

Can Spreadsheet Solvers Solve Demanding Optimization Problems?

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ABSTRACT: Practicing engineers resort to modular simulators or to algebraic tools such as GAMS or AMPL for performing complex process optimizations. These tools, however, have a significant learning curve unless they have been introduced at the undergraduate level beforehand. In this work we show how the Solver feature of the Excel spreadsheet can be used for the optimization of a fairly complex system, i.e., a classic solvent extraction/pollution prevention with heat integration process. The specific goal was the design optimization for continuous recovery of organic solvents (VOCs) using a gas absorption tower with solvent recovery in a stripper. It is shown that the Solver feature of the Excel spreadsheet can be used to converge on local optima for these complex systems, provided proper care is taken in the solution procedure. The complexities of optimization can also be demonstrated with this tool, as can several common pitfalls encountered during optimization. © 2001 John Wiley & Sons, Inc. *Comput Appl Eng Educ* 9: 49–56, 2001

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INTRODUCTION

With the advent of personal computers based on friendly environments with graphical interfaces such as Windows 95/98 or MacOS, and the widespread availability of powerful ‘what-if’ spreadsheets with optimization capabilities such as the EXCEL Solver from Microsoft Co., most engineering students are attracted to using these tools, which require a minimum amount of effort in building a typical simulation/optimization problem, in comparison with standard high level language coding. Since practicing engineers also use spreadsheets for many tasks, and

since process optimization is steadily becoming a common task, it is important to establish to what extent these tools are capable of solving demanding optimization problems.

An interesting optimization problem dealing with the concepts of process synthesis including heat integration and solvent recovery can be found in Umeda [1] and Umeda and Ichikawa [2]. The problem shown in this paper has been adapted from these authors, and Silverberg [3] shows that this process is widely in use.

The problem shown in this paper has been adapted for demonstration purposes in two courses, respectively, *Strategy of Chemical Processes* in the Chemical Engineering Department at the Universidade do Porto, and *Strategy of Process Engineering* in the

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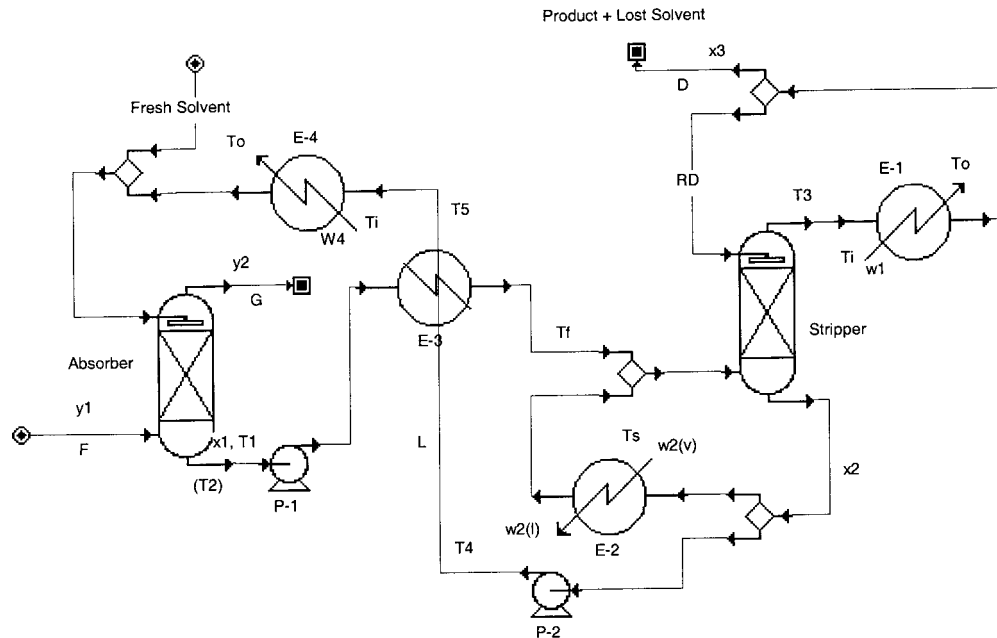


Figure 1 Schematic representation of the process.

