A Tool to Optimize VOC Removal During Absorption and Stripping

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Spreadsheet analysis offers a simpler and less costly alternative to simulators and algebraic tools

Practicing engineers routinely use modular simulators and algebraic tools to perform rigorous process optimizations. These complex tools, however, can have a significant learning curve. Meanwhile, spreadsheet programs are becoming a ubiquitous tool for performing calculations for many chemical process operations [*1-4*]. In this article, we show how the Solver feature of the Microsoft Excel spreadsheet program can be used to optimize a fairly complex system. In this case, the specific goal was to optimize the design of a gas-absorption tower paired with a solvent-recovery stripper for the continuous recovery of organic solvents (VOCs) from a contaminated stream. Two examples are given, with and without environmental emission constraints. The results show that Excel Solver can converge on local optima for these complex systems, as long as proper care is taken during the solution procedure.

Equations and constraints

With the widespread availability of powerful "what if" spreadsheet programs with optimization capabilities (such as Excel), many engineers and students can easily use these tools to solve a typical simulation or optimization problem. It is important to establish the extent to which these tools can solve demanding optimization problems.

The optimization problem discussed in detail here deals with the concepts of process synthesis, heat integration and solvent recovery, and details can be found in Umeda [*5*], and Umeda and Ichikawa [*6*]. The problem as discussed here has been adapted from these authors; Silverberg [*7*] shows that this process is widely in use.

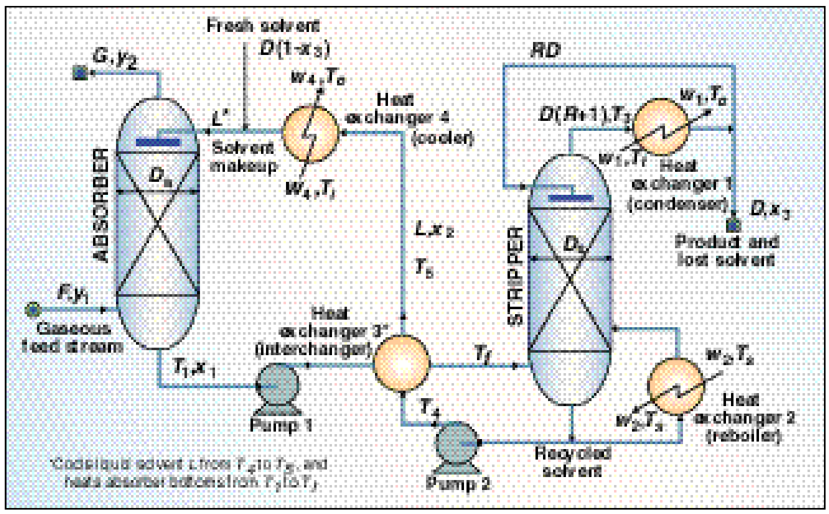

FIGURE 1. The continuous, steady-state process for solvent extraction and recovery shown here is the subject of this optimization study. All symbols are defined with appropriate units in Figure 2, and are computed by the equations in Table 1 or Table 3

Figure 1 shows the continuous and steady-state process under study here. It consists of a packed absorber column, a plate-tower stripper and integrated heat recovery. The gaseous stream *F*, with mole fraction y_1 of a contaminant to be recovered or removed is fed to the absorber, where a solvent, with flowrate *L,* is countercurrently enriched in the solute.

The extraction solvent is stripped in a plate tower, and the solute in the overhead vapors is condensed for recovery or further disposal. The cooled solvent is returned to the absorber, where fresh solvent is added to replaces losses in the overhead vapors.

