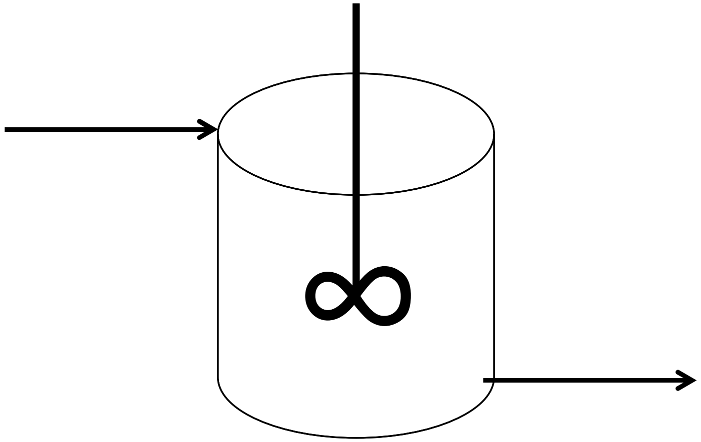
Balanço de Energia em Reatores CSTR

Exemplo de Aplicação:

Reator CSTR

Reação: A ➔ B, em fase líquida



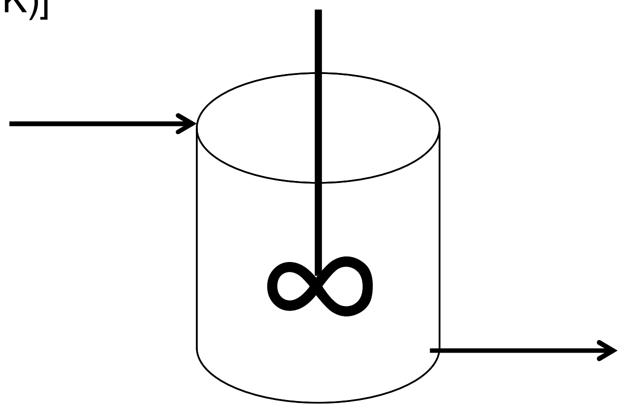
Exemplo:

Reator CSTR, volume V = 18 Litros;

Reação: A ➔ B, em fase líquida

$$(-r_A) = kC_A = k\left[C_{A0}(1-X_A)\right] \quad \text{[kmol/(m}^3\text{ s)]}$$

$$k = 4,48 \times 10^6 \exp\left[\frac{-62800}{RT}\right] \quad R \text{ em [J/(mol K)]}$$



$$\Delta H^0_{R,T_R} = -2,09 \times 10^8 \ \frac{\text{J}}{\text{kmol}}$$

$$\hat{c}_{p,A} = \hat{c}_{p,B} = \hat{c}_{p,solução} = 4,18 \ \frac{\text{kJ}}{\text{kg K}}$$

Densidade do fluido = 1000 kg m^{-3}

Calcular X_A e T supondo que o reator é **adiabático** e opera nas seguintes condições:

$\dot{Q} = 0$

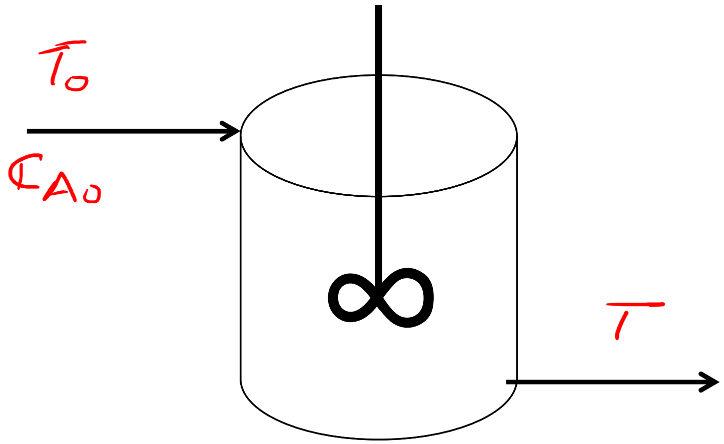
$\dot{W}_s \cong 0$

Corrente de Alimentação: solução líquida de A, com:

$v_0 = 60 \times 10^{-6}\ m^3/s$

$T_0 = 25^o\ C$

$C_{AO} = 3\ mol/L$ $\qquad C_{BO} = 0$



X_A
T ?

Aplicação da Eq. 21 a um reator CSTR:

$$\tilde{H}_{j,T} = \int_{T_{ref}}^{T} \tilde{C}p_j \, dT \simeq \tilde{C}p_j (T - T_{ref})$$

$$0 = \dot{Q} - \dot{W}_s + \sum_{j=1}^{n} F_{j0} (\tilde{H}_{j0} - \tilde{H}_j) - V \sum_{i=1}^{Q} r_i \Delta H_{R\,i,T}$$

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1 reação: $Q = 1$: $A \rightarrow B$ $(-r_A)$ ...

