Spreadsheets in Chemical Engineering Education—A Tool in Process Design and Process Integration*

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Recent developments in embedding numerical optimization procedures with linear and nonlinear solvers within a spreadsheet environment have greatly enhanced the use of these tools for teaching chemical process design and process integration. Student skills with respect to these topics are usually gained by complex and expensive modular simulators, e.g., ASPEN Plus® or algebraic tools such as GAMS® or AMPL®. However, modular simulators have a significant learning curve, and algebraic modeling languages are usually ignored once students commence careers. This paper demonstrates how the Solver feature of the Excel® spreadsheet is used for the optimization of several chemical engineering systems, including pollution prevention problems and mass-exchange networks. Three nonlinear problems are examined: the (a) recovery of benzene from a gaseous emission; (b) design of a chemical reactor network; and (c) solution of material balances in the production of vinyl chloride from ethylene. Dephenolization of aqueous wastes is presented as a linear case. The ease with which these and similar process problems can be formulated and solved within the Excel® environment constitutes a major step towards teaching practical optimization and design concepts for university students.

INTRODUCTION

UNDERGRADUATE ENGINEERING students are attracted to the powerful ‘what-if’ spreadsheets with optimization capabilities, such as the EXCEL® Solver (Microsoft Co.) and What’s Best (Lindo Systems, Inc.). They require a minimum amount of effort in building a typical simulation/optimization problem, in comparison with standard high level language coding such as GAMS® or AMPL®. Undergraduate instructors are adopting Excel Solver for introducing students to solving and optimizing process design and integration [1, 2]. In addition, several engineering textbooks now include coverage of the Excel Solver [3–6]. The new edition of the classical textbook Optimization of Chemical Processes [4] dedicates several pages to the use of Excel Solver as an optimization tool. The book includes a new co-author, Leon Lasdon, a recognized authority in operations research optimization software and implementation of the Excel Solver [7].

Practicing engineers also use spreadsheets for many tasks, and process optimization is steadily becoming a common task in process synthesis, design and integration. Therefore, it is important to establish to what extent these tools are capable of solving optimization problems.

The present authors studied recently an interesting problem dealing with the concepts of process synthesis including heat integration and solvent recovery [1, 2, 8]. The Solver feature of the Excel® spreadsheet is demonstrated for the optimization of several chemical engineering systems, including pollution prevention problems and mass-exchange networks in the current paper. Three nonlinear problems (the recovery of benzene from a gaseous emission; the design of a chemical reactor network; and the solution of material balances in the production of vinyl chloride from ethylene), and one linear problem (the dephenolization of aqueous wastes) are examined. These case studies have been adapted for demonstration purposes in two courses run by the authors.

THE EXCEL SOLVER

The Microsoft Excel® spreadsheet was used as a development framework, coupled with the Solver add-on—a companion of Excel since 1991 (version 3.0). The Excel Solver has two nonlinear unconstrained optimizers, a quasi-Newton method and a reduced gradient method. These are used within a

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Generalized Reduced Gradient algorithm [9] for solving constrained optimization problems. The linear simplex method with bounds on the variables, and the branch-and-bound method implemented by Fylstra et al. [7], can be used for solving linear and integer problems.

The approach used to obtain better initial estimates of the basic variables in each one-dimensional search can be specified in Solver options. Linear extrapolation from a tangent vector or quadratic extrapolation can be used, which may improve the results on highly nonlinear problems. It is also possible to specify the differencing method to estimate derivatives of the objective and constraint functions: ‘Forward’ when the constraint values change relatively slowly, or ‘Central’, used for problems when the constraints change rapidly, especially near the boundaries of the active constraints. It is possible to control:

a) the solution process by limiting the time taken and the number of interim calculations by the solution process;
b) the precision within which constraints are considered binding;
c) the convergence criteria for the solutions.

Example 1: Material balances in the production of vinyl chloride

This case study illustrates the use of Excel Solver in the solution of simultaneous nonlinear equations associated with material balances in the production of vinyl chloride from ethylene. DeLancey [10] solved this example using Scientific Notebook.
(MacKichan Software, Inc.) primarily oriented for solving systems of nonlinear equations.

The flow diagram in Fig. 1 represents the main steps in the production of vinyl chloride (C$_2$H$_3$Cl) from ethylene (C$_2$H$_4$).