The entire set of equality constraints is given in Table 1 (for definitions of the symbols in these well-known design equations, refer to Table 3 and Figure 1, and to standard textbooks). Each equation is set to zero, as is the convention with spreadsheet optimization. The absorber diameter (Equation f_9) is computed so that the vapor velocity is 75% of the flooding velocity. Estimate the stripper diameter (Equation f_{23}) by dividing the vapor load (defined in Equation 1)

$$V_v = \frac{Q_2}{\lambda M_l}\,\frac{22.4 T_4}{273.2} \quad (1)$$

by the superficial vapor velocity, as calculated by the Souders-Brown equation [*8*]

$$V_M = K\sqrt{\frac{\rho_l - \rho_g}{\rho_g}} \quad (2)$$

where *K* is an empirical constant, and Q_2 equals the heating duty of the reboiler (defined by Equation f_{32}). The Fenske-Underwood equations (Equations f_{24}–f_{25}) are used to compute the minimum number of plates and the minimum reflux ratio. The number of plates (Equations f_{26}–f_{27}) is computed from the Eduljee approximation to Gilliland's graphical method [*8*].

This is an economic optimization, so

TABLE 1. PROCESS DESIGN EQUATIONS

ABSORBER

$$f_1 = F - G - Dx_3 = 0$$

$$f_2 = Fy_1 + Lx_2 - (L + D)x_1 - Gy_2 = 0$$

$$f_3 = N_{og} - \frac{1}{1 - \frac{HG}{PL^*}} \ln\left[\left(1 - \frac{HG}{PL^*}\right)\left(\frac{y_1 - \frac{H}{p}x_2^*}{y_2 - \frac{H}{p}x_2^*}\right) + \frac{HG}{PL^*}\right] = 0$$

$$f_4 = H_{og} - H_g - \frac{HGH_l}{PL^*} = 0$$

$$f_5 = H_g - \alpha\left(\frac{FM_g}{A_a}\right)^{\beta}\sqrt{Sc_g}\Bigg/\left(\frac{(L + D)M_l}{A_a}\right)^{\gamma} = 0$$

$$f_6 = H_l - \left(\frac{(L + D)M_l}{A_a \varphi}\right)^{\delta}\varphi\sqrt{Sc_l} = 0$$

$$f_8 = A_a - \pi\frac{D_a^2}{4} = 0$$

$$f_9 = D_a - \sqrt{\frac{4GM_g}{0.75\pi G_f\, 3,600}} = 0$$

$$f_{10} = \log_{10}\left(G_f^2\left(\frac{a_p}{\varepsilon^3}\right)\left(\frac{1}{g\rho_g\rho_l}\right)\left(\frac{\alpha}{\alpha_g}\right)^{0.2}\right) - 1.74\left(\frac{L^*M_l}{GM_g}\right)^{0.25}\left(\frac{\rho_l}{\rho_g}\right)^{-0.125} = 0$$

PUMP NO. 1

$$f_{11} = HP_1 - K_{p1}(L + D)N = 0$$

PUMP NO. 2

$$f_{12} = HP_2 - K_{p2}LZ = 0$$

HEAT EXCHANGER NO. 4

$$f_{13} = Q_4 - Lc_p(T_5 - T_1) = 0$$

$$f_{14} = Q_4 - W_4c_{pw}(T_o - T_i) = 0$$

$$f_{15} = Q_4 - U_4A_4\Delta T_{lm4} = 0$$

$$f_{16} = \Delta T_{lm4} - \frac{(T_5 - T_o) - (T_1 - T_i)}{\ln\frac{T_5 - T_o}{T_1 - T_i}} = 0$$

HEAT EXCHANGER NO. 3

$$f_{17} = Q_3 - (L + D)c_p(T_f - T_1) = 0$$

$$f_{18} = Q_3 - Lc_p(T_4 - T_5) = 0$$

$$f_{19} = Q_3 - U_3A_3\Delta T_{lm3} = 0$$

$$f_{20} = \Delta T_{lm3} - \frac{(T_1 - T_5) - (T_f - T_4)}{\ln\frac{T_1 - T_5}{T_f - T_4}} = 0$$

