Simulación y Optimización

Modelado
Parte VI

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Estudio de estabilidad

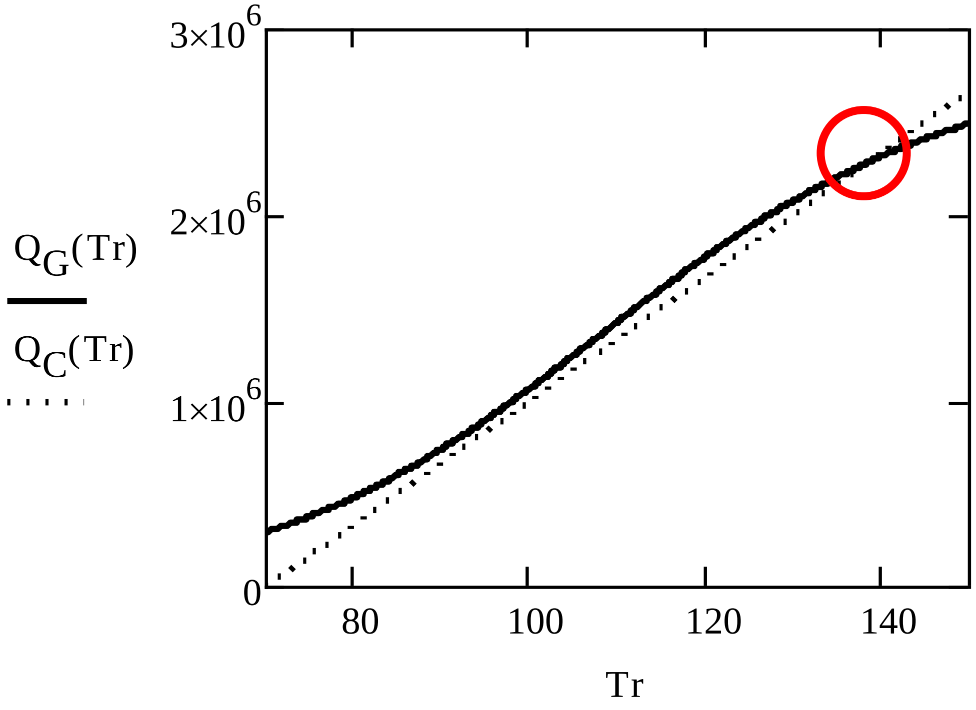
Estudio de estabilidad

Estado estacionario

$$0 = F_0\, C_0\, Cp_0\, (T_0 - T) + V\, r\, (-\Delta H) - Q$$

$$Q_G = V\, r\, (-\Delta H) \qquad r(T)$$

$$Q_C = F_0\, C_0\, Cp_0 \left(T - T_0\right) + Q \qquad Q(T)$$



Calor generado

$$Q_G = V\,r\,(-\Delta H)$$

$$r = \alpha\, e^{-\frac{E}{RT}} C_A$$

$$0 = \frac{F_0\left(C_{A0} - C_A\right)}{V} - r$$

$$r = \frac{\alpha\, e^{-\frac{E}{RT}} C_{A0}}{\frac{V}{F_0}\alpha\, e^{-\frac{E}{RT}} + 1}$$

$$Q_G = \frac{V\,\alpha\, e^{-\frac{E}{RT}} C_{A0}\,(-\Delta H)}{\frac{V}{F_0}\alpha\, e^{-\frac{E}{RT}} + 1}$$

Calor consumido

$$Q_C = F_0\, C_0\, Cp_0 \left(T - T_0\right) + Q$$

$$Q_C = F_0\, C_0\, Cp_0 \left(T - T_0\right) + N_{s0}\, Cp_{s0} \left(T - T_{s0}\right)\left(1 - e^{-\frac{UA}{N_{s0}\, Cp_{s0}}}\right)$$

$$Q = UA \frac{T_s - T_{s0}}{\ln\left(\frac{T - T_{s0}}{T - T_s}\right)}$$

$$Q = N_{s0}\, Cp_{s0} \left(T_s - T_{s0}\right)$$

$$Q = N_{s0}\, Cp_{s0} \left(T - T_{s0}\right)\left(1 - e^{-\frac{UA}{N_{s0}\, Cp_{s0}}}\right)$$

Estado estacionario

$$Q_C = F_0\, C_0\, Cp_0 \left(T - T_0\right) + N_{s0}\, Cp_{s0} \left(T - T_{s0}\right) \left(1 - e^{-\frac{UA}{N_{s0}\, Cp_{s0}}}\right)$$

$$Q_C = \left(F_0\, C_0\, Cp_0 + N_{s0}\, Cp_{s0} \left(1 - e^{-\frac{UA}{N_{s0}\, Cp_{s0}}}\right)\right) T - \left(F_0\, C_0\, Cp_0\, T_0 + N_{s0}\, Cp_{s0}\, T_{s0} \left(1 - e^{-\frac{UA}{N_{s0}\, Cp_{s0}}}\right)\right)$$

- No se puede modificar la pendiente sin modificar la distancia al origen; pero sí se puede modificar la distancia al origen sin alterar la pendiente variando T_0 y T_{s0}.

