Many practical problems in chemical engineering give rise to the need to solve systems of nonlinear algebraic equations (NLE). Typical examples include phase equilibrium and chemical equilibrium computations, steady state process simulation, flow distribution in pipeline networks, etc. Nowadays powerful mathematical software packages are available for solving systems of NLEs. Cutlip and Shacham,\textsuperscript{[1]} for example, demonstrate the use of the POLYMATH,\textsuperscript{[2]} and MATLAB\textsuperscript{[3]} software packages and the Excel\textsuperscript{[4]} spreadsheet for solving various NLE systems encountered in undergraduate and graduate chemical engineering education.

The availability of the powerful software packages and solved textbook examples that utilize these packages may be sufficient to enable students to tackle many ChE problems associated with solution of NLE systems. However, even if the students follow exactly the instructions of the NLE solver packages and the textbook examples, they still may find that using a particular problem formulation and a set of initial guesses for the unknowns, a solution is not reached and the program issues error messages (e.g., “division by zero”). Our experience has shown that to deal with such a situation, students need to learn to analyze the equation set and modify it, if necessary, to enable convergence to the solution. The objective of this paper is to present the analysis and the systematic modification process, along with examples that we have been using to educate students in the framework of mathematical modeling and numerical methods courses.

Even though there are so-called “globally convergent” methods for finding a solution (besides the trivial case of errors in the problem formulation) is the presence of discontinuities and/or regions where some of the functions are undefined.\textsuperscript{[6]} The impact of such discontinuities becomes most severe if they lie in the vicinity of the solution. Analysis of the system of NLEs in order to locate the discontinuities and the boundaries of the regions where some functions are undefined, is a much more complex task than finding a solution. The objective here is to propose and demonstrate a procedure for reformulating the NLE system so as to increase the probability of finding a solution and at the same time speeding up the solution process.

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DEFINITION OF EXAMPLE PROBLEM 1

The first example is the “VLE: Wilson’s Equation” problem provided in the LearnChemE website. In this example the bubble point temperature and the vapor phase composition of a non-ideal binary mixture have to be found using the modified Raoult’s law and the Wilson equation. The equations that need to be solved are shown in Table 1. There are 10 nonlinear equations with 10 unknowns: \( P_1^{\text{sat}} \) and \( P_2^{\text{sat}} \) (kPa) – saturation pressure values for components 1 and 2, \( T \) – temperature (K), \( y_1 \) and \( y_2 \) – mole fraction of components 1 and 2 in the gas phase, \( \gamma_1 \) and \( \gamma_2 \) – activity coefficients, and \( W, \Lambda_{12}, \Lambda_{21} \) – the Wilson parameters. In addition, the data provided include the liquid mole fraction of the first compound \( (x_0 = 0.85) \), pressure \( (P = 100 \text{kPa}) \) and the values of the Wilson parameters: \( a_{12} = 440 \text{cal/mol}, a_{21} = 1250 \text{cal/mol}, V_1 = 77 \text{cm}^3/\text{mol}, \) and \( V_2 = 18 \text{cm}^3/\text{mol}. \)

The equations in Table 1 are all written in the implicit form of \( f(x) = 0 \), of 10 equations with 10 unknowns. There are several mathematical software packages that can be used for solving such a system of equations. LearnChemE recommends the use of the POLYMATH. Introducing the equations of Table 1 into POLYMATH requires some changes in the notation as POLYMATH does not accept Greek letters, subscripts, and superscripts (the variable names as entered into POLYMATH are shown in Table 2). Additionally, the names of the constants and their numerical values, and initial guesses for the expected values of the 10 unknowns at the solution, need to be entered into POLYMATH.

The complete POLYMATH program for solving this problem is available at the website: <www.learncheme.com/student-resources/polymath>.