Bal. Molar (p/ A): $F_{A0} - F_A + r_A V = 0$

$\therefore F_{A0} X_A = (-r_A) V$

$$\underline{BE}: \quad \dot{Q} - \dot{W}_s + F_{A0} \sum_{j=1}^{n} \theta_j \tilde{c_{p}}_j (T_0 - T) - \underbrace{V(-r_A)}_{= F_{A0} X_A} \Delta H_{R_T} = 0$$

($\tilde{c_p}_j \simeq$ constante entre T_0 e T
ou $\simeq \tilde{c_p}_j$ médio nesse intervalo)

$$\theta_j = \frac{F_{j0}}{F_{A0}} \qquad F_{j0} = \theta_j \cdot F_{A0}$$

$$0 = \dot{Q} - \dot{W}_s - F_{A0} \left[\sum_{j=1}^{n} \theta_j \tilde{c_p}_j (T - T_0) + \Delta H_{R,T} X_A \right]$$

Balanço Molar:

$$F_{A0} - F_A + r_A V = 0$$

ou: $$F_{A0} X_A = (-r_A) V = k C_{A0} V (1 - X_A)$$

$$\tau = \frac{V}{v_0}$$

$$\boxed{X_A = \frac{k\tau}{1 + k\tau}}$$

$$k = 4,48 \times 10^6 \exp\left[\frac{-62800}{RT}\right]$$

Balanço de Energia:

$$0 = \dot{Q} - \dot{W}_s - F_{A0}\left[\sum_{j=1}^{n} \theta_j \tilde{c}_{pj}(T - T_0) + \Delta H_{R,T} X_A\right]$$

$$F_{j0} = F_{A0}\Theta_j$$

$$X_A = \frac{F_{A0}\sum_{j=1}^{n}\theta_j \tilde{c}_{pj}(T - T_0)}{-\Delta H_{Ri,T} F_{A0}}$$

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v_0 = 60x10^{-6} m^3/s   Densidade do fluido = 1000 kg m^{-3} $\hat{c}_{p,A} = \hat{c}_{p,B} = \hat{c}_{p,solução} = 4{,}18 \frac{k\,J}{kg\,K}$

Balanço de Energia:

$$0 = \dot{Q} - \dot{W}_s - F_{A0}\left[\sum_{j=1}^{n} \theta_j \tilde{c}_{pj} (T - T_0) + \Delta H_{R,T} X_A\right]$$

$$F_{j0} = F_{A0}\Theta_j$$

$$= \dot{m}\hat{c}_p$$

$$X_A = \frac{\boxed{F_{A0} \sum_{j=1}^{n} \theta_j \tilde{c}_{pj}} (T - T_0)}{-\Delta H_{Ri,T} F_{A0}}$$

v_0 = 60x10^{-6} m^3/s   Densidade do fluido = 1000 kg m^{-3} $\hat{c}_{p,A} = \hat{c}_{p,B} = \hat{c}_{p,solução} = 4{,}18 \dfrac{kJ}{kg\ K}$

Balanço Molar:

$$X_A = \frac{k\tau}{1 + k\tau} \qquad (1)$$

$$k = 4,48 \times 10^6 \exp\left[\frac{-62800}{RT}\right]$$

Balanço de Energia:

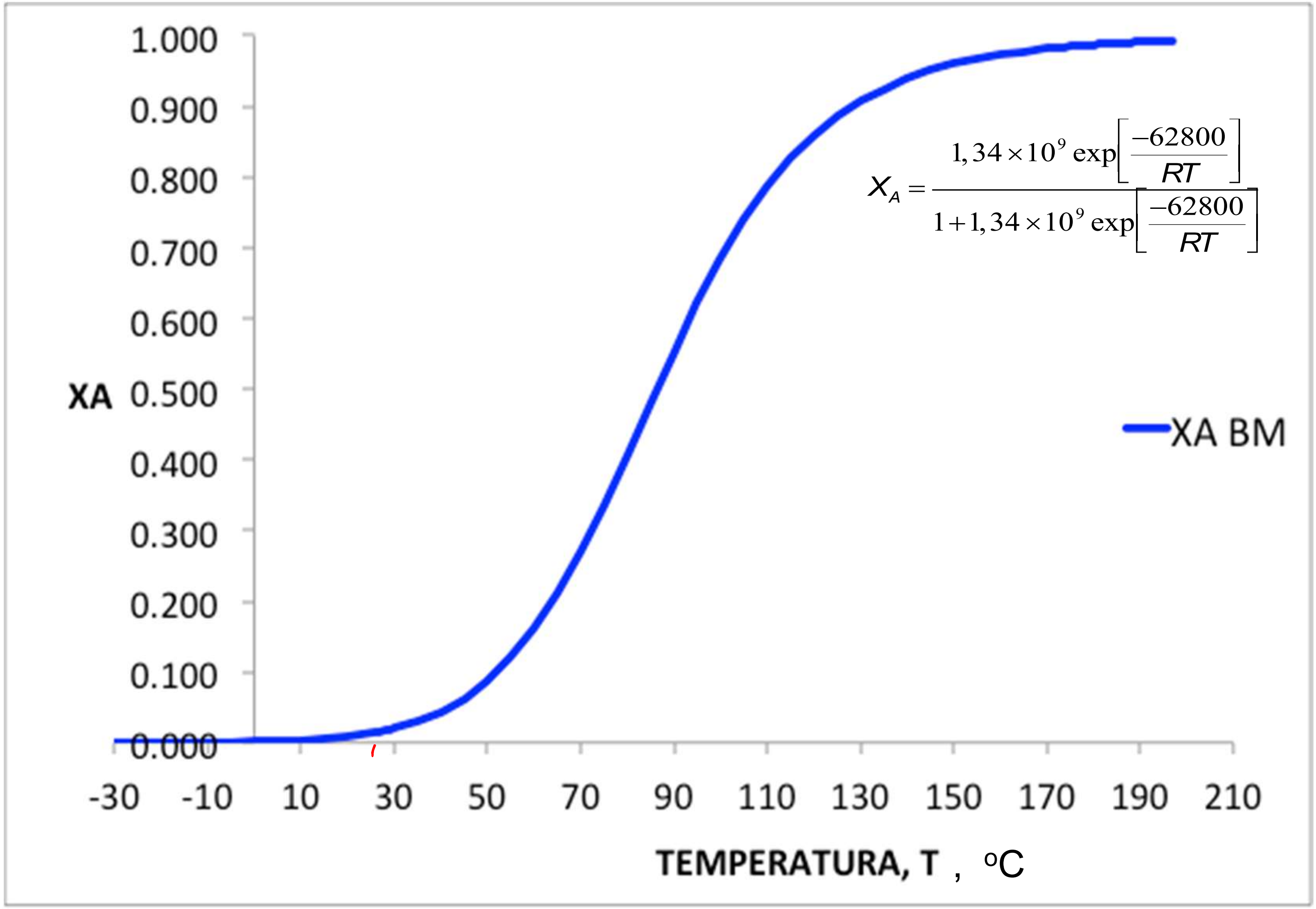
$$X_A = \frac{\dot{m}\hat{c}_p (T - T_0)}{-\Delta H_{R,T} F_{A0}} \qquad (2)$$

