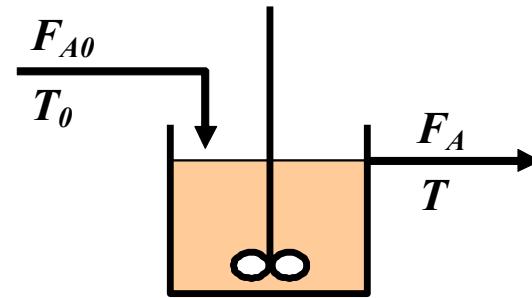


Operação não adiabática

Non-adiabatic operation

CSTR



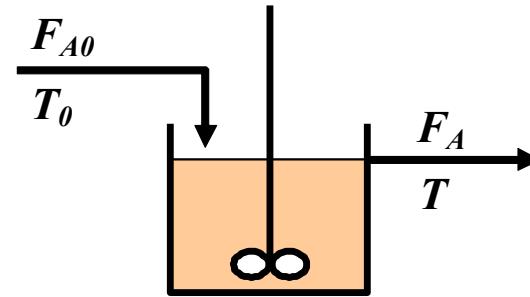
Operação não adiabática

Non-adiabatic operation

CSTR

Exemplo:

A → B



Operação não adiabática

Non-adiabatic operation

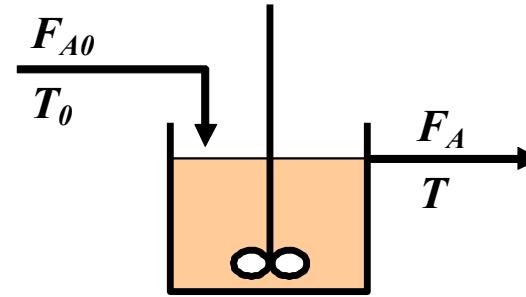
CSTR

Exemplo:



Lei cinética:
Kinetic law

$$-r_A = k C_A = k C_{A0} (1 - X)$$



Operação não adiabática

Non-adiabatic operation

CSTR

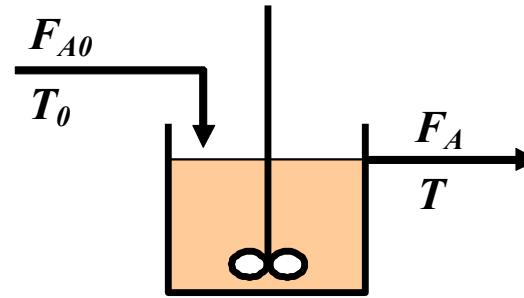
Exemplo:



$$k = k_0 e^{-\frac{E}{RT}}$$

Lei cinética:
Kinetic law

$$-r_A = k C_A = k C_{A0} (1 - X)$$



Operação não adiabática

Non-adiabatic operation

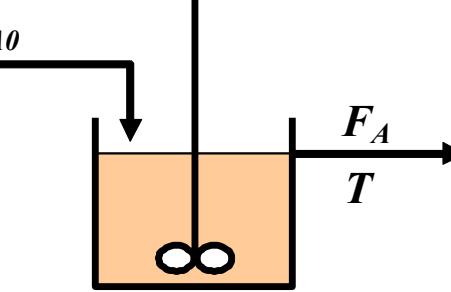
CSTR

Exemplo:



$$k = k_0 e^{-\frac{E}{RT}}$$

Lei cinética:
Kinetic law



$$-r_A = k C_A = k C_{A0} (1 - X)$$

$$k(T) = k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)}$$

Operação não adiabática

Non-adiabatic operation

CSTR

Exemplo:



$$k = k_0 e^{-\frac{E}{RT}}$$

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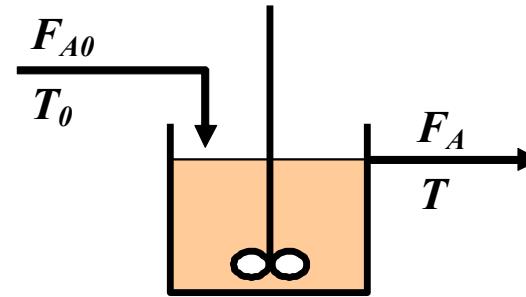
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Balanço molar:

Mole balance

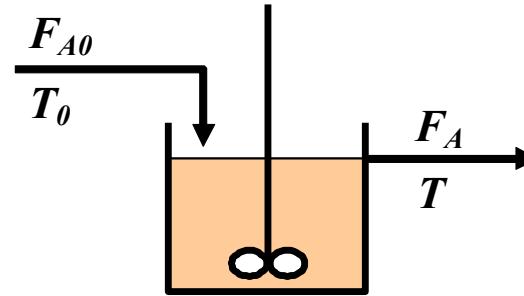
$$\tau = \frac{C_{A0} X}{(-r_A)} = \frac{C_{A0} X}{k C_{A0} (1 - X)} = \frac{X}{k (1 - X)}$$



Operação não adiabática

Non-adiabatic operation

CSTR



Exemplo:



$$k = k_0 e^{-\frac{E}{RT}}$$

Lei cinética:
Kinetic law

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Mole balance

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Operação não adiabática

Non-adiabatic operation

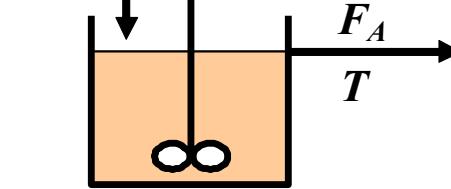
CSTR

Exemplo:



$$k = k_0 e^{-\frac{E}{RT}}$$

Lei cinética:
Kinetic law



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$$k(T) = k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)}$$

$$V = \frac{F_{A0} \cdot X}{(-r_A)}$$

Balanço molar:

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Operação não adiabática

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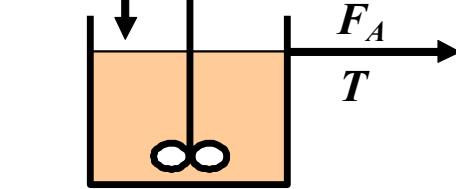
CSTR

Exemplo:



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Lei cinética:
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Operação não adiabática

Non-adiabatic operation

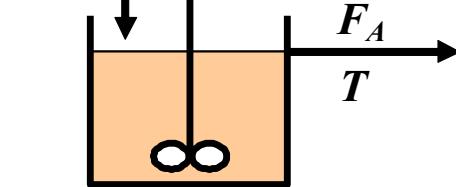
CSTR

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$$\boxed{\therefore \tau = C_{A0} \frac{X}{(-r_A)}}$$

Balanço de energia

Energy balance

$$\dot{Q} - F_{A0} \sum_i \theta_i C_{pi} (T - T_0) - F_{A0} \left[\Delta H_R^o + \sum_i \nu_i C_{pi} (T - T_R) \right] X = 0$$