The reactions taking place separately in each reactor are:

**Chlorination:**
\[ C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2 \]

**Oxyhydrochlorination:**
\[ C_2H_4 + 2HCl + \frac{1}{2}O_2 \rightarrow C_2H_4Cl_2 + H_2O \]

**Pyrolysis:**
\[ C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl \]

The ethylene feed, $F_1$, is 90% molar ethylene and the remainders are inerts. The chlorine and oxygen feeds, $F_2$ and $F_3$, respectively, are pure. All of the ethylene, oxygen, and chlorine react and the conversion of the hydrochloric acid (HCl) fed to the oxyhydrochlorination is complete.

Only 50% of the total dichloroethane (C$_2$H$_4$Cl$_2$) fed to the pyrolysis reactor is converted, with the remainder being separated and recycled with inerts in stream $F_{12}$. The inert concentration in the recycle stream is 50% molar. Pure hydrochloric acid (HCl) is recycled in stream $F_{13}$. The final product stream, $F_9$, consists only of vinyl chloride and water.

Setting $F_1 = 1$ mole/hr results in a problem with 24 independent (unknown) variables and 26 equations issued from material balances (Table 1), with no degrees of freedom. The EXCEL Solver was used to determine all of the unknown flow rates, $F_j$, and mole fractions, $x_{ij}$ (mole fraction $i$ in stream $j$). The species are labeled in Table 2.

The Solver is used to compute the root of one equation subject to several equality constraints (Fig. 2). Equation 1 ($C_{36}$) was set as ‘Target Cell’ with a required zero value and all the 26 equations were set as equality constraints. The initial values for the decision variables (‘By Changing Cells’) were 1.0 for all the flow rates ($F_j$) and 0.50 to all the mole fractions ($x_{ij}$). The solution is obtained almost instantaneously.

**Example 2: Dephenolization of aqueous wastes**

This example is used to illustrate the synthesis of mass-exchange networks based on a mathematical programming approach. For an overview of this technique the reader is referred to El-Halwagi [11].

An oil-recycling plant is demonstrated in Fig. 3 as adapted from [11]. Two types of waste oil are handled: gas and lube oils. The two streams are

<table>
<thead>
<tr>
<th>#</th>
<th>Equation</th>
<th>#</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$x_{1,1} + x_{6,1} = 1$</td>
<td>14</td>
<td>$0.50(x_{5,6}F_6 + x_{5,12}F_{12}) = x_{5,6}F_3$</td>
</tr>
<tr>
<td>2</td>
<td>$F_2 = x_{1,1}F_4$</td>
<td>15</td>
<td>$0.50(x_{5,6}F_6 + x_{5,12}F_{12}) = x_{5,6}F_3$</td>
</tr>
<tr>
<td>3</td>
<td>$F_3 = 0.5x_{6,1}F_4$</td>
<td>16</td>
<td>$0.50(x_{5,6}F_6 + x_{5,12}F_{12}) = x_{5,6}F_3$</td>
</tr>
<tr>
<td>4</td>
<td>$x_{6,6}F_6 = x_{1,1}F_4$</td>
<td>17</td>
<td>$x_{5,7}F_7 = x_{5,6}F_3$</td>
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<tr>
<td>5</td>
<td>$x_{6,6}F_6 = x_{1,1}F_4$</td>
<td>18</td>
<td>$x_{5,6}F_6 + x_{5,12}F_{12} = x_{5,6}F_3$</td>
</tr>
<tr>
<td>6</td>
<td>$x_{6,6}F_6 = x_{1,1}F_4$</td>
<td>19</td>
<td>$x_{5,6} + x_{6,0} + x_{6,6} + x_{5,7} + x_{5,8} = 1$</td>
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<tr>
<td>7</td>
<td>$x_{6,6} + x_{6,0} = 1$</td>
<td>20</td>
<td>$x_{5,6}F_6 = F_{13}$</td>
</tr>
<tr>
<td>8</td>
<td>$x_{7,7}F_7 = x_{1,1}F_4$</td>
<td>21</td>
<td>$x_{6,6}F_6 = x_{5,12}F_{10}$</td>
</tr>
<tr>
<td>9</td>
<td>$x_{6,7}F_7 = x_{1,1}F_4$</td>
<td>22</td>
<td>$x_{6,6}F_6 + x_{5,7}F_7 = x_{5,6}F_3$</td>
</tr>
<tr>
<td>10</td>
<td>$F_{13} = 2(x_{1,1}F_4)$</td>
<td>23</td>
<td>$x_{6,6}F_6 + x_{5,7}F_7 = x_{5,6}F_3$</td>
</tr>
<tr>
<td>11</td>
<td>$x_{6,7}F_7 + x_{9,7} = 1$</td>
<td>24</td>
<td>$x_{6,6}F_6 = x_{6,10}F_{10}$</td>
</tr>
<tr>
<td>12</td>
<td>$x_{5,12}F_{12} + x_{6,10}F_{10} = x_{5,12}F_{12}$</td>
<td>25</td>
<td>$x_{6,6} + x_{9,7} = 1$</td>
</tr>
<tr>
<td>13</td>
<td>$x_{6,6} + x_{6,0} = 1$</td>
<td>26</td>
<td>$F_{10} = F_{11} + F_{12}$</td>
</tr>
</tbody>
</table>

