Development of a Physical Property Management System (PPMS) to Support Clean Process Design [1]

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ABSTRACT

An obstacle to achieving clean, cost-effective chemical process designs is obtaining reliable physical property data and thermodynamic parameters. The PPMS (Physical Property Management System) software is intended to overcome this barrier by providing the design engineer with an expandable software interface capable of evaluating and delivering physical property and thermodynamic information. At the heart of PPMS are three tools for data access and management: PEARLS (Property Estimation And RetrievaL Software), DCUT (Data Conversion UTility), and SDAS (Structure Disassembly Advisory System). PEARLS provides transport, thermodynamic, fire/explosion, and partitioning/equilibrium data from experimental sources and predictive methods. Data from PEARLS can be transferred to other process design tools, simulators, word processors, or spreadsheets. The DCUT utility enables the user to link existing chemical databases such as DIPPR®801 and 911 to PEARLS. The SDAS algorithm generates group fragments that can be used in the structure-based UNIFAC and fire and explosion estimation methods available within PEARLS. By combining UNIFAC with methods for calculating the pure component vapor pressure, PEARLS can predict, from chemical structure alone, a number of useful phase partitioning properties involving vapor-liquid and liquid-liquid phases in equilibrium. PEARLS includes a UNIFAC parameter set developed by the authors specifically for aqueous mixtures which is particularly applicable to environmental air-water partitioning calculations.

To demonstrate PPMS in a conceptual process design, Henry's constant data from PEARLS are used to model a staged stripping column to remove toluene from water using steam. Data estimation and extrapolation methods within PEARLS were used to obtain values of Henry's constant at the average column temperature (90°C) used in the tower design and utility calculations. At 90°C, PEARLS identified one estimated value from the literature as an outlier which was clearly distinguished from four other independent values that agreed closely. An economic analysis showed that the incorrect published data value led to a tower design that underspecified the number of trays and increased the utility (i.e. steam and cooling water) requirements necessary to meet the toluene effluent concentration limit. By using PEARLS, inaccurate data were screened out at the design stage and the utility cost penalty avoided.

KEY WORDS: **physical property data, data delivery, property estimation, group contribution**

1.0 PHYSICAL PROPERTY MANAGEMENT SYSTEM (PPMS)

Process design has required engineers to accumulate relevant physical property data from a variety of sources and find appropriate estimation methods for any missing data (Carlson, 1996). PPMS eliminates much of the work involved in this process by providing a single platform from which the engineer can access and display physical property data in a matter of seconds. PPMS is a central information network containing tools to organize, display, estimate, and add physical property data. PPMS, written in Visual Basic™ version 4.0, currently consists of three main tools: Property Estimation And RetrievaL Software (PEARLS), Data Conversion Utility (DCUT), and Structure Disassembly Advisory System (SDAS).

1.1 Data Conversion UTility (DCUT)

A great deal of effort has been expended to develop a universal database standard for data transfer between academic and industrial databases, and process simulation software. Some older databases are stored as ASCII text files, but today, data are typically stored using commercial database software capable of managing large chemical data sets.

Two main problems impede the development of a universal data format. One is the way in which data are stored. For example, since Access® and Paradox® store databases in different formats, an Access® database cannot be read in directly from Paradox® without an internal conversion routine. The second problem is deciding on an optimum database structure. The DCUT module within PPMS is a model for a standard database design and provides a way to add customized conversion routines. Currently, DCUT can translate the DIPPR®801 (PSU, 1994 and 1995 versions) ASCII text database and the DIPPR®911 (MTU, 1997) Paradox® database into a

standard PPMS Access® format. Conversion routines to import other databases into the PPMS Access® format can be coded and added to DCUT.

1.2 Property Estimation And RetrievaL Software (PEARLS)

Data display, retrieval, estimation, printing, exporting, and graphing are currently handled under PPMS by PEARLS. Data from DIPPR®801 (PSU, 1993) and DIPPR®911 (MTU, 1997) can be accessed from PEARLS after using DCUT to convert the databases. By including the DIPPR® databases, users may access critically evaluated data for 36 thermophysical properties for over 2000 chemicals. Properties within PEARLS are organized by folders for seven different physical property areas: Chemical Information, General 1, General 2, Transport, Fire and Explosion, Oxygen Demand, and Partitioning/Equilibrium. Each group is displayed as a folder that facilitates easy access to any property within that group. Any other available sources for experimental or estimated data may be selected instead of the current value displayed under the folder. If the data sources are unsatisfactory or missing, the user may also specify one value for each property. All of the data sources displayed in PEARLS include original source references. Table I gives a concise listing of standard features of the PEARLS module.

Temperature and pressure values can be changed at any time with the affected properties being updated automatically. Also, estimated values are recalculated to maintain thermodynamic consistency. Property units may be changed between SI, CGS, English and other mixed units.