The solution obtained by POLYMATH for this problem is shown in Table 2. The results presented by POLYMATH include the names and values of the constants, the names, initial guesses, the values at the solution \( (x^*) \), and the value of \( f(x^*) \) at the solution for all the unknowns. Observe that all the function values are very close to zero (between \( 0 – 1.71\times10^{-12} \), in absolute value), thus at the solution all the implicit equations are satisfied with high accuracy. Initial guesses were entered for all 10 unknowns. For some of the variables (like \( P_1^{\text{sat}} \) and \( P_2^{\text{sat}} \), \( T, y_1 \), and \( y_2 \)) good initial estimates can be determined based on physical considerations, but for others (the Wilson’s equation parameters) this task is more difficult. Observe, for example, that the initial guess given for \( W \) is positive, while at the solution it attains a negative value. Providing inappropriate initial guesses may cause failure of the solution algorithm. Using some negative values as an initial estimate for A12 (such as \(-0.05\)) leads to an error message related to an attempt to calculate the logarithm of a negative number.

In the following section a systematic

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Equation set for Example 1: VLE – Wilson’s formulated as a system of 10 implicit NLE (source: LearnChemE website)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eq. No.</td>
<td>Equations</td>
</tr>
<tr>
<td>1</td>
<td>( f_1 = \ln(P_1^{\text{sat}}) - 17 + 3600/(T - 54) = 0 )</td>
</tr>
<tr>
<td>2</td>
<td>( f_2 = \ln(P_2^{\text{sat}}) - 16.5 + 3850/(T - 47) = 0 )</td>
</tr>
<tr>
<td>3</td>
<td>( f_3 = x_1 y_1 P_1^{\text{sat}} - y_1 P = 0 )</td>
</tr>
<tr>
<td>4</td>
<td>( f_4 = x_2 y_2 P_2^{\text{sat}} - y_2 P = 0 )</td>
</tr>
<tr>
<td>5</td>
<td>( f_5 = 1 - y_1 - y_2 = 0 )</td>
</tr>
<tr>
<td>6</td>
<td>( f_6 = \ln(\gamma_1) + \ln(x_1 + x_2 A_{12}) - x_2 W = 0 )</td>
</tr>
<tr>
<td>7</td>
<td>( f_7 = \ln(\gamma_2) + \ln(x_1 A_{21} + x_2) + x_1 W = 0 )</td>
</tr>
<tr>
<td>8</td>
<td>( f_8 = W - \frac{A_{12}}{x_1 + x_2 A_{12}} + \frac{A_{21}}{x_1 A_{21} + x_2} = 0 )</td>
</tr>
<tr>
<td>9</td>
<td>( f_9 = A_{12} - \frac{V_2}{V_1} \exp\left(-\frac{a_{12}}{RT}\right) = 0 )</td>
</tr>
<tr>
<td>10</td>
<td>( f_{10} = A_{21} - \frac{V_1}{V_2} \exp\left(-\frac{a_{21}}{RT}\right) = 0 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Results presented by POLYMATH for example problem 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Variables (Unknowns)</td>
</tr>
<tr>
<td></td>
<td>f(x)</td>
</tr>
<tr>
<td>1</td>
<td>G12</td>
</tr>
<tr>
<td>2</td>
<td>G21</td>
</tr>
<tr>
<td>3</td>
<td>gamma1</td>
</tr>
<tr>
<td>4</td>
<td>gamma2</td>
</tr>
<tr>
<td>5</td>
<td>P1sat</td>
</tr>
<tr>
<td>6</td>
<td>P2sat</td>
</tr>
<tr>
<td>7</td>
<td>T</td>
</tr>
<tr>
<td>8</td>
<td>W</td>
</tr>
<tr>
<td>9</td>
<td>y1</td>
</tr>
<tr>
<td>10</td>
<td>y2</td>
</tr>
</tbody>
</table>
NORTHERN AFGHANISTAN: 
ANALYSIS OF SOIL PROPERTIES AND THEIR IMPACT ON AGRICULTURAL YIELD

INTRODUCTION

The soil properties in Northern Afghanistan play a crucial role in determining the agricultural yield. This study aimed to analyze the soil properties and their impact on agricultural yield in the region.

METHODS

Soil samples were collected from different locations in Northern Afghanistan. The soil properties such as texture, pH, organic matter content, and available nutrients were determined using standard laboratory procedures. The agricultural yield was measured using the harvest data from various crops.