Biological Engineering Department at the Universidade do Minho, both in the north of Portugal.

PROCESS

The continuous and steady-state process under study is shown in figure 1. It consists of an absorber column (packing tower) and a stripper (plate tower), with heat recovery, with the objectives of solvent recovery and/or recovery of organic solvent (VOC) abatement.

Basically, the gaseous feeding F with a mole fraction y_1 of a gaseous solute to be recovered or removed, is fed to an absorber, where an appropriate solvent with flowrate L is counter currently enriched in the solute. For example, Silverberg [3] states that proper solvents (polyethylene glycol ethers) may remove up to 80 different VOCs. The extraction solvent is recovered in a plate tower by stripping, and the solute in the overhead vapors is condensed for recovery or further disposal. The extraction solvent is cooled and returned to the absorber, where some fresh solvent needs to be added to account for losses in the overhead vapors.

The entire set of equality constraints is given in the Table 1. The absorber diameter [Eq. (f₉ in Table 1)] was computed so that the vapor velocity is 75% of the flooding velocity. The stripper diameter can be estimated from the Souders-Brown equation [4]

$$V_M = K \sqrt{\frac{\rho_l - \rho_g}{\rho_g}},$$

where V_M is the superficial vapor velocity and K an empirical constant, and from the vapor load, $V_v = Q_2/\lambda\rho_g$. The Fenske-Underwood equations [Eqs. (f₂₄) and (f₂₅)] were used to compute the minimum number of plates and the minimum reflux ratio, and the number of plates [Eqs. (f₂₆) and (f₂₇)] was computed from the Eduljee approximation to Gilliland's graphical method [4].

The objective function is to maximize the profit and is given by the difference between sales from the recovered VOC and operating and annualized investment costs,

$$F_{\text{obj}} = P_p D M_1 x_3 - [C_g F M_g + C_1 D (1 - x_3) M_1 + C_w (w_1 + w_4) + C_s w_2 + C_e (HP_1 + HP_2) + \text{Inv} F_c],$$

where the investment costs are given by

$$\text{Inv} = C_z Z D_a^{1.0} + C_n N D_s^{1.085} + C_a (A_1^{0.556} + A_2^{0.556} + A_3^{0.556} + A_4^{0.556}) + C_{hp} (HP_1^{0.3} + HP_2^{0.3})$$

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

$$L < 300 \text{ kg mol.hr}^{-1} \text{ (maximum flowrate),}$$

$$R < 20 \text{ (maximum reflux)}$$

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

Table 1 Process Design Equation

Absorber

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

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

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

$$f_4 = H_{og} - H_g - \frac{HGH_1}{PL^*} = 0$$

$$f_5 = H_g - \alpha \left(\frac{FM_g}{A_a} \right)^\beta \sqrt{Sc_g} / \left(\frac{(L + D)M_1}{A_a} \right)^\gamma = 0$$

$$f_6 = H_1 - \left(\frac{(L + D)M_1}{A_a \mu_1} \right)^\delta \phi \sqrt{Sc_1} = 0$$

$$f_7 = Z - N_{og}H_{og} = 0$$

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

$$f_9 = D_a - \sqrt{\frac{4GM_g}{0.75\pi G_f 3600}} = 0$$

$$f_{10} = \log_{10} \left[G_f^2 \left(\frac{a_p}{\varepsilon^3} \right) \left(\frac{1}{g\rho_g\rho_l} \right) \left(\frac{\mu_l}{\mu_g} \right)^{0.2} \right] - 1.74 \left(\frac{L^*M_1}{GM_g} \right)^{0.25} \left(\frac{\rho_l}{\rho_g} \right)^{-0.125} = 0$$

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

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

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

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

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

Heat Exchanger no. 3

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

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

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

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

Stripper and heat exchangers

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

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

$$f_{23} = \pi \frac{D_s^2}{4} - \frac{22.4Q_2T_4}{273.2 \times 3600 \lambda M_1 K \sqrt{(\rho_1 - \rho_g)/\rho_g}} = 0$$

