SPREADSHEET APPROACH FOR THE DESIGN OF AIR STRIPPING OF VOLATILE ORGANIC CONTAMINANTS (VOCs) FROM WATER

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INTRODUCTION

Air stripping is a unit process often used for removing volatile organic chemicals from water. Mathematical models of this process have been well developed. Nomographs, although less common, have been suggested as an alternative to mathematical models. In addition to being convenient, a major advantage of using nomographs is that the sensitivity of the air stripping process to different design parameters and critical ranges can be readily observed. However, finding answers or obtaining values from nomographs is a tedious and time-consuming process. As an alternative, a well designed spreadsheet program running on personal computers can offer the combined advantages of both nomographs and mathematical models.

Engineering design can be greatly simplified with Computer-Aided Design (CAD) programs. However, the development of a CAD program using computer languages such as FORTRAN, PL1, or PASCAL is oftentimes a major undertaking (Holtz, 1987). Using a spreadsheet program, limited capability CAD programs can be easily developed and the time needed to do so can be greatly reduced. In a spreadsheet program, the working sheet is divided into rows and columns whose intersections are cells. Each cell can hold a data item or an equation and its value is automatically displayed in the cell. The content of any cell can be referenced by its location. Hence it is extremely simple to develop an application template, i.e., a program, for a user to input data items, perform a set of operations, and display the results. This template approach has been used by some researchers and practioners to a limited extent for mathematical modeling and engineering design (Chao & Liu, 1985; Jewell, 1985; Keith, 1986; Miles & Heaney, 1986; Rossmiller, 1985; Thurston et al. 1985; Wu, 1986).

As with any other application program, the template approach of the spreadsheet may not be considered user-friendly if the user is not familiar with the program. Using the macro commands, a user-friendly spreadsheet can be developed (Yu & Tisdale, 1986). In this paper, modifications of the template approach for spreadsheet programming using macro commands are presented in a modular fashion, thereby facilitating the development of menus and help information that can assist the user.

Input data items such as load, temperature, etc. are unique to each design and must be provided by the user for each design problem. Some others, such as material properties and their dimensions and/or properties can be obtained from published technical reports, design manuals, and/or papers once the design

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is defined or the material is selected. But obtaining such design data from these sources is a slow and time-consuming process. Thus, in many cases the user may not initially have all the data items he needs and this may inhibit execution of the program. The modular approach proposed herein is further improved to include a database containing all the data common to the design as well as a method for retrieving the needed data from the database, thus allowing for virtually effortless data input. Such improvements make the resulting program more user-friendly and self-adaptive, thereby enhancing its application and use. The modular approach has been used herein to develop a program for the design of air stripping of Volatile Organic Contaminant (VOC) from water.

DESIGN OF THE AIR STRIPPING PROCESS

According to Henry's law, the quantity of a gas or a volatile substance dissolved in water is proportional to its partial pressure in the air above the liquid. Thus, if the liquid containing a gas or volatile contaminant is dispersed in fresh air where the partial pressure of the dissolved gas (or volatile contaminant) is nearly zero, the dissolved gas (or volatile contaminant) is transferred from water to the surrounding air. The dispersion of water in air for removal of dissolved gas or volatile contaminant is termed air stripping. The most efficient method of dispersing the liquid in air is to use a counter-current spray tower with air blown through it. Packing materials are provided inside the tower to minimize the film resistance to gas transfer, thus maximizing the removal efficiency. Design of the air stripping process involves determining the number of spray towers, their height, the air volume requirement, the blower horsepower, and the pump horsepower for achieving a certain removal efficiency with a given set of operating conditions.

Manual design of this process is based on a strong theoretical foundation and the design considerations proposed by Roberts et al. (1985). Speece et al. (1987) constructed nomographs to assist in the preliminary air stripping process design. The design equations for the air stripping process as outlined by Speece et al. (1987) are given below.