The 23 estimation methods currently included in PEARLS were selected as the best models for a given property by a thorough literature search and model evaluation. This number is continuing to grow. Most important to environmental calculations are the partitioning/equilibrium properties and parameters available in PEARLS. PEARLS contains a group of algorithms, based

upon those developed by Arbuckle (1983, 1986) for dilute aqueous systems, specifically built to accommodate equilibrium calculations at various operating conditions. Equilibrium calculations include procedures for determining activity coefficients at infinite dilution, Henry's law constants, aqueous solubilities, and octanol/water partitioning coefficients. These are all based upon simple thermodynamic relationships using the infinite dilution activity coefficient calculated from UNIFAC. The utility of using UNIFAC within PEARLS is that no other property information is required other than the structure of the chemical.

Four UNIFAC functional group binary interaction parameter databases are available within PEARLS. The original vapor-liquid (e.g. AVLE, Fredenslund et al. (1975) and several subsequent revisions and extensions) and liquid-liquid (e.g. ALLE, Magnussen et al. (1981)) databases are available in addition to two new datasets (e.g., AENV and AGLB) developed by Rogers (1994) for dilute aqueous mixtures. The environmental AENV set is a revised version of the original AVLE set tailored to aromatics, aliphatics, and halogenated derivatives at dilute aqueous concentrations. The ALLE set was created as a companion to the original AVLE set and is applicable to liquid-liquid mixtures at various concentrations. The fourth set, AGLB, announced here for the first time, is an entirely new set of interaction parameters based solely on carefully evaluated Henry's law constant data and designed for aqueous dilute mixtures of organics of all types. General recommendations for selecting an appropriate parameter set are listed in Table II and built into the PEARLS calculation hierarchy.

1.3 Structure Disassembly Advisory System (SDAS)

The structure of PEARLS is designed to allow additional properties and estimation methods to be added later. Group contribution models, in which a property is estimated from the

contribution of group fragments which make up that structure, are particularly attractive. UNIFAC is the first group contribution calculation in PEARLS. Other models, such as the MTU Fire and Explosion and MTU Vapor Pressure models, are being implemented. SDAS suggests to the PPMS user how to divide a chemical structure into the fragments for a given model, greatly reducing the work required to do this by hand. To use SDAS, a chemical's SMILES (Simplified Molecular Input Line Entry System) string must be entered. The SMILES string is then broken into suggested group contribution fragments for any of several structure-based algorithms. These fragments can be accepted or modified for use in the group contribution routine(s) in PEARLS.

2.0 APPLYING PPMS TO THE DESIGN OF A STEAM STRIPPER

2.1 Goals of the Analysis

To demonstrate the utility of PPMS in conceptual design, Henry's constant data from PEARLS were used to facilitate the design of a plate steam stripping column to remove toluene from water. The two main goals of the study were: (1) to show that PPMS can supply reliable physical property data in the conceptual process design stage; and (2) to demonstrate the utility of PPMS as a data screening tool to avoid faulty designs and possible economic penalties.

2.2 Steam Stripping of Dilute Aqueous Wastes

Steam stripping is used typically in the petrochemical industry to remove volatile organic contaminants (VOCs) from wastewater or groundwater streams. The Best Available Technology Economically Achievable (BATEA, 40 CFR Part 414.101) effluent limits for toluene are 74 µg/L as a maximum daily concentration, and a maximum monthly average concentration of 28 µg/L

(Potter, 1990). These limits were established by the EPA for the Organic Chemical, Plastics, and Synthetic Fibers (OCPSF) category using steam stripping as the standard removal technology (Reith, 1991).

A typical steam stripper operating at atmospheric pressure (Spencer, 1996) is presented in Figure 1. The contaminated water is preheated by the treated stream leaving the bottom of the column. Contaminated water enters the top of the column and flows down through the stripping section. Steam is injected countercurrently up the column. The temperature difference between the top and bottom of the column usually differs by less than 5°C (Potter, 1990). As the organics vaporize they are transferred from the liquid to the gas phase. As the steam travels up the column the concentration of organics increases. Steam exiting the top of the column is sent to a condenser where it undergoes a phase change to a liquid. Since the liquid is supersaturated with organics, a separate organic phase forms in the decanter. The aqueous phase can be sent back to the main feed mixing tank or refluxed back to the top of the column. The organic phase is then drawn off for reuse or is sold as a product.

2.3 Design Equations and Economic Assumptions

A performance and economic analysis was performed on the steam stripping system shown in Figure 1. A 100 kmol/hr wastewater stream containing 550 ppm(wt.) toluene is to be stripped down to the BATEA daily effluent limit of 74 µg/L (0.074 ppm(wt.)). Table III lists technical specifications and engineering assumptions for the steam stripping process and economic data are listed in Table IV. In this analysis the stripping column was considered to consist of a series of stacked trays with the toluene rich feed entering the top of the column and pure steam

injected countercurrently from the bottom.

