C.2 ACTIVITY COEFFICIENT (GAMMA-PHI) METHOD

The equation that must be solved is:

\[ y^V_i P = x^V_i \phi_i P_{i sat} \exp \left( \frac{V_i^L (P - P_{i sat})}{RT} \right) \]

Bubble P

1. Know \( x_i, T \)  
   Calc \( \phi_i P_{i sat} \). Assume modified Raoult’s law for first \( P, y_i \) calculation.

2. Calc \( \phi_i \)'s. Poynting correction.

3. \( y_i = x_i \phi_i P_{i sat} = x_i K_i \)

4. \( y_T = \sum y_i \)

5. \( y_T \) changed? Yes for first inner loop pass.  
   No

6. \( y_i = y_T/y_T \)  
   Calc \( \phi_i \) at new \( y_i \)

7. \( y_T = 1? \)
   Yes
   No

8. if \( y_T > 1, P \uparrow \)  
   if \( y_T < 1, P \downarrow \)

9. Guess \( P \)

10. Bubble \( P \) and \( y_i \) found

Inner loop can often be eliminated, and step 6 moved here.
**Bubble T**

1. Know $x_i, P$
   Assume Raoult’s law for first $T_i, y_i$ calculation.

2. Calc $\phi_i^{sat}, \gamma_i, P_i^{sat}, \phi_i^\gamma$  
   Poynting correction.

3. $y_i = \frac{x_i \gamma_i \phi_i^\gamma}{P}$

4. $y_T = \sum_{i} y_i$

5. $y_T$ changed? Yes for first inner loop pass.

6. $y_i = \frac{y_i}{y_T}$
   Calc $\phi_i^\gamma$ at new $y_i$

7. $y_T = 1$? 
   Yes
   No

8. if $y_T > 1$, $P \downarrow$
   if $y_T < 1$, $P \uparrow$

9. Guess $T$

10. Bubble $T$ and $y_i$ found

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**Dew P**

1. Know $y_i, T$
   Calc $\phi_i^{sat}, P_i^{sat}$. Assume Raoult’s law for first $P, x_i$
   calculation, then calc $\gamma_i$ at $x_i$.

2. Calc $\phi_i^\gamma$, Poynting correction.

3. $x_i = \frac{y_i \phi_i^\gamma}{\gamma_i \phi_i^{sat}}$

4. $x_T = \sum_{i} x_i$

5. $x_T$ changed? Yes for first inner loop pass.

6. $x_i = \frac{x_i}{x_T}$
   Calc $\gamma_i$ at new $x_i$

7. $x_T = 1$? 
   Yes
   No

8. if $x_T > 1$, $P \downarrow$
   if $x_T < 1$, $P \uparrow$

9. Guess $P$

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For ideal vapor mixture, inner loop not required

Inner loop can often be eliminated, and step 6 moved here.