- <u>Equações de Balanço de Massa por Componente</u>

$$\frac{dm_{i,j}}{dt} = L_{j-1} \cdot x_{i,j-1} - L_j \cdot x_{i,j} + V_{j+1} \cdot y_{i,j+1} - V_j \cdot y_{i,j}$$

sendo: $m_{i,j} = M_j \cdot x_{i,j}$ ou $x_{i,j} = \frac{m_{i,j}}{M_j} = \frac{m_{i,j}}{\sum_{i=1}^{N_C} m_{i,j}}$, para $j = 1, 2, \cdots, N \quad (j \neq N_F)$ e $i = 1, 2, \cdots, N_C$

- <u>Equações de Balanço de Energia</u>

$$\frac{d\left(M_j \cdot H_j^{(L)}\right)}{dt} = L_{j-1} \cdot H_{j-1}^{(L)} - L_j \cdot H_j^{(L)} + V_{j+1} \cdot H_{j+1}^{(V)} - V_j \cdot H_j^{(V)}$$

sendo: $H_j^{(L)} = \sum_{i=1}^{N_c} x_{i,j} \cdot h_i^{(L)}$ e $H_j^{(V)} = \sum_{i=1}^{N_c} y_{i,j} \cdot h_i^{(V)}$, para $j = 2, 3, \cdots, N-1 \quad (j \neq N_F)$.

- <u>Equações de Balanço de Massa por Componente no Prato de Alimentação</u>

$$\frac{dm_{i,N_F}}{dt} = L_{N_F-1} \cdot x_{i,N_F-1} - L_{N_F} \cdot x_{i,N_F} + V_{N_F+1} \cdot y_{i,N_F+1} - V_{N_F} \cdot y_{i,N_F} + F \cdot z_i$$

sendo: $m_{i,N_F} = M_{N_F} \cdot x_{i,N_F}$ ou $x_{i,N_F} = \frac{m_{i,N_F}}{M_{N_F}} = \frac{m_{i,N_F}}{\sum_{i=1}^{N_C} m_{i,N_F}}$, para $i = 1, 2, \cdots, N_C$

- <u>Equações de Balanço de Energia no Prato de Alimentação</u>

$$\frac{d\left(M_{N_F} \cdot H_{N_F}^{(L)}\right)}{dt} = L_{N_F-1} \cdot H_{N_F-1}^{(L)} + V_{N_F+1} \cdot H_{N_F+1}^{(V)} - \left(L_{N_F} \cdot H_{N_F}^{(L)} + V_{N_F} \cdot H_{N_F}^{(V)}\right) + F \cdot H_{Feed}^{(L)}$$

sendo: $H_{N_F}^{(L)} = \sum_{i=1}^{N_c} x_{i,N_F} \cdot h_i^{(L)}$ e $H_{N_F}^{(V)} = \sum_{i=1}^{N_c} y_{i,N_F} \cdot h_i^{(V)}$.

- <u>Equações de Balanço de Massa por Componente no Condensador</u>

$$\frac{dm_{i,0}}{dt} = -L_0 \cdot x_{i,0} + V_1 \cdot y_{i,1} - D \cdot x_{i,d}$$

sendo: $m_{i,0} = M_0 \cdot x_{i,0}$ ou $x_{i,0} = \frac{m_{i,0}}{M_0} = \frac{m_{i,0}}{\sum_{i=1}^{N_C} m_{i,0}}$, para $i = 1, 2, \cdots, N_C$

- <u>Equações de Balanço de Energia no Condensador</u>

$$\frac{d\left(M_0 \cdot H_0^{(L)}\right)}{dt} = -L_0 \cdot H_0^{(L)} + V_1 \cdot H_1^{(V)} - D \cdot H_d^{(L)} - Q_c$$

sendo: $H_0^{(L)} = \sum_{i=1}^{N_c} x_{i,0} \cdot h_i^{(L)}$, $H_1^{(V)} = \sum_{i=1}^{N_c} y_{i,1} \cdot h_i^{(V)}$ e $H_d^{(L)} = \sum_{i=1}^{N_c} x_{i,d} \cdot h_i^{(L)}$.