The fixed capital investment (FCI) for the entire steam stripping process was calculated using Equation (1):

$$FCI = (C_T + C_C + C_P + C_D + C_{BP})(F_{Lang}) \quad \textbf{(1)}$$

where:

FCI = Fixed Capital Investment, ($)
C_T = Cost of trays, ($)
C_C = Cost of condenser, ($)
C_P = Cost of preheater, ($)
C_D = Cost of decanter, ($)
C_P = Cost of bottoms pump, ($)
F_{Lang} = Lang factor (4.8 for a fluid-processing plant)

Using the column design equations and fixed capital costs, the next step in the overall analysis was to determine the optimum steam flow rate. The net present value, NPV, of the total investment based on the total fixed capital investment and operating costs was computed for steam flow rates of 1.0 to 5.0 kmol/h. The optimum design was taken at a maximum NPV, neglecting any income for the recovered toluene. The NPV was most significantly affected by steam and cooling water utility costs.

Table VII summarizes the tray-by-tray iteration procedure used to determine the optimum column design. At each steam flow rate, the integer number of ideal trays is determined so that the toluene concentration of the treated water is equal to or lower than the target effluent concentration of 0.074 ppm(wt.). A discounted cash flow analysis is performed to calculate the NPV for each steam flow rate, and the steam rate is incremented, and the process repeated, up to a steam flow rate of 5.0 kmol/h.

2.4 Design Data Retrieval and Comparison Using PEARLS

2.4.1 General Property Data

Physical property data required for the steam stripper design calculations were obtained from the PEARLS software, the primary source being critically evaluated DIPPR®801 experimental data or correlations. The data used in this design study are the highest rated values available among the PEARLS data resources.

2.4.2 Toluene-Water Henry's Law Constant Data

2.4.2.1 *UNIFAC Calculations*

Data for toluene-water vapor-liquid partitioning were obtained using several estimation methods within PEARLS. The AENV binary interaction database was chosen for the UNIFAC infinite dilution activity coefficient calculation because it was derived for aromatics, aliphatics, and halogenated derivatives of these at dilute concentrations (Rogers, 1994). The values from this estimation technique were compared against other literature values and estimates displayed by the PEARLS software.

2.4.2.2 *Ratio of Vapor Pressure to Solubility*

Solubility data for toluene in water from Stephenson (1992) and Chen and Wagner (1994) were used in conjunction with the vapor pressure correlations from DIPPR®801 to calculate Henry's constant at temperatures from ambient to 90°C. Henry's constant can be described as the partial pressure of the solute in the gas phase over the solute concentration in the liquid phase. The Henry's law relationship (Carroll, 1991) is often applicable for hydrophobic solutes, at near-ambient conditions, up to the point at which two phases form:

$$H = \frac{P_{vap}}{S} \qquad \textbf{(2)}$$

where:

H = Henry's law constant, {atm}
P_{vap} = Vapor pressure of chemical, {atm}
S = Solubility limit of chemical in water, {mole fraction}

This method assumes that Equation (2) remains valid for toluene in water at elevated temperatures and that the solubility limit of water in the chemical is negligibly small.

2.4.2.3 *Product of Vapor Pressure and Infinite Dilution Activity Coefficient*

Infinite dilution activity coefficient data from the literature were also multiplied by vapor pressures to obtain Henry's constant estimates. Gmehling (1994) and Hwang (1992a, 1992b) provide infinite dilution activity coefficients at 25°C. These data, along with the vapor pressure value from PEARLS given in Table VIII, were used to calculate Henry's law constant at 25°C.

2.4.2.4 *Linear van't Hoff Data Regression*

Direct Henry's constant measurements from 10 to 30°C made at Research Triangle Institute (RTI; see Ashworth et al., 1988) were also displayed by PEARLS. Temperature regression equations were computed for the 45 chemicals studied, using a van't Hoff equation format (i.e., $\ln H' = A/T + B$). Parameters (A and B) for the 45 chemicals were correlated over a 10 to 30°C range using this relationship. The correlation format presented by Ashworth et al. (1988), along with his parameters for toluene, is shown below in Equation (3):

$$\ln H' = \frac{A}{T} + B \qquad \textbf{(3)}$$

where:

H′ = Henry's law constant, {atm-m^3/mol}
T = Temperature, {K}

A = -3024 for toluene
B = 5.133 for toluene

A similar two-parameter correlation by Persichetti (1990) was developed using low temperature liquid-liquid miscibility data from Gmehling (1979, 1986, and 1988). The slope and intercept presented by Persichetti for the toluene-water Henry's constant are A=-4400.91 and B=-20.647, with Henry's constant units of {atm} and T in {K}. Persichetti (1990) used this correlation as an extrapolation tool for obtaining toluene-water Henry's constant estimates at higher temperatures.

2.4.2.5 *Data Comparison and Discrimination*

All of the literature and calculated Henry's constant values were stored in the PPMS default database. Within PEARLS, values from the literature were compared on-screen to validate the PEARLS (UNIFAC-AENV) estimated value at ambient and steam stripping conditions. Tables VIII, IX, and X summarize the values displayed on-screen in PEARLS at 25, 30, and 90°C, respectively. At 25 and 30°C all of the values agree closely and no severe outliers are seen. Further analysis at steam stripping conditions (90°C) also indicates a close agreement of all values with the exception of the Persichetti value (Persichetti, 1990). The extrapolated RTI data tend to support UNIFAC-AENV at this temperature. Experimental data taken at MTU (Rogers et al., 1994) also agree with the PEARLS (UNIFAC-AENV) value, as shown in Figure 2. The RTI extrapolation shows nearly exact agreement with UNIFAC-AENV up to about 50°C.

