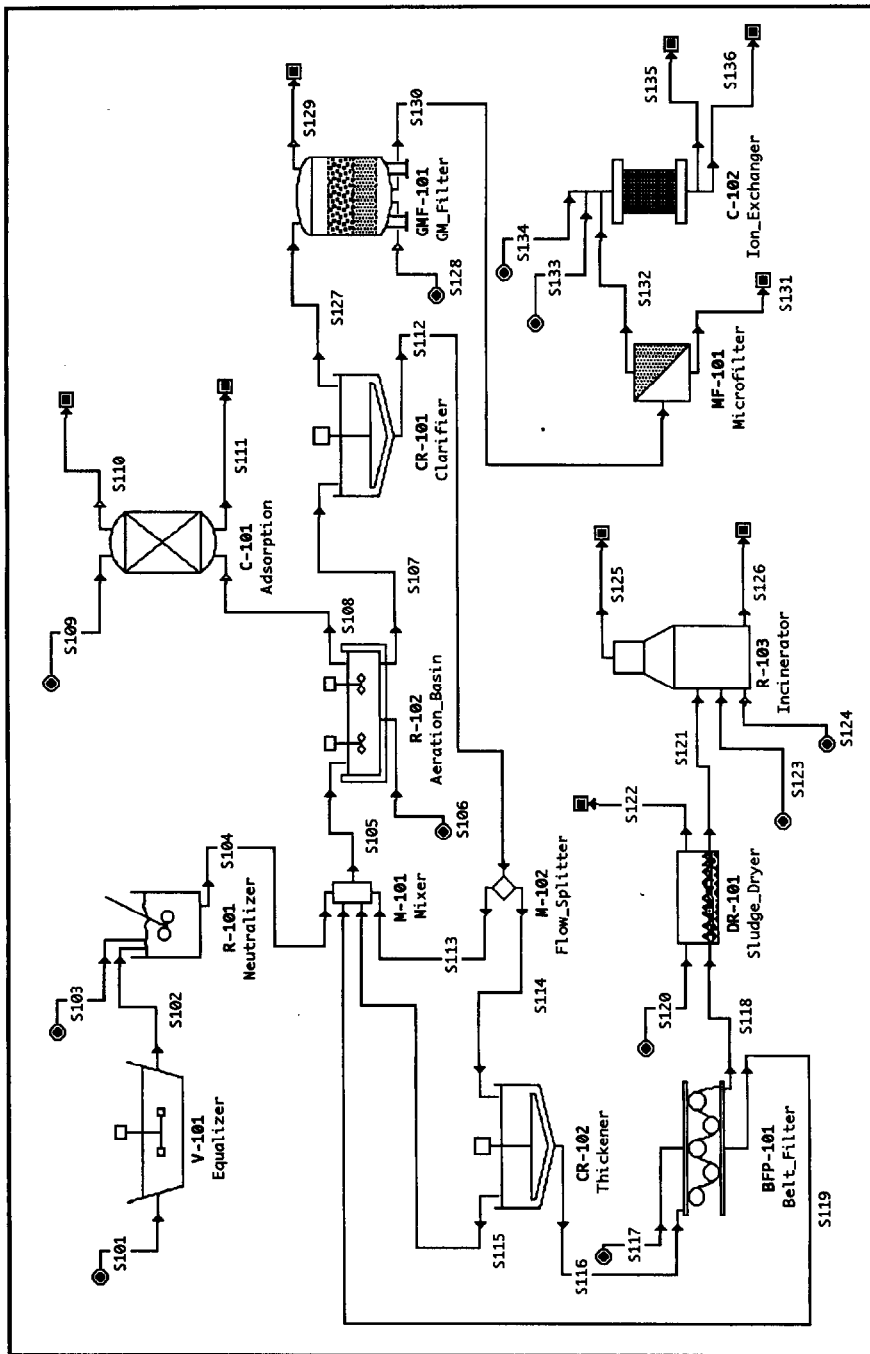
Fig. 9. Modified treatment plant to control VOCs and heavy metals.