STRIPPER & HEAT EXCHANGERS

$$f_{21} = (L + D)x_1 - Lx_2 - Dx_3 = 0$$

$$f_{22} = (L + D)c_pT_f + Q_2 - Dc_pT_3 - Lc_pT_4 - Q_1 = 0$$

$$f_{23} = \pi\frac{D_s^2}{4} - \frac{22.4Q_2T_4}{273.2 \times 3,600\lambda M_lK_v\sqrt{(\rho_l - \rho_g)/\rho_g}} = 0$$

$$f_{24} = R_m - \frac{1}{\alpha - 1}\left[\frac{x_3}{x_1} - \alpha\frac{(1 - x_3)}{(1 - x_1)}\right] = 0$$

$$f_{25} = N_m - \ln\left[\frac{x_3}{(1 - x_3)}\frac{(1 - x_2)}{x_2}\right]\Big/\ln\alpha = 0$$

$$f_{26} = N - \frac{(N_m + X)}{(1 - X)} = 0$$

$$f_{27} = X - 0.75\left[1 - \left(\frac{R - R_m}{R + 1}\right)^{0.5668}\right] = 0$$

$$f_{29} = Q_1 - W_1c_{pw}(T_o - T_i) = 0$$

$$f_{30} = Q_1 - U_1A_1\Delta T_{lm1} = 0$$

$$f_{31} = \Delta T_{lm1} - \frac{(T_3 - T_o) - (T_3 - T_i)}{\ln\left(\frac{T_3 - T_o}{T_3 - T_i}\right)} = 0$$

$$f_{32} = Q_2 - W_2\lambda_w = 0$$

$$f_{33} = Q_2 - U_2A_2\Delta T_{lm2} = 0$$

$$f_{34} = \Delta T_{lm2} - (T_s - T_4) = 0$$

$$f_{35} = x_2e^{\left(A_1 - B_1/(T_s + T_{c1})\right)} + (1 - x_2)e^{\left(A_2 - B_2/(T_s + T_{c2})\right)} - P = 0$$

$$f_{36} = \frac{Px_3}{e^{\left(A_1 - B_1/(T_3 + T_{c1})\right)}} + \frac{P(1 - x_3)}{e^{\left(A_2 - B_2/(T_3 + T_{c2})\right)}} - 1 = 0$$

$$f_{37} = T_f - T_2 - (q - 1)\lambda/c_p = 0$$

$$f_{38} = x_1e^{\left(A_1 - B_1/(T_1 + T_{c1})\right)} + (1 - x_1)e^{\left(A_2 - B_2/(T_1 + T_{c2})\right)} - P = 0$$

MAKEUP

$$f_{39} = x_2^* - \frac{Lx_2}{L + D(1 - x_3)} = 0$$

$$f_{40} = L^* - D(1 - x_3) - L = 0$$

the objective is to maximize the profit, which is the difference between revenue from the sale of recovered VOCs, and annual capital and operating costs of the system:

$$F_{obj} = P_pDM_lx_3 - C_gFM_g + C_lD(1 - x_3)M_l + C_w(w_1 + w_4) + C_sw_2 + C_e(HP_1 + HP_2) + InvF_c] \quad (3)$$

where investment costs (the last symbol in Equation 3) are given by:

$$\text{Inv} = C_zZD_a^{1.0} + C_nND_s^{1.085} + C_a(A_1^{0.556} + A_2^{0.556} + A_3^{0.556} + A_4^{0.556}) + C_{hp}(HP_1^{0.3} + HP_2^{0.3}) \quad (4)$$

The problem is subject to the 40 equality constraints shown in Table 1, as well as to the following process inequality constraints:

$L < 300$ Kg·mole/h (maximum flowrate) **(5)**

$R < 20$ (maximum reflux in stripper) **(6)**

Thus, this problem, as formulated, has 45 independent (unknown) variables and 40 equations, with a total of 5 degrees of freedom.

(Continues on p. 96)