2.4.2.6 *Henry's Constant as a Function of Temperature*

Henry's constant tends to follow the linear relationship shown in Equation (3) over a relatively narrow temperature range. At higher temperatures, as may be the case at steam stripping conditions, the solubility limit of toluene in water is known to increase as the water

solvent expands. One must be cautious when approximating Henry's constant with Equation (2) at elevated temperatures. Since aqueous solubility is a strong function of temperature and is difficult to measure experimentally, extrapolations with a van't Hoff type model may tend to a large degree of inaccuracy. Neglecting the solvent swelling at elevated temperatures may have caused the correlation of Persichetti (1990) to overestimate γ^{∞} and thus over predict Henry's constant. Hydrophobic solutes exhibit a maximum in Henry's constant with temperature (e.g., at T_{max}), beyond which Henry's law constant decreases as temperature increases (i.e., increased solubility of the solute overcomes the rise in the solute vapor pressure). Data from Tsonopoulos and Wilson (1983, 1985) verify this effect at elevated temperatures (Figure 3).

Based on these observations, an extended form of Equation (3) for correlating Henry's law constant as a function of temperature has been suggested for hydrophobic solutes by Nirmalakhandan and Speece (1988):

$$\ln H = \frac{A}{T} + B + C \ln T \qquad \textbf{(4)}$$

where:

H = Henry's law constant, {atm}
T = Absolute temperature, {K}
A,B,C = semi-empirical adjustable correlating parameters

The adjustable parameters in Equation (4) have physical significance, as demonstrated by Pierotti (1963). Furthermore, the A and C parameters are related by an expression derived by setting the first derivative of Equation (4) equal to zero and solving for T_{max}, the temperature at which the

Henry's law constant goes through a maximum value:

$$T_{max} = A / C \quad \textbf{(5)}$$

The C parameter is negative, causing the third term in Equation (4) to dominate as the temperature becomes large. Unfortunately, to accurately determine the adjustable C parameter in Equation (4) requires Henry's constant (e.g., activity coefficient) versus temperature data at or near the maximum value, which is where predictions are most needed. Typically, T_{max} is not known for a given solute, and the temperature dependence of Henry's law constant must come from direct measurements, extrapolations of near-ambient data, or predictive models.

From the solutes displayed in Figure 3, benzene and ethyl benzene would be expected to have thermodynamic properties close to those of toluene since the structures of benzene, toluene, and ethyl benzene differ by only one methyl group. This suggests that the Henry's constant of toluene might fall between those of benzene and ethyl benzene. The Henry's constants of 1.02 and 2.13 for benzene and ethyl benzene respectively at 90°C should bracket the value for toluene. Taking an arithmetic mean of the data for benzene and ethyl benzene gives a value of 1.58 unit-less, close to the PEARLS (UNIFAC-AENV) value of 1.4 unit-less, and indirectly supporting the PEARLS (UNIFAC-AENV) recommended value.

2.4.2.7 *Recommended PEARLS Henry's Law Constant Data for Toluene*

In summary, a comparison and evaluation of all data sources of toluene-water VLE data concluded that the recommended PEARLS (UNIFAC-AENV) value of 1.4 unit-less is correct at 90°C for steam stripping calculations. The analysis led to the following observations: (1) RTI extrapolated data agreed with the PEARLS correlated and predicted values at low and elevated temperatures; (2) Tsonopoulos and Wilson data suggest only slight curvature of ln H versus 1/T

up to 90°C, implying that the linear van't Hoff relationship for toluene is applicable in this region; (3) MTU static cell ebulliometer experiments confirm the elevated temperature result; and (4) the Persichetti Henry's constant estimate of 3.06 unit-less at 90°C appears to be an outlier and should not be used in steam stripper design calculations.

2.5 Column Specifications using PEARLS Recommended Data

To show the value of PEARLS as a data comparison and discrimination tool, a steam stripping system was designed to treat toluene-contaminated water using both the recommended PEARLS (UNIFAC-AENV) and Persichetti (1990) values of Henry's law constant. The procedure outlined in Section 2.3 was used along with each Henry's constant value to determine the effect on overall economics. Using the Persichetti value, the NPV values for steam flow rates from 1.0 to 5.0 kmol/h were calculated, and the optimum design corresponds to the maximum NPV. At this optimum steam flow rate, the remaining design parameters were obtained, and these are listed in Table XI. Keeping the same number of trays, the actual utility requirements for the steam stripping system were calculated using the PEARLS (UNIFAC-AENV) value for Henry's constant. Table XII shows the optimum design parameters based on the PEARLS value.

Of the two cases examined, the design based on the Persichetti (1990) Henry's constant value failed to meet the effluent target of 74 µg/L of toluene because the toluene volatility was overestimated. To meet the effluent target, the steam rate must be raised from 1.7 to 3.75 kmol/h, leading to an increased treatment cost of $0.23/Mg of wastewater treated. The design based on the PEARLS (UNIFAC-AENV) Henry's constant value is more economical, having a lower NPV than that calculated for the Persichetti design.