Balanço de energia

Energy balance

$$\dot{Q} - F_{A0} \sum_i \theta_i C_{pi} (T - T_0) - F_{A0} \left[\Delta H_R^o + \sum_i \nu_i C_{pi} (T - T_R) \right] X = 0$$

Caso 1: Temperatura externa constante (ex: vapor saturado; inexistência de camisa)

Case 1: constant external temperature (ex.: saturated vapour; non-jacketed reactor)

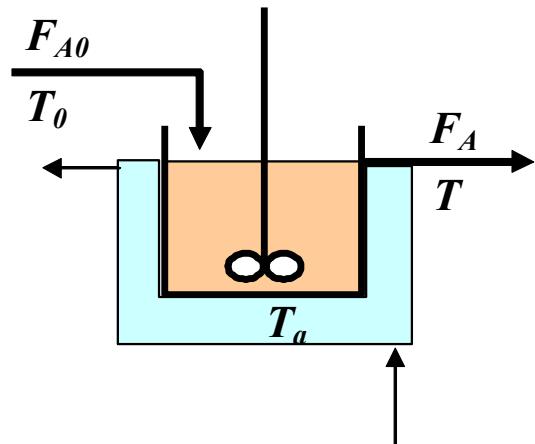
Balanço de energia

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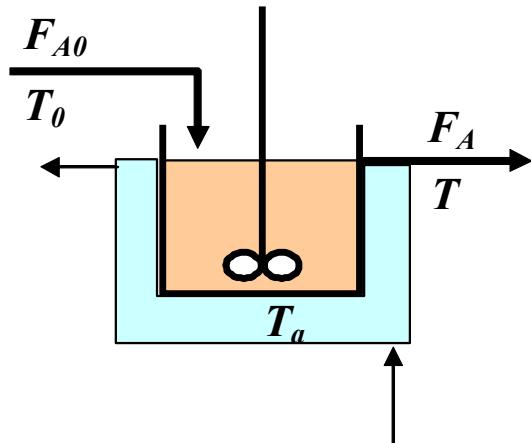
Balanço de energia

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$$\dot{Q} - F_{A0} \sum_i \theta_i C_{pi} (T - T_0) - F_{A0} \left[\Delta H_R^o + \sum_i \nu_i C_{pi} (T - T_R) \right] X = 0$$

Caso 1: Temperatura externa constante (ex: vapor saturado; inexistência de camisa)

Case 1: constant external temperature (ex.: saturated vapour; non-jacketed reactor)



$$\dot{Q} = U A (T_a - T)$$

Balanço de energia

Energy balance

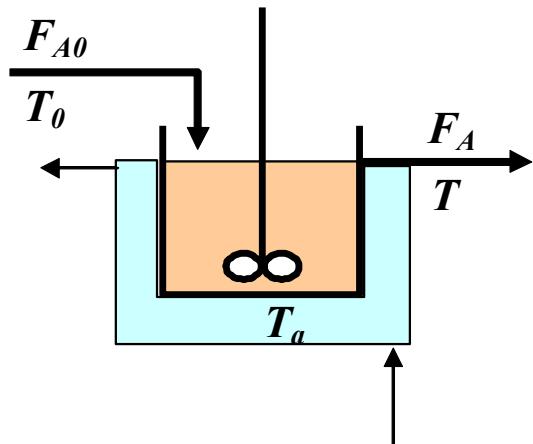
$$\dot{Q} - F_{A0} \sum_i \theta_i C_{pi} (T - T_0) - F_{A0} \left[\Delta H_R^o + \sum_i \nu_i C_{pi} (T - T_R) \right] X = 0$$

Caso 1: Temperatura externa constante (ex: vapor saturado; inexistência de camisa)

Case 1: constant external temperature (ex.: saturated vapour; non-jacketed reactor)

Caso 2: a temperatura externa varia entre a entrada e a saída da camisa

Case 2: external temperature changes between the jacket entrance and the jacket exit.



$$\dot{Q} = U A (T_a - T)$$

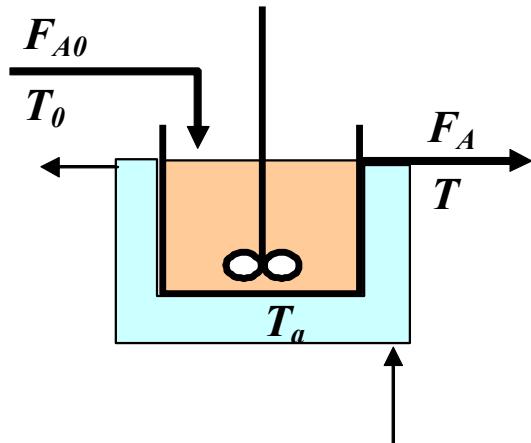
Balanço de energia

Energy balance

$$\dot{Q} - F_{A0} \sum_i \theta_i C_{pi} (T - T_0) - F_{A0} \left[\Delta H_R^o + \sum_i \nu_i C_{pi} (T - T_R) \right] X = 0$$

Caso 1: Temperatura externa constante (ex: vapor saturado; inexistência de camisa)

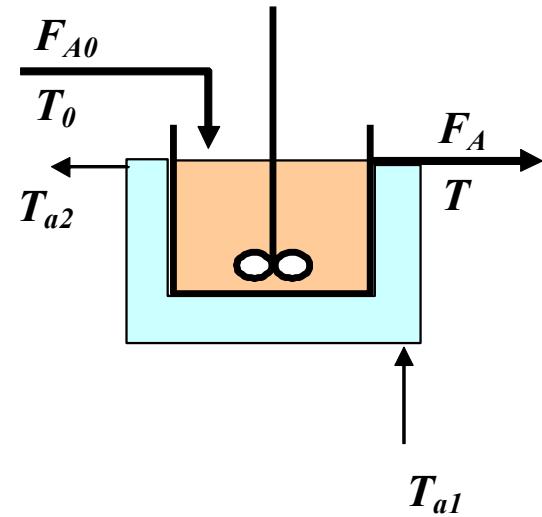
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Caso 2: a temperatura externa varia entre a entrada e a saída da camisa

Case 2: external temperature changes between the jacket entrance and the jacket exit.



