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Optimization of Wastewater Treatment Facilities Using Process Simulation

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Abstract
The role of process simulation in designing, evaluating, and optimizing wastewater treatment facilities is discussed. Alternatives for controlling VOC emissions from treatment plants and removing dissolved solids from clarified effluent streams are evaluated. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords: Wastewater Treatment, Computer-Aided Process Design, Process Modeling, Process Simulation, Environmental Impact Assessment, Waste Minimization.

Introduction

The increasingly stringent environmental regulations on discharge standards have rendered the optimal design and operation of industrial and publicly owned treatment works (POTWs) a challenging task. Such new requirements include:

1) The need to track the fate of volatile organic compounds (VOCs). VOCs when present in influent streams tend to volatilize from open tanks and end up in the atmosphere. Current regulations limit VOC emissions from treatment plants to no more than 25 tons per year (Van Durme, 1993). A key question concerning the environmental engineer is how to estimate and effectively control emissions from treatment plants.
2) The need to track the fate of heavy metals and other hazardous chemicals in integrated treatment processes. Heavy metals tend to associate with solids and accumulate in sludge. How can we predict this? How can we make sure we meet regulatory standards?
3) The recently introduced, strict biological nutrient removal regulations create additional problems. More specifically, most existing treatment facilities do not meet the new nutrient removal standards and will need to be revamped in the next few years. The question is how can we design and operate treatment facilities that can 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 have reached the level of manufacturing operations, 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 wastewater 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 (constituents) 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 pollutants are present at very low concentrations requiring more accurate material balances that can predict trace contaminant levels.

To address the current industrial needs for efficient design, evaluation, and operation of integrated environmental processes, engineers at Intelligen, Inc. developed and commercialized EnviroPro Designer,