Table 2. Labeling of components

<table>
<thead>
<tr>
<th>Index</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species</td>
<td>C$_2$H$_4$</td>
<td>Cl$_2$</td>
<td>HCl</td>
<td>O$_2$</td>
<td>C$_2$H$_4$Cl$_2$</td>
<td>C$_2$H$_3$Cl</td>
<td>H$_2$O</td>
<td>Inerts</td>
</tr>
</tbody>
</table>
first de-ashed and de-metallized. Atmospheric distillation is used to obtain light gases, gas oil, and a heavy product. The heavy product is distilled under vacuum to yield lube oil. The gas and the lube oils can be further processed to attain other properties. The gas oil is steam stripped to remove light and sulphur impurities, then hydrotreated. The lube oil is dewaxed/deasphalted using solvent extraction followed by steam stripping. The process has two main sources of waste water. These are the condensate streams from the steam strippers.

The principal pollutant in both wastewater streams is phenol that can be separated using several techniques. Solvent extraction using gas oil (S1) or lube oil (S2) as process Mass Separation Agents (MSA) is an option. The data for the waste streams and the process MSA are given in Tables 3 and 4 respectively.

Three external technologies are also considered for the removal of phenol. These processes include adsorption using activated carbon, S3, ion exchange using a polymeric resin, S4, and stripping using air.

Table 3. Data on waste streams for the dephenolization example [11]

<table>
<thead>
<tr>
<th>Stream</th>
<th>Description</th>
<th>Flow rate G, kg/s</th>
<th>Supply composition</th>
<th>Target composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Condensate from first stripper</td>
<td>2</td>
<td>0.050</td>
<td>0.010</td>
</tr>
<tr>
<td>R2</td>
<td>Condensate from second stripper</td>
<td>1</td>
<td>0.030</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Fig. 2. Solving simultaneous nonlinear equation associated with material balances in the production of vinyl chloride from ethylene.

Fig. 3. Dephenolization of aqueous wastes in an oil recycling plant.
The equilibrium data for the transfer of phenol to the jth lean stream is given by 
\[ y^\grave{}_{mj} = \frac{y}{x_j} \]
where the values of \( m_j \) are given in Table 4. Also, listed are the supply and target compositions and unit cost data for each MSA. Throughout this example, a minimum allowable composition difference, \( \varepsilon_j \), of 0.001 (kg phenol)/(kg MSA) is used.

An analysis based on ‘pinch diagrams’ (see [11] for details) indicates that 0.0184 kg phenol/s is the excess capacity for the process MSA and that 0.0124 kg phenol/s are to be removed using an external MSA.

The problem of minimizing the operating cost of mass separation agents was formulated in [11] by adopting the linear-programming approach solved using the LINGO package (Lindo Systems, Inc.).

The objective function is:

\[
\min\{0.081L_3 + 0.214L_4 + 0.060L_5\}
\]

subject to:

\[
\begin{align*}
\delta_1 & = 0.0052 \\
\delta_2 - \delta_1 + 0.0101L_2 & = 0.0308 \\
\delta_3 - \delta_2 + 0.0010L_4 + 0.0013L_2 & = 0.0040 \\
\delta_4 - \delta_3 + 0.00066L_1 + 0.0086L_2 & = 0.0396 \\
\delta_5 - \delta_4 + 0.0024L_1 + 0.0537L_4 & = 0.0144 \\
\delta_6 - \delta_5 + 0.0222L_4 & = 0.0060 \\
\delta_7 - \delta_6 + 0.0444L_4 & = 0.0040 \\
\delta_8 - \delta_7 + 0.0420L_4 & = 0.0000 \\
\delta_9 - \delta_8 + 0.0510L_3 + 0.0114L_4 & = 0.0000
\end{align*}
\]