3.2. Process modifications

To bring the plant in compliance with the US EPA standards, process modifications were evaluated for controlling VOC emission from the aeration basin and removing heavy metals from the water effluent stream. Fig. 9 shows the modified flowsheet. An activated carbon adsorption unit was considered for VOC removal. It was assumed that the basin is covered with a roof to collect the exiting gases. The carbon column was designed to remove at least 98% of the combined VOCs and reduce the total annual emissions to less than 25 t. For heavy metals removal, a train of two filtration units and an ion exchanger were employed. The granular media filter (GF-101) removes most of the particulate material (primarily biomass) and colloidal solids that escape the clarifier. The 0.45 μm pore size membrane microfilter (MF-101) removes the remaining small amount of particulate material to prevent biomass growth in the ion exchanger that may lead to clogging.

3.3. Economic evaluation of alternatives

EnviroCAD was used to evaluate the economic performance of the base case as well as the modified flowsheet. In addition, two more cases were evaluated, one with VOC control only (no heavy metals control) and another with VOC and heavy metals control but without the membrane filters.

Key assumptions made for the simulation and economic evaluation include:

(a) an increase of 30% in the capital cost of the aeration basin, to account for the addition of the roofs on the equalizer, neutralizer and aeration basin required to collect all exiting gases and direct them to the adsorption unit;

(b) an average disposal cost of $0.75/kg of VOCs for the mixture of organic solvents recovered by the activated carbon adsorption unit;

(c) for the stabilization of the heavy metals-containing incinerator ash, an average cost of $0.3/kg of ash;

(d) for the disposal of the heavy metals recovered by the ion exchanger, a cost of $1/kg of solution (heavy metals concentration was 0.95% w/w);

(e) to reduce the cost impact of membrane filtration, an optimistic purchase cost of $15000 per equipment unit (the current average purchase cost of a similar unit for manufacturing applications is at least twice as much). Each unit has a membrane area of 80 m^2 and an average filtrate flux of 60 l/m^2 h. The membrane is replaced every 4000 h of operation and the average membrane cost is $100/$m^2$;

(f) for the activated carbon adsorption unit, a carbon cost of $3/kg and a replacement frequency of once every 40000 h;

(g) for the ion exchanger, a resin unit cost of $10/l and a replacement frequency of once every 4 y,

(h) for the sludge dryer, use medium pressure steam for heating;

(i) for the incinerator there is no need for an absorber to treat the flue gas stream;

(j) a value of 20% (of the total purchase equipment cost) for the cost of the unlisted equipment. The cost of pumps, some process tanks not shown on the flowsheet, etc., go under this category.

Table 6
Capital and operating cost of the four alternatives

Case no.	Direct fixed capital ($M)	Operating cost ($M/year)	Operating cost ($/kg of BOD_5 removed)
1	27.8	7.2	0.70
2	29.2	8.5	0.83
3	36.1	10.3	0.99
4	50.2	18.1	1.73

Case 1. Base case shown in Fig. 8.
Case 2. With VOC but without heavy metals control.
Case 3. With VOC and heavy metals control but without membrane filters.
Case 4. With VOC and heavy metals control as shown in Fig. 9.

Table 7
Major equipment specification and FOB cost (1994 prices)