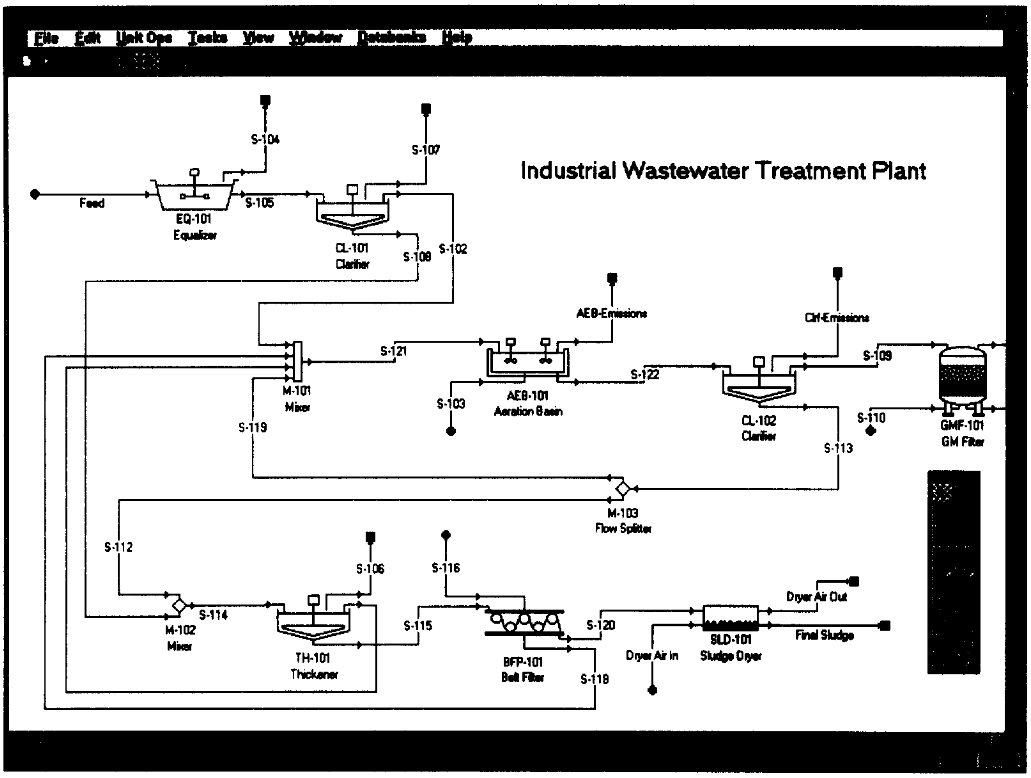

Figure 1. Main Window of EnviroPro Designer

a comprehensive process simulator for environmental applications. In the development of EnviroPro, particular emphasis was placed on the requirement to carry out material balances on consituents and predict the fate of hazardous chemicals (e.g., heavy metals and VOCs) in integrated environmental processes. This is particularly important for industrial wastewater because the U.S. Environmental Protection Agency (EPA) regulates the amount and concentration of discharged priority pollutants (various organic chemicals, heavy metals and ions).

Description of EnviroPro Designer

System Architecture and User Interface
The general structure of the software consists of the graphical user interface, the process simulation module, and the economic evaluation module. EnviroPro 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 unit operations from the "Unit_Ops" menu and drawing the material streams that connect the units. All input-output information is provided/displayed through dialog windows. Figure 1 shows how information about a flowsheet is displayed on the main window. Figure 2 shows a typical input dialog window for initializing unit operation models.

Process Simulation
The process simulation module of EnviroPro assists the engineer to interactively develop and analyze integrated flowsheets for waste recycling, treatment and disposal processes. Flowsheets consist of unit operations, material streams, and chemical components. A flowsheet in EnviroPro can have any number of these objects.

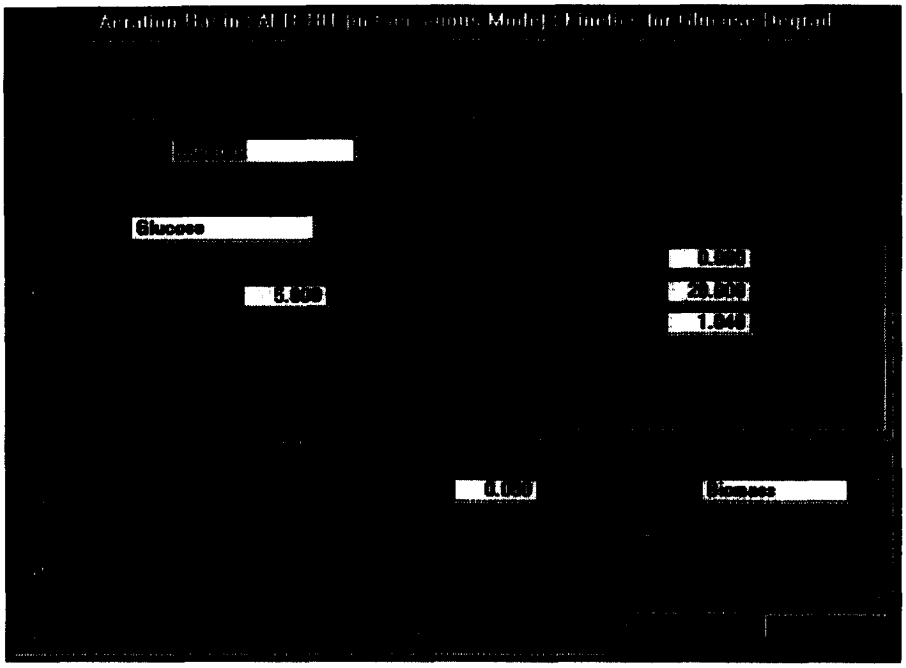

Figure 2. Reaction Kinetics Input/Output Dialog Window of the Aeration Basin Model

Chemical components are used to describe flow and composition of material in streams. EnviroPro distinguishes between conventional components, which are 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, critical pressure and temperature, accentric factor, vapor pressure, Henry's law constant, octanol-water coefficient, density, specific heat, and particle size), environmental (contributions to COD, TOC, BOD_5/COD, TSS, etc.) and regulatory properties (e.g., SARA Title III chemical) for around four hundred 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 lumped stream properties (BOD, COD, TSS, etc.) based on stream composition.