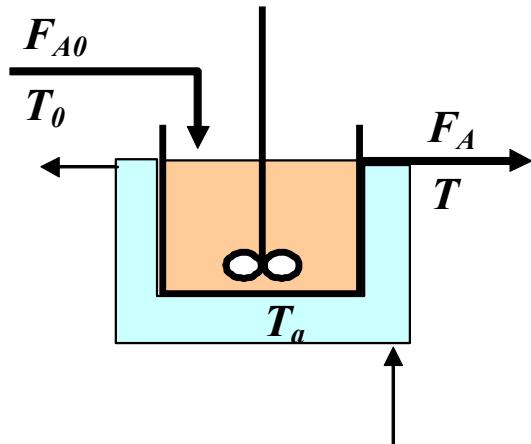
Balanço de energia

Energy balance

$$\dot{Q} - F_{A0} \sum_i \theta_i C_{pi} (T - T_0) - F_{A0} \left[\Delta H_R^o + \sum_i \nu_i C_{pi} (T - T_R) \right] X = 0$$

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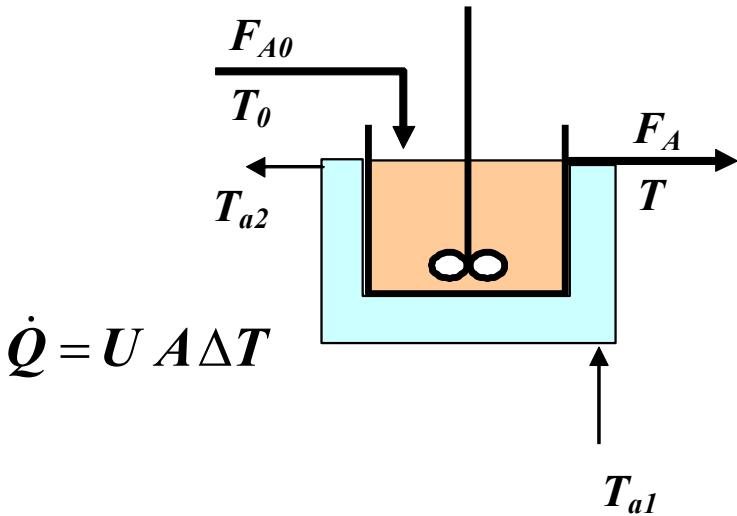
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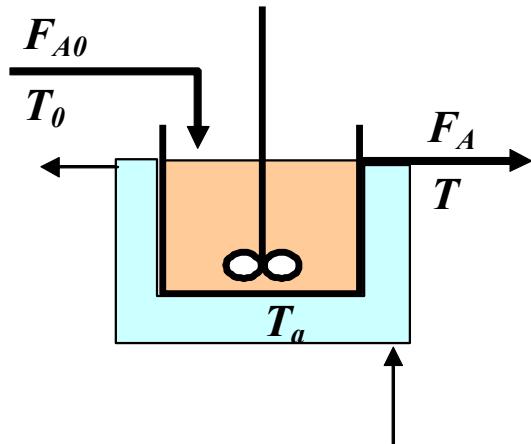
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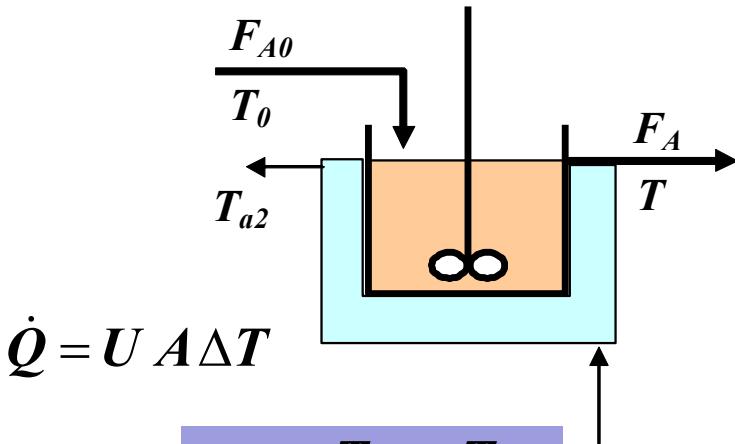
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$$\dot{Q} = U A (T_a - T)$$

Caso 2: a temperatura externa varia entre a entrada e a saída da camisa

Case 2: external temperature changes between the jacket entrance and the jacket exit.



$$\dot{Q} = U A \Delta T$$

$$\Delta T = \frac{T_{a1} - T_{a2}}{\ln \frac{T_{a1} - T}{T_{a2} - T}} \quad T_{a1}$$

Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:

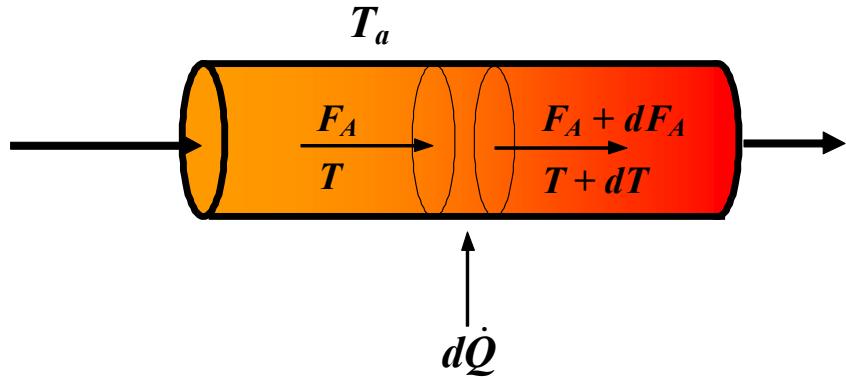


Lei cinética:

Kinetic law

$$-r_A = k C_A = k C_{A0} (1 - X)$$

$$k = k_0 e^{-\frac{E}{RT}} \quad k(T) = k(T_R) e^{-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}$$



Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



Lei cinética:

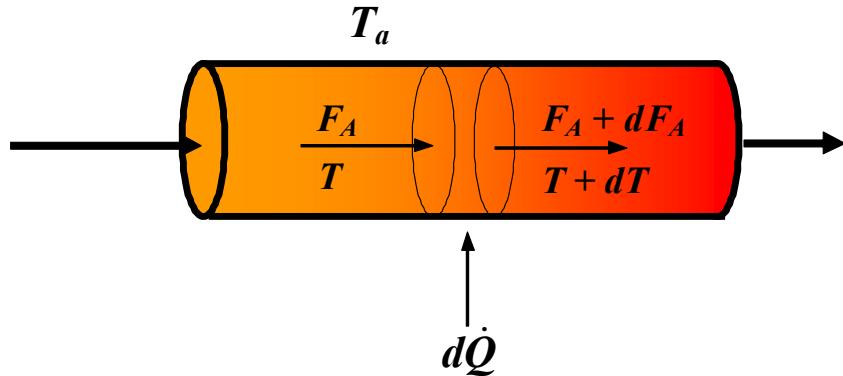
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Balanço molar:

Mole balance:



Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



Lei cinética:

Kinetic law

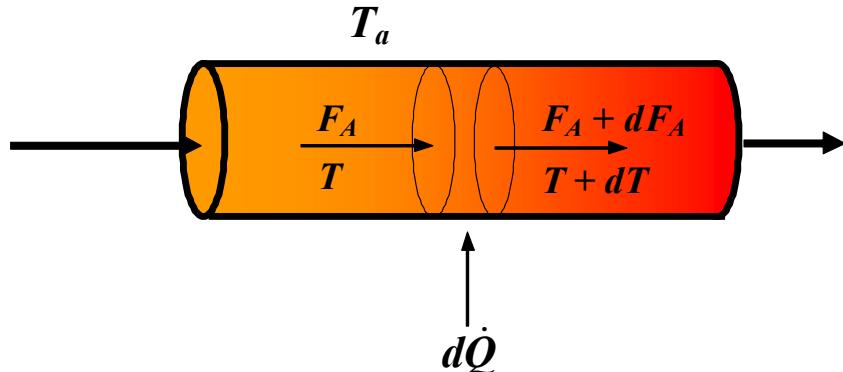
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Mole balance:

$$F_A - (F_A + dF_A) + r_A dV = 0$$



Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



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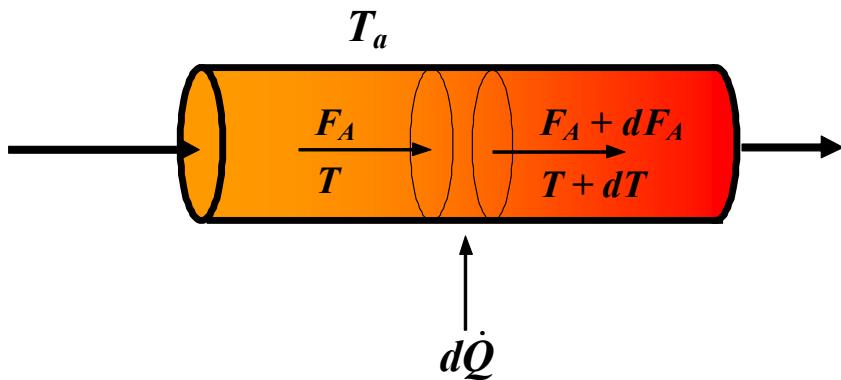
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$$F_A - (F_A + dF_A) + r_A dV = 0$$

$$\therefore -dF_A + r_A dV = 0$$



Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



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Kinetic law

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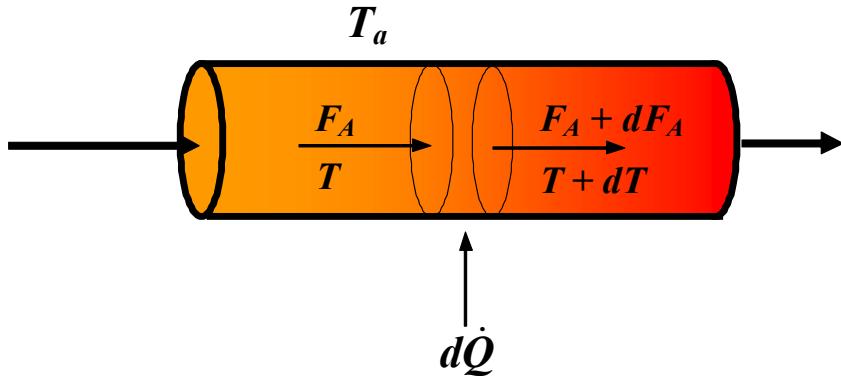
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Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



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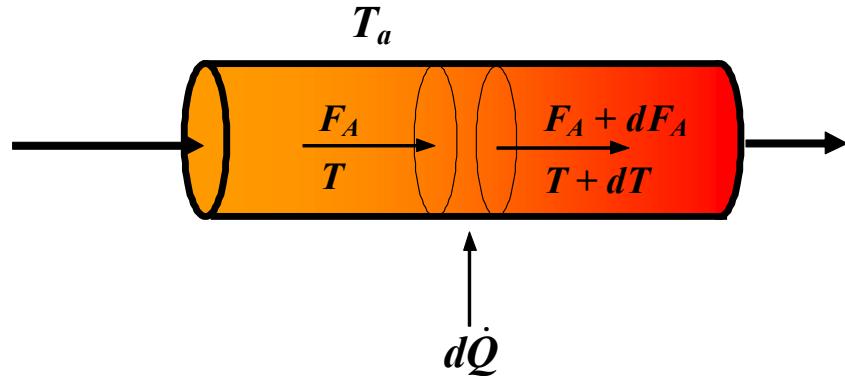
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$$\therefore \frac{dX}{dV} = \frac{(-r_A)}{F_{A0}}$$

Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



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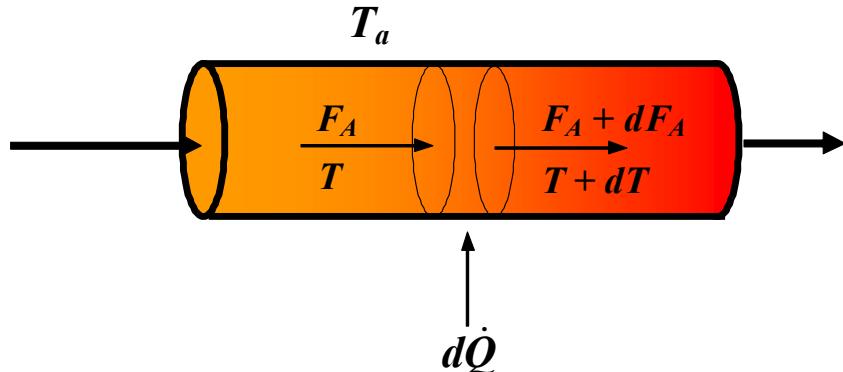
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Balanço de energia:

Energy balance;

Operação não adiabática

Non-adiabatic operation

PFR

Exemplo:



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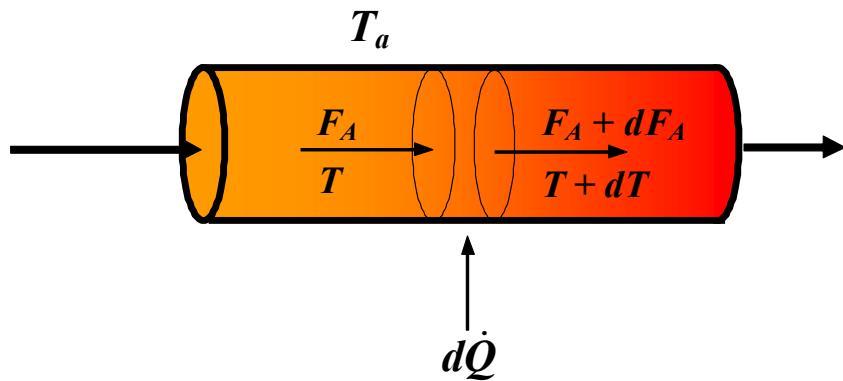
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Balanço de energia:

Energy balance;

Tal como o balanço molar, o balanço de energia é feito a um elemento de volume dV :

Similarly to the mole balance, the energy balanced is performed on a elemental volume dV

Operação não adiabática

Non-adiabatic operation

PFR

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Balanço molar:

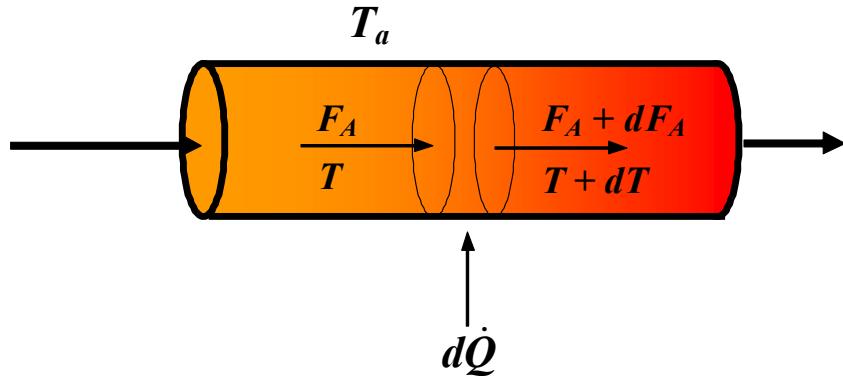
Mole balance:

$$F_A - (F_A + dF_A) + r_A dV = 0$$

$$\therefore -dF_A + r_A dV = 0$$

$$\therefore F_{A0} dX + r_A dV = 0$$

$$\therefore \frac{dX}{dV} = \frac{(-r_A)}{F_{A0}}$$



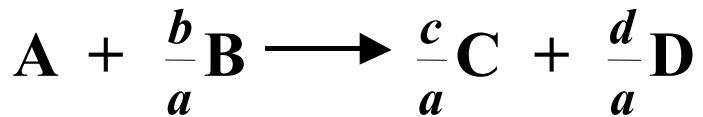
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$$d\dot{Q} + \sum_i F_i H_i - \sum_i (F_i + dF_i)(H_i + dH_i) = 0$$



$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i\big(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i\big)\!=\!0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$d\dot{Q}+F_A\,H_A+F_B\,H_B+F_C\,H_C+F_D\,H_D-F_A\,H_A-F_A\,dH_A-H_A\,dF_A-\\-dH_A\,dF_A-F_B\,H_B-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-F_C\,H_C-F_C\,dH_C-\\-H_C\,dF_C-dH_C\,dF_C-F_D\,H_D-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$d\dot{Q}+\cancel{F_A H_A}+F_B\,H_B+F_C\,H_C+F_D\,H_D-\cancel{F_A H_A}-F_A\,dH_A-H_A\,dF_A-\\-dH_A\,dF_A-F_B\,H_B-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-F_C\,H_C-F_C\,dH_C-\\-H_C\,dF_C-dH_C\,dF_C-F_D\,H_D-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$d\dot{Q}+\cancel{F_A H_A}+\cancel{F_B H_B}+F_C\,H_C+F_D\,H_D-\cancel{F_A H_A}-F_A\,dH_A-H_A\,dF_A-\\-dH_A\,dF_A-\cancel{F_B H_B}-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-F_C\,H_C-F_C\,dH_C-\\-H_C\,dF_C-dH_C\,dF_C-F_D\,H_D-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$\cancel{d\dot{Q}+F_A\cancel{H_A}+F_B\cancel{H_B}+F_C\cancel{H_C}+F_D\,H_D-\cancel{F_A}\cancel{H_A}-F_A\,dH_A-H_A\,dF_A-}\\ -dH_A\,dF_A-\cancel{F_B}\cancel{H_B}-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-\cancel{F_C}\cancel{H_C}-F_C\,dH_C-\\ -H_C\,dF_C-dH_C\,dF_C-F_D\,H_D-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$\cancel{d\dot{Q}+F_A\cancel{H_A}+F_B\cancel{H_B}+F_C\cancel{H_C}+F_D\,H_D-\cancel{F_A}\cancel{H_A}-F_A\,dH_A-H_A\,dF_A-}\\ -dH_A\,dF_A-\cancel{F_B}\cancel{H_B}-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-\cancel{F_C}\cancel{H_C}-F_C\,dH_C-\\ -H_C\,dF_C-dH_C\,dF_C-F_D\,H_D-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$\cancel{d\dot{Q}+F_A\cancel{H_A}+F_B\cancel{H_B}+F_C\cancel{H_C}+F_D\,H_D-\cancel{F_A}\cancel{H_A}-F_A\,dH_A-H_A\,dF_A-}\\ -dH_A\,dF_A-\cancel{F_B}\cancel{H_B}-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-\cancel{F_C}\cancel{H_C}-F_C\,dH_C-\\ -H_C\,dF_C-dH_C\,dF_C-F_D\,H_D-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\textbf{A} \; + \; \frac{b}{a}\textbf{B} \longrightarrow \frac{c}{a}\textbf{C} \; + \; \frac{d}{a}\textbf{D}$$

$$d\dot{Q}+\sum_iF_i\,H_i-\sum_i(F_i\,H_i+F_i\,dH_i+H_i\,dF_i+dH_i\,dF_i)=0$$

$$\cancel{d\dot{Q}+F_A\cancel{H_A}+F_B\cancel{H_B}+F_C\cancel{H_C}+F_D\cancel{H_D}-F_A\cancel{H_A}-F_A\,dH_A-H_A\,dF_A-}\\ -dH_A\,dF_A-\cancel{F_B\cancel{H_B}}-F_B\,dH_B-H_B\,dF_B-dH_B\,dF_B-\cancel{F_C\cancel{H_C}}-F_C\,dH_C-\\ -H_C\,dF_C-dH_C\,dF_C-\cancel{F_D\cancel{H_D}}-F_D\,dH_D-H_D\,dF_D-dH_D\,dF_D=0$$

$$\mathbf{A} + \frac{b}{a}\mathbf{B} \longrightarrow \frac{c}{a}\mathbf{C} + \frac{d}{a}\mathbf{D}$$

$$d\dot{Q} + \sum_i F_i H_i - \sum_i (F_i H_i + F_i dH_i + H_i dF_i + dH_i dF_i) = 0$$

$$\begin{aligned} d\dot{Q} &+ \cancel{F_A H_A} + \cancel{F_B H_B} + \cancel{F_C H_C} + \cancel{F_D H_D} - \cancel{F_A H_A} - F_A dH_A - H_A dF_A - \\ &- dH_A dF_A - \cancel{F_B H_B} - F_B dH_B - H_B dF_B - dH_B dF_B - \cancel{F_C H_C} - F_C dH_C - \\ &- H_C dF_C - dH_C dF_C - \cancel{F_D H_D} - F_D dH_D - H_D dF_D - dH_D dF_D = 0 \end{aligned}$$

$$\therefore d\dot{Q} - F_A dH_A - H_A dF_A - dH_A dF_A - F_B dH_B - H_B dF_B - dH_B dF_B - \\ - F_C dH_C - H_C dF_C - dH_C dF_C - F_D dH_D - H_D dF_D - dH_D dF_D = 0$$

$$\mathbf{A} + \frac{b}{a}\mathbf{B} \longrightarrow \frac{c}{a}\mathbf{C} + \frac{d}{a}\mathbf{D}$$