Quantity/stand-by		Description	Unit cost ($)	Cost ($)
1/0	V-101	Equalizer volume = 200.00 m^3	592 000	592 000
2/0	R-101	Neutralizer CS, volume = 473.35 m^3	190 000	380 000
1/0	CR-101	Clarifier Vol. = 1626.02 m^3, depth = 8.00 m	115 000	115 000
12/0	GF-101	Granular media filter Diam = 2.95 m, flux = 160.00 l/m^2 min	80 000	960 000
162/0	MF-101	Membrane microfilter Area = 80.0 m^2, 16.00 kW	15 000	2 430 000
1/0	C-102	Ion exchange unit L = 4.00 m, D = 0.75 m	256 000	256 000
1/0	CR-102	Thickener Area = 27.77 m^2	71 000	71 000
1/0	BFP-101	Belt filter Width = 1.54 m	106 000	106 000
1/0	DR-101	Sludge dryer Concrete, Duty = 112 9275 kcal/h	592 000	592 000
1/0	R-103	Incinerator Waste flow = 1525.48 kg/h Fuel flow = 0.00 kg/h	2 771 000	2 771 000
1/0	R-102	Aeration basin Volume = 6630.00 m^3 Loading = 41371.75 kg BOD_5/day	707 000	707 000
2/0	C-101	Adsorption column Diam = 1.82 m, Length = 0.32 m	27 000	54 000
		Cost of unlisted equipment 20.0% of total		2 258 000
Total equipment purchase cost				11 129 000

Table 6 shows the capital and operating cost of each case. The results of the economic evaluation clearly show that the use of membrane filtration should be avoided because it is too costly. This may be feasible if a fluidized bed ion exchanger is used instead of a packed column that can tolerate some amount of solids. Membrane filters and other expensive unit operations should be used to process concentrated streams of low flow rates aiming at material reclamation and reuse.

Tables 7–9 are excerpts from the economic evaluation report generated by the program for case #4 (with VOC and heavy metals control including membrane filtration). Table 7 shows a list of equipment with some descriptive information and the purchase cost for each piece. The total equipment purchase cost is around $11.3 million. The incinerator is the most expensive piece of equipment followed by the membrane filters in the second place and the granular media filters in the third position.

The autothermal combustion of the sludge results in a negligible operating cost for the incinerator. On the other hand, the operating cost associated with the membrane filters is substantial because of the requirement for membrane replacement every 4000 h of operation and of pumping power. Among the more traditional wastewater

Table 8
Fixed capital estimate summary (1994 prices)

Total Plant Direct Cost (TPDC) (physical cost)		
1. Equipment purchase cost	(PC)	$11 292 000
2. Installation	(0.39 × PC)	4 379 000
3. Process piping	(0.35 × PC)	3 952 000
4. Instrumentation	(0.15 × PC)	1 694 000
5. Insulation	(0.03 × PC)	339 000
6. Electrical	(0.10 × PC)	1 129 000
7. Buildings	(0.15 × PC)	1 694 000
8. Yard improvement	(0.10 × PC)	1 129 000
9. Auxiliary facilities	(0.15 × PC)	1 694 000
		TPDC = 27 302 000
Total Plant Indirect Cost (TPIC)		
10. Engineering	(0.25 × TPDC)	6 825 000
11. Construction	(0.35 × TPDC)	9 556 000
		TPIC = 16 381 000
Total Plant Cost (TPDC + *TPIC*)		TPC = 43 683 000
12. Contractor's fee	(0.05 × TPC)	2 184 000
13. Contingency	(0.10 × TPC)	4 368 000
		$\sum$(12 + 13) = 6 552 000
Direct Fixed Capital (DFC) TPC + 12 + 13		50 235 000

Table 9
Annual operating cost (1994 prices)

DFC-dependent items (DFC = $50 235 000)		
Depreciation		$4 772 000
Maintenance material	(0.03 × DFC)	1 507 000
Insurance	(0.01 × DFC)	502 000
Local Taxes	(0.02 × DFC)	1 005 000
Factory expense	(0.05 × DFC)	2 512 000
		10 298 000
Labor-dependent items		
Operating labor	(14460 h × 20.0 $/h)	289 000
Maintenance labor	(0.01 × DFC)	502 000
Fringe benefits	(0.40 × (a + b))	316 000
Supervision	(0.20 × (a + b))	158 000
Operating supplies	(0.10 × a)	29 000
Laboratory	(0.15 × a)	43 000
		1 337 000
Administration and overhead expense (0.6 × (a + b + c))		569 000
Raw materials		99 000
Other consumables		2 572 000
Utilities		1 827 000
Waste disposal		1 366 000
Total annual operating cost		
Including depreciation		18 068 000
Excluding depreciation		13 296 000