- Equações de Balanço de Massa por Componente no Refervedor

$$\frac{dm_{i,N+1}}{dt} = L_N \cdot x_{i,N} - V_{N+1} \cdot y_{i,N+1} - B \cdot x_{i,b}$$

sendo: $m_{i,N+1} = M_{N+1} \cdot x_{i,N+1}$ ou $x_{i,N+1} = \frac{m_{i,N+1}}{M_{N+1}} = \frac{m_{i,N+1}}{\sum_{i=1}^{N_C} m_{i,N+1}}$, para $i = 1, 2, \cdots, N_C$

- Equações de Balanço de Energia no Refervedor

$$\frac{d\left(M_{N+1} \cdot H_{N+1}^{(L)}\right)}{dt} = L_N \cdot H_N^{(L)} - V_{N+1} \cdot H_{N+1}^{(V)} - B \cdot H_b^{(L)} + Q_r$$

sendo: $H_N^{(L)} = \sum_{i=1}^{N_c} x_{i,N} \cdot h_i^{(L)}$, $H_{N+1}^{(V)} = \sum_{i=1}^{N_c} y_{i,N+1} \cdot h_i^{(V)}$ e $H_b^{(L)} = \sum_{i=1}^{N_c} x_{i,b} \cdot h_i^{(L)}$.

- Relação de Equilíbrio Termodinâmico

  $y_{i,j} = K_{i,j} \cdot x_{i,j}$ para $j = 0, 1, 2, \cdots, N+1$ e $i = 1, 2, \cdots, N_C$

- Equação da Hidráulica do Prato

  $L_j = \Psi\left(M_j\right)$ para $j = 0, 1, 2, \cdots, N+1$.

Aproximações Polinomiais por Seção $y_{i,j} = K_{i,j} \cdot x_{i,j}$ para $j = 0, 1, 2, \cdots, N+1$ e $i = 1, 2, \cdots, N_C$

Seção de Retificação: $s^{(1)} = \frac{j-1}{N_F - 1}$ para $j = 0, 1, 2, \cdots, N_F$

$X_j(t) \cong X^{(n+1)}\left(s^{(1)}, t\right) = \sum_{k=0}^{n+1} \ell_k\left(s^{(1)}\right) \cdot X^{(n+1)}\left(s_k^{(1)}, t\right)$, sendo: $s_0^{(1)} = -\frac{1}{N_F}$; $s_{n+1}^{(1)} = 1$ e $-\frac{1}{N_F} < s_1^{(1)} < s_2^{(1)} < \cdots < s_n^{(1)} < 1$ as n raízes do polinômio da Hahn: $P_n^{(N_F-1)}\left(s^{(1)}\right)$,

com a propriedade: $\sum_{j=1}^{N_F-1} \left(s^{(1)}\right)^k \cdot P_n^{(N_F-1)}\left(s^{(1)}\right) = 0$ para $k = 0, 1, \ldots n-1$.

Seção de Esgotamento: $s^{(2)} = \frac{j-1-N_F}{N-N_F}$ para $j = N_F, N_F+1, \cdots N, N+1$

$X_j(t) \cong X^{(m+1)}\left(s^{(2)}, t\right) = \sum_{k=0}^{m+1} \ell_k\left(s^{(2)}\right) \cdot X^{(m+1)}\left(s_k^{(2)}, t\right)$, sendo: $s_0^{(2)} = -\frac{1}{N-N_F}$;

$s_{m+1}^{(2)}=1$ e $-\dfrac{1}{N-N_F}<s_1^{(2)}<s_2^{(2)}<\cdots<s_m^{(2)}<1$ as m raízes do polinômio da Hahn:

$P_m^{(N-N_F)}\left(s^{(2)}\right)$, com a propriedade: $\sum_{j=N_F+1}^{N}\left(s^{(2)}\right)^k\cdot P_n^{(N-N_F)}\left(s^{(2)}\right)=0$ para k = 0, 1,... $m-1$.

A aplicação do método dos momentos nas duas seções dá origem a:

- Equações de Balanço na Seção de Retificação

$$\frac{dM_{i,j}(t)}{dt}=\sum_{k=0}^{n+1}B_{j,k}^{(-)}\cdot L_k(t)\cdot x_{i,k}(t)+\sum_{k=0}^{n+1}B_{j,k}^{(+)}\cdot V_k(t)\cdot y_{i,k}(t)-Y_{i,j}(t),$$

$$\frac{d\hat{H}_j(t)}{dt}=\sum_{k=0}^{n+1}B_{j,k}^{(-)}\cdot L_k(t)\cdot H_k^{(L)}(t)+\sum_{k=0}^{n+1}B_{j,k}^{(+)}\cdot V_k(t)\cdot H_k^{(V)}(t)-R_j(t)$$

$y_{i,j}=K_{i,j}\cdot x_{i,j}$ e $L_j=\Psi\left(M_j\right)$ para $j=1,\ 2,\ \cdots,\ n$ e $i=\ 1,\ 2,\ \cdots,\ N_C$