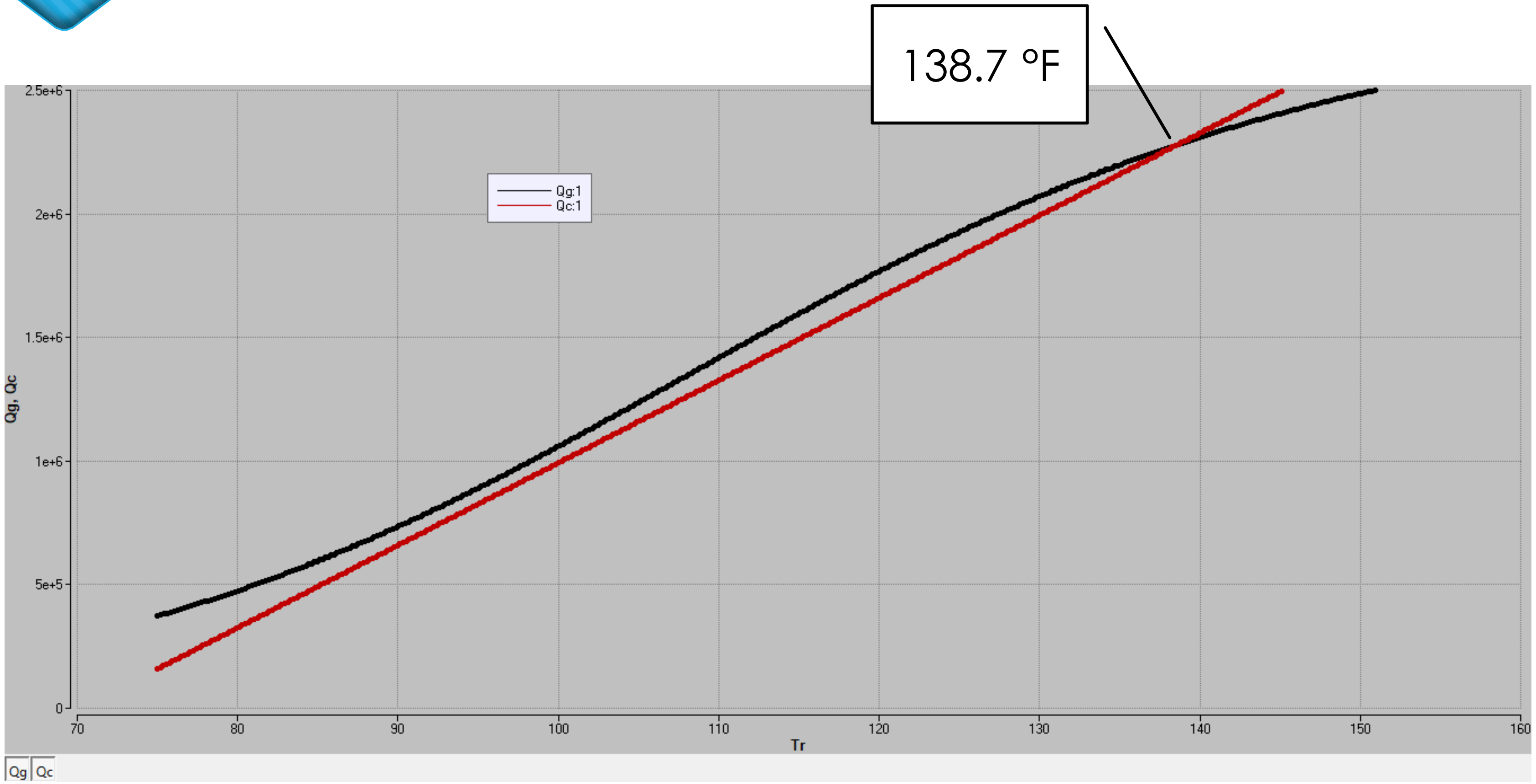
- Q_C depende de la corriente de enfriamiento, mientras que Q_G no.

Calor generado y consumido

$$Q_G = \frac{V \alpha e^{-\frac{E}{RT}} C_{A0} (-\Delta H)}{\frac{V}{F_0} \alpha e^{-\frac{E}{RT}} + 1}$$

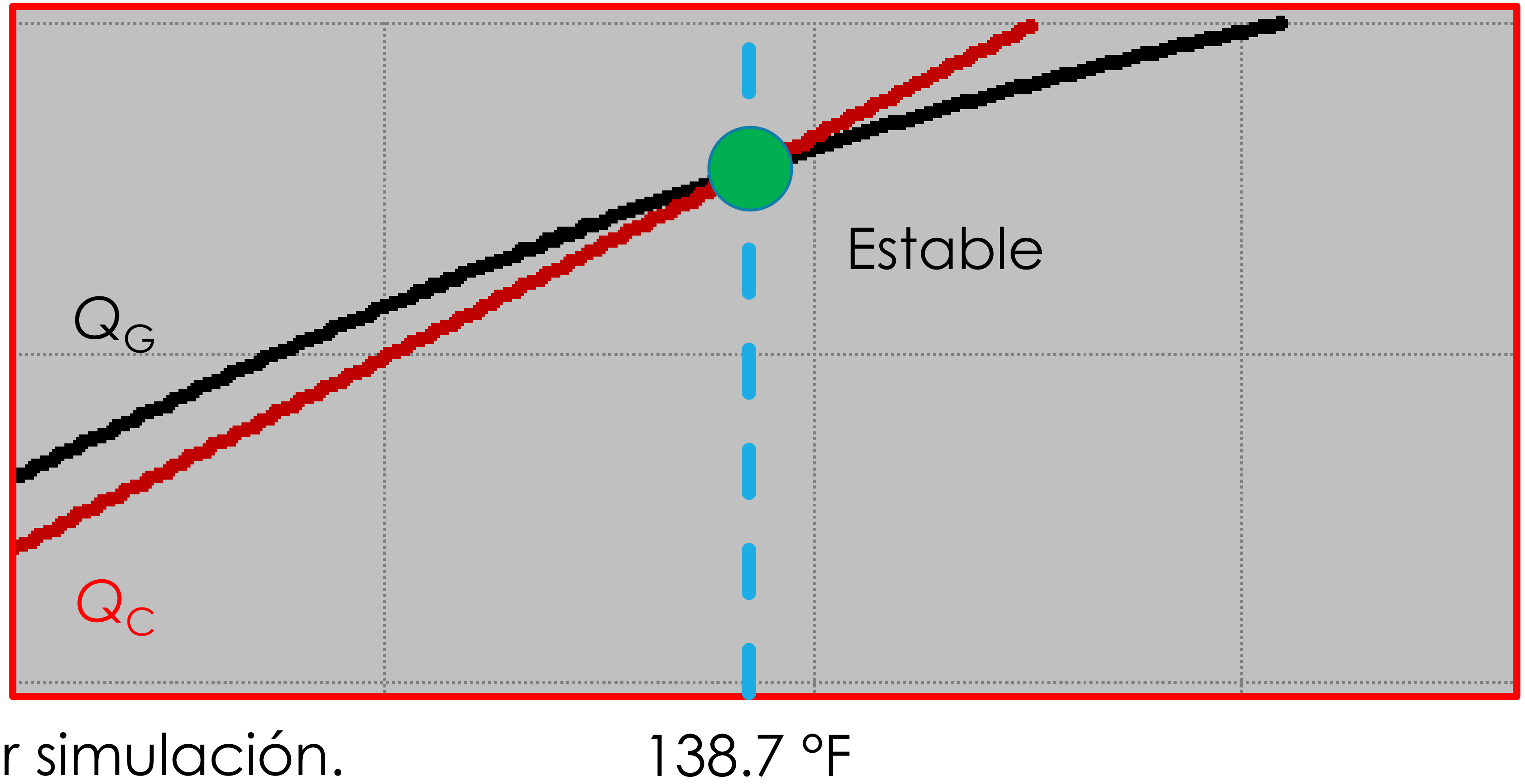
$$Q_C = F_0 C_0 Cp_0 (T - T_0) + N_{s0} Cp_{s0} (T - T_{s0}) \left(1 - e^{-\frac{UA}{N_{s0} Cp_{s0}}} \right)$$