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

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

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

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

Table 1. (Continued)

$$f_{28} = Q_1 - D\lambda(R + 1) = 0$$

$$f_{29} = Q_1 - W_1 c_{pw}(T_o - T_i) = 0$$

$$f_{30} = Q_1 - U_1 A_1 \Delta T_{lm1} = 0$$

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

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

$$f_{33} = Q_2 - U_2 A_2 \Delta T_{lm2} = 0$$

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

$$f_{35} = x_2 e^{(A_1 - B_1)/(T_4 + T_{ref})} + (1 - x_2) e^{(A_2 - B_2)/(T_4 + T_{ref})} - P = 0$$

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

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

$$f_{38} = x_1 e^{(A_1 - B_1)/(T_2 + T_{ref})} + (1 - x_1) e^{(A_2 - B_2)/(T_2 + T_{ref})} - P = 0$$

Make-up

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

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

SIMULATION

To use the EXCEL application, it is necessary to specify a sequence for the simulation step, i.e., what variables are to be computed from which equation, and on which order. A preprocessing step was applied to this example, where the number of theoretical stages (N) and the bubble points (T_2 , T_4) were *a priori* chosen as decision variables. This makes it possible to define this problem as a mixed integer nonlinear programming (MINLP) problem (although not strictly necessary here) and to linearize two equations [Eqs. (f₃₅) and (f₃₈)] to avoid the iterative calculation of two temperatures. A serial solution could easily be obtained [5], and the corresponding solution procedure is given in Table 2.

The remaining degrees of freedom correspond to the variables $\{W_4, A_1\}$. The corresponding FORTRAN 77 code of this sequencing was interfaced with an adaptive random search MINLP optimizer [6,7] for

comparison with the solver capabilities built within the EXCEL environment.

SPREADSHEET SOFTWARE

Spreadsheet programs are becoming nowadays a ubiquitous tool in Chemical Engineering mathematical calculation [8,9,10] due to its popularity and availability. The Microsoft Excel spreadsheet, a Microsoft Office family member, was used as a development framework, coupled with the Solver tool, a companion of Excel since 1991 (version 3.0). The Excel solver has two nonlinear optimizers, respectively, a quasi-Newton method and a generalized reduced gradient algorithm [11]. Linear and integer problems use the linear simplex method with bounds on the variables, and the branch-and-bound method, implemented by Fylstra et al. [12].

The solver options allow one to specify the approach used to obtain better initial estimates of

Table 2 Serial Solution Procedure with $\{N, W_4, T_4, T_2$, and $A_1\}$ as Decision Variables

Equation (variable)

$$f_{36}(T_3), f_{14}(Q_4), f_{34}(\Delta T_{lm2}), f_{35}(x_2), f_{25}(N_m), f_{26}(X), f_{31}(\Delta T_{lm1}), f_{30}(Q_1), f_{29}(W_1), f_{38}(x_1),$$

$$f_{24}(R_m), f_{27}(R), f_{28}(D), f_1(G), f_{21}(L), f_2(y_2), f_{11}(HP_1), f_{13}(T_5), f_{16}(\Delta T_{lm4}), f_{15}(A_4), f_{18}(Q_3),$$

$$f_{17}(T_f), f_{20}(\Delta T_{lm3}), f_{19}(A_3), f_{22}(Q_2), f_{23}(D_s), f_{32}(W_2), f_{33}(A_2), f_{37}(q), f_{39}(x_2^*), f_{40}(L^*),$$

$$f_3(N_{og}), f_{10}(G_f), f_9(D_a), f_8(A_a), f_5(H_g), f_6(H_1), f_4(H_{og}), f_{12}(HP_2)$$

the basic variables in each one-dimensional search, either using linear extrapolation from a tangent vector or quadratic extrapolation, which may improve the results on highly nonlinear problems. It is also possible to specify the differencing method used to estimate derivatives of the objective and constraint functions: forward in which the constraint values change relatively slowly, or central method used for problems in which the constraints change rapidly, especially near the boundaries of the active constraints. It is possible to control the solution process by limiting the time taken and the number of interim calculations by the solution process; it is also possible to control the precision within which constraints are considered binding and the convergence criteria for the solutions.