Sendo: $M_{i,j}=m_{i,j}+G_{j,0}\cdot m_{i,0}+G_{j,1}\cdot m_{i,n+1}$,

$\hat{H}_j(t)=M_j\cdot H_j^{(L)}+G_{j,0}\cdot M_0\cdot H_0^{(L)}+G_{j,1}\cdot M_{n+1}\cdot H_{n+1}^{(L)}$,

$$Y_{i,j}(t)=L_j(t)\cdot x_{i,j}(t)+V_j(t)\cdot y_{i,j}(t)+G_{j,0}\cdot\left[L_0(t)\cdot x_{i,0}(t)+V_0(t)\cdot y_{i,0}(t)\right]+$$
$$+G_{j,1}\cdot\left[L_{n+1}(t)\cdot x_{i,n+1}(t)+V_j(t)\cdot y_{i,n+1}(t)\right],$$

$$R_j(t)=L_j(t)\cdot H_j^{(L)}(t)+V_j(t)\cdot H_j^{(V)}(t)+G_{j,0}\cdot\left[L_0(t)\cdot H_0^{(L)}(t)+V_0(t)\cdot H_0^{(V)}(t)\right]+$$
$$+G_{j,1}\cdot\left[L_{n+1}(t)\cdot H_{n+1}^{(L)}(t)+V_{n+1}(t)\cdot H_{n+1}^{(V)}(t)\right]$$

$m_{i,j}=M_j\cdot x_{i,j}$, $x_{i,j}=\dfrac{m_{i,j}}{M_j}=\dfrac{m_{i,j}}{\sum_{i=1}^{N_C}m_{i,j}}$,

- Equações de Balanço na Seção de Esgotamento

$$\frac{d\boldsymbol{M}_{i,j}(t)}{dt}=\sum_{k=0}^{m+1}\boldsymbol{B}_{j,k}^{(-)}\cdot\boldsymbol{L}_k(t)\cdot\boldsymbol{x}_{i,k}(t)+\sum_{k=0}^{m+1}\boldsymbol{B}_{j,k}^{(+)}\cdot\boldsymbol{V}_k(t)\cdot\boldsymbol{y}_{i,k}(t)-\boldsymbol{Y}_{i,j}(t),$$

$$\frac{d\hat{\boldsymbol{H}}_j(t)}{dt}=\sum_{k=0}^{m+1}\boldsymbol{B}_{j,k}^{(-)}\cdot\boldsymbol{L}_k(t)\cdot\boldsymbol{H}_k^{(L)}(t)+\sum_{k=0}^{m+1}\boldsymbol{B}_{j,k}^{(+)}\cdot\boldsymbol{V}_k(t)\cdot\boldsymbol{H}_k^{(V)}(t)-\boldsymbol{R}_j(t)$$

$\boldsymbol{y}_{i,j}=\boldsymbol{K}_{i,j}\cdot\boldsymbol{x}_{i,j}$ e $\boldsymbol{L}_j=\Psi\left(\boldsymbol{M}_j\right)$ para $j=1,\ 2,\ \cdots,\ m$ e $i=\ 1,\ 2,\ \cdots,\ N_C$

Sendo: $\boldsymbol{M}_{i,j}=\boldsymbol{m}_{i,j}+\boldsymbol{G}_{j,0}\cdot\boldsymbol{m}_{i,0}+\boldsymbol{G}_{j,1}\cdot\boldsymbol{m}_{i,m+1}$,

$$\hat{\boldsymbol{H}}_j(t) = \boldsymbol{M}_j \cdot \boldsymbol{H}_j^{(L)} + \boldsymbol{G}_{j,0} \cdot \boldsymbol{M}_0 \cdot \boldsymbol{H}_0^{(L)} + \boldsymbol{G}_{j,1} \cdot \boldsymbol{M}_{m+1} \cdot \boldsymbol{H}_{m+1}^{(L)} \quad ,$$

$$\boldsymbol{Y}_{i,j}(t) = \boldsymbol{L}_j(t) \cdot \boldsymbol{x}_{i,j}(t) + \boldsymbol{V}_j(t) \cdot \boldsymbol{y}_{i,j}(t) + \boldsymbol{G}_{j,0} \cdot \left[\boldsymbol{L}_0(t) \cdot \boldsymbol{x}_{i,0}(t) + \boldsymbol{V}_0(t) \cdot \boldsymbol{y}_{i,0}(t)\right] + \\ + \boldsymbol{G}_{j,1} \cdot \left[\boldsymbol{L}_{m+1}(t) \cdot \boldsymbol{x}_{i,m+1}(t) + \boldsymbol{V}_{m+1}(t) \cdot \boldsymbol{y}_{i,m+1}(t)\right] \quad ,$$