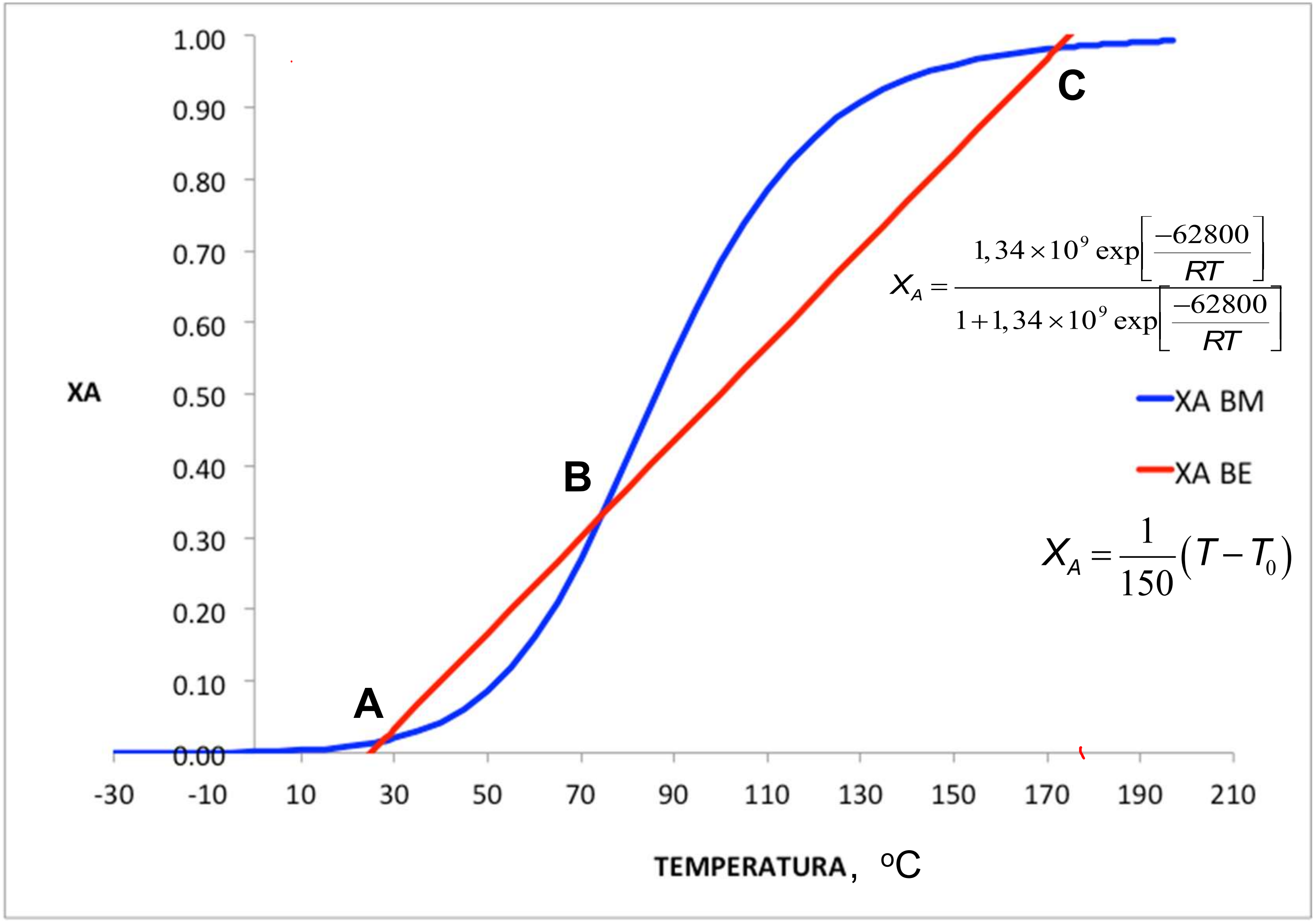
Balanço Molar (com os valores numéricos):

$$X_A = \frac{1,34\times 10^9 \exp\left[\frac{-62800}{RT}\right]}{1+1,34\times 10^9 \exp\left[\frac{-62800}{RT}\right]} \qquad (1)$$