$$d\dot{Q} + \sum_i F_i H_i - \sum_i (F_i H_i + F_i dH_i + H_i dF_i + dH_i dF_i) = 0$$

$$\begin{aligned} & d\dot{Q} + \cancel{F_A H_A} + \cancel{F_B H_B} + \cancel{F_C H_C} + \cancel{F_D H_D} - \cancel{F_A H_A} - F_A dH_A - H_A dF_A - \\ & - dH_A dF_A - \cancel{F_B H_B} - F_B dH_B - H_B dF_B - dH_B dF_B - \cancel{F_C H_C} - F_C dH_C - \\ & - H_C dF_C - dH_C dF_C - \cancel{F_D H_D} - F_D dH_D - H_D dF_D - dH_D dF_D = 0 \end{aligned}$$

$$\begin{aligned} \therefore & d\dot{Q} - F_A dH_A - H_A dF_A - dH_A dF_A - F_B dH_B - H_B dF_B - dH_B dF_B - \\ & - F_C dH_C - H_C dF_C - dH_C dF_C - F_D dH_D - H_D dF_D - dH_D dF_D = 0 \end{aligned}$$

$$\begin{aligned} \therefore & d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\ & + H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\ & - dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0 \end{aligned}$$

$$\mathbf{A} + \frac{b}{a}\mathbf{B} \longrightarrow \frac{c}{a}\mathbf{C} + \frac{d}{a}\mathbf{D}$$

$$d\dot{Q} + \sum_i F_i H_i - \sum_i (F_i H_i + F_i dH_i + H_i dF_i + dH_i dF_i) = 0$$

$$\begin{aligned} & d\dot{Q} + \cancel{F_A H_A} + \cancel{F_B H_B} + \cancel{F_C H_C} + \cancel{F_D H_D} - \cancel{F_A H_A} - F_A dH_A - H_A dF_A - \\ & - dH_A dF_A - \cancel{F_B H_B} - F_B dH_B - H_B dF_B - dH_B dF_B - \cancel{F_C H_C} - F_C dH_C - \\ & - H_C dF_C - dH_C dF_C - \cancel{F_D H_D} - F_D dH_D - H_D dF_D - dH_D dF_D = 0 \end{aligned}$$

$$\begin{aligned} \therefore & d\dot{Q} - F_A dH_A - H_A dF_A - dH_A dF_A - F_B dH_B - H_B dF_B - dH_B dF_B - \\ & - F_C dH_C - H_C dF_C - dH_C dF_C - F_D dH_D - H_D dF_D - dH_D dF_D = 0 \end{aligned}$$

$$\begin{aligned} \therefore & d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\ & + H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\ & - dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0 \end{aligned}$$

$$\begin{aligned}
d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\
+ H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\
- dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0
\end{aligned}$$

$$\begin{aligned}
d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\
+ H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\
- dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0
\end{aligned}$$

$$d\dot{Q}=Ua(T_a-T)dV$$

$$\begin{aligned}
d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\
+ H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\
- dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0
\end{aligned}$$

$$d\dot{Q} = U a (T_a - T) dV \quad dH_i = C p_i dT$$

$$\begin{aligned}
d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\
+ H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\
- dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0
\end{aligned}$$

$$d\dot{Q} = U a (T_a - T) dV \quad dH_i = Cp_i dT$$

$$\begin{aligned}
U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\
- \left(-Cp_A - \frac{b}{a}Cp_B + \frac{c}{a}Cp_C + \frac{d}{a}Cp_D \right) F_{A0} X dT - \left(-H_A - \frac{b}{a}H_B + \frac{c}{a}H_C + \frac{d}{a}H_D \right) F_{A0} dX \\
- \left(-dH_A - \frac{b}{a}dH_B + \frac{c}{a}dH_C + \frac{d}{a}dH_D \right) F_{A0} dX = 0
\end{aligned}$$

$$\begin{aligned}
d\dot{Q} - F_{A0}(1-X)dH_A + H_A F_{A0} dX + dH_A F_{A0} dX - F_{A0} \left(\theta_B - \frac{b}{a}X \right) dH_B + \\
+ H_B F_{A0} \frac{b}{a} dX + dH_B F_{A0} \frac{b}{a} dX - F_{A0} \left(\theta_C + \frac{c}{a}X \right) dH_C - H_C F_{A0} \frac{c}{a} dX - \\
- dH_C F_{A0} \frac{c}{a} dX - F_{A0} \left(\theta_D + \frac{d}{a}X \right) dH_D - H_D F_{A0} \frac{d}{a} dX - dH_D F_{A0} \frac{d}{a} dX = 0
\end{aligned}$$

$$d\dot{Q} = U a (T_a - T) dV \quad dH_i = Cp_i dT$$

$$\begin{aligned}
U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\
- \left(-Cp_A - \frac{b}{a}Cp_B + \frac{c}{a}Cp_C + \frac{d}{a}Cp_D \right) F_{A0} X dT - \left(-H_A - \frac{b}{a}H_B + \frac{c}{a}H_C + \frac{d}{a}H_D \right) F_{A0} dX \\
- \left(-dH_A - \frac{b}{a}dH_B + \frac{c}{a}dH_C + \frac{d}{a}dH_D \right) F_{A0} dX = 0
\end{aligned}$$

$$\begin{aligned}
U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\
- \left(-Cp_A - \frac{b}{a}Cp_B + \frac{c}{a}Cp_C + \frac{d}{a}Cp_D \right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0
\end{aligned}$$

$$U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\ - \left(-Cp_A - \frac{b}{a} Cp_B + \frac{c}{a} Cp_C + \frac{d}{a} Cp_D \right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0$$

$$U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\ - \left(-Cp_A - \frac{b}{a} Cp_B + \frac{c}{a} Cp_C + \frac{d}{a} Cp_D \right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0$$

$$- d(\Delta H_R) F_{A0} dX$$

$$U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT -$$
$$-\left(-Cp_A - \frac{b}{a}Cp_B + \frac{c}{a}Cp_C + \frac{d}{a}Cp_D\right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0$$