3.0 CONCLUSIONS

PPMS is a tool for obtaining and comparing physical and thermophysical property data for use in conceptual design. All of the tools needed to retrieve physical property information are available from a single software interface. Critically evaluated data sources, such as DIPPR®801 and DIPPR®911, can be converted by the DCUT module for use in PPMS. Within PPMS, the PEARLS module provides retrieval, display, storage, and report features for organizing and managing physical property data. Properties may be estimated when little or no data are available using built-in group contribution models. To assist in building group fragments for these methods, the SDAS module contains a disassembly engine which converts a chemical structure from SMILES into a set of possible fragments. The PEARLS interface allows all experimental and estimated values to be displayed simultaneously on one screen for easy comparison.

PPMS was demonstrated by supplying physical property data to the design of a steam stripper to remove toluene from water. Henry's constant data were obtained from a PEARLS estimation method (UNIFAC-AENV) and validated within PEARLS at low and high temperatures with literature data values. One apparent outlier value at steam stripping conditions (approximately 90°C) was calculated from a correlation by Persichetti (1990). Supporting data confirm the PEARLS (UNIFAC-AENV) value over the Persichetti value. The effect on the column design of using both the recommended PEARLS (UNIFAC-AENV) and Persichetti values was studied, revealing an annual operating cost penalty of $0.23/Mg of water treated. PEARLS was successfully applied to screen out the inaccurate data points and estimates at the elevated temperatures of interest and thereby avoid an operating cost penalty.

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This paper has not been reviewed by these organizations prior to submittal and no official endorsement of its contents should be inferred.

Figure Captions:

Figure 1. Steam stripping process flow diagram.

Figure 2. MTU and RTI experimental data compared to Henry's law constants from PEARLS (UNIFAC-AENV).

Figure 3. Dependence of Henry's law constant on temperature for various hydrophobic organic solutes in a water solvent.

TABLE I. Features Available in PEARLS Version 1.00

Access 36 unique physical properties for over 2000 chemicals
Calculate properties at different operating conditions
Estimate properties using 21 predictive methods plus two group contribution models
Change property input values for estimated properties
Compare all estimated and experimental data on-screen
Display primary reference source for any value
Store one user input value per property per chemical
Store user f(T) parameters for DIPPR® correlations
Convert units for any property between SI, English, CGS and other mixed units
Graph up to 10 chemicals for a single DIPPR® f(T) property over a specified
Set default preferences for units, UNIFAC binary interaction parameter databases, and
Save and load data for a user specified list of up to 20 chemicals
Sort the chemical or user list alphabetically in ascending or descending order
Search the chemical or user list by name, CAS number, family group, source list name,
Filter the chemical list by name, CAS number, family group, source list name, formula,
Export data to a delimited ASCII text file for use in wordprocessors, spreadsheets,
Print selected properties grouped by chemical or property
Access DIPPR®911 rating and citation information

TABLE II. Default UNIFAC Binary Interaction Parameter Database Hierarchy

Property	**Order of Decreasing Preference**
Activity Coefficient at Infinite Dilution	AGLB, AENV, AVLE, ALLE
Solubility	ALLE, AGLB, AENV, AVLE
Octanol-Water Partitioning Coefficient	AGLB, ALLE, AVLE, AENV

TABLE III. Steam Stripping Process Specifications and Assumptions

Average temperature over the column length	90°C (194°F)
Concentration of toluene in feed	550 ppm(wt.)
Concentration limit of toluene in effluent	0.074 ppm(wt.)
Tray type	Stainless steel sieve trays (5-ft dia.)
Feed flow rate	100 kmol/h (8 gpm)
Overall tray efficiency	40% (Geankoplis, 1983)
Cooling water temperature entering condenser	27°C (80°F)
Cooling water temperature leaving condenser	49°C (120°F)
Temperature of feed wastewater	58°C (92°F)
Temperature of treated water	100°C (212°F)
Temperature of treated water after preheater	78°C (172°F)
Overall heat transfer coefficient for condenser	1420 W/m^2-K (Geankoplis, 1983)
Overall heat transfer coefficient for preheater	1140 W/m^2-K (Geankoplis, 1983)
Holdup time for decanter	12 h

TABLE IV. Process Economic Data (Peters and Timmerhaus, 1991)

Service factor	0.8
Cost of steam	\$3.20/1000 lb_m
Cost of cooling water (clean well water)	\$0.50/1000 gal
Cost per tray (installed)	\$1250
Lang factor for fluid-processing plant	4.8
Depreciation	MACRS (7-yr)
Corporate tax rate	34%
Operating labor	\$15/h
Number of posts	1
Working capital	15% of FCI

TABLE V. Summary of Costs for Process Equipment, Excluding the Tray Cost

Item	Cost
Column skirt and shell, plus auxiliaries	$81,500
Condenser	$ 7,000
Preheater	$ 3,000
Bottoms Pump	$10,500
Decanter	$20,000

TABLE VI. Miscellaneous Operating Expenses (Peters and Timmerhaus, 1991)