With known temperature, calculation of Henry's Coefficient (H) is:

$$\log H = \frac{A}{R*T} + B \qquad (1)$$

Where:
- A,B = Characteristic constants of contaminant
- H = Henry's coefficient (atm)
- R = Gas constant (0.08207 atm-l/mole-^{o}K)
- T = Absolute temperature (^{o}K)

Equation (1) shows that H is dependent on the type of VOC and on the liquid temperature. Knowing H, the stripping factor (S) can be calculated from the molar gas/liquid ratio:

$$S = \left(\frac{H}{P_t}\right)\left(\frac{G}{L}\right) \qquad (2)$$

Where: H = Henry's coefficient (atm)

G = Gas molar flow rate (Moles/s)
L = Liquid molar flow rate (Moles/s)
P_t = Total pressure (atm)

After S is determined, the number of transfer units (NTU) is calculated to be:

$$NTU = \left(\frac{S}{S-1}\right) \ln \left[\frac{\left(C_{L,2} - \frac{C_{G,1}}{H}\right)(S-1)}{\left(C_{L,1} - \frac{C_{G,1}}{H}\right) S} + \left(\frac{1}{S}\right)\right] \quad \ldots.(3)$$

Where:
S = Stripping factor (Dimensionless)
NTU = Number of transfer units
$C_{L,2}$ = Influent liquid solute concentration (Kg/M^3)
$C_{L,1}$ = Effluent liquid solute concentration (Kg/M^3)
$C_{G,1}$ = Influent gas solute concentration (Kg/M^3)

The ratio of wetted area to total area (A_w/A_t) is then determined using the following equation:

$$\frac{A_w}{A_t} = 1-\exp\left[-1.45\left(\frac{D_c}{D_l}\right)^{0.75}\left(\frac{L_m}{A_t * U_l}\right)^{0.1}\left(\frac{R_l{}^2 * G}{L_m{}^2 * A_t}\right)^{0.05}\left(\frac{L_m{}^2}{R_L * D_L * A_t}\right)^{0.2}\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(4)$$

Where:
A_w = Specific wetted packing area (M^2/M^3)
A_t = Specific total packing area (M^2/M^3)
R_l = Liquid density (kg/M^3)
U_l = Liquid viscosity (kg/M-s)
G = Gravity acceleration (M/s^2)
L_m = Liquid mass flux (kg/M^2-s)

Subsequently, the liquid phase mass transfer coefficient (k_l) can be calculated using the following equation:

$$k_l \left[\frac{R_l}{U_l * G}\right]^{1/3} = 0.0051 \left[\frac{L_m}{A_w * U_l}\right]^{2/3} \left[\frac{U_l}{R_l * D_l}\right]^{-0.5} [A_t * D_p]^{0.4} \quad \ldots\ldots(5)$$

Where:
k_l = Liquid film mass transfer coefficient (M/s)
D_l = Diffusivity of VOCs in liquid
D_p = Nominal diameter of packing material (M)
A_w = Specific wetted packing area (M^2/M^3)
A_t = Specific total packing area (M^2/M^3)

The gas phase transfer coefficient equation is:

$$k_g = A_t * D_g \left[\frac{G_m}{A_t * U_g}\right]^{0.7} \left[\frac{U_g}{R_g * D_g}\right]^{1/3} (A_t * D_p)^{-2} \quad \ldots\ldots\ldots\ldots(6)$$

Where: k_g = Gas phase mass transfer coefficient (M/s)

D_g = Diffusivity of VOCs in gas phase
G_m = Air flow rate per unit area (kg/M^2-s)
U_g = Viscosity of air (kg/M-s)
R_g = Viscosity of air (kg/M-s)

And the overall resistance ($1/K_L$) is the sum of the gas and liquid phase resistances as follows:

$$\frac{1}{K_L} = \frac{1}{k_g{*}H_c{}^n} + \frac{1}{k_1} \qquad (7)$$

$$K_L{}^a = K_L{*}A_w \qquad (8)$$

Where:
Hc^n = Non-dimensional Henry's coefficient
k_1 = Liquid film mass transfer coefficient (M/s)
$K_L{}^a$ = Overall mass transfer coefficient (1/s)
K_L = Overall mass transfer coefficient (M/s)
A_w = Specific wetted packing area (M^2/M^3)

The height of a transfer unit (HTU) is then calculated using the following equation:

$$HTU = \left(\frac{Lm}{R_1{*}K_L{}^a}\right) \qquad (9)$$

Where:
HTU = Height of a single transfer unit (M)
$K_L{}^a$ = Overall mass transfer coefficient (1/s)
Lm = Liquid mass flux (kg/M^2-s)
R_1 = Liquid density (kg/M^3)

and the tower height (Z) is as follows:

$$Z = HTU{*}NTU \qquad (10)$$

Where:
Z = Total tower height (M)
HTU = Height of a single transfer unit (M)
NTU = Number of transfer units (Dimensionless)