treatment units, the aeration basin, the equalizer, and the sludge dryer are the most expensive ones in terms of capital cost. Table 8 shows a summary of the fixed capital investment which for case #4 is around $50.2 million. The multipliers used in Table 8 were adapted and modified from projects for manufacturing processes. Validation of these multipliers has not been completed.

A summary of the annual operating cost is presented in Table 9. All the multipliers used to estimate various items of the operating cost can be modified by the user. Finally, Table 10 shows a breakdown of the operating cost for all four cases. Clearly, the direct-fixed-capital (DFC) dependent cost is the most important item followed by the labor-dependent cost. Depreciation was calculated over a 10-yr period assuming a 5% salvage value for the entire plant. A $20/h rate was assumed for operating labor.

The cost of raw materials includes the cost of $Ca(OH)_2$ (at $0.2/kg) used in the neutralizer while the cost of consumables includes primarily the cost of membrane for the membrane filters. The cost of the resin (for the ion exchanger) and the cost of the carbon (for the activated carbon column) came out rather small because of infrequent replacement. The cost of utilities includes primarily electricity for the aeration basin (with a unit power consumption of 0.03 kW/m^3 of liquid) and the membrane filters and steam for the sludge dryer.

Table 10
Breakdown of operating cost

Cost item	Case 1	Case 2	Case 3	Case 4
DFC-dependent	79.5	70.2	71.9	57.0
Labor-dependent	8.6	7.6	8.5	7.4
Administration	3.8	3.3	3.7	3.2
Raw materials	1.3	1.1	0.9	0.5
Consumables	0.0	0.0	0.0	14.2
Utilities	2.1	1.8	1.7	10.1
Waste disposal	4.7	16	13.3	7.6

The waste disposal cost includes the stabilization of ash (in all four cases), the disposal of the VOCs recovered by the adsorption column (in cases 2, 3, and 4) and the stabilization of the heavy metals removed by the ion exchange (cases 3 and 4).

This example clearly shows that the wastewater treatment cost of a manufacturing facility, especially in cases where volatile organics and heavy metals are present in the feed stream, can be quite substantial, contributing a major fraction of the overall operating cost. Instead of trying to remove such hazardous chemicals from dilute wastewater streams, emphasis should be placed on their recovery and recycling inside the manufacturing battery limits. Also, this cost is an incentive to design new as well as existing facilities so that they produce less waste.

4. Conclusions

The architecture and features of a prototype environmental simulator have been presented. The example illustrates how such tools can be used to track the fate of VOCs and hazardous chemicals in integrated waste treatment facilities. The fate of VOCs is of great importance to industry and to publicly owned treatment works (POTWs) that are being confronted with increasingly stricter regulations. The example also illustrates how environmental simulators can be used to evaluate process modifications and extensions necessitated by new regulations. This can be used by regulatory agencies and industry to estimate the economic burden of stricter environmental regulations. The results of such analyses can also act as incentives for pollution prevention strategies that reduce waste generation at the source and minimize the need for investment in pollution control.

Tools such as EnviroCAD can also play a role in educating students and engineers how to optimize a process with environmental constraints during the early stages of process development and design, when there is still room for process modifications. The interactive interface stimulates a dialog between the user and the computer resulting in effective training and refined final designs.

Since EnviroCAD is still a research prototype, a number of improvements and extensions are needed to make it more complete and effective. Development of more

rigorous biotreatment unit operation models is of high priority. These models will be based on fundamental principles for estimating the extent of biodegration, sorption and stripping for a compound that enters a biotreatment reactor. However, limited availability of fundamental models and data may prove to be an impediment to the progress.

Acknowledgements

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