Operating labor	(4 1/3)(# Posts)(Labor wage ($/h))
Supervisory and other labor	15% of Operating labor
Maintenance labor	1.7% of FCI
Maintenance materials	1.9% of FCI
Contract labor	0.5% of FCI
Operating supplies	0.1% of FCI
General supplies	3.5% of FCI
Control lab and experimental auxiliaries	1% of FCI
Auxiliary garage	10% of Operating labor
Auxiliary pumping	20% of Operating labor
Employee benefits	40% of Total labor
Administration	15% of Operating and maintenance
Mechanical overhead	54% of Maintenance labor
Technical	1% of FCI
Corporate overhead	1% of all above items plus utilities
Ad valorem tax	4% of FCI
Research expenses	2% of FCI

TABLE VII. Tray-by-Tray Calculation Used to Determine Optimum Design

1. Start with a steam flow rate of 0.1 kmol/h.
2. Set x_j to influent liquid concentration (550 ppm(wt.)).
3. Calculate y_{j+1} at x_j using operating line.
4. Determine new x_{j+1} from equilibrium line using y_{j+1}.
5. Repeat steps 2 and 3 until x_j meets or exceeds the target effluent concentration at which point j + 1 is equal to the number of ideal trays for the given steam flow rate.
6. If a solution is not found, increment the steam flow rate and restart at step 2.
7. Compute the FCI and operating costs for each valid steam flow rate.
8. Perform a cash flow analysis to compute NPV.
9. Increment steam rate by 0.05 kmol/h and repeat steps 2 through 8 to a steam flow rate of 5 kmol/h.
10. Optimum design taken at maximum NPV on a plot of NPV versus steam flow rate.

TABLE VIII. Henry's Constant Values from PEARLS at 25°C

Source	Value (unit-less)	Type of Data
911 Database (RTI)	0.262	Data
Ashworth	0.272	Data
Yaws	0.258	Data
Superfund	0.258	Data
Gmehling	0.229	Data
Persichetti	0.265	Estimated
Hwang	0.302	Data
ASPEN (AENV)	0.297	Estimated
PEARLS (AENV)	0.281	Estimated

TABLE IX. Henry's Constant Values from PEARLS at 30°C

Source	Value (unit-less)	Type of Data
RTI	0.324	Data
Ashworth	0.317	Estimated
Stephenson	0.220	Data
Chen and Wagner	0.299	Data
Persichetti	0.333	Estimated
PEARLS (AENV)	0.329	Estimated

TABLE X. Henry's Constant Values from PEARLS at 90°C

Source	Value (unit-less)	Type of Data
Ashworth	1.375	Estimated
Stephenson	1.382	Data
Chen and Wagner	1.391	Data
Persichetti	3.057	Estimated
PEARLS (AENV)	1.404	Estimated

TABLE XI. Operating Costs for Steam Stripping Tower Design Based on Persichetti Henry's Law Constant Value at 90°C

Data Source for Utilities	Steam Flow Rate (kmol/h)	Cooling Water Flow Rate (kmol/h)	# Actual Trays	Opera-ting Cost	Total Invest-ment	NPV, MM$
Persi-chetti (1990)	1.70[(a)]	42.08	3	$529,600	$195,200	-3.9622
PEARLS (AENV)	3.75[(b)]	92.87	---	$532,500	-----	-3.9835

(a) Assumes Persichetti value is correct; therefore, effluent target concentration is not met.

(b) Larger steam rate needed for Persichetti tower design to meet effluent target concentration.

TABLE XII. Optimum Steam Stripper Design Specifications Based on PEARLS (UNIFAC-AENV) Henry's Law Constant Value at 90°C

Steam Flow Rate (kmol/h)	Cooling Water Flow Rate (kmol/h)	# Actual Trays	Operating Cost	Total Investment	NPV
0.85	21.02	4	$530,200	$209,300	-$3,975,200