RESULTS

The results showed that the soil texture varied from sandy loam to clay loam, with the majority being sandy loam. The pH values ranged from 6.5 to 7.5, indicating a neutral to slightly alkaline soil. The organic matter content was found to be low, ranging from 0.5% to 1.5%. The available nutrients were also found to be low, with nitrogen ranging from 0.1 to 0.3% and phosphorus from 0.01 to 0.05%.

DISCUSSION

The low nutrient availability and organic matter content may be contributing to the low agricultural yield in the region. Improving soil fertility through the application of organic amendments and fertilizers is recommended to enhance the agricultural yield.

CONCLUSIONS

The soil properties in Northern Afghanistan need improvement to increase the agricultural yield. Further research is needed to develop effective strategies for soil fertility improvement.

REFERENCES


Acknowledgements

This study was supported by the Ministry of Agriculture, Forestry and Fisheries of Japan, and the University of Tokyo.
has to be specified and they are denoted as “tear” variables. In this particular example the variable T is a single input variable in four explicit equations, consequently it is designated as a “tear” variable. Assigning a trial value for T enables calculating the output variables: \( P_{1}^{\text{sat}} \) (Eq. 1), \( P_{2}^{\text{sat}} \) (Eq. 2), \( \Lambda_{12} \) (Eq. 9) and \( \Lambda_{21} \) (Eq. 10). These operations are recorded in the computation sequence: (T) 1, 2, 9, 10 indicating that T is the tear variable, and upon assigning a value to T, the explicit Equations 1, 2, 9, 10 can be solved in the order specified.

In step 2 of the sequencing procedure the equations that were already included in the computational sequence are removed from the table, and the input variables that were calculated in the previous step are marked (in bold letters). Observe that the two input variables to Eq. 8 are known. Consequently the output variable W can be calculated and Eq. 8 can be added to the calculation sequence. With the known W value, the output variables \( \gamma_{1} \) and \( \gamma_{2} \) can be calculated from Eqs. 6 and 7, respectively (step 3 in Table 4), whereby these equations can be added to the computation sequence. In the last step (4) the variables \( y_{1} \) and \( y_{2} \) are calculated from the explicit Eqs. 3 and 4, and finally the value of \( f(T) \) is calculated from Eq. 5, yielding the final computation sequence: (T) 1, 2, 9, 10, 8, 6, 7, 3, 4, 5(f(T)). This way the system of 10 equations and 10 unknowns can be easily solved, as there is only one implicit equation with one unknown: T.

**Stage 4.** In Figure 1 the function value of the revised NLE system (Eq. 5 in Table 5) in the 200 K – 400 K temperature range is shown. Observe that there is only one root (with \( f(T) = 0 \)) in the region of interest. The numerical value of T at the solution is 344.2265 K, with \( f(T) = -1.535e-11 \). Using this T value the explicit equations in Table 5 provide the values of the rest of the unknowns at the solution. Introducing these unknown values into the original (implicit) set of NLE in Table 1 yields function absolute values in the range of 0 – 1.77e-17. Thus, the revised system of equations and the solution

![Figure 1. Function value (Eq. 5 in Table 5) in the 200 K – 400 K temperature range.](image)

**TABLE 4**

<table>
<thead>
<tr>
<th>Computation sequencing with the variable mapping table</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Step 1.</strong> Computation sequencing with the variable mapping table</td>
</tr>
<tr>
<td>Input Variable/s</td>
</tr>
<tr>
<td>------------------</td>
</tr>
<tr>
<td>T</td>
</tr>
<tr>
<td>T</td>
</tr>
<tr>
<td>( \gamma_{1}, P_{1}^{\text{sat}} )</td>
</tr>
<tr>
<td>( \gamma_{2}, P_{2}^{\text{sat}} )</td>
</tr>
<tr>
<td>( y_{1}, y_{2} )</td>
</tr>
<tr>
<td>( A_{12}, W )</td>
</tr>
<tr>
<td>( A_{21}, W )</td>
</tr>
<tr>
<td>( A_{12}, A_{21} )</td>
</tr>
<tr>
<td>T</td>
</tr>
<tr>
<td>T</td>
</tr>
<tr>
<td>Computational sequence: (T) 1, 2, 9,10</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Step 2.</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda_{12}, \Lambda_{21} )</td>
</tr>
<tr>
<td>Computational sequence: (T) 1, 2, 9,10, 8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Step 3.</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda_{12}, W )</td>
</tr>
<tr>
<td>( \Lambda_{21}, W )</td>
</tr>
<tr>
<td>Computational sequence: (T) 1, 2, 9,10, 8, 6, 7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Step 4.</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>( \gamma_{1}, P_{1}^{\text{sat}} )</td>
</tr>
<tr>
<td>( \gamma_{2}, P_{2}^{\text{sat}} )</td>
</tr>
<tr>
<td>( y_{1}, y_{2} )</td>
</tr>
<tr>
<td>Compt. sequence: (T) 1, 2, 9,10, 8, 6, 7, 3, 4, 5(f(T))</td>
</tr>
</tbody>
</table>
The objective here is to propose and demonstrate a procedure for reformulating the NLE system to increase the probability of finding a solution and at the same time speeding up the solution process.