Assuming a pressure drop of 0.1 in of water per foot of column height, the adiabatic compression equation is :

$$HP_{air} = \frac{144\ Q_a(P_1 - P_2)}{33000\ E} \qquad (11)$$

Where:
Q_a = Air flow rate (cu-ft/min)
P_1 = Inlet air pressure (lb/sq in)
P_2 = Outlet air pressure (lb/sq in)
E = Efficiency (assuming 80%)
HP_{air} = Blower horsepower (hp)

and the liquid pumping horsepower per unit tower area is:

$$HP_{liquid} = \frac{62.4\ Z^{*}Q_w}{550\ E} \quad \text{.........................}(12)$$

Where HP_{liquid} = Pump horsepower (hp)
Z = Tower packing height (ft)
Q_w = Liquid applying rate (ft^3/ft^2-s)

THE MODULAR APPROACH TO SPREADSHEET PROGRAMMING

The proposed modular approach is implemented using a LOTUS-123 spreadsheet but can be applied to other types of spreadsheet programs as well. In this approach, the spreadsheet is divided into several subsheets or modules: the worksheet, error and directive messages, macro commands, and supporting databases. All modules except the worksheet are transparent to the user. The worksheet is used to interact with the user for data input and output, and to display intermediate and final results. All initial input data items, intermediate and final results, and descriptive messages are arranged in a tabular format on the worksheet. Hard copies of the current design, ncluding the worksheet, the database, or the steps of calculations that generate intermediate results can be obtained from a direct printout of the worksheet.

The macro commands module is the programming component of the spreadsheet. Macro commands are used to activate the functions of subsheet modules and to combine functions from different modules. The error and directive messages module contains the messages which will be displayed to warn the user or to guide him through the subsequent steps to continue executing the design program. Supporting design data items are organized in a form similiar to relational database tables and are stored in the database module. Macro commands are used to retrieve the needed data items and place them in the proper cell locations on the worksheet. Such a modular partitioning of process control and data fully utilizes the capacity and functionality of a spreadsheet program. In the following sections each of these modules is further discussed and examples of their use are provided.

The Worksheet

The worksheet contains all the input and output data items in a template format that is easy to view, comprehend, and check by the user. Table 1 shows the worksheet of one air stripping design program. It consists of three groups of data items: the input data, the derived data, and the output data.

INPUT DATA

Contaminant =	Chloroform	
Temperature =	15.00	C
Efficiency of removal =	99.00	%
Hydraulic loading =	20.00	gpm/sq-ft
Air/water ratio =	25.00	vol/vol
Packing material =	Tripak-1"	

DERIVED DATA

Liquid density (kg/cu-m)	=	9.990E+02
Liquid viscosity (kg/m-s)	=	1.139E-03
Liquid surface tension (kg/sq-s)	=	7.349E-02
Air density (kg/cb-m)	=	1.226E+00
Viscosity of air (kg/m-s)	=	1.807E-05
Stripping factor	=	2.45

OUTPUT DATA

Henry's coefficient (atm)	=	0.10
Overall Transfer coefficient (KLa)	=	0.02 1/s
Number of transfer units (NTU)	=	6.90
Height of transfer unit (HTU)	=	0.76 M
	=	2.49 ft
Tower height (Z)	=	5.27 M
	=	17.29 ft
Air requirement	=	66.67 $ft^3/min/ft^2$
	=	20.32 $M^3/min/M^2$
Blower horsepower	=	2.26E-02 HP/ft^2
	=	1.18E-03 KWH/M^2
Pump horsepower	=	1.34E-01 HP/ft^2
	=	6.97E-03 KWH/M^2

Table 1: Worksheet for Input and Output

The input data are those provided and keyed in directly by the user. Of these, temperature, efficiency of removal, hydraulic loading rate, and air/water ratio are numerical while contaminant and packing material are alphanumeric descriptive names. The program checks numerical input data items and accepts their values if they are within the ranges specified in Table 2.

Temperature	0 - 35 ^oC (32 - 95 ^oF)
Henry's constant	0 - 2400 atm
Air/water ratios	1.25 - 50 (V/V)
Stripping factor	1 - 5
Removal efficiency	50 - 99.9 %
Hydraulic loading	1.18 - 63.3 gpm/ft^2 (0.8-43 $kg/S/M^2$)

Table 2: Sample Value Ranges for Numerical Input Data Items

Descriptive input data such as Volatile Organic Contaminants (VOCs) and packing materials are limited to those that have been included in the database. To assist the user in selecting the proper type of VOCs and packing materials, two databases are provided; one for the VOCs and one for the packing materials. A portion of the content of these databases is shown in Table 3.