Estado estacionario



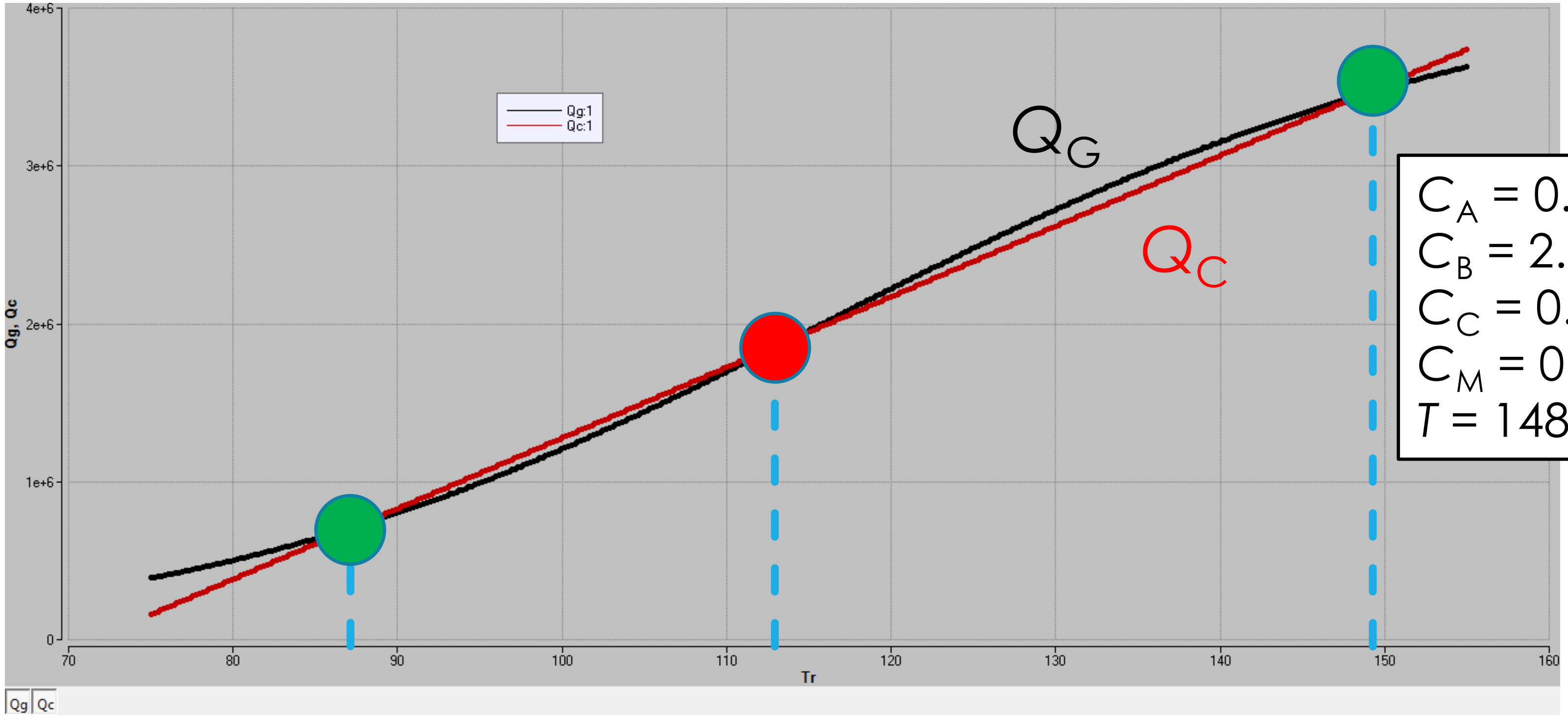
[Simulación de un reactor CSTR]

Estabilidad



Verificar por simulación.

Estabilidad, 50 % de aumento en F_0

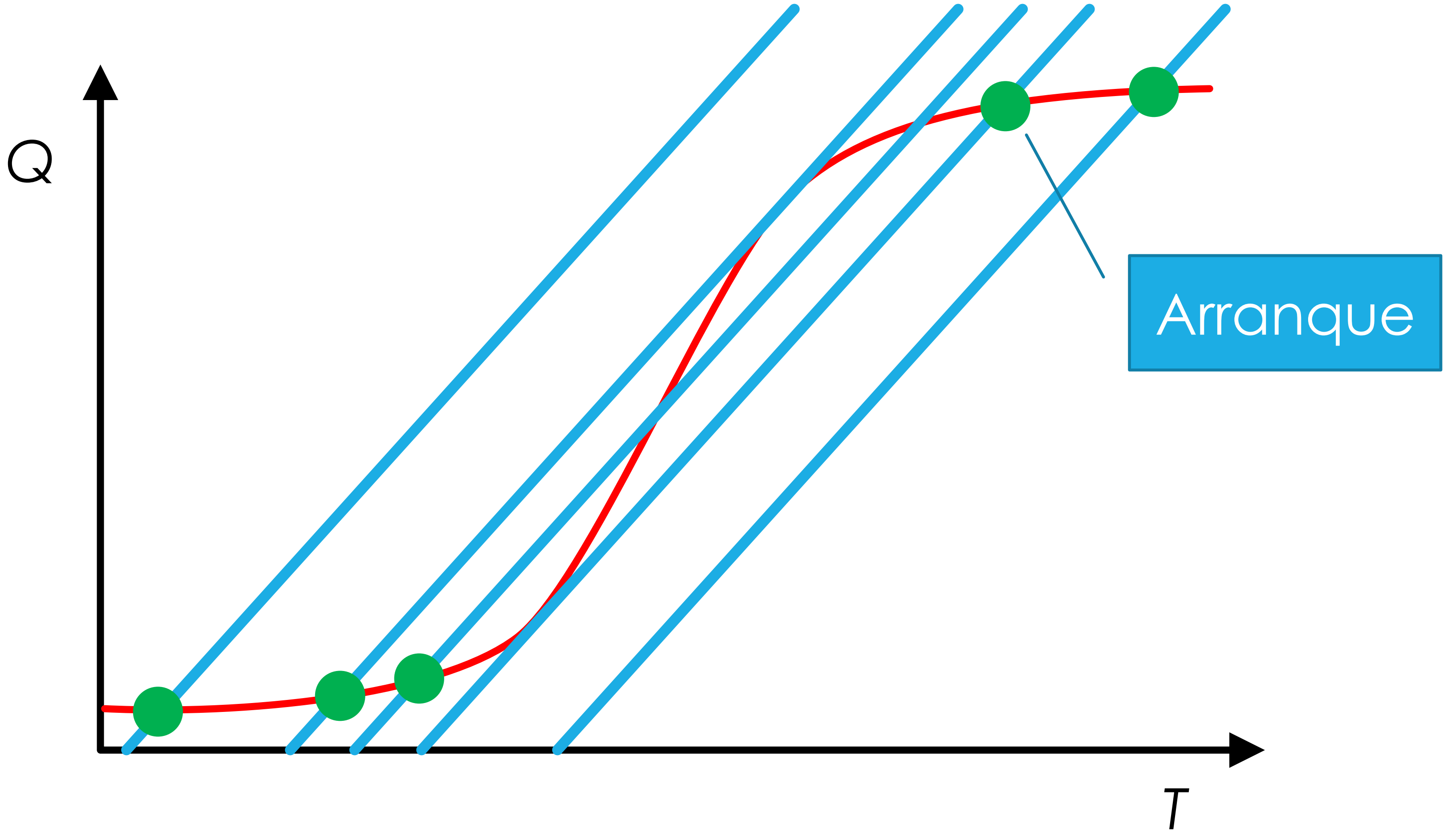


C_A = 0.0365 lb-mol/ft^3
C_B = 2.1245 lb-mol/ft^3
C_C = 0.1451 lb-mol/ft^3
C_M = 0.2269 lb-mol/ft^3
T = 148.6 °F