~~$- d(\Delta H_R) F_{A0} dX$~~

$$\begin{aligned}
& U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\
& - \left(-Cp_A - \frac{b}{a} Cp_B + \frac{c}{a} Cp_C + \frac{d}{a} Cp_D \right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0 \\
& \quad \cancel{- d(\Delta H_R) F_{A0} dX}
\end{aligned}$$

$$U a (T_a - T) dV - \sum_i \theta_i Cp_i F_{A0} dT - \sum_i v_i Cp_i F_{A0} X dT - \Delta H_R F_{A0} dX = 0$$

$$\begin{aligned}
& \mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - (\mathbf{Cp}_A + \theta_B \mathbf{Cp}_B + \theta_C \mathbf{Cp}_C + \theta_D \mathbf{Cp}_D + \theta_I \mathbf{Cp}_I) \mathbf{F}_{A0} dT - \\
& - \left(-\mathbf{Cp}_A - \frac{b}{a} \mathbf{Cp}_B + \frac{c}{a} \mathbf{Cp}_C + \frac{d}{a} \mathbf{Cp}_D \right) \mathbf{F}_{A0} X dT - \Delta \mathbf{H}_R \mathbf{F}_{A0} dX - \cancel{d(\Delta \mathbf{H}_R) \mathbf{F}_{A0} dX} = 0
\end{aligned}$$

$$\mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - \sum_i \theta_i \mathbf{Cp}_i \mathbf{F}_{A0} dT - \sum_i \nu_i \mathbf{Cp}_i \mathbf{F}_{A0} X dT - \Delta \mathbf{H}_R \mathbf{F}_{A0} dX = 0$$

$$\therefore \mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - \left[\mathbf{F}_{A0} \left(\sum_i \theta_i \mathbf{Cp}_i + X \sum_i \nu_i \mathbf{Cp}_i \right) \right] dT - \Delta \mathbf{H}_R \mathbf{F}_{A0} dX = 0$$

$$\begin{aligned}
& U a (T_a - T) dV - (Cp_A + \theta_B Cp_B + \theta_C Cp_C + \theta_D Cp_D + \theta_I Cp_I) F_{A0} dT - \\
& - \left(-Cp_A - \frac{b}{a} Cp_B + \frac{c}{a} Cp_C + \frac{d}{a} Cp_D \right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0 \\
& \quad \cancel{- d(\Delta H_R) F_{A0} dX}
\end{aligned}$$

$$U a (T_a - T) dV - \sum_i \theta_i Cp_i F_{A0} dT - \sum_i \nu_i Cp_i F_{A0} X dT - \Delta H_R F_{A0} dX = 0$$

$$\therefore U a (T_a - T) dV - \left[F_{A0} \left(\sum_i \theta_i Cp_i + X \sum_i \nu_i Cp_i \right) \right] dT - \Delta H_R F_{A0} dX = 0$$

$$\therefore U a (T_a - T) - \left[F_{A0} \left(\sum_i \theta_i Cp_i + X \sum_i \nu_i Cp_i \right) \right] \frac{dT}{dV} - \Delta H_R F_{A0} \frac{dX}{dV} = 0$$

$$\begin{aligned}
& \mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - (\mathbf{Cp}_A + \theta_B \mathbf{Cp}_B + \theta_C \mathbf{Cp}_C + \theta_D \mathbf{Cp}_D + \theta_I \mathbf{Cp}_I) F_{A0} dT - \\
& - \left(-\mathbf{Cp}_A - \frac{b}{a} \mathbf{Cp}_B + \frac{c}{a} \mathbf{Cp}_C + \frac{d}{a} \mathbf{Cp}_D \right) F_{A0} X dT - \Delta \mathbf{H}_R F_{A0} dX - d(\Delta \mathbf{H}_R) F_{A0} dX = 0 \\
& \quad \cancel{- d(\Delta \mathbf{H}_R) F_{A0} dX}
\end{aligned}$$

$$\mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - \sum_i \theta_i \mathbf{Cp}_i F_{A0} dT - \sum_i \nu_i \mathbf{Cp}_i F_{A0} X dT - \Delta \mathbf{H}_R F_{A0} dX = 0$$

$$\therefore \mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - \left[F_{A0} \left(\sum_i \theta_i \mathbf{Cp}_i + X \sum_i \nu_i \mathbf{Cp}_i \right) \right] dT - \Delta \mathbf{H}_R F_{A0} dX = 0$$

$$\therefore \mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) - \left[F_{A0} \left(\sum_i \theta_i \mathbf{Cp}_i + X \sum_i \nu_i \mathbf{Cp}_i \right) \right] \frac{dT}{dV} - \Delta \mathbf{H}_R F_{A0} \frac{dX}{dV} = 0$$

$$\mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) - \left[F_{A0} \left(\sum_i \theta_i \mathbf{Cp}_i + X \sum_i \nu_i \mathbf{Cp}_i \right) \right] \frac{dT}{dV} - \Delta \mathbf{H}_R \underbrace{\left(-r_A \right)}_{F_{A0} \frac{dX}{dV}} = 0$$

$$\begin{aligned}
& \mathbf{U} \mathbf{a} (\mathbf{T}_a - \mathbf{T}) dV - (\mathbf{Cp}_A + \theta_B \mathbf{Cp}_B + \theta_C \mathbf{Cp}_C + \theta_D \mathbf{Cp}_D + \theta_I \mathbf{Cp}_I) F_{A0} dT - \\
& - \left(-\mathbf{Cp}_A - \frac{b}{a} \mathbf{Cp}_B + \frac{c}{a} \mathbf{Cp}_C + \frac{d}{a} \mathbf{Cp}_D \right) F_{A0} X dT - \Delta H_R F_{A0} dX - d(\Delta H_R) F_{A0} dX = 0 \\
& \quad \cancel{- d(\Delta H_R) F_{A0} dX}
\end{aligned}$$

$$U a (T_a - T) dV - \sum_i \theta_i Cp_i F_{A0} dT - \sum_i v_i Cp_i F_{A0} X dT - \Delta H_R F_{A0} dX = 0$$

$$\therefore U a (T_a - T) dV - \left[F_{A0} \left(\sum_i \theta_i Cp_i + X \sum_i v_i Cp_i \right) \right] dT - \Delta H_R F_{A0} dX = 0$$

$$\therefore U a (T_a - T) - \left[F_{A0} \left(\sum_i \theta_i Cp_i + X \sum_i v_i Cp_i \right) \right] \frac{dT}{dV} - \Delta H_R F_{A0} \frac{dX}{dV} = 0$$

$$U a (T_a - T) - \left[F_{A0} \left(\sum_i \theta_i Cp_i + X \sum_i v_i Cp_i \right) \right] \frac{dT}{dV} - \Delta H_R \underbrace{\left(-r_A \right)}_{F_{A0} \frac{dX}{dV}} = 0$$

$$\therefore \frac{dT}{dV} = \frac{U a (T_a - T) + [-\Delta H_R (T)] (-r_A)}{F_{A0} \left(\sum_i \theta_i Cp_i + X \sum_i v_i Cp_i \right)}$$

$$\left\{ \begin{array}{l} \frac{dT}{dV} = \frac{U a (T_a - T) + [-\Delta H_R(T)](-r_A)}{F_{A0} \left(\sum_i \theta_i C_{pi} + X \sum_i v_i C_{pi} \right)} \\ \frac{dX}{dV} = \frac{(-r_A)}{F_{A0}} \end{array} \right.$$

A reacção de 1^a ordem, em fase líquida, A → B, é conduzida num reactor PFR de 5 mm de diâmetro interno e 50 cm de comprimento. A alimentação ao reactor, a um caudal volumétrico de 0.004 dm³/min., é constituída por A(11.1 mol%) e por um inerte I .