Contaminant (VOC)	Packing Material
Benzene	Flexiring-5/8"
Bromoform	Flexiring-1"

Chloroform	Flexiring-3/2"
Tetrachloroethylene	Flexiring-2"
Trichloroethylene	Flexisaddles-1"
1,1-Dichloroethane	Flexisaddles-2"
1,2-Dichloroethane	Tri-packs(no. 1)-2"
1,1,1-Trichloroethane	Tripak-1"
Carbon dioxide	Flexpac(type 2)-7/8"
Carbon tetrachloride	
Chlorine	
Chloromethane	
Sulfur dioxide	

Table 3: Available VOCs and Packing Materials

Using a macro command, the program user can display the above VOCs or packing materials. The user can then select a proper VOC or packing material from the displayed list by moving the cursor, highlighting the item, and selecting it with the return key.

Derived and output data items are those which are calculated using the input data, using data items retrieved from the internal database, or both. For example, when the type of contaminant is selected, and the temperature is specified, values of A, B, D_l and D_g are automatically retrieved from the contaminant database. When the packing material is selected by the user, values of A_t and D_p are automatically retrieved from the packing material database. Liquid density, liquid viscosity, surface tension, air density, and air viscosity can then be automatically calculated using the temperature provided. Afterwards, all of Equations (1) through (12) are executed and the results are displayed in the "OUTPUT DATA" section of the worksheet as shown in Table 1.

The Macro Module

Using macro codes provided by LOTUS-123, the manual steps that are required to perform a sequence of calculations and/or tasks can be grouped and activated with a single command. The groups of macro commands used in this program are shown in Table 4.

Command	Functions
Alt-A:	Select contaminant compound
Alt-C:	Input temperature in degree C
Alt-F:	Input temperature in degree F
Alt-G:	Input hydraulic loading in gpm/sq-ft
Alt-K:	Input hydraulic loading in kg/s/sq-m
Alt-H:	HELP
Alt-P:	Print to obtain hard copies
Alt-Q:	Quit 123 system
Alt-S:	Save the file in 123 system

Table 4: Macro Commands

Codes for each macro command are programmed and are stored in remote cells so that they will not be accidentally changed or modified by the user.

As an example, Table 5 shows the macro codes for selecting the contaminant using the Alt-A command.

Name	Code	Comment line
\a	{GOTO}INPUT~	Move cursor to cell INPUT.........(1)
	{GOTO}CONTAM~	Move cursor to cell CONTAM........(2)
	/rem3..m16~	Erase range M3 to M16............(3)
	/reo4..o16~	Erase range O4 toO16.............(4)
	/ren13..n20~	Erase range N13 to N20...........(5)
	/ren24..n41~	Erase range N24 to N41...........(6)
	{GOTO}MESSAGE1~	Move cursor to cell MESSAGE1......(7)
	{?}~	MESSAGE1 is displayed until user enter an entry such as RETURN...(8)
	{GOTO}INDEX1~	Move cursor to cell INDEX1 to display list of VOCs ....(9)
	{GOTO}INDEX1IT1~	Move cursor to first VOC item....(10)
	{?}~	Accept the item selected by user.(11)
	/c~CONTAM~	Copy the selected item to CONTAM.(12)
	{GOTO}INPUT~	Move cursor to cell INPUT ....(13)
	{GOTO}CONTAM~	Move cursor to cell CONTAM.......(14)
	{GOTO}MESSAGE2~	Move cursor to cell MESSAGE2.....(15)
	{QUIT}	End of Macro.....................(16)

Table 5: Macro Codes for Selecting a VOC

Sixteen steps are involved in this macro. When Alt-A is activated, codes (1) and (2) bring the worksheet to the screen and move the cursor to the cell for VOC in the worksheet. All previous data items are then cleared by codes (3) - (6). Codes (7) and (8) display the message to instruct the user to select a VOC. The message is displayed until the user types in any input item such as a RETURN. The table of VOCs is then displayed by codes (9) and (10). After the user selects a VOC by code (11), the selected item is copied to the worksheet by code (12). Next, the screen displays menus to complete the data entry process.