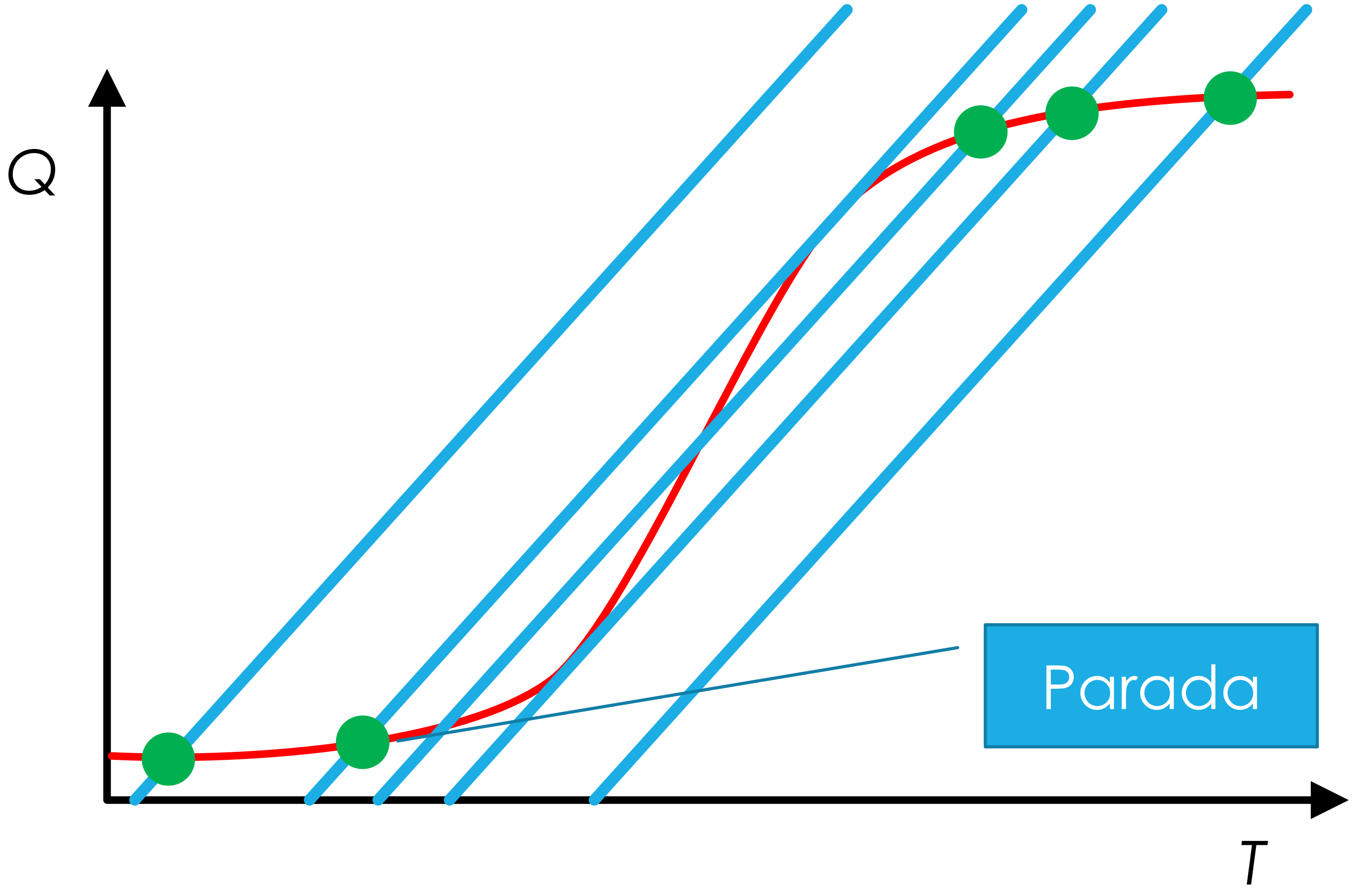
87.54 °F　　113.72 °F　　148.6 °F

Verificar por simulación.