* Including regeneration and make-up costs.
Fig. 5. Recovery of benzene from a gaseous emission.
\[ \delta_L - \delta_y + 0.0555L_3 + 0.0123L_4 + 0.0277L_5 = 0.0144 \]
\[ \delta_L - \delta_y + 0.0025L_3 + 0.0013L_5 = 0.0000 \]
\[ -\delta_L + 0.0010L_3 = 0.0000 \]
\[ \delta_k \leq 0, k = 1, 2, \ldots, 11 \]
\[ L_j \geq 0, j = 1, 2, \ldots, 7 \]
\[ L_j \leq 5, \]
\[ L_j \leq 3. \]

where \( L_j \) is the flow rate of the \( j \)th MSA, \( \delta_k \) and \( \delta_k \) are the residual masses of the key pollutant entering and leaving the \( k \)th interval. The first set of 11 equality constraints represents successive material balances around each composition interval. Setting \( \delta_k \geq 0 \) enables the waste streams to pass the mass of the pollutant downwards if it does not fully exchange it with the MSAs in a given interval. Setting \( L_j \geq 0 \) guarantees that the optimal flow rate of each MSA is non-negative. The last two constraints are upper bounds on flow rates less than the total available quantity of the corresponding lean stream.

The EXCEL Solver is used to optimize the objective function, which was set as the ‘Target Cell’ for minimization (Fig. 4). The initial values for the variables were set to 1.0 for all the flow rates \( (L_j) \) and to 0.001 for all the mole fractions \( (\delta_k) \). The solution is quickly obtained by selecting the ‘Linear Model’ option in the Solver Parameters since all relationships are linear as is the objective function. The binding of the equality constraints determines the residual masses of the key pollutant entering and leaving the \( k \)th interval \( (\delta_k) \). The solution for the MSA optimized flow rates is \( \{L_1, L_2, L_3, L_4, L_5\} = \{5.0000, 2.0800, 0.1127, 0.0000, 0.0000\} \). Therefore, activated carbon \( (L_3) \) is the optimum external MSA. The same minimum operating cost can also be achieved by other combinations of the process MSA, since both \( L_1 \) and \( L_2 \) are inexpensive.

**Example 3: Recovery of Benzene from a Gaseous Emission**

This example is used to illustrate the application of the EXCEL Solver to solution of a nonlinear optimization problem [11] which is to remove benzene from a gaseous emission by contact with an absorbent (wash oil, molecular weight 300). The gas flow rate is 0.2 kmole/s and it contains 0.1% molar (1000 ppm) of benzene. The molar mass of the gas is 29 g/mole, its temperature is 300 K, at a pressure of 141 kPa. It is desired to reduce the benzene to 0.01 mole/mole% using the system shown in Fig. 5, where benzene is first absorbed into oil. The oil is then fed to a regeneration system in which it is heated and passed on to a flash column that recovers benzene as a top product. The bottom product is the regenerated oil, which contains 0.08 mole/mole% benzene. Finally, the regenerated oil is cooled and pumped back to the absorber.

The EXCEL Solver is used to assess the optimal flow rate of recirculating oil that minimizes the total annualized cost (TAC) of the system.

The design equations for this process follow:

- **Cost equations:**
  - Annual operating cost, \( \text{AOC} = C_aL_j(8000 \text{ yrs/annum}) \)
  - Fixed cost of installed shell and auxiliaries, \( \text{FCI} = 2300H^{0.85}D^{0.95} \)
  - Cost of packing, \( \text{FC2} = 800(\pi/4)HD^2 \)
  - Annualized Fixed Cost, \( \text{AFC} = (\text{FCI} + \text{FC2})/\text{Depreciation} \)
  - Total Annualized Cost, \( \text{TAC} = \text{AOC} + \text{AFC} \)

**Constraints:**

- Mass velocity of oil, \( \frac{L_j M_{\text{oil}}}{4D^2} \geq 2.7 \text{ kg/m}^2/\text{s} \)
- \( \varepsilon_j \leq 0.005 \)
- \( \varepsilon_j \geq 0.00072 \)