DEFINITION OF EXAMPLE PROBLEM 2

This example involves calculation of reaction equilibrium by minimization of the Gibbs energy. The example was introduced by Balzisher, et al.\(^8\) and is discussed in detail by Cutlip and Shacham.\(^1^1\) Ethane is steam cracked to form hydrogen over a cracking catalyst at temperature \(T = 1000\) K and pressure of \(P = 1\) atm. The feed contains 4 moles of \(\text{H}_2\text{O}\) per mole of \(\text{C}_2\text{H}_6\). It is assumed\(^8\) that only the compounds 1. \(\text{CH}_4\), 3. \(\text{C}_2\text{H}_6\), 4. \(\text{CO}_2\), 5. \(\text{CO}\), 6. \(\text{O}_2\), 7. \(\text{H}_2\), 8. \(\text{H}_2\text{O}\) and 9. \(\text{C}_2\text{H}_4\) are present in the equilibrium mixture (assuming that no carbon is deposited). The Gibbs energies of formation of the various compounds at the reaction temperature of 1000 K are available in the reference.\(^1^1\) Example problem 2 involves the calculation of the equilibrium composition of the effluent mixture.

The solution of this problem involves the minimization of the total Gibbs energy given by

\[
\min \frac{G}{RT} = \sum_{i=1}^{c} n_i \left( \frac{G_i^0}{RT} + \ln \left( \frac{n_i}{n_1} \right) \right) \tag{2.1}
\]

where \(n_i\) is the number of moles of component \(i\), \(c\) is the total number of compounds, \(R\) is the gas constant and \(G_i^0\) is the Gibbs energy of pure component \(i\) at temperature \(T\). The minimization of Eq. (2.1) is carried out subject to atom balance constraints:

- Oxygen balance \(g_1 = 2n_O + n_H + 2n_O + n_H - 4 = 0\) \tag{2.2}
- Hydrogen balance \(g_2 = 4n_H + 4n_H + 2n_O + 2n_O + 6n_O - 14 = 0\) \tag{2.3}
- Carbon balance \(g_3 = n_C + 2n_C + 2n_C + n_C + 2n_C - 2 = 0\) \tag{2.4}

where \(n_i\) represents amount (moles) of a compound \(i\) (\(i\) corresponds to the component number provided in the list above). The three constraints can be introduced into the objective functions using Lagrange multipliers: \(\lambda_1, \lambda_2,\) and \(\lambda_3\). The extended objective function is

\[
\min F = \sum_{i=1}^{c} n_i \left( \frac{G_i^0}{RT} + \ln \left( \frac{n_i}{n_1} \right) \right) + \lambda_1 g_1 + \lambda_2 g_2 + \lambda_3 g_3 \tag{2.5}
\]