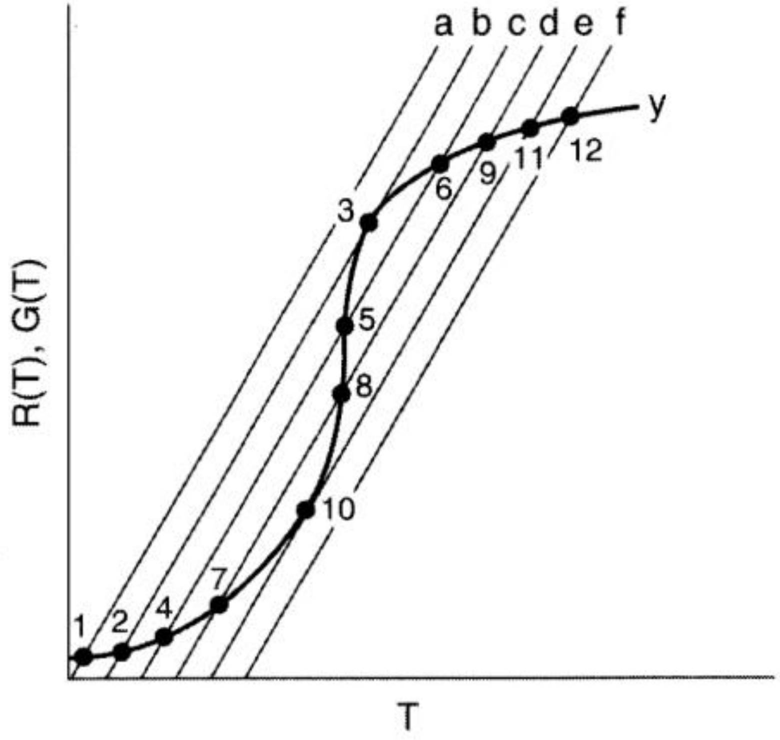
Arranque aumentando T_0



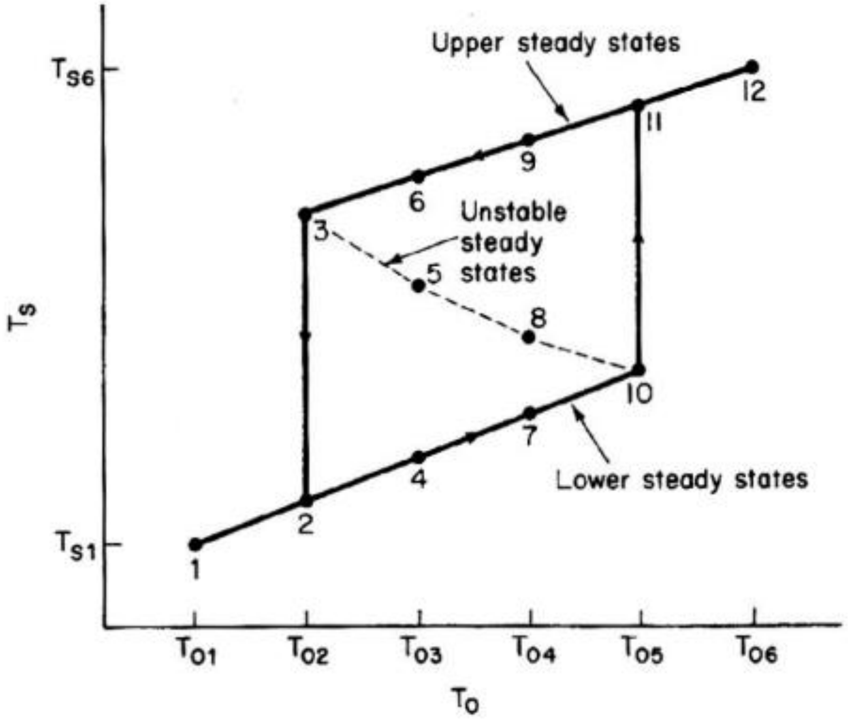
Parada disminuyendo T_0



Histéresis

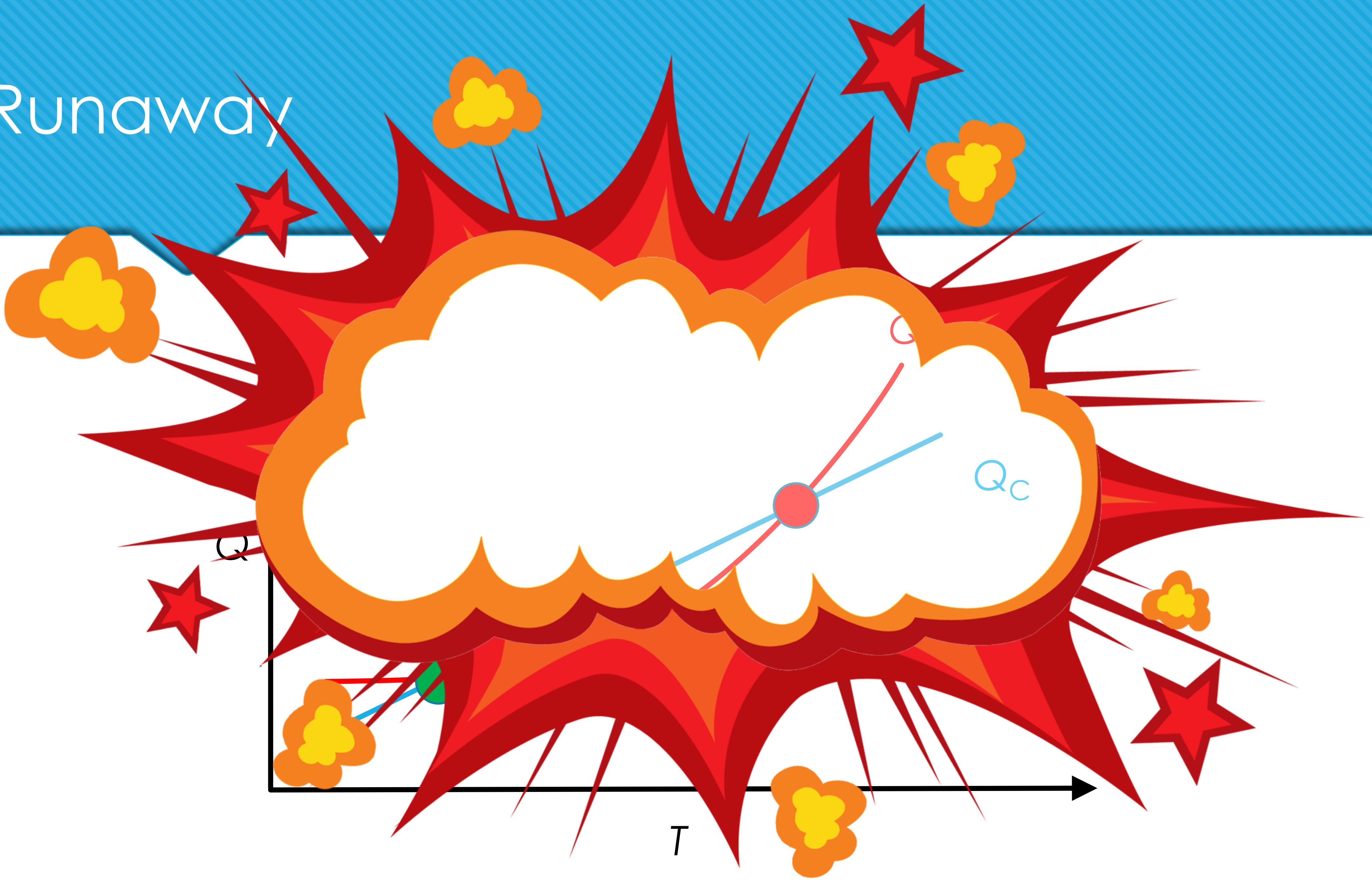


a b c d e f
y
1
2
4
7
10
8
5
3
6
9
11
12
R(T), G(T)
T



Upper steady states
Unstable steady states
Lower steady states
T_{S6}
T_{S1}
T_S
T_{01} T_{02} T_{03} T_{04} T_{05} T_{06}
T_0
1
2
3
4
5
6
7
8
9
10
11
12