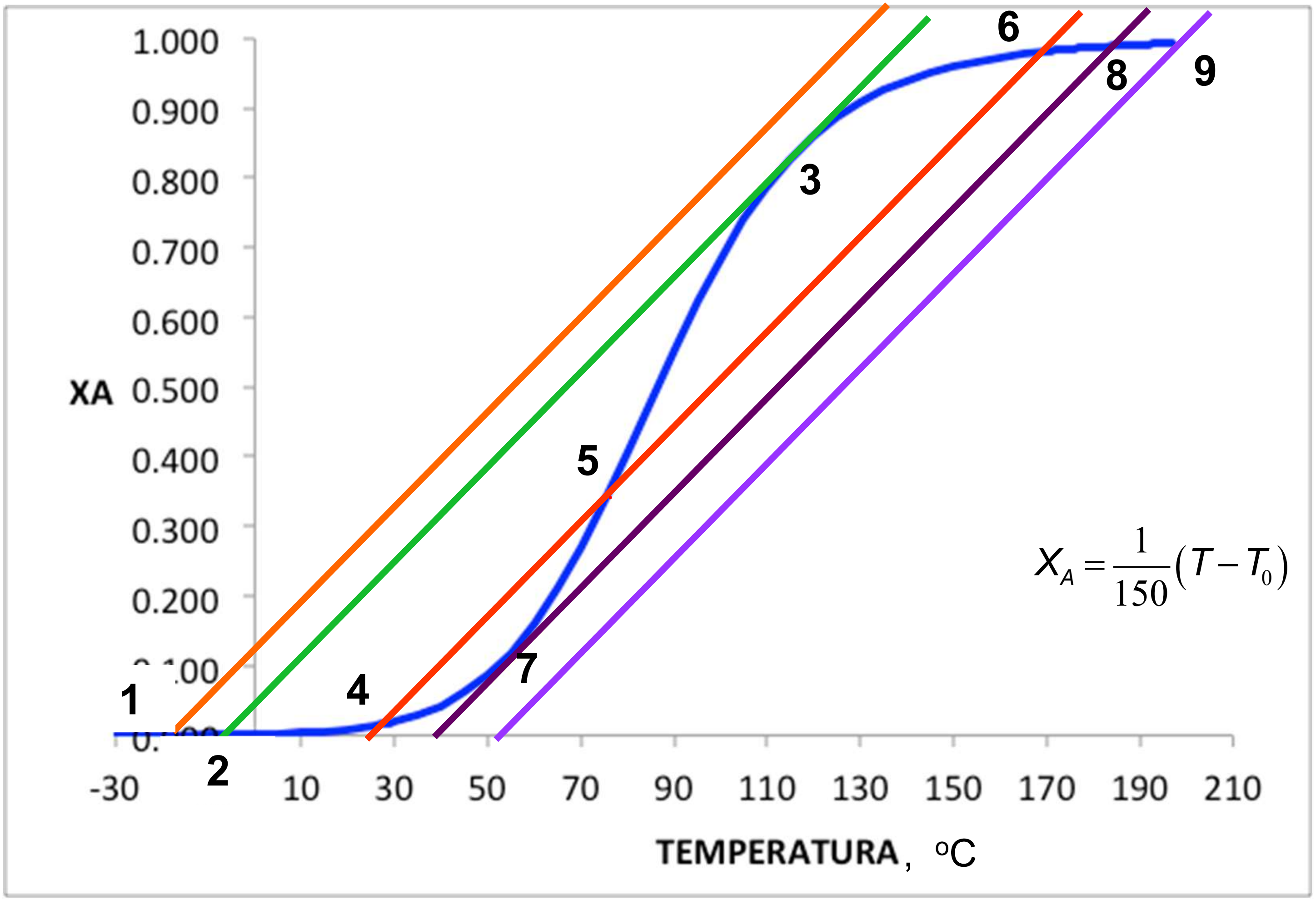
Balanço de Energia (com os valores numéricos):

$$X_A = \frac{1}{150}\left(T - T_0\right) \qquad (2)$$


1.000
0.900
0.800
0.700
0.600
XA
0.500
0.400
0.300
0.200
0.100
0.000
-30
-10
10
30
50
70
90
110
130
150
170
190
210
TEMPERATURA, T , °C
XA BM
$X_A = \dfrac{1,34\times10^9 \exp\left[\dfrac{-62800}{RT}\right]}{1+1,34\times10^9 \exp\left[\dfrac{-62800}{RT}\right]}$



1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
XA
-30
-10
10
30
50
70
90
110
130
150
170
190
210
TEMPERATURA, °C
A
B
C
$X_A = \dfrac{1,34\times10^9 \exp\left[\dfrac{-62800}{RT}\right]}{1+1,34\times10^9 \exp\left[\dfrac{-62800}{RT}\right]}$
XA BM
XA BE
$X_A = \dfrac{1}{150}(T - T_0)$