The condition for minimum of this function at a particular point is that all the partial derivatives of \(F\) with respect to \(n_i\) and \(\lambda\) vanish at this point. Taking the derivatives of Eq. (2.5) and putting them in a POLYMATH program, together with Eqs. (2.2), (2.3), and (2.4) and initial estimates for all the unknown \(n_i\) yields the program shown in Table 6 (next page). The POLYMATH model (including the “comments,” which start with the # sign) provides complete documentation of the equations, the values of the constants, and the initial estimates used for the 12 unknowns. The 12 implicit algebraic equations [associated with Eqs. (2.2), (2.3), and (2.4) and the nine partial derivatives of \(F\) in Eq.(2.5)] are shown in rows 3 through 14 of Table 6. It is assumed that at the solution these equations should be equal to zero. For the sake of clarity, in the POLYMATH input the \(n_i\) is represented by the formula of the compound. Initial estimates for the 12 unknowns are specified in rows 16 through 27. Those are based on the values suggested by Balzisher, et al.,\(^8\) and Cutlip and Shacham.\(^1^1\)

This system of equations is very difficult to solve as the functions are undefined for \(n_i \leq 0\) and for some of the compounds the amount in the effluent is very close to zero. Non-constrained equation solvers may overstep the zero value, requiring calculation of the logarithm of a negative value, which stops the computation. With constrained equation solvers it is difficult to determine how close to zero the constraints should be specified. If the constraints are set too far from a zero value, incorrect results may be obtained. Cutlip and Shacham attempted to solve this system of equations using the POLYMATH,

<table>
<thead>
<tr>
<th>Table 5</th>
<th>Equation set of Example 1 rewritten as a system of 9 explicit and 1 implicit NLEs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eq. No.</td>
<td>Equations</td>
</tr>
<tr>
<td>1</td>
<td>(P_1^{\text{Sat}} = \exp[17 - 3600/(T - 54)])</td>
</tr>
<tr>
<td>2</td>
<td>(P_2^{\text{Sat}} = \exp[16.5 - 3850/(T - 47)])</td>
</tr>
<tr>
<td>9</td>
<td>(A_{12} = \frac{V_1}{V_i} \exp \left(-\frac{a_{12}}{RT} \right))</td>
</tr>
<tr>
<td>10</td>
<td>(A_{21} = \frac{V_1}{V_2} \exp \left(-\frac{a_{21}}{RT} \right))</td>
</tr>
<tr>
<td>8</td>
<td>(W = \frac{A_{12}}{(x_1 + x_5 A_{12})} - \frac{A_{21}}{(x_1 A_{21} + x_2)})</td>
</tr>
<tr>
<td>6</td>
<td>(y_1 = \exp(x_2 W)/(x_1 + x_5 A_{12}))</td>
</tr>
<tr>
<td>7</td>
<td>(y_2 = \exp(x_2 W)/(x_1 A_{21} + x_2))</td>
</tr>
<tr>
<td>3</td>
<td>(y_1 = x_1 y_1 P_1^{\text{Sat}} / P)</td>
</tr>
<tr>
<td>4</td>
<td>(y_2 = x_1 y_2 P_2^{\text{Sat}} / P)</td>
</tr>
<tr>
<td>5</td>
<td>(f_1 = y_1 + y_2 - 1 = 0)</td>
</tr>
</tbody>
</table>

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MATLAB, and Excel packages. None of the programs was able to solve the problem in the form it is presented in Table 6. Solution of the problem was obtained in a “trial and error” process, where the particular equation that caused the failure was modified in order to enable further progress of the solution process.

REARRANGEMENT AND SOLUTION OF EXAMPLE PROBLEM 2

Stage 1. The regions where the functions are undefined can be eliminated by modifying the equations in rows 6 through 14 (Table 6) so that the calculations of logarithms of very small numbers are avoided. Essentially, the modification involves replacement of the logarithm operation with exponentiation. For example, the equation in row 6 of Table 6 can be replaced by the following equation: 

\[ CH_4 = \exp(-4.61/R - 4 \times \text{lamda2} - \text{lamda3})\times \text{sum} \]

Another modification that can be very beneficial is the replacement of the explicit equation for calculating \( \text{sum} \) by an implicit equation: 

\[ f(\text{sum}) = \text{sum} - (H_2 + O_2 + CO + CO_2 + CH_4 + C_2H_6 + C_2H_4 + C_2H_2) \]

This modification enables the selection of output variables from several implicit equations, which would be otherwise impossible.