Streams represent the flow of material from one unit operation to the next and are displayed as polylines on the computer screen. A stream object stores component specific information, such as mass and mole flowrate, the partition between sludge and water, the weight or mole percentage as well as the total mass or mole flowrate, the stream name, and several other properties (temperature, pressure, activity, etc.).

Environmental characterization of streams. Based on stream composition, EnviroPro calculates and displays the following environmental stream properties: Total Organic Carbon (TOC), Total Phosphorus (TP), Total Kjeldahl Nitrogen (TKN), Ammonia Nitrogen (NH3-N), Nitrate-Nitrite Nitrogen (NO3-NO2-N), Chemical Oxygen Demand (COD), Theoretical Oxygen Demand (ThOD), Biological Oxygen Demand (BOD5 and BODu), Total Solids (TS), Total Suspended Solids (TSS), Volatile Suspended Solids (VSS), Biodegradable Volatile Suspended Solids (DVSS), Total Dissolved Solids (TDS), Volatile Dissolved Solids (VDS), and Biodegradable Volatile Dissolved Solids (DVDS). These properties apply to liquid waste streams and are indicators of environmental impact on the receiving water body. To estimate these properties, EnviroPro 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 predicted) come from experimental data retrieved from the database or provided by the user. In other words, EnviroPro carries out material balances on individual chemical components (constituents) and estimates the lumped environmental stream properties (e.g., BOD, TSS, etc.) based on stream composition. This feature 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 EnviroPro 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 information. The primary function of a unit operation model is to carry out the material and energy balances around a process step and estimate outlet stream variables given inlet stream variables and operating specifications. The user provides engineering information during initialization of unit operations through unit specific dialog windows (see Figure 2). 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 EnviroPro are estimated in a sequential modular approach. 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. In the implementation of unit operation models in EnviroPro a serious effort was made to balance ease of use with engineering rigorousness. The mathematical model of the aeration basin, a typical unit operation in wastewater treatment, is described in the following section to illustrate the modeling approach.

Aeration Basin Mathematical Model

The aeration basin is modeled as a well-mixed reactor with versatile kinetic expressions. Any number of reactions can be specified that may represent biochemical oxidation, hydrolysis, chemical oxidation, photolysis, nitrification, etc. The stoichiometry of a reaction is specified on a mass or molar basis while the reaction rate is specified by selecting appropriate expressions for the substrate term, the other term (e.g., oxygen), and the biomass term (see Figure 2). The reaction rate constant is either specified by the user or retrieved from the component databank for biochemical oxidation reactions that follow Monod-type kinetics. The various reactions may be based on different biomass components. For instance, heterotrophic biomass may be used for biochemical oxidation and denitrification reactions and autotrophic biomass for nitrification reactions. Biomass death and hydrolysis reactions may be written to keep track of the active and dead fractions of biomass components. The aeration basin model handles VOC emission calculations. Different models exist for surface and diffused aeration that are mass transfer and equilibrium limited, respectively.

In terms of sorption of chemicals on sludge, the user may specify the fraction of a component that adsorbs on the primary biomass component. The program, then, keeps track of the fraction in solution throughout the flowsheet.

For steady-state operation of a well-mixed aeration basin, the general material balance equation for a component that biodegrades and is emitted is given by the following equation:

$$0 = (\mathit{Input}) - (\mathit{Output}) - \begin{pmatrix} \mathit{Biochemical} \\ \mathit{Oxidation} \end{pmatrix} - \begin{pmatrix} \mathit{Surface} \\ \mathit{Volatilization} \end{pmatrix} - \begin{pmatrix} \mathit{Diffused} \\ \mathit{Air} \\ \mathit{Stripping} \end{pmatrix}$$

or

$$0 = QC_{in} - QC - Vr_b - K_L aVC - Q_a K_{eq} CF_{st}$$

Where Q is the liquid flow rate, V is the reactor volume, C_{in} is the inlet concentration, C is the outlet concentration which is the same as the concentration in the reactor, r_b is the biodegradation rate, K_La is the overall mass transfer coefficient, Q_a is the air flow rate (in case of diffused aeration), K_{eq} is the equilibrium constant, and F_{st} is the saturation term (it represents the extent of saturation of the exiting gas stream). In general, the biodegradation rate is a function of substrate concentration, oxygen concentration, and biomass concentration. Various expressions are available to account for the effect of substrate. The overall equation with a Monod-type substrate expression is written as follows:

$$r_b = K_{\max}\left(\frac{C}{K_s + C}\right)\left(\frac{C_O}{K_O + C_O}\right)X$$