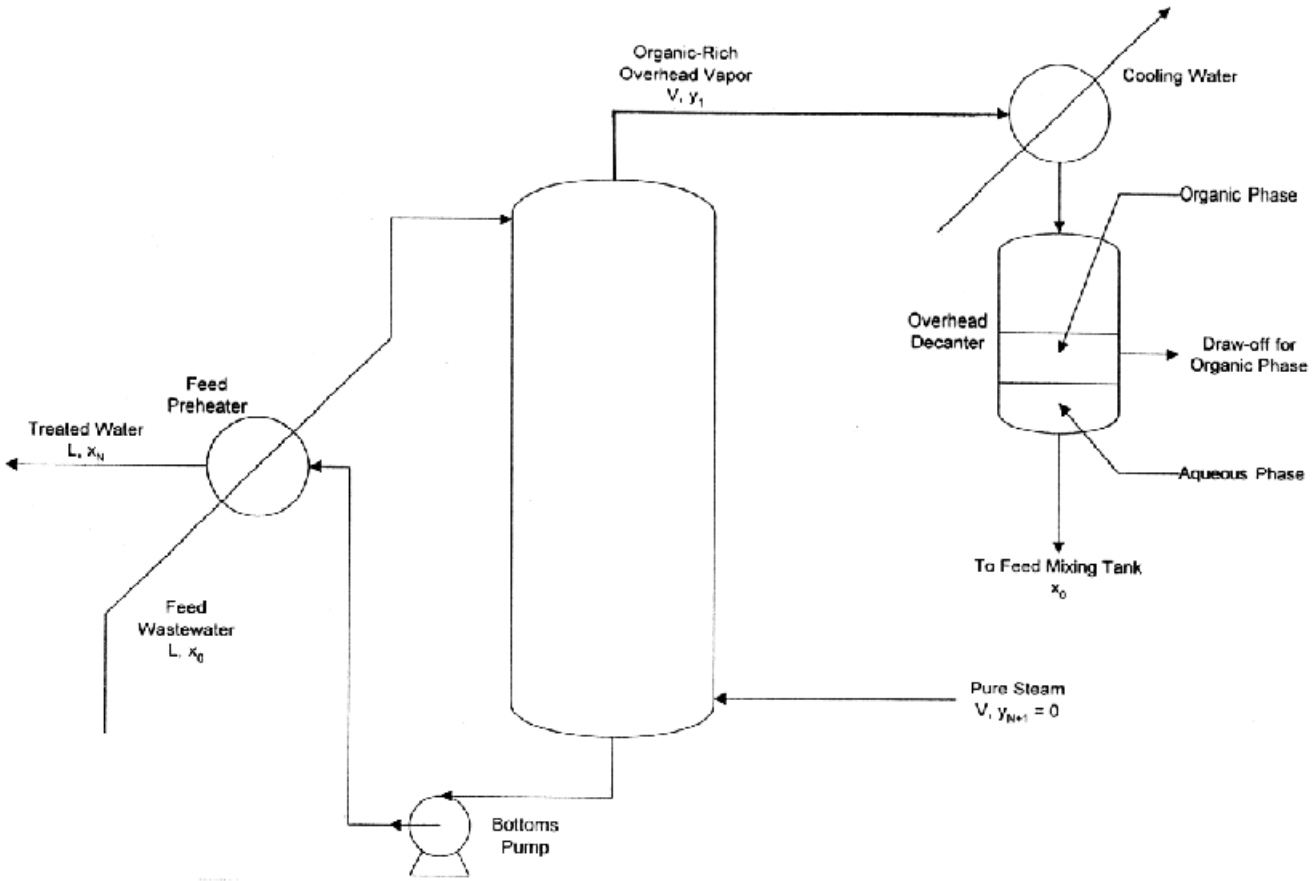

Figure 1. Steam stripping process flow diagram.