Instead of manually invoking repeatedly the Solver dialog box in the Tools menu (a time-consuming, repetitive action), we have automated this task by

creating and running a single macro. A macro is a series of commands and instructions grouped together as a single command to accomplish a task automatically. The macro is created invoking the macro recorder that saves the series of commands in the *Visual Basic for Applications* programming language [13,14]. A recorded macro can be opened in the *Visual Basic Editor* to modify the source code. Macros may be assigned to a toolbar, a menu, shortcut keys, or a button (see Fig. 2). Running the macro is as simple as clicking the button.

Temperature T_3 was estimated using the Excel "Goal Seek" feature to solve iteratively the nonlinear equation f_{36} since this is the only unknown variable from this equation. Goal Seek permits one to find a specific result for a cell by adjusting the value of any one other cell. Equation (f_{36}) was written in the goal cell and a starting (initial) value to T_3 was assigned in another cell (see Fig. 3). This dialog box was also

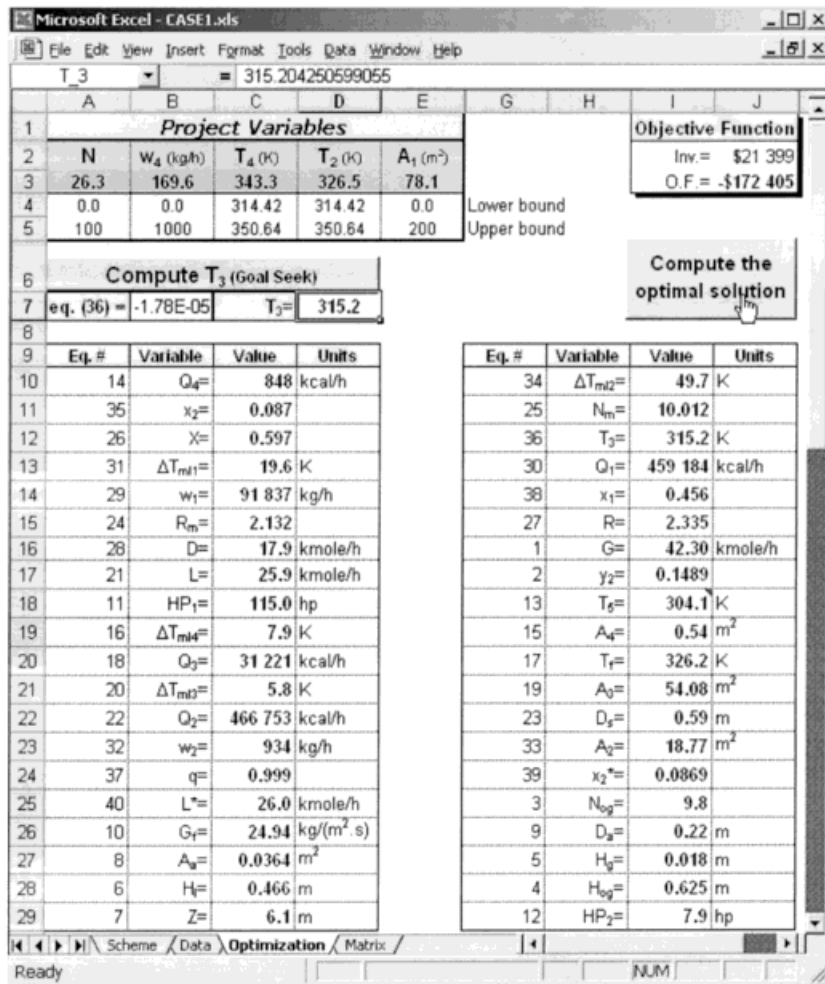


Figure 2 Snapshot of the Excel screen: results for case1 optimization.

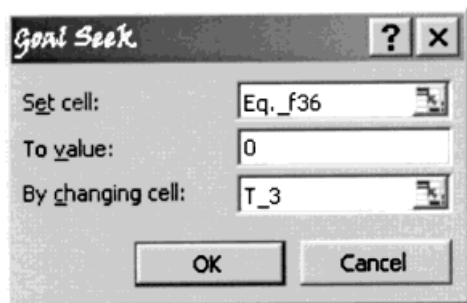


Figure 3 Solving a nonlinear equation by using “Goal Seek”.

automated by creating a macro assigned to the “Compute T_3 ” button.