TABLE 2. SERIAL SOLUTION PROCEDURE WITH {N, W_4, T_4, T_2 AND A_1} AS DECISION VARIABLES

Equation(Variable) $f_{36}(T_3)$, $f_{14}(Q_4)$, $f_{34}(\Delta T_{lm2})$, $f_{35}(x_2)$, $f_{25}(N_m)$, $f_{26}(X)$, $f_{31}(\Delta T_{lm1})$, $f_{30}(Q_1)$, $f_{29}(W_1)$, $f_{38}(x_1)$, $f_{24}(R_m)$, $f_{27}(R)$, $f_{28}(D)$, $f_1(G)$, $f_{21}(L)$, $f_2(y_2)$, $f_{11}(HP_1)$, $f_{13}(T_5)$, $f_{16}(\Delta T_{lm4})$, $f_{15}(A_4)$, $f_{18}(Q_3)$, $f_{17}(T_f)$, $f_{20}(\Delta T_{lm3})$, $f_{19}(A_3)$, $f_{22}(Q_2)$, $f_{23}(D_s)$, $f_{32}(W_2)$, $f_{33}(A_2)$, $f_{37}(q)$, $f_{39}(x_2^*)$, $f_{40}(L^*)$, $f_3(N_{og})$, $f_{10}(G_f)$, $f_9(D_a)$, $f_8(A_a)$, $f_5(H_g)$, $f_6(H_l)$, $f_4(H_{og})$, $f_7(Z)$, $f_{12}(HP_2)$

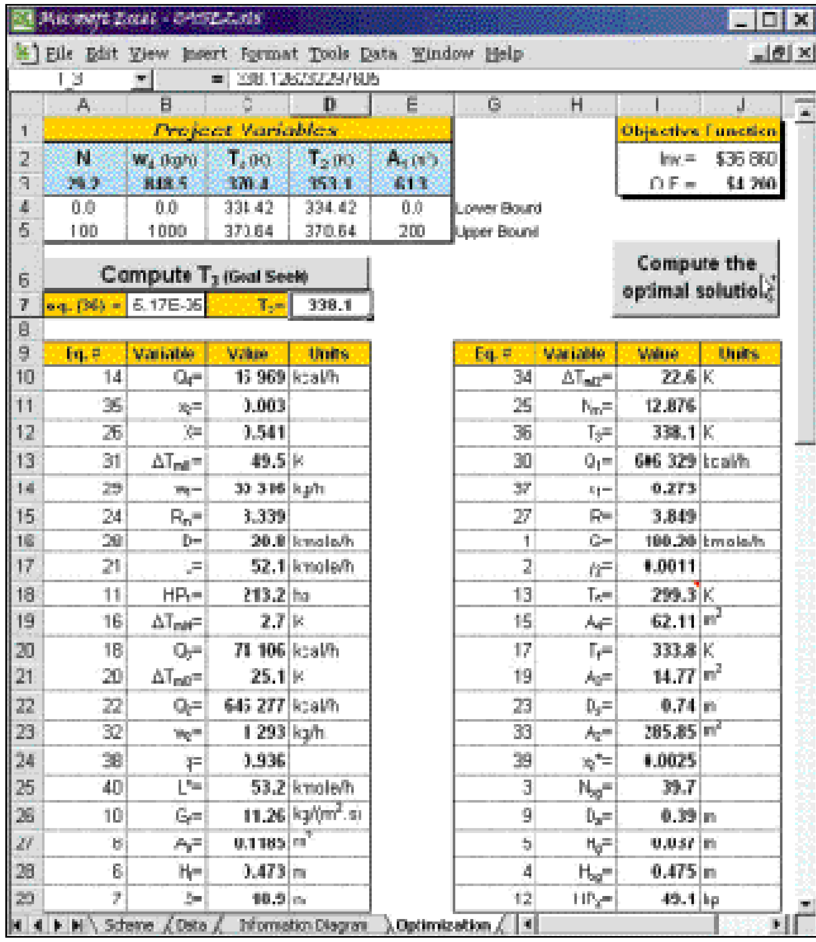

FIGURE 2. The authors created a macro to automate the iterative calculation process. Once such a macro is created, it can be assigned to a toolbar, a menu, a shortcut key, or a button, so that running the macro is as simple as clicking a button

Solver saves the day

The sequence we programmed for the order of solution is shown in Table 2. In addition to the data, there are five convenient decision variables [N, T_2, T, W_4, A_1], since this produces a serial solution [9]. Table 2 indicates that the first equation solved is Equation f_{36}, for varible T_3, and then Equation f_{14} for Q_4, finishing finally with Equation f_{12}. The corresponding Fortran 77 code of this sequencing was interfaced with an adaptive, random search optimizer [*10,11*] for comparison with the Solver capabilities built into the Excel environment.