Stage 2 and 3. Unique output variables can be selected for nine out of the (now) 13 equations. Upon selecting \( \lambda_1, \lambda_2, \) and \( \lambda_3 \) as output variables, \( H_2O, H_2, CO \) and \( \text{sum} \) need to be selected as “tear” variables. With these tear variables the remaining nine explicit equations can be sequenced following the route outlined in Example 1. The reformulated and rearranged equation set is shown in Table 7. Observe that in this case initial estimates are needed only for four variables (the initial estimates values shown in Table 6 were used). Using this formulation, a converged solution (Table 8) was obtained by POLYMATH, MATLAB, and Excel without any difficulties.

With POLYMATH the safenewt algorithm was used for the solution. This algorithm is based on the newt subroutine provided by Press, et al.\(^5\) It uses the Newton-Raphson method with line search to ensure reduction of the norm of the function values in every iteration. For solution with MATLAB the fsolve function was used. In this function one of the available methods: the trust-region dogleg method (based on Powell’s dogleg method)\(^9\) was utilized. Using the Excel’s Solver to solve the problem, the sum of squares of the function values is minimized using the GRG\(^10\) (Generalized Reduced Gradient) method. Identical solutions were obtained by the three software tools.

Stage 4. Introducing the variable values shown in Table 8 into the original equations of Table 6 yields function absolute values in the range of 4.44e-16 – 1.37e-13. Thus the revised system is identical to the original one. A MATLAB program: GibbsEnergy.m, that solves the revised NLE system and introduces the solution into the original system is available at <ftp://ftp.bgu.ac.il/shacham/NLE_CEE16/>.

USING THE EXAMPLES IN THE CLASSROOM

The subject of numerical solution of NLE systems is included in the Numerical Methods 3rd-year required course
and in the Process Simulation 4th-year elective course for undergraduate chemical engineering students at the Ben-Gurion University of the Negev. The Numerical Methods course is described in some detail by Shacham, et al.\(^{11}\) and the Process Simulation course is described in detail by Shacham.\(^{12}\) The procedure for reformulation and rearrangement of NLE systems is discussed in class and occasionally homework assignments related to this issue are given. Examples for “difficult to solve” NLE systems are usually taken from References 6 and 13. The examples presented here have been recently added to the assignments of these courses.

CONCLUSIONS

The examples presented here demonstrate that the solution of some NLE systems may represent a challenge even if the problem formulation is correct and state of the art “globally convergent” methods are used for solution.

It has been shown that the proposed method for reformulation and rearrangement of the NLE systems can reduce the dimension of the system, remove discontinuities, and considerably simplify the task of finding initial estimates for the unknowns so that solution is obtained. This is demonstrated in particular in example 2: by following the proposed procedure, three software packages (POLYMATH, MATLAB, and Excel) were able to find the solution from the same initial estimate that caused them to fail with the original problem formulation.

This material can be very helpful for undergraduate and graduate students and practicing engineers who are involved in mathematical modeling, which often requires solution of nonlinear equations.

REFERENCES

2. POLYMATH is a product of Polymath Software (<http://www.polymath-software.com>)
3. MATLAB is a trademark of The Math Works, Inc. (<http://www.mathworks.com>)
4. Excel is a trademark of Microsoft Corporation (<http://www.microsoft.com>)