The workspace architecture of Excel allows one to integrate multisheets in the same file. In this example, we have put together the scheme (Fig. 1), the data sheet, the information matrix, the algorithm, and the macro module with source coding in the Visual Basic editor. This Excel workbook file is available for download on the World Wide Web at http://www.de-b.uminho.pt/ecferreira/download/abs_str.zip

RESULTS AND DISCUSSION

We have studied two cases, one corresponding to solvent recovery (Case 1) and the other to air pollution abatement (Case 2). The differences rely on the addition of a constraint for the absorption tower collection efficiency, i.e.,

$$1 - \frac{Gy_2}{Fy_1} > 0.99$$

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

The search space for the decision variables $\{N, W_4, A_1\}$ was set quite wide, respectively, $[0, 100]$, $[0, 1000 \text{ kg h}^{-1}]$, and $[0, 200 \text{ m}^2]$, to minimize the chance of missing the global optimum. As the number of theoretical plates does not, in general, reflect the number of real plates, all decision variables were considered continuous. This also avoids difficulties in defining a MINLP solution strategy within the EXCEL spreadsheet since this environment does not have MINLP optimization capabilities. The search intervals for T_2 and T_4 were estimated from the boiling points of the pure components giving, respectively, $[314.4, 350.6 \text{ K}]$ and $[334.4, 370.6 \text{ K}]$ for Cases 1 and 2.

The MSGA algorithm [6,7] was applied to both the cases and, irrespective of the starting point, always arrived at feasible points very close to the global optimum. The EXCEL spreadsheet was applied to both the cases and, in general, the following conclusions could be taken:

- (1) A feasible starting point should first be obtained by trial and error to avoid trapping the solver with mathematical inconsistencies, i.e., negative arguments of logarithmic functions from which it cannot recover. This can be easily performed by simply changing the values of the decision variables and immediately seeing the impact on the simulation/optimization procedure.
- (2) Not all initial values that obey 1 will converge to the global optimum, or will converge at all.

So, what are the possible benefits of using the EXCEL spreadsheet to solve optimization problems? For one, it is easier to build a typical simulation/optimization problem in the EXCEL environment rather than coding it in high level languages, or learning a new algebraic environment. It is also very convenient to have an integrated workbook whereby the process diagram, data, flowsheets, occurrence matrices, and simulation procedure are all interconnected and easily visualized. This concept is not possible with the other approaches and allows one to easily add new constraints and process specifications. The physical and economic data can be easily changed and its effect can be immediately reflected in the simulation/optimization results.

CONCLUSIONS

The problem analyzed in this paper is of sufficient complexity to allow the observation of several convergence problems within the EXCEL solver. It is our opinion that irrespective of the problem statement, an initial feasible point is required for progress toward a local optimum. Since the optimizers within the EXCEL environment are local search algorithms [12], convergence to the global optimum is only guaranteed with convex problems.

Although the EXCEL solver is not comparable with robust optimizers such as the MSGA [6,7] or other global search algorithms [15], it has, from the point of view of practicing engineers, the distinct advantage of providing an integrated framework for problem setting, visualization, inspection, and solving.