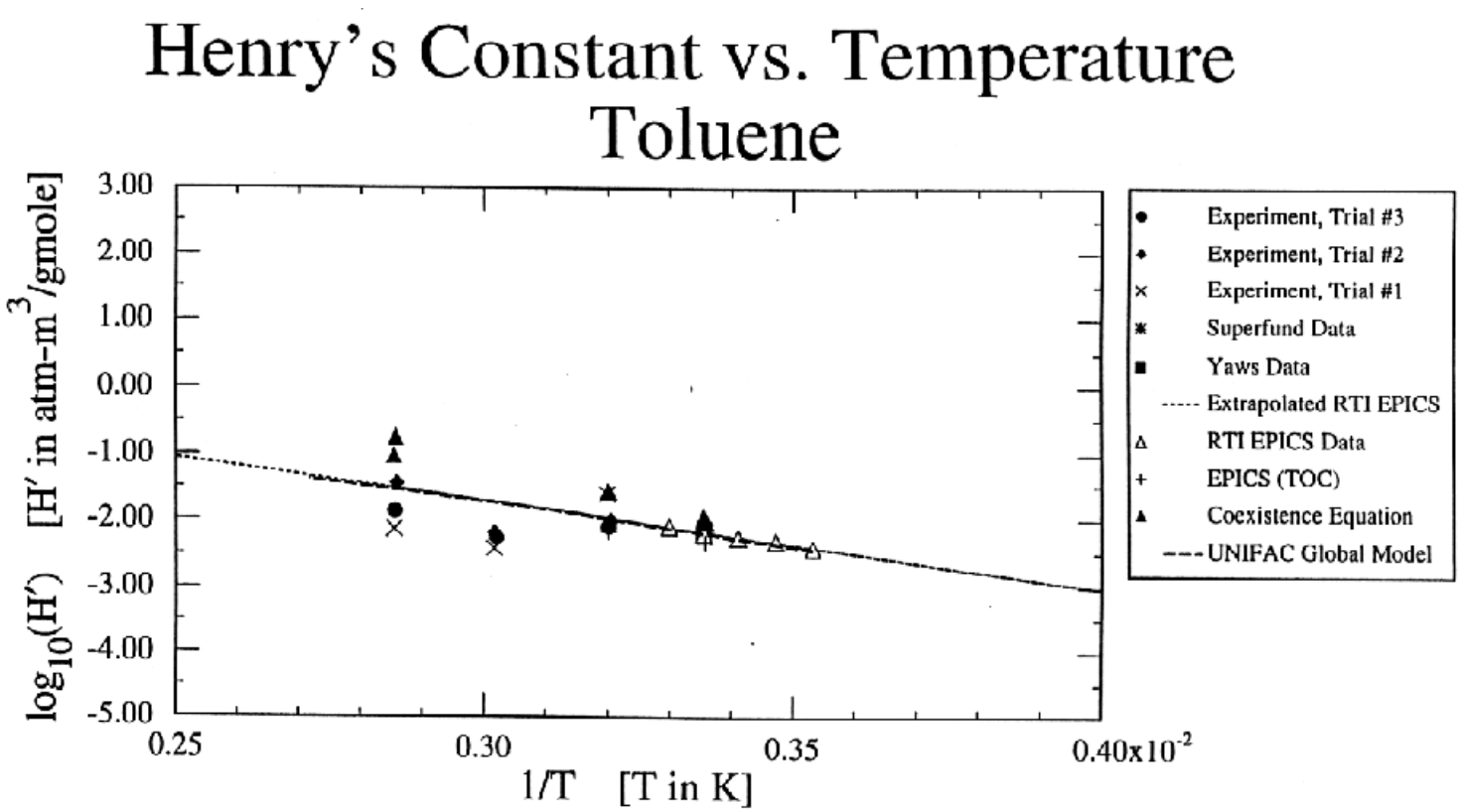

Figure 2. MTU and RTI experimental data compared to Henry's law constants from PEARLS (UNIFAC-AENV).

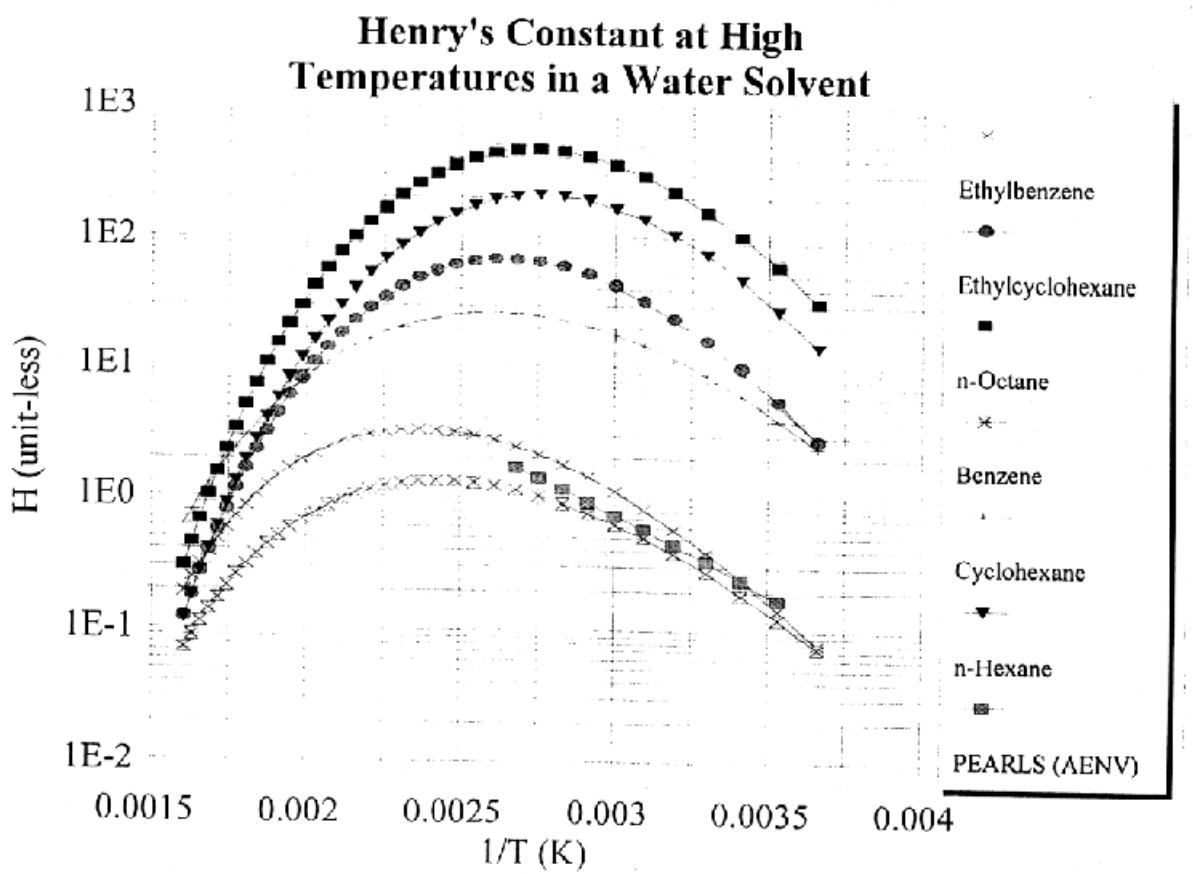

Figure 3. Dependence of Henry's law constant on temperature for various hydrophobic organic solutes in a water solvent.