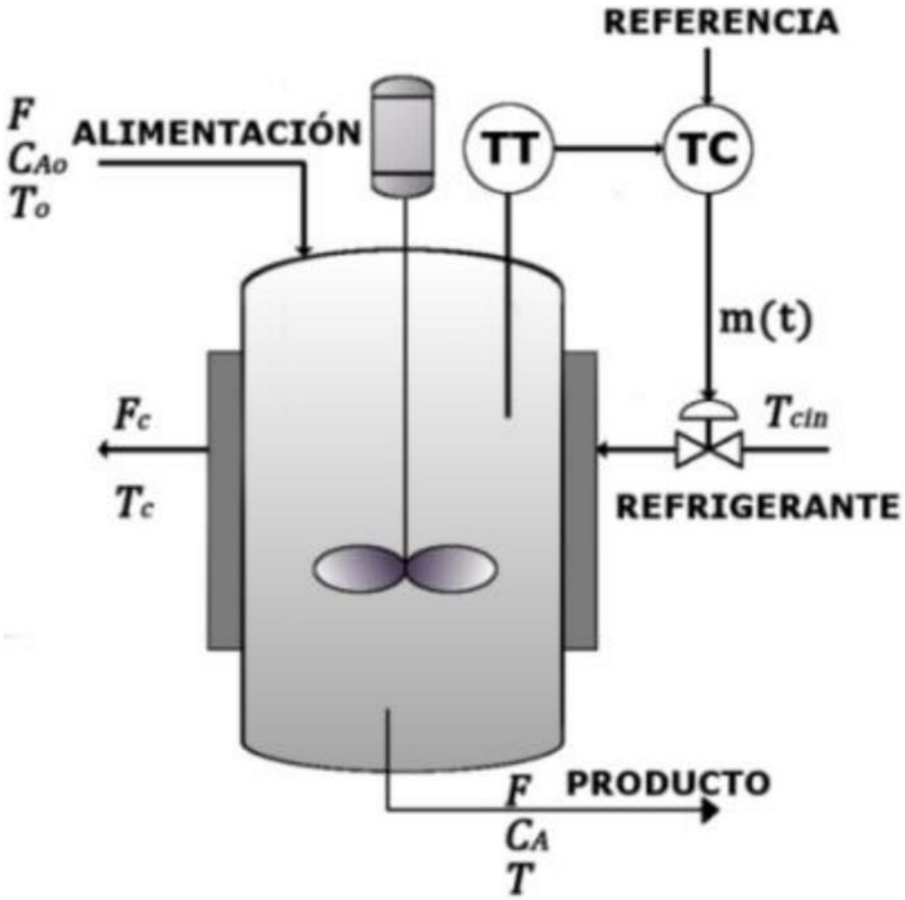
Runaway



Instalación de un controlador de temperatura

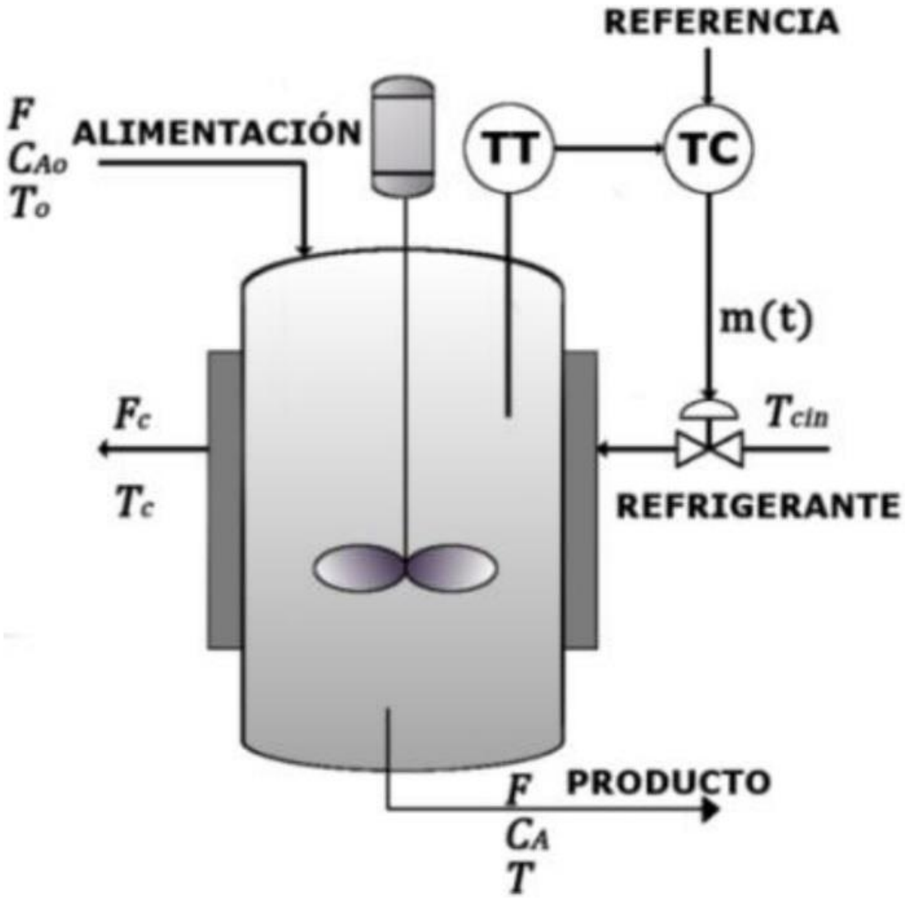
Selección de acción en modo servo

1. Acción inversa y válvula NA
2. *Set point* $T_{sp}(+)$
3. $T_{sp}(+) \rightarrow e(+) \rightarrow Ac(+) \rightarrow x(-) \rightarrow N_{s0}(-) \rightarrow Q(-) \rightarrow T(+)$
4. Si $T(+)$, aceptar la acción.



Selección de acción en modo regulador

1. Acción inversa y válvula NA
2. $T(+)$
3. $T(+) \rightarrow e(-) \rightarrow Ac(-) \rightarrow x(+) \rightarrow N_{s0}(+) \rightarrow Q(+) \rightarrow T(-)$
4. Si $T(-)$, aceptar la acción.



Instalación de un control PI para T

Modelo original

$$Ac = Ab + Kp\left(e + \frac{1}{\tau i}Ai\right)$$

$$e = T_{sp} - T$$

$$Ai = \int_0^t e\,dt$$

$$x_s = \begin{cases} 1 & Ac < 0 \\ 0 & Ac > 1 \\ 1 - Ac & \text{en otro caso} \end{cases}$$

Modelo simplificado

$$\frac{dAi}{dt} = e$$

$$e = T_{sp} - T$$

$$Ac = Ab + Kp\left(e + \frac{1}{\tau i}Ai\right)$$

$$x_s = \begin{cases} 1 & Ac < 0 \\ 0 & Ac > 1 \\ 1 - Ac & \text{en otro caso} \end{cases}$$

Cálculo de N_{s0}

$$F_{s0} = C_{vs}\, X_s \sqrt{\frac{\Delta P_{vs}}{\rho_s / \rho_w}}$$

$$N_{s0} = \frac{F_{s0}\, \rho_s}{PM_s}$$

Modelo de CT

$$\frac{dAi}{dt} = e$$

$$e = T_{sp} - T$$

$$Ac = Ab + Kp\left(e + \frac{1}{\tau i} Ai\right)$$

$$x_s = \begin{cases} 1 & Ac < 0 \\ 0 & Ac > 1 \\ 1 - Ac & \text{en otro caso} \end{cases}$$

$$F_{s0} = C_{vs}\, x_s \sqrt{\frac{\Delta P_{vs}}{\rho_s / \rho_w}}$$

$$N_{s0} = \frac{F_{s0}\, \rho_s}{PM_s}$$

Parámetros en sistema inglés

- $Kp = 4.25\times10^{-3}$ °F^{-1}
- $Ab = 0.5$
- $\tau i = 0.152$ h
- $T_{sp} = 138.7$ °F
- $Ai(0) = 0$
- $\rho_s = \rho_w$, $\rho_s = 62.43$ lb/ft^3
- $PM_s = 18$ lb/lb-mol
- $\Delta P_{vs} = 4.383\times10^{11}$ lb/(ft·h^2).
- $C_{vs} = 8.71\times10^{-4}$ ft$^{3.5}$/lb$^{0.5}$

