**Iteration Concept**

Let's use a simple example of a cubic equation to illustrate the iteration concept. Although this example equation can be factor to reveal its three roots, we will examine it from a graphical viewpoint to see how manual iterations are done.

**Cubic Equation Example:**

\[
\frac{1}{4}x^3 + \frac{3}{4}x^2 - \frac{3}{2}x - 2 = 0
\]

\[
\frac{1}{4}(x + 4)(x + 1)(x - 2) = 0
\]

Thus, roots of -4, -1, and 2

Iteration can be done on a scalar or single variable (i.e., one algebraic equation in one unknown), or it can be done on a vector of variables (i.e., "n" algebraic equations with "n" unknowns, where "n" is the number of unknowns). For either case, two iteration forms exists: “ \( f(x) = 0 \)” and “ \( g(x) = x \)”.

**Scalar Iteration Variable:**

In scalar iteration, one unknown variable is iterated on in one algebraic equation.

<table>
<thead>
<tr>
<th>( f(x) = 0 ) Iteration Form</th>
<th>( g(x) = x ) Iteration Form</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ITERATE</strong> ( x ) <strong>IN</strong></td>
<td><strong>ITERATE</strong> ( x ) <strong>IN</strong></td>
</tr>
<tr>
<td>( f(x) \leftarrow \frac{1}{4}x^3 + \frac{3}{4}x^2 - \frac{3}{2}x - 2 )</td>
<td>( g(x) \leftarrow \frac{1}{6}x^3 + \frac{1}{2}x^2 - \frac{2}{3}x )</td>
</tr>
<tr>
<td><strong>UNTIL</strong> ( f(x) = 0 )</td>
<td><strong>UNTIL</strong> ( g(x) = x )</td>
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**Vector Iteration Variable:**

Vector iteration is similar to scalar iteration; however, "n" unknown variables are simultaneously iterated on in "n" algebraic equations.

<table>
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<tbody>
<tr>
<td><strong>ITERATE</strong> ( \bar{x} ) <strong>IN</strong></td>
<td><strong>ITERATE</strong> ( \bar{x} ) <strong>IN</strong></td>
</tr>
<tr>
<td>( f_1(\bar{x}) \leftarrow \text{expression}_1 )</td>
<td>( g_1(\bar{x}) \leftarrow \text{expression}_1 )</td>
</tr>
<tr>
<td>( f_2(\bar{x}) \leftarrow \text{expression}_2 )</td>
<td>( g_2(\bar{x}) \leftarrow \text{expression}_2 )</td>
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<tr>
<td>( \vdots )</td>
<td>( \vdots )</td>
</tr>
<tr>
<td>( f_n(\bar{x}) \leftarrow \text{expression}_n )</td>
<td>( g_n(\bar{x}) \leftarrow \text{expression}_n )</td>
</tr>
<tr>
<td><strong>UNTIL</strong> ( \bar{f}(\bar{x}) = 0 ) Vector form used in E-Z Solve and HYSYS</td>
<td><strong>UNTIL</strong> ( \bar{g}(\bar{x}) = \bar{x} ) Vector form used in HYSYS</td>
</tr>
</tbody>
</table>

**where** \( \bar{x} \equiv x_1, x_2, x_3, \ldots, x_n \)

In Aspen HYSYS, the vector \( f(x) \) form is used in ADJUST operators where two or more variables are iterated upon simultaneously. The vector \( g(x) \) form is used in the HYSYS RECYCLE operator to iterate on the process state of a material stream. In the ADJUST operator, the scalar \( f(x) \) form is used when iterating on a single variable and that ADJUST operator is not part of a simultaneous iteration with other ADJUST operators.
B. The \( f(x) \) and \( g(x) \) forms for the example cubic equation are shown graphically below.

How do you manually conduct the iteration technique for each of these forms?

Manually applying the \( f(x) \) iteration is just a trial-and-error procedure.

You guess a value for \( x \), calculate \( f(x) \), and examine how close \( f(x) \) is to zero. If it is not close enough to zero, then you guess another value for \( x \).

You repeat this process until \( f(x) \) is close enough to zero, and the last two guesses for \( x \) are also close enough in value.

Manually applying the \( g(x) \) iteration is called successive substitution.

You guess a value for \( x \), calculate \( g(x) \), and examine how close \( g(x) \) is to \( x \). If it is not close enough to \( x \) then you use \( g(x) \) as your next value for \( x \).

You repeat this process until \( g(x) \) is close enough to the last \( x \), and the last two guesses for \( x \) are also close enough in value.

In summary, you are guaranteed to converged to a root when you bracket that root in a \( f(x) \) iteration. However, you are not guaranteed to converged to a root in a \( g(x) \) iteration when you pick the first guess for the unknown variable. You must use the context of the problem you are solving to estimate a realistic first guess for the unknown variable. Click here to download an E-Z Solve file, open that file from within E-Z solve, and practice manually solving the cubic equation using the \( f(x) \) and \( g(x) \) iteration techniques.
C. In Aspen HYSYS, the iteration to close the mass and energy balances of a recycle loop is a g(x) form. Conceptually, what does the g(x) iteration look like on the styrene monomer flowsheet?

The process state of a material stream is defined by (nc+3) quantities, where "nc" is the number of chemical compounds in that stream. Once (nc+3) quantities are defined, all other quantities of a process stream can be determined. When doing a g(x_bar) iteration, Aspen HYSYS uses molar enthalpy, pressure, molar flow rate, and mole fractions as the x_bar for the process state to check for convergence, instead of temperature, pressure, molar flow rate, and mole fractions.
D. Why does the HYSYS Recycle operator use the molar enthalpy, pressure, molar flow rate, and mole fractions to converge the mass and energy balances of a recycle loop?

Methanol Alkylation of Toluene to produce Styrene Monomer

HYSYS Process Stream Convergence using the Recycle Block:
Why molar enthalpy, pressure, molar flow rate, and mole fractions and not temperature, pressure, molar flow rate, and mole fractions?

Hint: $nc = 1$ versus $nc > 1$; that is, the chemical mixture for a process material stream may contain only one compound or multiple compounds. Also, the mole fraction of one chemical compound in a multi-component mixture could be 1.0 while all of the rest are zero, in which case the mixture is just a pure compound.
E. Let’s examine the temperature-enthalpy (TH) diagrams for pure hexane and a hexane-octane mixture. What does the Gibbs phase rule predict about the isobars in the dome region of the two diagrams?

Gibbs Rule: \( \text{dof} = \text{nc} + P - 2 = 1+2-2 = 1 \)  
Thus, isobar is horizontal and T is constant in dome region.

For a material mixture that is just a pure chemical compound, the molar enthalpy, pressure, and mole fractions of that mixture uniquely define its material state in a HYSYS simulation.

Gibbs Rule: \( \text{dof} = \text{nc} + P - 2 = 2+2-2 = 2 \)  
Thus, isobar is not horizontal and T changes in dome region.

Click here to download and open a HYSYS file that generated the above two TH diagrams.