![Fig. 6. Using ‘Goal Seek’ to find the value 2.70 for the mass velocity of oil (SIS47) by adjusting \( \varepsilon_j \).](image-url)
These last constraints on the minimum allowable composition difference at the lean end of the mass exchanger are upper and lower bounds to the search space. The lower bound,

$$j \geq 0.00072,$$

is equivalent to the constraint on mass velocity of oil being less than 2.7 kg m\(^{-2}\) s\(^{-1}\) and was calculated using the ‘Goal Seek’ tool available in EXCEL. This feature allows one to find a specific result for a cell by adjusting the value of any other cell by solving iteratively the sequence of nonlinear equations. The goal cell (mass velocity of oil) was set to 2.7 by changing the \(j\) cell value (see Fig. 6).
Table 5. Local optima for the reactor network optimization [12]

<table>
<thead>
<tr>
<th>Variables</th>
<th>Local 1</th>
<th>Local 2</th>
<th>Local 3</th>
<th>Local 4</th>
<th>Global</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
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<td>5.097112</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0.374617</td>
<td>0.386745</td>
<td>0.388102</td>
<td>0.388811</td>
<td></td>
</tr>
</tbody>
</table>

The EXCEL Solver was then used to find the best value of $F_{\theta}$ to minimize the total annualized cost. The initial value of $F_{\theta}$ was set to $5 \times 10^{-4}$ and the optimum one was $1.25 \times 10^{-3}$ which corresponds to a minimum TAC of $41,386/yr. In [11] an optimum of $41,560/yr was found by trying several initial values of $F_{\theta}$ until a minimum TAC was identified.

By limiting the search space for $F_{\theta}$ with upper and lower bounds, the EXCEL Solver converges to the optimum irrespectively of the initial value for this parameter. A previous attempt without these bounds, and using only the constraint on mass velocity of oil, was too sensitive to the initial value of $F_{\theta}$.

Example 4: Design of a chemical reaction network

The optimal way to solve network problems is by specifying binary variables that multiply in an appropriate (logical) way the continuous variables, such that nonexistent units (corresponding to a zero binary variable associated with that unit) are treated with mathematical consistency. Thus, a network problem becomes a mixed integer nonlinear programming (MINLP) problem. However, there are many examples of such problems that are specified as pure nonlinear programming (NLP) problems, e.g. Fig. 7 [12].

The reactions are first order, the reactors are perfectly mixed (steady-state) and there is no variation in density of the reacting mixture. The problem may be formulated as follows:

$$F_{obj} = \max \{ C_{B9} \} = \max \left\{ \frac{F_5 C_{B5} + F_6 C_{B6}}{F_9} \right\}$$

subject to:

$$F_1 + F_2 - F_0 = 0$$
$$F_1 + F_8 - F_3 = 0$$
$$F_2 + F_7 - F_4 = 0$$
$$F_3 + F_7 - F_5 = 0$$
$$F_6 + F_8 - F_4 = 0$$
$$F_1 C_{A0} + F_3 C_{A6} - F_3 C_{A3} = 0$$
$$F_1 C_{B0} + F_5 C_{B6} - F_3 C_{B3} = 0$$
$$F_2 C_{A0} + F_5 C_{A5} - F_3 C_{A4} = 0$$
$$F_2 C_{B0} + F_5 C_{B5} - F_3 C_{B4} = 0$$
$$F_3 (C_{A3} - C_{A5}) - k_1 V_1 C_{A5} = 0$$
$$F_3 (C_{B3} - C_{B5}) + (k_2 C_{A5} - k_3 C_{B5}) V_1 = 0$$
$$F_4 (C_{A4} - C_{A6}) - k_2 V_2 C_{A6} = 0$$
$$F_4 (C_{B4} - C_{B6}) + (k_2 C_{A6} - k_3 C_{B6}) V_2 = 0$$
$$k_1 = 0.09755988 \ h^{-1}$$
$$k_2 = 0.99 k_1 \ h^{-1}$$
$$k_3 = 0.0391908 k_1 \ h^{-1}$$
$$k_4 = 0.90 k_1 \ h^{-1}$$
$$C_{A0} = 1 \ kg.m^{-3}$$
$$C_{B0} = 0 \ kg.m^{-3}$$
$$F_0 = 1 \ m^3.h^{-1}$$

and to the inequality constraints:

$$0 \leq F_i \leq 1 \ (volumetric \ flow \ rates, \ m^3.h^{-1});$$
$$i = 1, \ldots, 9$$

$$0 \leq C_{Ai}, C_{Bi} \leq 1 \ (concentrations, \ kg.m^{-3});$$
$$i = 1, \ldots, 9$$

$$0 \leq V_i \leq 16 \ (reactor \ volumes, \ m^3);$$
$$i = 1, 2$$

$$V_i^{0.3} + V_j^{0.3} \leq 4$$

The $k_i$ are 1st order rate constants.