Condiciones iniciales

$C_A = 0.0377$ lb-mol/ft^3
$C_B = 2.1256$ lb-mol/ft^3
$C_C = 0.1439$ lb-mol/ft^3
$C_M = 0.2269$ lb-mol/ft^3
$T = 138.7$ °F

Listado en Berkeley Madonna

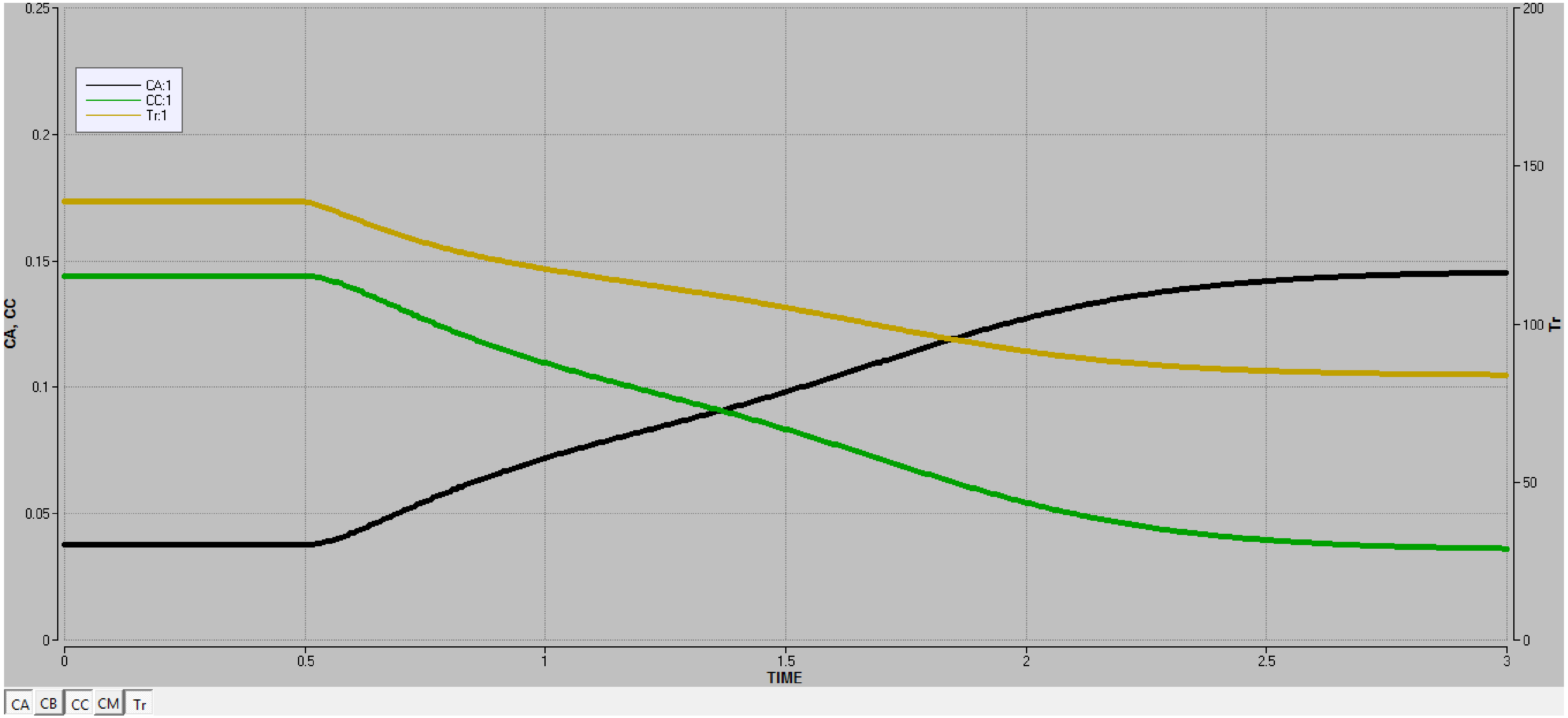
```
{Reactor de propilenglicol con CT}

METHOD RK4
STARTTIME = 0
STOPTIME = 3
DT = 0.01

; Inicialización
INIT CA = 0.0377
INIT CB = 2.1256
INIT CC = 0.1439
INIT CM = 0.2269
INIT Tr = 138.7
INIT Ai = 0

; Sistema ODEs
CA' = F0*(CA0-CA)/V-r
CB' = F0*(CB0-CB)/V-r
CC' = F0*(CC0-CC)/V+r
CM' = F0*(CM0-CM)/V
Tr' = (F0*C0*Cp0*(T0-Tr)+V*r*(-DH)-Q)/(V*C*Cp)
Ai' = e
```

```
; Sistema AEs
r = alpha*exp(-Ea/(Rg*(Tr+460)))*CA

Ts = Ts0+(Tr-Ts0)*(1-exp(-UA/(Ns0*Cps0)))
Q = Ns0*Cps0*(Tr-Ts0)*(1-exp(-UA/(Ns0*Cps0)))

C = CA+CB+CC+CM
Cp = (CA*CpA0+CB*CpB0+CC*CpC0+CM*CpM0)/C
C0 = CA0+CB0+CC0+CM0
Cp0 = (CA0*CpA0+CB0*CpB0+CC0*CpC0+CM0*CpM0)/C0

e = Tsp-Tr
Ac = Ab+Kp*(e+Ai/taui)
xs = 1-Ac
LIMIT xs >= 0
LIMIT xs <= 1
Fs0 = Cvs*xs*sqrt(DPs)
Ns0 = Fs0*rhos/PMs
```