### TABLE 7

<table>
<thead>
<tr>
<th>No.</th>
<th>Equation # Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>R = 1.9872</td>
</tr>
<tr>
<td>2</td>
<td>( f(\text{sum}) = \text{sum} - (H2 + O2 + H2O + CO + CO2 + CH4 + C2H6 + C2H4 + C2H2) )</td>
</tr>
<tr>
<td>3</td>
<td>( f(H2O) = 2 * CO2 + CO + 2 * O2 + H2O - 6 ) # Oxygen balance</td>
</tr>
<tr>
<td>4</td>
<td>( f(H2) = 4 * CH4 + 4 * C2H4 + 2 * CH2 + 2 * H2 + 2 * H2O + 6 * C2H6 - 14 ) # Hydrogen balance</td>
</tr>
<tr>
<td>5</td>
<td>( f(CO) = CH4 + 2 * C2H4 + 2 * C2H2 + CO2 + CO + 2 * C2H6 - 2 ) # Carbon balance</td>
</tr>
<tr>
<td>6</td>
<td>( \lambda_2 = -\ln(H2 / \text{sum}) / 2 )</td>
</tr>
<tr>
<td>7</td>
<td>( \lambda_1 = 46.03 / R - (\ln(H2O / \text{sum}) + 2 * \lambda_2) )</td>
</tr>
<tr>
<td>8</td>
<td>( \lambda_3 = 47.942 / R - (\ln(CO / \text{sum}) + \lambda_1) )</td>
</tr>
<tr>
<td>9</td>
<td>( CH4 = \exp(-4.61 / R - 4 * \lambda_2 - \lambda_3) ) * ( \text{sum} )</td>
</tr>
<tr>
<td>10</td>
<td>( C2H4 = \exp(-28.249 / R - 4 * \lambda_2 - 2 * \lambda_3) ) * ( \text{sum} )</td>
</tr>
<tr>
<td>11</td>
<td>( C2H2 = \exp(-40.604 / R - 2 * \lambda_2 - 2 * \lambda_3) ) * ( \text{sum} )</td>
</tr>
<tr>
<td>12</td>
<td>( CO2 = \exp(94.61 / R - 2 * \lambda_1 - \lambda_3) ) * ( \text{sum} )</td>
</tr>
<tr>
<td>13</td>
<td>( O2 = \exp(-2 * \lambda_1) ) * ( \text{sum} )</td>
</tr>
<tr>
<td>14</td>
<td>( C2H6 = \exp(-26.13 / R - 6 * \lambda_2 - 2 * \lambda_3) ) * ( \text{sum} )</td>
</tr>
<tr>
<td>15</td>
<td># Initial estimates</td>
</tr>
<tr>
<td>16</td>
<td>sum(0)=8</td>
</tr>
<tr>
<td>17</td>
<td>CO(0)=1</td>
</tr>
<tr>
<td>18</td>
<td>H2(0)=5.992</td>
</tr>
<tr>
<td>19</td>
<td>H2O(0)=1</td>
</tr>
</tbody>
</table>

### TABLE 8

<table>
<thead>
<tr>
<th>Variables (Implicit Equations)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
</tr>
<tr>
<td>------</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables (Explicit Equations)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
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<tr>
<td>------</td>
</tr>
<tr>
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</tr>
<tr>
<td>6</td>
</tr>
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<td>12</td>
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<tr>
<td>13</td>
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<tr>
<td>14</td>
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</tbody>
</table>

APPENDIX A

Examples of Equation Modification for Discontinuity Removal

In Table A-1 three pairs of equations are presented where the first equation in the pair contains discontinuity and the second equation in the pair is in a modified form, where the discontinuity has been removed. For example in Eq. (1.1), due to the division by \((1-x)\), the function is undefined for \(x = 1\). This discontinuity is removed upon multiplying the two terms of the equation by \((1-x)\), Eq. 1.2. It can be seen that the solution of the two versions of the NLE are identical.

TABLE A-1

<table>
<thead>
<tr>
<th>No.</th>
<th>Function</th>
<th>Undefined for</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>(f(x) = 2x^2 - 1/(1-x) = 0)</td>
<td>(x = 1)</td>
<td>-0.5651977</td>
</tr>
<tr>
<td>1.2</td>
<td>(f(x) = 2x^2 - (1-x) - 1 = 0)</td>
<td>-</td>
<td>-0.5651977</td>
</tr>
<tr>
<td>2.1</td>
<td>(f(x) = x/5 - \ln(x) = 0)</td>
<td>(x \leq 0)</td>
<td>12.71321</td>
</tr>
<tr>
<td>2.2</td>
<td>(f(x) = \exp(x/5) - x = 0)</td>
<td>-</td>
<td>12.71321</td>
</tr>
<tr>
<td>3.1</td>
<td>(f(x) = x/5 - (x+2))</td>
<td>(x \leq -2)</td>
<td>26.86141</td>
</tr>
<tr>
<td>3.2</td>
<td>(f(x) = (x/5)^2 - (x+2) = 0)</td>
<td>-</td>
<td>26.86141</td>
</tr>
</tbody>
</table>