Where K_{max} is the maximum rate constant, K_s is the half saturation constant for the substrate, C_O is the oxygen concentration, K_O is the half saturation constant for oxygen, and X is the biomass concentration. Alternative expressions for the substrate and oxygen terms are also available. The component databank includes data for K_{max} and K_S for a large number of chemical components.

The overall mass transfer coefficient of a VOC component is estimated as a function of the oxygen mass transfer coefficient in wastewater, using a proportionality coefficient, ψ_M. In other words,

$$(K_La)_{VOC} = \psi_M (K_La)_{O2}$$

The value of $(K_La)_{O2}$ in the wastewater is a user input to the program. ψ_M is given by the following equation (Hsieh et. al., 1993):

$$\psi_M = \psi \left(1 + \frac{1}{H_c \frac{k_g a}{k_l a}}\right)^{-1}$$

ψ is the dimensionless transfer coefficient proportionality constant and is calculated by the following equation (Corsi and Card, 1991):

$$\psi = \left(\frac{D_{VOC}}{D_{O_2}}\right)^n$$

Where D_{VOC} and D_{O2} are the liquid diffusion coefficients for a VOC and oxygen in (m^2/s), respectively. The exponent n varies from 0.5 for penetration and surface renewal theories to 1.0 for two-film theory (Corsi and Card, 1991) and is typically 0.5 to 0.6 (Mihelcic et. al., 1993). The diffusion coefficients of VOC components are retrieved from the component databank of the program. k_ga and k_la are the individual mass transfer coefficients of the VOC in the gas and liquid phases, respectively, in (s^{-1}). For mechanically aerated systems, the value of k_ga/k_la is estimated using the following empirical equation (Hsieh et. al., 1993):

$$\log \left(\frac{k_g a}{k_l a}\right) = -0.39664 \log_{10} (P/V) + 2.6776$$

(P/V) represents the mechanical power consumed for surface aeration divided by the liquid volume of the aeration basin and is calculated by the program. Alternatively, the user has the option to set the value of $k_ga/$.

For diffused aeration systems, the F_{st} term is calculated by the following equation:

$$F_{st} = 1 - \exp\left(\frac{\psi_M (K_La)_{O_2} V}{H_c Q_g}\right)$$

To calculate ψ_M, the user has the option to set either the k_ga/k_la ratio or the entire term in parenthesis. The equilibrium constant is estimated by:

$$K_{eq} = \frac{H_C}{RT}$$

Where H_C is Henry's law constant, R is the universal gas constant and T is temperature. The above equations are written for each chemical component entering a well mixed aeration basin and constitute a set of non-linear equations which is solved numerically to calculate the exit concentration and the emission rate of each component.

Economic Evaluation

For an integrated waste treatment process, EnviroPro 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, material 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 (U.S. EPA, 1980; Garrett, 1989; Peters and Timmerhaus, 1991; and Cooper and Alley, 1994). The fixed capital investment is calculated based on the total purchase cost of equipment using multipliers, which users can modify. The annual operating cost includes cost of process chemicals and consumables, labor, utilities, equipment 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.

Computer Implementation

EnviroPro runs on personal computers and is written in Microsoft Visual C++ 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 EnviroPro can be used in practice follows.

Simulation and Economic Evaluation Example

This example focuses on the retrofit design of an industrial wastewater treatment plant that services a petrochemical facility located in the Pacific Rim. Figure 1 shows the flowsheet of the current facility, which has been slightly modified to hide confidential information.