The liquid phase 1st order reaction A→B is carried out in a 50 cm length by 5 mm cross-section diameter. A (11.1 mole %) and an inert I are fed to the reactor at a volumetric flow rate of 0.004 dm³/min.

**k(300 K) = 0.4 min⁻¹; ΔH_R = -22.5 kcal/mol; E = 10 kcal/mol;
 Cp_A = Cp_B = 8 cal/mol.K; Cp_I = 6 cal/mol.K; R = 1.987 cal mol⁻¹ K⁻¹.
 U = 9x10⁻⁵ cal m⁻² min⁻¹ K⁻¹**

$$\left\{ \begin{array}{l} \frac{dT}{dV} = \frac{U a (T_a - T) + [-\Delta H_R(T)] k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} (1-X)}{v_0 (Cp_A + \theta_I Cp_I + X (-Cp_A + Cp_B))} \\ \\ \frac{dX}{dV} = \frac{k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} (1-X)}{v_0} \end{array} \right.$$

$$\left\{ \begin{array}{l} \dfrac{dT}{dV} = \dfrac{\displaystyle U a \left(T_a - T \right) + \left[- \Delta H_R(T) \right] k(T_R) e^{- \dfrac{E}{R} \left(\dfrac{1}{T} - \dfrac{1}{T_R} \right)} \left(1 - X \right)}{\displaystyle v_0 \left(Cp_A + \theta_I \, Cp_I + X \left(-Cp_A + Cp_B \right) \right)} \\ \\ \dfrac{dX}{dV} = \dfrac{k(T_R) e^{- \dfrac{E}{R} \left(\dfrac{1}{T} - \dfrac{1}{T_R} \right)} \left(1 - X \right)}{v_0} \end{array} \right.$$

$$a=\frac{2\,\pi\,r\,L}{\pi\,r^2\,L}=\frac{2}{r}=\frac{2}{\frac{d}{2}}=\frac{4}{d}$$

$$\left\{ \begin{array}{l} \dfrac{dT}{dV} = \dfrac{\textcolor{black}{Ua}\left(T_a-T\right) + \left[-\Delta H_R(T)\right]k(T_R)e^{-\dfrac{E}{R}\left(\dfrac{1}{T}-\dfrac{1}{T_R}\right)}\left(1-X\right)}{v_0\left(Cp_A+\theta_I\,Cp_I+X\left(-Cp_A+Cp_B\right)\right)} \\ \\ \dfrac{dX}{dV} = \dfrac{k(T_R)e^{-\dfrac{E}{R}\left(\dfrac{1}{T}-\dfrac{1}{T_R}\right)}\left(1-X\right)}{v_0} \end{array} \right.$$

$$a=\frac{2\,\pi\,r\,L}{\pi\,r^2\,L}=\frac{2}{r}=\frac{2}{\frac{d}{2}}=\frac{4}{d}$$

$$\theta_I = \frac{F_{I0}}{F_{A0}} = \frac{y_{I0}}{y_{A0}} = \frac{1 - 0.111}{0.111} = 8.01$$

$$\left\{ \begin{array}{l} \dfrac{dT}{dV} = \dfrac{\displaystyle U \, a \, (T_a - T) + \left[- \Delta H_R^0(T) \right] k(T_R) e^{- \displaystyle \dfrac{E}{R} \left(\dfrac{1}{T} - \dfrac{1}{T_R} \right)} (1-X)}{\nu_0 \left(Cp_A + \theta_I \, Cp_I + X \left(-Cp_A + Cp_B \right) \right)} \\ \\ \dfrac{dX}{dV} = \dfrac{k(T_R) e^{- \displaystyle \dfrac{E}{R} \left(\dfrac{1}{T} - \dfrac{1}{T_R} \right)} (1-X)}{\nu_0} \end{array} \right.$$

$$a=\frac{2\,\pi\,r\,L}{\pi\,r^2\,L}=\frac{2}{r}=\frac{2}{\frac{d}{2}}=\frac{4}{d}$$

$$\theta_I = \frac{F_{I0}}{F_{A0}} = \frac{y_{I0}}{y_{A0}} = \frac{1-0.111}{0.111} = 8.01$$

$$\left\{ \begin{array}{l} \dfrac{dT}{A_c dz} = \dfrac{\displaystyle U \, a \, (T_a - T) + \left[- \Delta H_R^0(T_R) \right] k(T_R) e^{- \displaystyle \dfrac{E}{R} \left(\dfrac{1}{T} - \dfrac{1}{T_R} \right)} (1-X)}{\nu_0 \left(Cp_A + \theta_I \, Cp_I \right)} \\ \\ \dfrac{dX}{A_c dz} = \dfrac{k(T_R) e^{- \displaystyle \dfrac{E}{R} \left(\dfrac{1}{T} - \dfrac{1}{T_R} \right)} (1-X)}{\nu_0} \end{array} \right.$$

$$\left\{\begin{array}{l}\dfrac{dT}{dz}=\dfrac{U\,a\,(T_a-T)+\left[-\Delta H_R^0(T_R)\right]k(T_R)e^{-\dfrac{E}{R}\left(\dfrac{1}{T}-\dfrac{1}{T_R}\right)}(1-X)}{v_0\left(Cp_A+\theta_I\,Cp_I\right)}A_c\\ \\ \dfrac{dX}{dz}=\dfrac{k(T_R)e^{-\dfrac{E}{R}\left(\dfrac{1}{T}-\dfrac{1}{T_R}\right)}(1-X)}{v_0}A_c\end{array}\right.$$

$$\begin{cases} \frac{dT}{dz} = \frac{U a (T_a - T) + [-\Delta H_R^0(T_R)] k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} (1-X) A_c}{v_0 (Cp_A + \theta_I Cp_I)} \\ \\ \frac{dX}{dz} = \frac{k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} (1-X) A_c}{v_0} \end{cases}$$

Método de Euler:

Euler method

$$\begin{cases} \frac{dT}{dz} = \frac{U a (T_a - T) + [-\Delta H_R^0(T_R)] k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} (1-X) A_c}{v_0 (Cp_A + \theta_I Cp_I)} \\ \\ \frac{dX}{dz} = \frac{k(T_R) e^{-\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} (1-X) A_c}{v_0} \end{cases}$$

Método de Euler:

Euler method

$$\begin{cases} T_{i+1} = T_i + \frac{800 U (298 - T_i) + 22500 \times k(T_R) e^{-\frac{10000}{1.987} \left(\frac{1}{T_i} - \frac{1}{300} \right)} (1-X_i) \pi \frac{d^2}{4} \Delta z}{v_0 (8 + 8.01 \times 6)} \\ \\ X_{i+1} = X_i + \frac{k(T_R) e^{-\frac{10000}{1.987} \left(\frac{1}{T_i} - \frac{1}{300} \right)} (1-X_i) \pi \frac{d^2}{4} \Delta z}{v_0} \end{cases}$$

Folha de Cálculo