1.000
0.900
0.800
0.700
0.600
XA
0.500
0.400
0.300
0.200
1
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6
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-30
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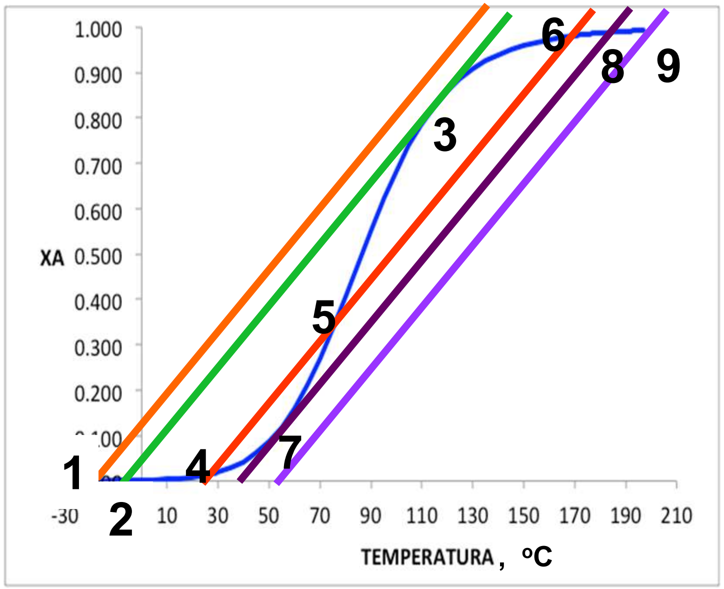
150
170
190
210
TEMPERATURA, ºC
$X_A = \frac{1}{150}(T - T_0)$


1.000
0.900
0.800
0.700
0.600
XA 0.500
0.400
0.300
0.200
-30 10 30 50 70 90 110 130 150 170 190 210
TEMPERATURA , ºC
1
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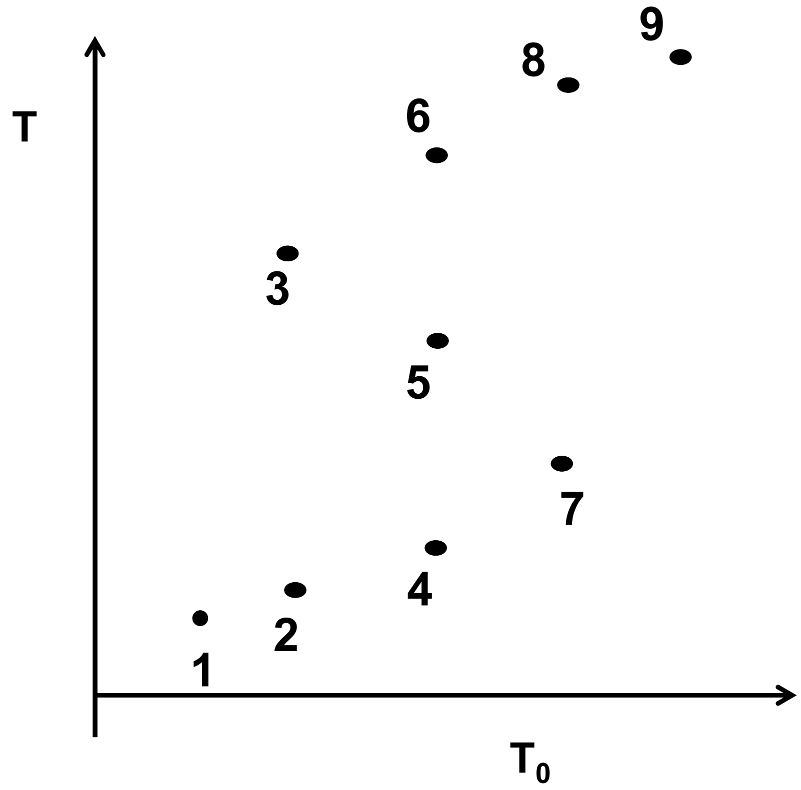
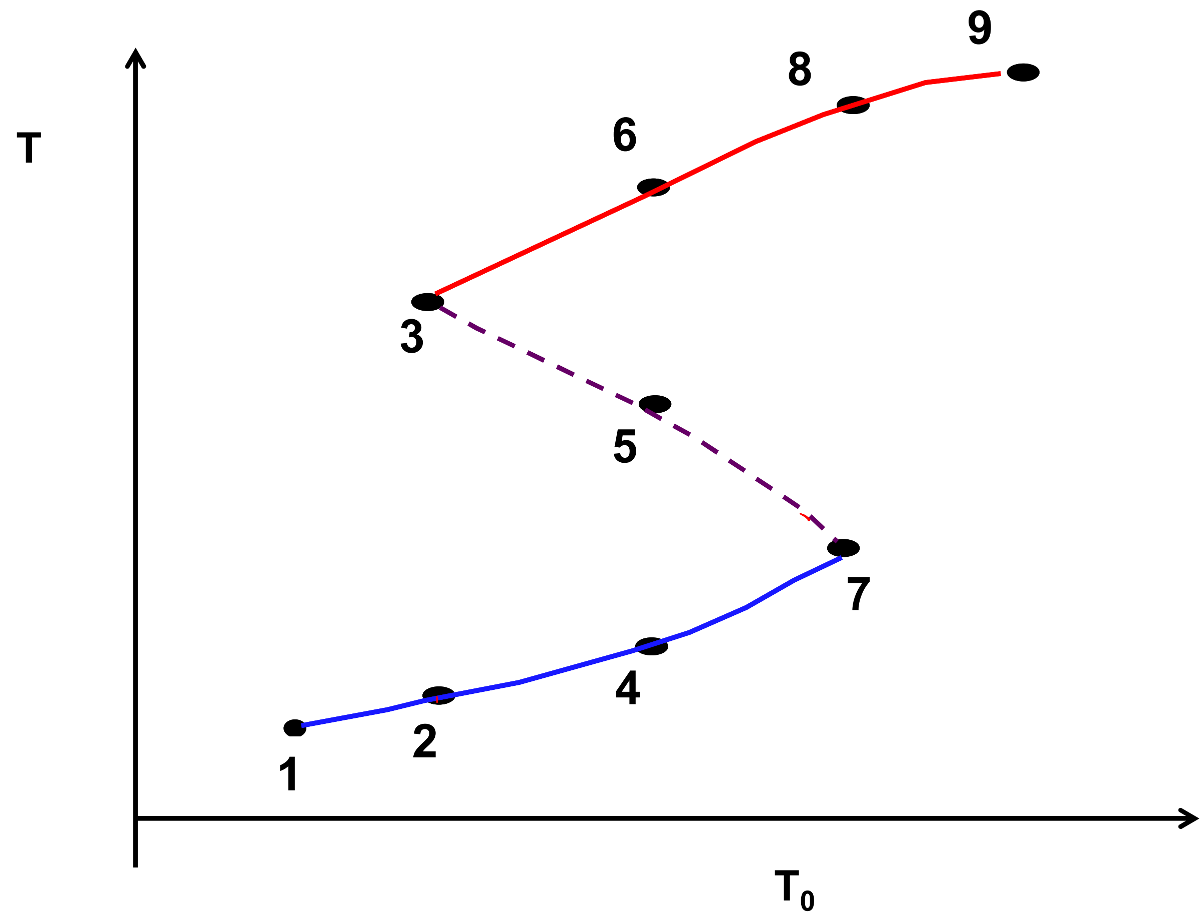
9