Table 3 Data

	Case 1	Case 2	Units
Operating Variables			
Feed flowrate	$F = 60$	200	kmol h^{-1}
Pressure	$P = 760$	760	mm Hg
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	$T_{\text{ref}} = 230$	210	K
Physical properties			
Liquid density	$\rho_l = 1500$	900	kg m^{-3}
Gas density	$\rho_g = 5$	2	kg m^{-3}
Molar weight	$M_1 = 154$	100	kg mol^{-1}
Molar weight	$M_g = 58$	20	kg mol^{-1}
Specific heat (streams W_1 and W_4)	$c_{pw} = 1$	1	$\text{kcal kg}^{-1} \text{K}^{-1}$
Specific heat (heat exchangers 3 and 4)	$c_p = 0.2$	0.2	$\text{kcal kg}^{-1} \text{K}^{-1}$
Liquid latent heat (from stripper)	$\lambda = 50$	60	kcal Kg^{-1}
Water latent heat (stream w_2)	$\lambda_w = 500$	500	kcal Kg^{-1}
Liquid viscosity	$\mu_l = 1.00 \times 10^{-3}$	1.00×10^{-3}	$\text{kg m}^{-1} \text{s}^{-1}$
Gas viscosity	$\mu_g = 1.85 \times 10^{-5}$	1.85×10^{-5}	$\text{kg m}^{-1} \text{s}^{-1}$
Liquid diffusivity	$D_l = 2.0 \times 10^{-9}$	2.0×10^{-9}	$\text{m}^2 \text{s}^{-1}$
Gas diffusivity	$D_g = 2.2 \times 10^{-5}$	2.2×10^{-1}	$\text{m}^2 \text{s}^{-1}$
Antoine parameter	$A_1 = 32.9$	32.9	
Antoine parameter	$B_1 = 14300$	14300	K
Antoine parameter	$A_2 = 30.4$	30.4	
Antoine parameter	$B_2 = 13800$	13800	K
H_g parameter	$\alpha = 0.557$	0.557	
H_g parameter	$\beta = 0.32$	0.32	
H_g parameter	$\gamma = 0.51$	0.51	
H_g parameter	$\delta = 0.22$	0.22	
H_g parameter	$\phi = 0.00235$	0.00235	$\text{m}^{1+\delta}$
Empirical constant (Souders-Brown equation)	$K = 0.10$	0.10	m s^{-1}
Specific area of fillings	$a_p/\epsilon^3 = 490$	490	$\text{m}^2 \text{m}^{-3}$
Relative volatility	$a = 2$	2	
Global heat transfer coefficient	$U_1 = 300$	200	$\text{kcal m}^{-2} \text{h}^{-1} \text{K}^{-1}$
Global heat transfer coefficient	$U_2 = 500$	100	$\text{kcal m}^{-2} \text{h}^{-1} \text{K}^{-1}$
Global heat transfer coefficient	$U_3 = 100$	200	$\text{kcal m}^{-2} \text{h}^{-1} \text{K}^{-1}$
Global heat transfer coefficient	$U_4 = 200$	100	$\text{kcal m}^{-2} \text{h}^{-1} \text{K}^{-1}$
Henry's constant	$H = 608$	208	mm Hg
Cost factors			
Feed F	$C_g = 50$	10	$\$ \text{h year}^{-1} \text{kg}^{-1}$
Product Dx_3	$P_p = 20$	65	$\$ \text{h year}^{-1} \text{kg}^{-1}$
Water	$C_w = 0.0635$	0.0635	$\$ \text{h year}^{-1} \text{kg}^{-1}$
Vapor (reboiler)	$C_s = 35.2$	35.2	$\$ \text{h year}^{-1} \text{kg}^{-1}$
Solvent	$C_1 = 5$	100	$\$ \text{h year}^{-1} \text{kg}^{-1}$
Electricity	$C_e = 89.7$	89.7	$\$ \text{h year}^{-1} \text{kg}^{-1}$
Heat exchangers	$C_a = 350$	350	$\$ (\text{m}^{-2})^{0.556}$
Pumps	$C_{hp} = 1000$	1000	$\$ \text{hp}^{-0.30}$
Absorber	$C_z = 600$	600	$\$ \text{m}^{-2}$
Stripper	$C_n = 363$	363	$\$ \text{N}^{-1} (\text{m width})^{-1.085}$
Return of investment	$F_c = 0.14286$	0.08	$\$ \text{year}^{-1}$
Pump Characteristics			
Pump 1	$kp_1 = 0.10$	0.10	$\text{hp h N}^{-1} \text{kmol}^{-1}$
Pump 2	$kp_2 = 0.05$	0.05	$\text{hp h (m high)}^{-1} \text{kmol}^{-1}$

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BIOGRAPHIES



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