The Database

Two regions of the spreadsheet have been identified for storing data in a relational database format; one for the VOCs and another for the packing materials. The VOC database contains values of A, B, D_l, and D_g of VOCs using the VOC name as the key. Table 6 illustrates the content of the VOC database.

VOC	A	B	D_l (at 20°C)	D_g (at 20°C)
Benzene	-3680.00	8.68	9.57E-10	9.32E-06
Bromoform	-7167.00	14.00	9.37E-10	7.67E-06
Chloroform	-4000.00	9.10	1.04E-09	8.88E-06
Tetrachloroethylene	-4290.00	10.38	8.54E-10	7.97E-06
Trichloroethylene	-3410.00	8.59	9.45E-10	8.75E-06
1,1-Dichloroethane	-3780.00	8.87	9.72E-10	9.19E-06
1,2-Dichloroethane	-3620.00	7.92	9.72E-10	9.07E-06
1,1,1-Trichloroethane	-3960.00	9.39	9.04E-10	7.94E-06
Carbon dioxide	-2070.00	6.73	1.78E-09	1.52E-05

Carbon Tetrachloride	-4050.00	10.06	9.28E-10	8.28E-06
Chlorine	-1740.00	5.75	1.50E-09	1.21E-05
Chloromethane	-2480.00	6.93	8.67E-10	1.29E-05
Sulfur dioxide	-2400.00	5.68	1.53E-09	1.25E-05

Table 6: Database for VOCs

The database of the packing materials includes values of A_t and D_p with the packing material (label being used as the key). Table 7 illustrates the entries in the packing materials database.

Packing Material	A_t (sq-m/cb-m)	D_p (in)
Flexiring-5/8"	341.00	0.63
Flexiring-1"	207.00	1.00
Flexiring-3/2"	128.00	1.50
Flexiring-2"	102.00	2.00
Flexisaddles-1"	207.00	1.00
Flexisaddles-2"	108.00	2.00
Tri-packs(NO.1)-2"	138.00	2.00
Tripak-1"	279.00	1.00
Flexpac(type 2)-7/8"	246.00	0.88

Table 7: Database for Packing Materials

Both of the above tables use the data items in the first column as the key for retrieving information. When the input data macro commands are activated, the keys are displayed and the user can move the cursor to highlight the item needed. Once the key item is accepted, other data items in the same row are automatically copied to the appropriate cells with the LOTUS-123 @HLOOKUP or @VLOOKUP commands. Data entry is thus greatly simplified.

The Error and Directive Message Module

Error and directive messages assist the user in avoiding errors and provide help and guidance on how to proceed. For example, ranges of numerical input data are displayed when an input item exceeds it proper value range as shown below.

```
   Input the Suitable Range Values and Return

   Range of Values Used in This Program are:

Temperature:         0 - 35 °C (32 - 95 °F)
Removal efficiency: 50 - 99.9 %
Hydraulic loading:  1.18 - 63.3 gpm/ft² (0.8-43 kg/s/m²)
```

Help messages, including those to assist the user in using the macro commands, are shown in Table 8.

```
Alt-A: Select Contaminant Compound
Alt-C: Input Temperature in Degree C
Alt-F: Input Temperature in Degree F
Alt-G: Input Hydraulic Loading in gpm/sq-ft
Alt-K: Input Hydraulic Loading in kg/s/sq-m
Alt-H: HELP
Alt-P: Print I/O or Table or calculate procedures
Alt-Q: Quit LOTUS-123
Alt-S: Save the File
```

Table 8: Example Content of Help Messages

Error messages are included to warn the user about the status of the printer when hard copies are being printed or about the disk drive when files are being loaded or saved. If the printer or the disk drive is not ready, the regular LOTUS program will run into a deadlock. With macro commands deadlock is avoided and the user is prompted for remedial steps to continue executing the design commands.

EVALUATION OF THE SPREADSHEET PROGRAM FOR ENGINEERING APPLICATIONS

The modular approach of the spreadsheet program for engineering design of air stripping of VOC from water provides the designer with significant utility and efficiency in his design task. When using this program, the designer is guided in his selection of VOCs and packing materials. These are specified as input data items along with the input design conditions of temperature, removal efficiency, hydraulic loading and air/water ratio. Afterwards, the results are quickly displayed in an organized fashion for the designer to view. The designer can also obtain hard copies of the worksheet (Shown as Table 1) and the intermediate results. Compared to the manual method of solving equations or using nomographs, this approach is an excellent design aid that provides accurate results with ease and speed.

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