T
T_0
1
2
3
4
5
6
7
8
9



T
T0
1
2
3
4
5
6
7
8
9

Voltando ao Balanço de Energia:

$$\dot{Q} - \dot{W}_s + F_{A0}\sum_{j=1}^{n}\theta_j\,\tilde{c}_{pj}\,(T_0 - T) - V\sum_{i=1}^{Q} r_j\,\Delta H_{Ri,T} = 0$$

$$UA(T_a - T) + F_{A0}\sum_{j=1}^{n}\theta_j\,\tilde{c}_{pj}\,(T_0 - T) - V(-r_A)\Delta H_{R,T} = 0$$

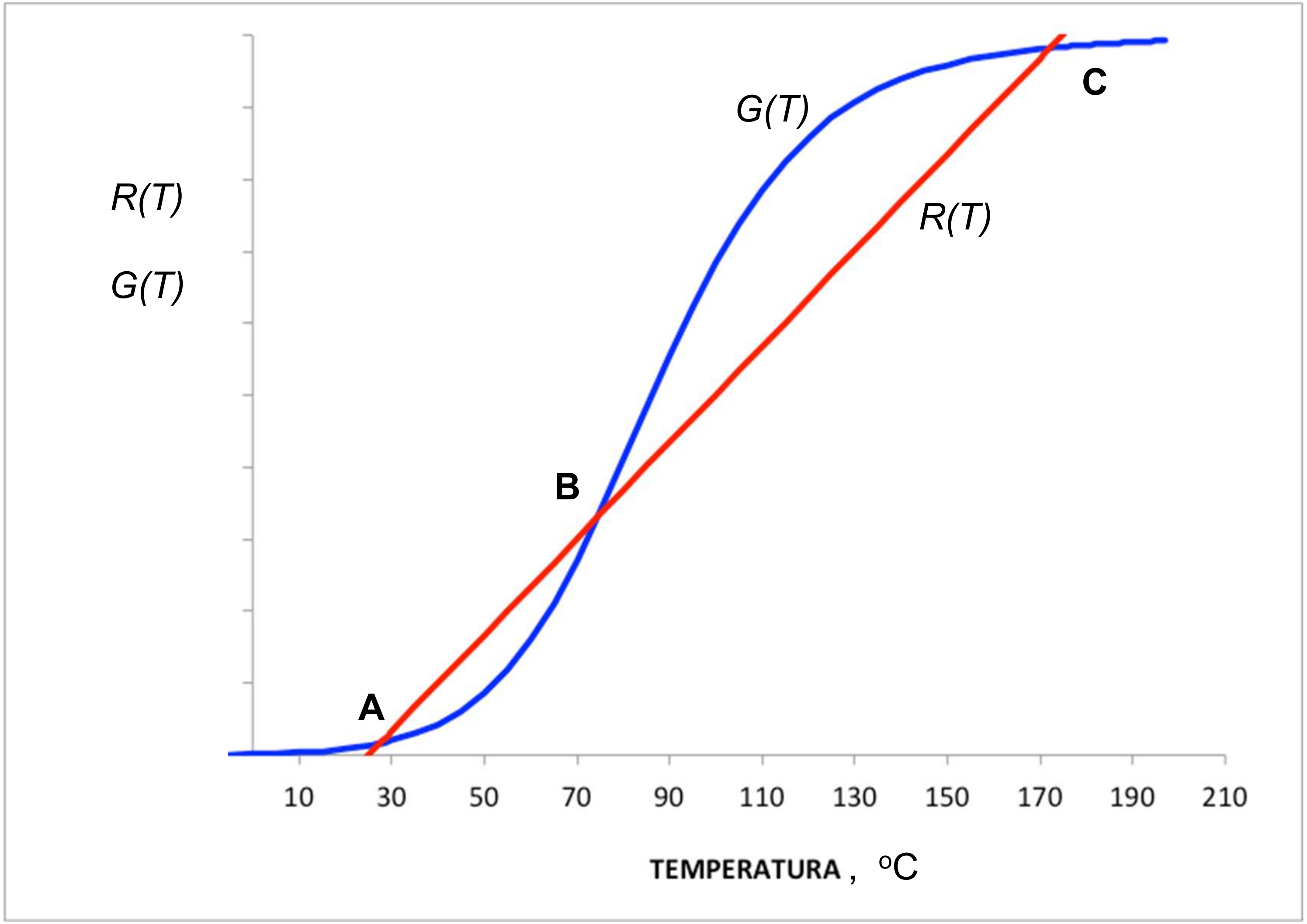
$$UA(T_a - T) + F_{A0}\sum_{j=1}^{n}\theta_j\,\tilde{c}_{pj}\,(T_0 - T) = V(-r_A)\Delta H_{R,T}$$

$$UA(T - T_a) + F_{A0} \sum_{j=1}^{n} \theta_j \, \tilde{c}_{pj} \, (T - T_0) = -V(-r_A)\Delta H_{R,T}$$