$$\boldsymbol{R}_j(t) = \boldsymbol{L}_j(t) \cdot \boldsymbol{H}_j^{(L)}(t) + \boldsymbol{V}_j(t) \cdot \boldsymbol{H}_j^{(V)}(t) + \boldsymbol{G}_{j,0} \cdot \left[\boldsymbol{L}_0(t) \cdot \boldsymbol{H}_0^{(L)}(t) + \boldsymbol{V}_0(t) \cdot \boldsymbol{H}_0^{(V)}(t)\right] + \\ + \boldsymbol{G}_{j,1} \cdot \left[\boldsymbol{L}_{m+1}(t) \cdot \boldsymbol{H}_{m+1}^{(L)}(t) + \boldsymbol{V}_{m+1}(t) \cdot \boldsymbol{H}_{m+1}^{(V)}(t)\right]$$

$$\boldsymbol{m}_{i,j} = \boldsymbol{M}_j \cdot \boldsymbol{x}_{i,j} \, , \; \boldsymbol{x}_{i,j} = \frac{\boldsymbol{m}_{i,j}}{\boldsymbol{M}_j} = \frac{\boldsymbol{m}_{i,j}}{\sum_{i=1}^{N_C} \boldsymbol{m}_{i,j}} \, .$$

- <u>Equações de Balanço no Prato de Alimentação</u>

$$\frac{dm_{i,N_F}}{dt} = \sum_{k=0}^{n+1} A_{n+1,k}^{(-)} \cdot L_k(t) \cdot x_{i,k}(t) + \sum_{k=0}^{m+1} \boldsymbol{A}_{0,k}^{(+)} \cdot \boldsymbol{V}_k(t) \cdot \boldsymbol{y}_{i,k}(t) - \left(L_{N_F} \cdot x_{i,N_F} + V_{N_F} \cdot y_{i,N_F}\right) + F \cdot z_i$$

$$\frac{d\left(M_{N_F} \cdot H_{N_F}^{(L)}\right)}{dt} = \sum_{k=0}^{n+1} A_{n+1,k}^{(-)} \cdot L_k(t) \cdot H_k^{(L)}(t) + \sum_{k=0}^{m+1} \boldsymbol{A}_{0,k}^{(+)} \cdot \boldsymbol{V}_k(t) \cdot \boldsymbol{H}_k^{(V)}(t) - \left(L_{N_F} \cdot H_{N_F}^{(L)} + V_{N_F} \cdot H_{N_F}^{(V)}\right) \\ + F \cdot H_{Feed}^{(L)}$$

$y_{i,N_F} = K_{i,N_F} \cdot x_{i,N_F}$ e $L_{N_F} = \Psi\left(M_{N_F}\right)$ para $i = 1, 2, \cdots, N_C$

Sendo: $m_{i,N_F} = M_{N_F} \cdot x_{i.N_F}$, $m_{i,N_F} = \dfrac{m_{i,N_F}}{M_{N_F}} = \dfrac{m_{i,N_F}}{\sum_{j=1}^{N_C} m_{j,N_F}}$, $m_{i,N_F} = m_{i,n+1} = \boldsymbol{m}_{i,0}$,

$x_{i,N_F} = x_{i,n+1} = \boldsymbol{x}_{i,0}$, $y_{i,N_F} = y_{i,n+1} = \boldsymbol{y}_{i,0}$, $K_{i,N_F} = K_{i,n+1} = \boldsymbol{K}_{i,0}$, $L_{N_F} = L_{n+1} = \boldsymbol{L}_0$,

$V_{N_F} = V_{n+1} = \boldsymbol{V}_0$, $M_{N_F} = M_{n+1} = \boldsymbol{M}_0$,

$$H_{N_F}^{(L)} = H_{n+1}^{(L)} = \boldsymbol{H}_0^{(L)} = \sum_{i=1}^{N_c} x_{i,N_F} \cdot h_i^{(L)} = \sum_{i=1}^{N_c} x_{i,n+1} \cdot h_i^{(L)} = \sum_{i=1}^{N_c} \boldsymbol{x}_{i,0} \cdot \boldsymbol{h}_i^{(L)} \text{ e}$$

$$H_{N_F}^{(V)} = H_{n+1}^{(V)} = \boldsymbol{H}_0^{(V)} = \sum_{i=1}^{N_c} y_{i,N_F} \cdot h_i^{(V)} = \sum_{i=1}^{N_c} y_{i,n+1} \cdot h_i^{(V)} = \sum_{i=1}^{N_c} \boldsymbol{y}_{i,0} \cdot \boldsymbol{h}_i^{(V)} \, .$$