The Excel spreadsheet Solver function has two nonlinear optimizers: a quasi-Newton method and a Generalized Reduced-Gradient algorithm [*12,13*]. With them, is possible to control the solution process by limiting the time taken and the number of interim calculations performed during the solution. It is also possible to control the precision within which constraints are binding, and the convergence criteria for the solutions.

Instead of manually invoking the Solver dialog box in the Tools menu, we have automated this task by creating a single macro. This is done by invoking the macro recorder, which saves the series of commands in the Visual Basic for Applications language [*14*]. Macros may then be assigned to a toolbar, menu, shortcut key, or button (Figure 2).

For this optimization, temperature T_3 — the only unknown variable from this equation — was estimated using the Excel "Goal Seek" feature to iteratively solve the nonlinear Equation f_{36}. "Goal Seek" lets the user find a specific result for one cell by adjusting the value of any other single cell. In this case, Equation *f36* was written in the goal cell and an initial value for T_3 was assigned to another cell (Figure 3). This was also automated by creating a macro, which was assigned to a button called "Compute T_3".

Excel's workspace architecture allows one to integrate multiple datasheets in the same file. In this example, we have put together the flow-

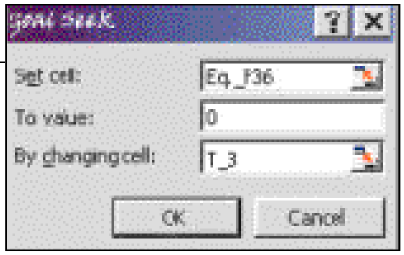

FIGURE 3. For this optimization, temperature, T_3, was estimated using the Excel "Goal Seek" feature to iteratively solve the nonlinear Equation f_{36} — the only unknown variable from this equation. Goal Seek lets the user find a specific result for one cell by adjusting the value of any other single cell. This process was automated by creating a macro assigned to a button labeled "Compute T_3"

sheet (Figure 1), data sheet, information matrix, algorithm, and macro module with source coding in the Visual Basic editor. Interested parties can go to www. deb.uminho.pt/ecferreira/download/abs_str.zip to download this Excel workbook file.

Results and discussion

We studied two cases (solvent recovery and air-pollution abatement). The differences pertain to the addition of a constraint for the collection efficiency of the absorption tower (in this case, $1\text{-}Gy_2/Fy_1 > 0.99$), and to the pertinent physical and economical data used during the calculations.

Case 2 (the air-pollution problem) is much more difficult to solve, since it is harder to find an initial feasible point, due to the highly constrained search space. The pertinent data for both cases are given in Table 3.

The search space for the decision variables $\{N, W_4, A_1\}$ was set quite wide, respectively [0, 100], [0, 1,000 kg/h] and [0, 200 m^2], to minimize the chance of missing the global optimum. The search intervals for T_2 and T_4 were estimated from the boiling points of the pure components, giving respectively [314.4, 350.6 K] and [334.4, 370.6 K] for Cases 1 and 2.

For comparison, the MSGA algorithm [*10, 11*] was applied to both cases and, irrespective of the starting point, always arrived at feasible points that were very close to the global optimum. The spreadsheet was then applied to both cases, and the following conclusions reached:

1. Trial-and-error testing should be done to obtain a feasible starting point. This will avoid trapping the solver with mathematical inconsistencies, such as negative arguments of logarithmic functions, from which it