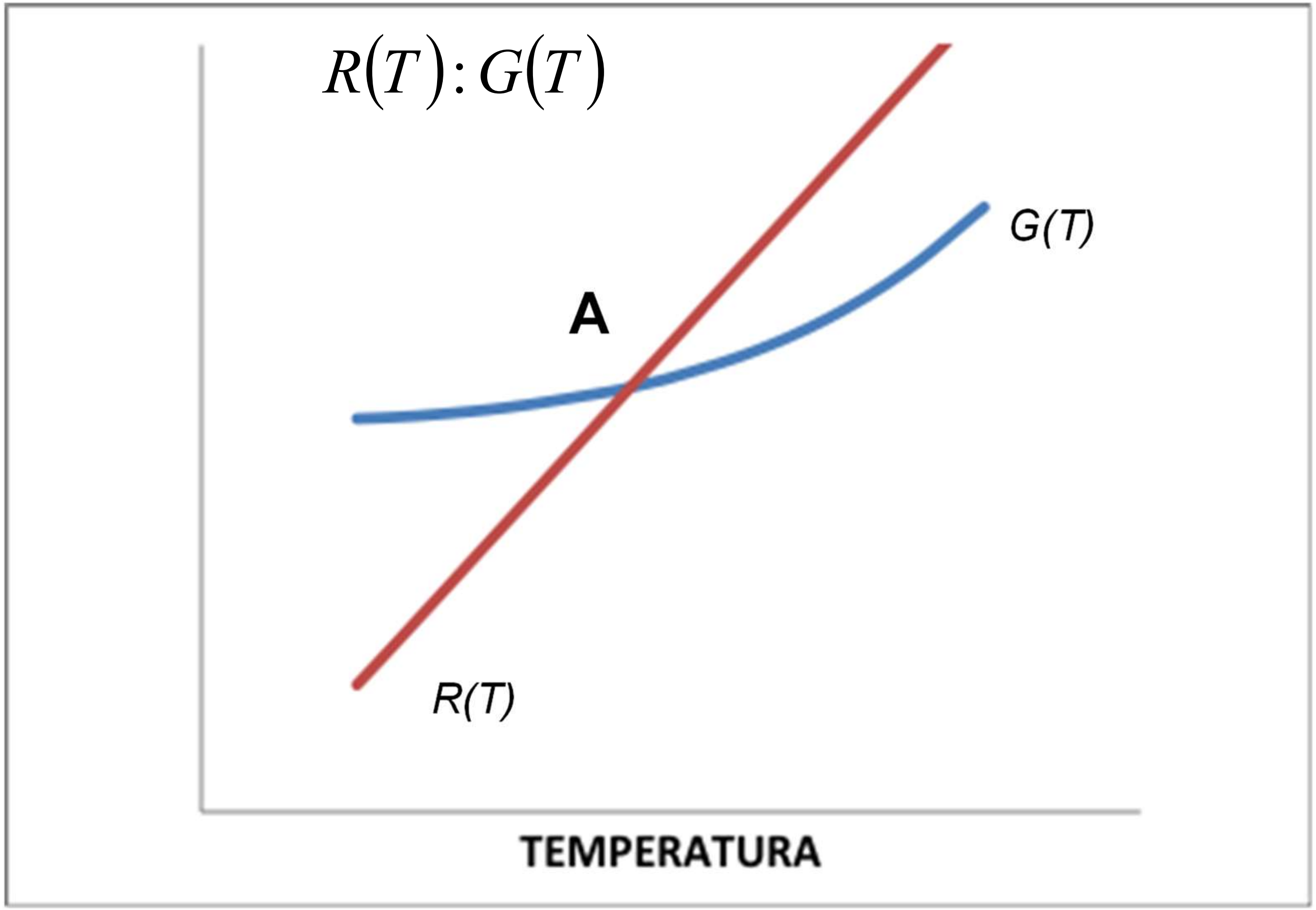
$$UA(T - T_a) + F_{A0} \sum_{j=1}^{n} \theta_j \, \tilde{c}_{pj} \, (T - T_0) = -\Delta H_{R,T} F_{A0} X_A$$