This problem has 5 degrees of freedom, and a decomposition algorithm can be employed to optimize the simulation step [13]. A sequential

Table 6. Comparison between GAMS and the EXCEL Solver for the reactor network optimization

<table>
<thead>
<tr>
<th>Starting point</th>
<th>Lower bounds $(10^{-3})$</th>
<th>Upper bounds</th>
<th>Midpoints</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>GAMS Solvers:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MINOS</td>
<td>Local2</td>
<td>Local3</td>
<td>Global</td>
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<tr>
<td>MINOS5</td>
<td>Local4</td>
<td>Local3</td>
<td>Local3</td>
</tr>
<tr>
<td>SNOPT</td>
<td>Local2</td>
<td>Local2</td>
<td>Local4</td>
</tr>
<tr>
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<td>Global</td>
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<td>Global</td>
</tr>
<tr>
<td>CONOPT2</td>
<td>Global</td>
<td>Local4</td>
<td>Local4</td>
</tr>
<tr>
<td><strong>EXCEL Solver:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Quasi-Newton</td>
<td>Non-feasible</td>
<td>Global</td>
<td>Global</td>
</tr>
<tr>
<td>Conjugate gradient</td>
<td>Non-feasible</td>
<td>Local3</td>
<td>Global</td>
</tr>
</tbody>
</table>
solution is not possible, no matter what the choice of decision variables, and several solutions with a subsystem of a minimum of 4 equations were encountered [14]. This subsystem is linear and readily solved. However, since in this example we compare the results obtained by the EXCEL Solver to the optimizers available within GAMS [15], the full nonlinear set of equations was solved as an alternative. The problem was solved starting from 3 different solution vectors, corresponding respectively to the lower bounds (assumed \(10^{-2}\) in order to avoid numerical difficulties with the optimizers), to the upper bounds and to the midpoints of the search intervals. Table 5 demonstrates the four local optima obtained by [12] using a systematic search coupled with deterministic algorithms for some selected variables corresponding to the 5 degrees of freedom. Also shown is another local optima obtained with GAMS in a previous study [14], which simply corresponds to no reaction and to the closure of the mass balances (Table 6). Thus, in only 27% of the runs was the global optimum obtained with the algorithms available within GAMS. The EXCEL Solver found it in 50% of the runs. However, GAMS could always find some local optimum, while the EXCEL Solver failed to find feasible solutions in 33% of the runs, irrespective of the options available (derivatives and step sizes). This behavior cannot be extrapolated to other problems, and many more examples are required to compare these solvers.

This example also demonstrates how the Excel Solver may handle floating point exceptions (violations on the equality or inequality mathematical domain, viz., divisions by zero and forbidden arguments of transcendental functions). This may be simply circumvented by checking for forbidden operations or values before the expression is evaluated. If a violation occurs, a flag is enforced and the objective function is penalized directly, and avoids premature stoppage of the optimization procedure. This approach may be easily verified by downloading Example 4 and specifying as initial vector \([10^{-2}, \ldots, 10^{-2}]^T\) in both worksheets available.

**CONCLUSIONS**

The problems analyzed in this paper are of sufficient complexity to allow the observation of some convergence problems within the EXCEL Solver. The solution may be dependent on the initialization and is in general a local optimum. Since the optimizers within the EXCEL environment are local search algorithms [7], convergence to the global optimum is only guaranteed with convex problems. This is also applicable to the nonlinear optimizers available within GAMS [15]. However, initializations that correspond to reasonable and practical designs generally progress towards feasible and locally optimal solutions.

The EXCEL Solver is not as good as robust global optimizers [14]. However, it does provide an integrated framework for problem setting, visualization, inspection and solving of particular utility for practicing engineers. The ease with which these and similar process problems can be formulated and solved within the Excel environment constitutes a major step towards teaching practical optimization and design concepts, ultimately benefiting students with knowledge acquisition procedures and later in an effortless continuing practice throughout careers.

Despite these benefits, the use of modular simulators such as ASPEN Plus is probably warranted for complex processes that need detailed stage calculations and extensive use of physical and thermodynamic data libraries.

All these Excel workbook files and other examples are available for download on the Internet at www.deb.uminho.pt/ecferreira/download.

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