Process Description

During primary treatment, the flowrates and concentrations of the inlet streams are equalized in a basin (EQ-101) and large particles are removed using a clarifier (CL-101). The secondary treatment includes an aeration basin (AEB-101) for the biological oxidation of organic materials and a clarifier (CL-102) for the removal of sludge and carried-over solids. The aeration basin operates at an average hydraulic residence time of 6 hours, an average sludge residence time of 24 hours, and a minimum dissolved oxygen concentration of 2,000 mg/liter. A fraction of the sludge (70%) is recycled to maintain a biomass concentration in the aeration basin of 2,250 mg/liter. The excess sludge (S-112) is sent to the sludge treatment section. The sludge is thickened in a thickener (TH-101) to a solids concentration of 3% w/w, dewatered in a belt filter press (BFP-101) to a solids concentration of 15% w/w, and dried in a sludge dryer (SLD-101) to a final solids concentration of around 35% w/w. The dried sludge is disposed off in a landfill.

Table 2 shows the average composition and flowrate of the feed stream to the treatment facility. This is a rather small treatment facility with an average throughput of 1.4 MGD. The feed stream to this plant includes a number of regulated chemicals (e.g., dichlorobenzene, butyraldehyde, ethylene glycol, and phenol). Glucose is used to represent the readily biodegradable organic compounds. The 'Salts' component represents the large amount (3.43 g/L or 750 kg/h) of non-degradable dissolved solids, such as sodium chloride, that are present in the feed stream.

Table 2. Influent Stream Composition

Component	Flowrate (kg/h)	ppm
Butyraldehyde	122.80	561.5
Dichlorobenzene	41.50	189.8
Ethylene Glycol	237.00	1,083.8
Glucose	135.40	619.2
Phenol	8.00	36.6
Salts	750.00	3,429.6
Water	217,441.10	994,315.9

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. Water soluble and non-degradable compounds will remain in the liquid effluent stream. 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. Plant Performance

Stream Property	% Removed
TOC	98.7
COD	98.6
BOD (5-day)	98.7
BOD (ultimate)	98.7
TSS	87.3
TDS	15.6

Table 3 shows the overall performance of the plant based on removal of TOC, COD, BODu, BOD_5, TSS, TDS, etc. according to the simulation results which were in good agreement with actual plant data. The plant performance is high in terms of BOD, COD, and TSS removal but rather poor in terms of TDS removal. This can be explained by the fact that most of the TDS is due to the non-degradable dissolved solids (Salts) that remain in the liquid effluent. This plant also performs rather poorly as far as emissions of VOCs are concerned. Table 4 presents the composition of the gas stream exiting the aeration basin (AEB-Emissions). A total of approximately 86.3 kg/h or 2,072 kg/day of VOCs are emitted from the aeration basin.

Table 4. Aeration Basin Gas Outlet Stream

Component	Flowrate (kg/h)	% Emitted
Butyraldehyde	55.187	44.63
Dichlorobenzene	28.762	68.46
Ethylene Glycol	2.341	0.99
Phenol	0.036	0.45
VOCs Total	**86.326**	**21.02**

Small amounts of VOCs are also emitted from the equalizer (EQ-101), the primary clarifier (CL-101), and the secondary clarifier (CL-102). If this plant were located in the U.S.A., it would be considered a major source of VOC emissions according to the 1990 Clean Air Act Amendments (Van Durme, 1993 and McInnes, 1993). To comply with the current limit of 25 tons/yr, 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 (Lahiere et al., 1993), thermal destruction, and biodegradation (biofilter or bioscrubber).

Table 5 presents the final liquid effluent stream. The dissolved solids concentration is 3.44 g/liter. To reduce wastewater as well as process water, facility managers wanted to evaluate wastewater treatment and purification technologies that would allow treated effluent to be recycled onsite.

Table 5. Clarified Liquid Effluent Stream

Component	Flowrate (kg/h)	ppm
Biomass	0.124	0.6
Butyraldehyde	3.046	14.0
Dichlorobenzene	1.838	8.5
Ethylene Glycol	0.115	0.5
Glucose	0.463	2.1
Phenol	0.002	0.0
Salts	746.718	3,435.1
Water	216,627.140	996,538.6
Total	217,379.449	1,000,000.0