- <u>Equações de Balanço no Condensador</u>

$$\frac{dm_{i,0}}{dt} = -L_0 \cdot x_{i,0} + \sum_{k=0}^{n+1} A_{0,k}^{(+)} \cdot V_k(t) \cdot y_{i,k}(t) - D \cdot x_{i,d}$$

$$\frac{d\left(M_0 \cdot H_0^{(L)}\right)}{dt} = -L_0 \cdot H_0^{(L)} + \sum_{k=0}^{n+1} A_{0,k}^{(+)} \cdot V_k(t) \cdot H_k^{(V)}(t) - D \cdot H_d^{(L)} - Q_c$$

$y_{i,0} = K_{i,0} \cdot x_{i,0}$ e $L_0 = \Psi\left(M_0\right)$ para $i = 1, 2, \cdots, N_C$

Sendo: $m_{i,0} = M_0 \cdot x_{i,0}$ ou $x_{i,0} = \frac{m_{i,0}}{M_0} = \frac{m_{i,0}}{\sum_{i=1}^{N_C} m_{i,0}}$, para $i =$ 1, 2, $\cdots$, N_C

- <u>Equações de Balanço no Refervedor</u>

$$\frac{d\boldsymbol{m}_{i,m+1}}{dt} = \sum_{k=0}^{m+1} \boldsymbol{A}_{m+1,k}^{(-)} \cdot \boldsymbol{L}_k(t) \cdot \boldsymbol{x}_{i,k}(t) - \boldsymbol{V}_{m+1} \cdot \boldsymbol{y}_{i,m+1} - B \cdot \boldsymbol{x}_{i,b}$$

$$\frac{d\left(\boldsymbol{M}_{m+1} \cdot \boldsymbol{H}_{m+1}^{(L)}\right)}{dt} = \sum_{k=0}^{m+1} \boldsymbol{A}_{m+1,k}^{(-)} \cdot \boldsymbol{L}_k(t) \cdot \boldsymbol{H}_k^{(L)}(t) - \boldsymbol{V}_{m+1} \cdot \boldsymbol{H}_{m+1}^{(V)} - B \cdot \boldsymbol{H}_b^{(L)} + Q_r$$

$\boldsymbol{y}_{i,m+1} = \boldsymbol{K}_{i,m+1} \cdot \boldsymbol{x}_{i,m+1}$ e $\boldsymbol{L}_{m+1} = \Psi\left(\boldsymbol{M}_{m+1}\right)$ para $i =$ 1, 2, $\cdots$, N_C

Sendo: $\boldsymbol{m}_{i,m+1} = \boldsymbol{M}_{m+1} \cdot \boldsymbol{x}_{i,m+1}$, $\boldsymbol{x}_{i,m+1} = \frac{\boldsymbol{m}_{i,m+1}}{\boldsymbol{M}_{m+1}} = \frac{\boldsymbol{m}_{i,m+1}}{\sum_{i=1}^{N_C} \boldsymbol{m}_{i,m+1}}$, para $i =$ 1, 2, $\cdots$, N_C

Adaptive collocation on finite elements models for the optimization of multistage distillation units

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Chemical Engineering Science -Volume 49, Issue 9, May 1994, Pages 1369-1382

Abstract

The size of the model for multistage distillation processes can be reduced by orthogonal collocation on finite elements (OCFE) techniques. The accuracy of the OCFE models can be improved by adaptively placing the breakpoints between the elements so that the approximation error is equally distributed among the elements within each column section. The location of the breakpoints depends on the features of the composition and temperature profiles in the column. Two different approaches are used for the estimation of the approximation error resulting from the OCFE solution. The first approach is based on the equidistribution of the residuals of the material and energy balances around envelopes that include predefined regions in the column. The additional constraints, generated by the adaptive grid procedure, are embedded into the economic optimization problem. Both the optimal operating conditions and the optimal breakpoint sequence are determined simultaneously. The second method uses the derivatives of the approximate solution and determines the element lengths by equidistributing the estimated error in an iterative procedure. The residual-based approach is more efficient than the derivative method in determining an element partition that results in a feasible optimal solution close to the optimal solution obtained by a tray-by-tray model. The

adaptive placement of the breakpoints allows a more compact OCFE model for which an optimal solution exists. Multiple locally optimal element partitions may be obtained using the residual-based approach.