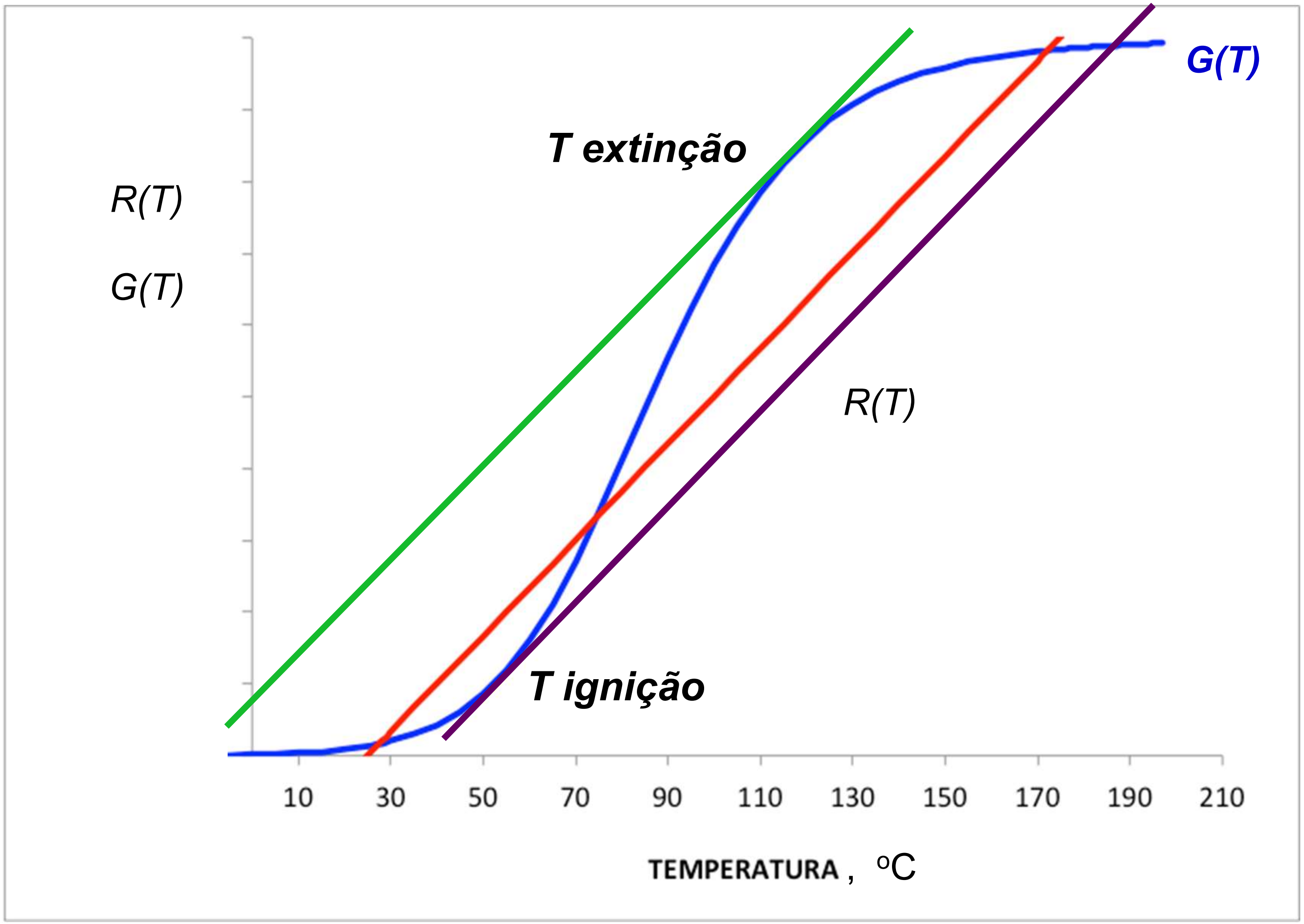
$$\boxed{X_A = \frac{k\tau}{1 + k\tau}}$$

$$\boxed{R(T) = G(T)}$$


R(T)
G(T)
G(T)
R(T)
A
B
C
10
30
50
70
90
110
130
150
170
190
210
TEMPERATURA , °C

Análise de Estabilidade das Soluções




G(T)
T extinção
R(T)
G(T)
R(T)
T ignição
10
30
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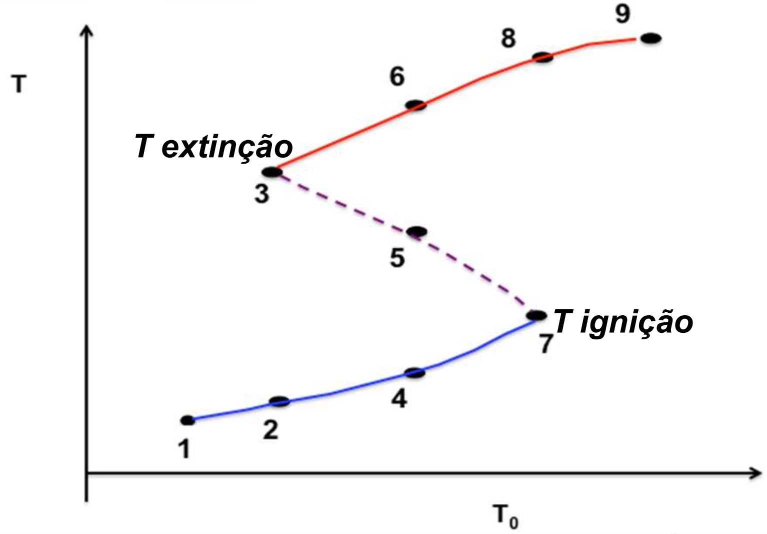
150
170
190
210
TEMPERATURA , °C

Condições das soluções:

$$R(T) = G(T)$$



Para T_{ign} ou T_{ext}:

$$\frac{dR}{dT} = \frac{dG}{dT}$$

$$\frac{d^2R}{dT^2} < \frac{d^2G}{dT^2} \qquad T_{ign}$$

$$\frac{d^2R}{dT^2} > \frac{d^2G}{dT^2} \qquad T_{ext}$$