Process Modifications

Engineers used EnviroPro Designer to bring the plant into compliance with EPA standards for VOC emissions and to meet wastewater purity specifications for recycling. To do this, they evaluated process modifications for controlling VOC emissions from the aeration basin and removing dissolved solids from effluent. 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 99% of the combined VOCs and reduce the total annual emissions to less than 25 tons. For dissolved solids removal, a combination of a reverse osmosis unit, an evaporator, and a crystallizer were evaluated. The clarified and filtered liquid effluent is processed by the reverse osmosis unit, which retains the vast majority of the dissolved solids. The retentate is further concentrated using an evaporator and the salts are precipitated in a crystallizer. The filtrate stream of the reverse osmosis unit is highly purified water and can be reused as process water. The vapor from the evaporator and the crystallizer is highly purified water vapor, which can be condensed and utilized elsewhere in the plant.

Economic Evaluation of Alternatives

EnviroPro was used to evaluate the economic performance of the base case as well as the modified flowsheet. In addition, a case with VOC control only (no dissolved solids removal) was evaluated. Key assumptions made for the modeling and economic evaluation include: (a) an installed capital cost of $250,000 for the roof of the aeration basin; (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) an average disposal cost of $0.02/kg for the concentrated and dried biological sludge; (d) an average disposal cost of $0.10/kg for the crystallized/precipitated dissolved salts; (e) to reduce the cost impact of reverse osmosis, an optimistic purchase cost of $40,000 per equipment unit. Each unit has a membrane area of 116 m^2 and an average filtrate flux of 80 liter/m^2-hour. The membrane is replaced every 8,000 hours 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 40,000 hours; (g) for the sludge dryer, medium pressure steam was assumed for heating; (h) 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 shows the capital and operating cost of each case (DFC stands for Direct Fixed Capital). The results of the economic evaluation clearly show that removal of dissolved solids is an expensive operation. Reverse osmosis and other costly unit operations should be used to process concentrated streams of low flowrates aiming at material reclamation and reuse.

Table 6. Capital and Operating Cost

Case #	DFC ($M)	Oper. Cost ($M/year)	Oper. Cost ($/kg of BOD_5)
1	14.5	4.0	1.24
2	16.7	5.3	1.64
3	22.2	8.9	2.76

Case #1: Base case shown in Figure 1.
Case #2: With VOC but without dissolved solids removal.
Case #3: With VOC and dissolved solids removal.

Table 7 shows a breakdown of the operating cost for all three cases. Clearly, the direct-fixed-capital (DFC) dependent cost is the most important item followed by the labor-dependent cost in Case 1 and the waste disposal cost in Cases 2 and 3. Depreciation was calculated over a ten-year period assuming a 5% salvage value for the entire plant. A $20/hour rate was assumed for operating labor. For treatment plants that have already been depreciated, labor and waste disposal costs will dominate the annual operating cost. The cost of 'Waste Treatment/Disposal' is primarily due to the disposal of the recovered VOCs and the disposal of the removed dissolved solids. The cost of utilities is primarily due to the power consumption by the reverse osmosis units and the aeration basin. The cost of consumables is due to the need for replacement of the reverse osmosis membranes every 8,000 hours of operation.

Table 7. Breakdown of Operating Cost

Cost Item	Case #1 %	Case # 2 %	Case # 3 %
DFC-Dependent	68.8	60.3	47.5
Labor-Dependent	18.6	14.8	11.6
Administration	9.1	7.3	5.6
Consumables	0.0	0.0	3.0
Utilities	2.6	2.0	15.0
Waste Disposal	1.0	15.5	17.3

This example clearly shows that the wastewater treatment cost of a manufacturing facility, especially in cases where volatile organics and large amounts of dissolved solids 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 unwanted chemicals from dilute wastewater streams, emphasis should be placed on their recovery and recycling inside the manufacturing battery limits.

Conclusions

The architecture and features of a comprehensive environmental simulation and design tool have been described. An example was presented to illustrate how such tools can be used to track the fate of VOCs and other 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. Such evaluations can be used by regulatory agencies and industry to estimate the economic burden of stricter environmental regulations. The results of such analyses can 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 EnviroPro can also play a role in educating students and engineers on how to design and operate processes within environmental constraints. The interactive interface stimulates a dialog between the user and the computer resulting in effective training.

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