TABLE 3. DATA

Operating variables:		CASE 1	CASE 2	Units
Feed flowrate	$F =$	60	200	Kmol/h
Pressure	$P =$	760	760	mmHg
Composition	$y_1 =$	0.4	0.1	
Composition	$x_3 =$	0.99	0.95	
Temperature	$T_1 =$	303	283	K
Temperature	$T_i =$	293	278	K
Temperature	$T_o =$	298	298	K
Temperature	$T_s =$	393	393	K
Reference temperature	$T_{ref} =$	230	210	K
Physical properties:				
Liquid density	$\rho_l =$	1,500	900	kg/m^3
Gas density	$\rho_g =$	5	2	kg/m^3
Molar weight	$M_l =$	154	100	kg/kmol
Molar weight	$M_g =$	58	20	kg/kmol
Specific heat (streams w_1 and w_4)	$c_{pw} =$	1	1	kcal/kg·K
Specific heat (heat exchangers 3 &4)	$c_p =$	0.2	0.2	kcal/kg·K
Liquid latent heat (from stripper)	$\lambda =$	50	60	kcal/kg
Water latent heat (stream w_2)	$\lambda_w =$	500	500	kcal/kg
Liquid viscosity	$\mu_l =$	1.00×10^{-3}	1.00×10^{-3}	kg/m·s
Gas viscosity	$\mu g =$	1.85×10^{-5}	1.85×10^{-5}	kg/m·s
Liquid diffusivity	$D_l =$	2.0×10^{-9}	2.0×10^{-9}	m^2/s
Gas diffusivity	$D_g =$	2.2×10^{-5}	2.2×10^{-5}	m^2/s
Antoine parameter	$A'_1 =$	32.9	32.9	
Antoine parameter	$B'_1 =$	14,300	14,300	K
Antoine parameter	$A'_2 =$	30.4	30.4	
Antoine parameter	$B'_2 =$	13,800	13,800	K
H_g parameter	$\alpha =$	0.557	0.557	
H_g parameter	$\beta =$	0.32	0.32	

Physical properties:		CASE 1	CASE 2	Units
H_g parameter	$\gamma =$	0.51	0.51	
H_g parameter	$\delta =$	0.22	0.22	
H_g parameter	$\varphi =$	0.00235	0.00235	m^{1+d}
Empiral constant (Souders- Brown Eq.)	$K =$	0.10	0.10	m/s
Specific area, fillings	$a_p/\varepsilon^3 =$	490	490	m^2/m
Relative volatility	$a =$	2	2	
Global heat transfer coefficient	$U_1 =$	300	200	kcal/m^2·h·K
Global heat transfer coefficient	$U_2 =$	500	100	kcal/m^2·h·K
Global heat transfer coefficient	$U_3 =$	100	200	kcal/m^2·h·K
Global heat transfer coefficient	$U_4 =$	200	100	kcal/m^2·h·K
Henry's constant	$H =$	608	208	mmHg
Cost factors:				
Feed F	$C_g =$	50	10	\$·h/yr·kg
Product Dx_3	$P_p =$	20	65	\$·h/yr·kg
Water	$C_w =$	0.0635	0.0635	\$·h/yr·kg
Vapor (reboiler)	$C_s =$	35.2	35.2	\$·h/yr·kg
Solvent	$C_l =$	5	100	\$·h/yr·kg
Electricity	$C_e =$	89.7	89.7	\$·h/yr·kg
Heat exchangers	$C_a =$	350	350	\$/(m^2)$^{0.556}$
Pumps	$C_{hp} =$	1,000	1,000	\$/hp$^{0.30}$
Absorber	$C_z =$	600	600	\$/m^2
Stripper	$C_n =$	363	363	\$/N·(m width)$^{-1.085}$
Return of investment	$F_c =$	0.14286	0.08	\$/\$·yr
Pump characteristics:				
Pump 1	$kp_1 =$	0.10	0.10	hp·h/N·kmol
Pump 2	$kp_2 =$	0.05	0.05	hp·h/(m high)·kmol

cannot recover. This can be performed by changing the values of the decision variables and seeing the impact on the simulation or optimization.

2. Unfortunately, not all initial values that obey (1) will converge to the global optimum, or will converge at all.

The possible benefits of using spreadsheets to solve optimization problems include the following:

- It is easier to build a simulation or optimization problem in Excel, which is available on many desktops, rather than coding the problem in a high-level language, or learning a new algebraic environment
- It is convenient to have a workbook in which the diagram, data, flowsheet, occurrence matrices and simulation procedure are interconnected and easily visualized

This interconnectivity allows one to easily add new constraints and specifications during the evaluation. Physical and economic data can also be easily changed, with the effect immediately reflected. Although the Excel solver is not comparable with more-robust optimizers [*10,11*] or other algorithms [*15*], it does provide an integrated framework for problem setting, visualization, inspection and solving. ■

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