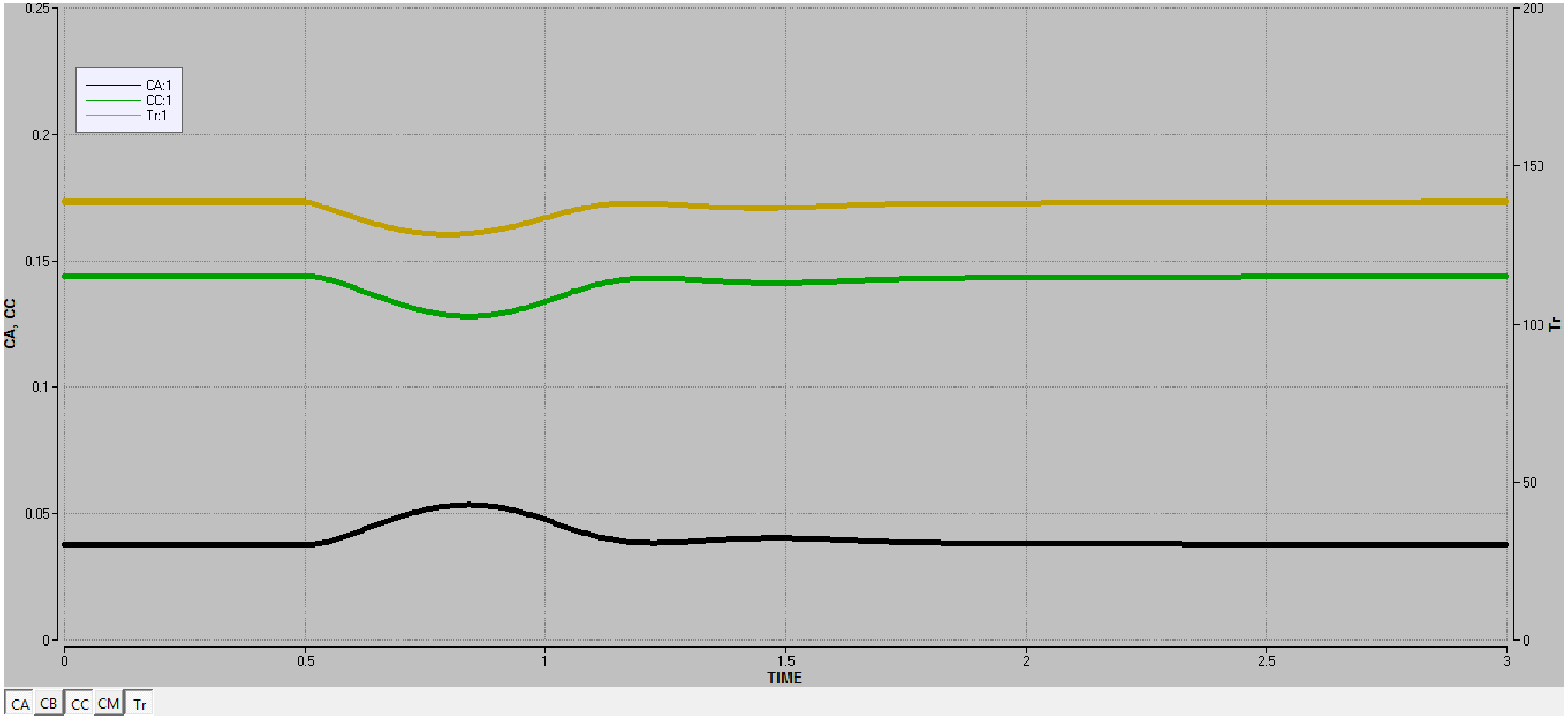
```
; Datos
V = 66.84

F0 = 440.63
T0 = 70
CA0 = 0.1816
CB0 = 2.2695
CC0 = 0
CM0 = 0.2269

CpA0 = 35
CpB0 = 18
CpC0 = 46
CpM0 = 19.5

Ts0 = 60
Cps0 = 18
UA = 16000

DH = -36000
alpha = 16.96E12
Ea = 32400
Rg = 1.987

Tsp = 138.7
Ab = 0.5
Kp = 4.25E-3
taui = 0.152

rhos = 62.43
PMs = 18
DPs = 4.383E11
Cvs = 8.71E-4
```

Ver Reactor con CT.mmd

Sin CT, $T_0 = 75 - \text{step}(5,0.5)$



Con CT, $T_0 = 75 - \text{step}(5,0.5)$

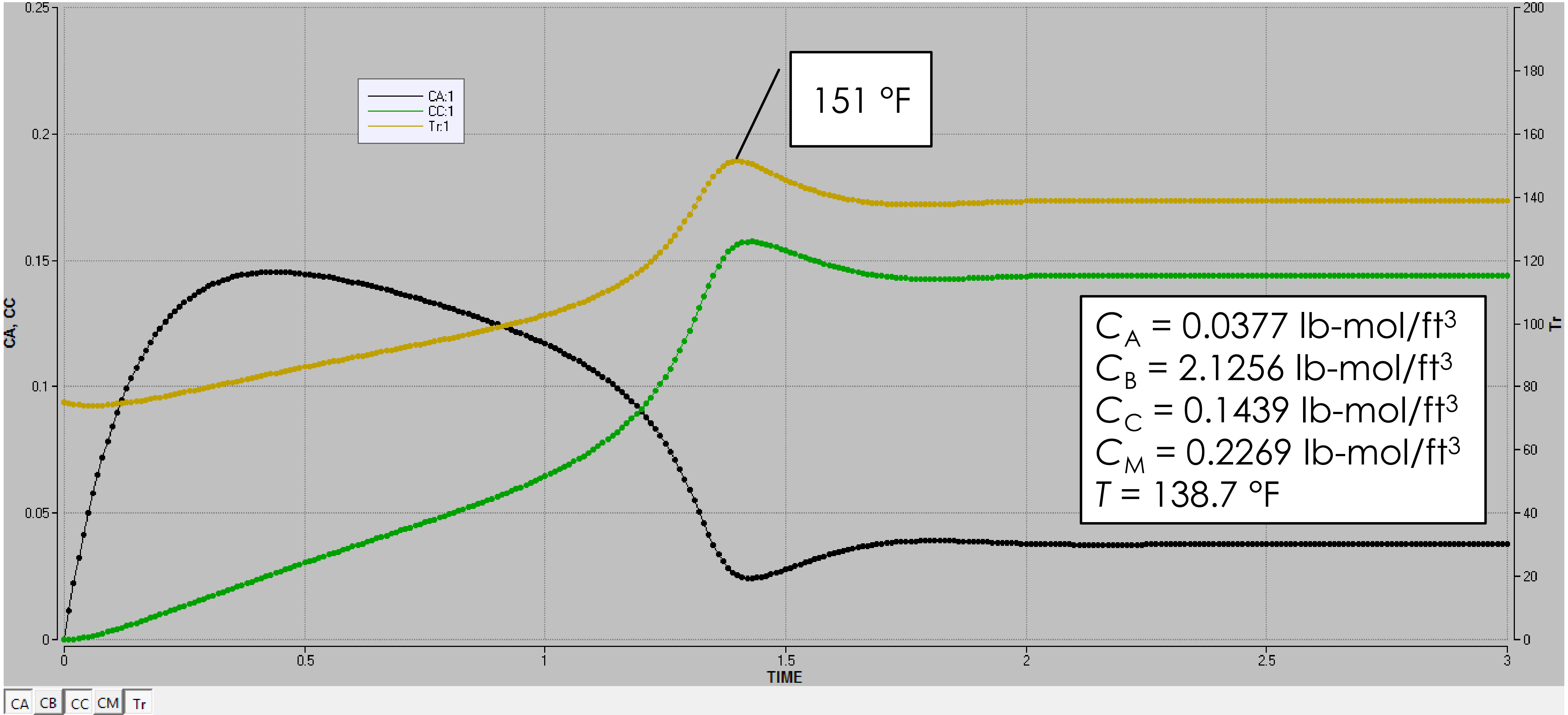


Puesta en marcha sin CT

- Inicialmente, agua a 75° F.
- Serpentín funcionando.

- C_A = 0 lb-mol/ft^3
- C_B = 3.45 lb-mol/ft^3
- C_C = 0 lb-mol/ft^3
- C_M = 0 lb-mol/ft^3
- T = 75 °F
- Kp = 0 °F^{-1}

Puesta en marcha sin CT



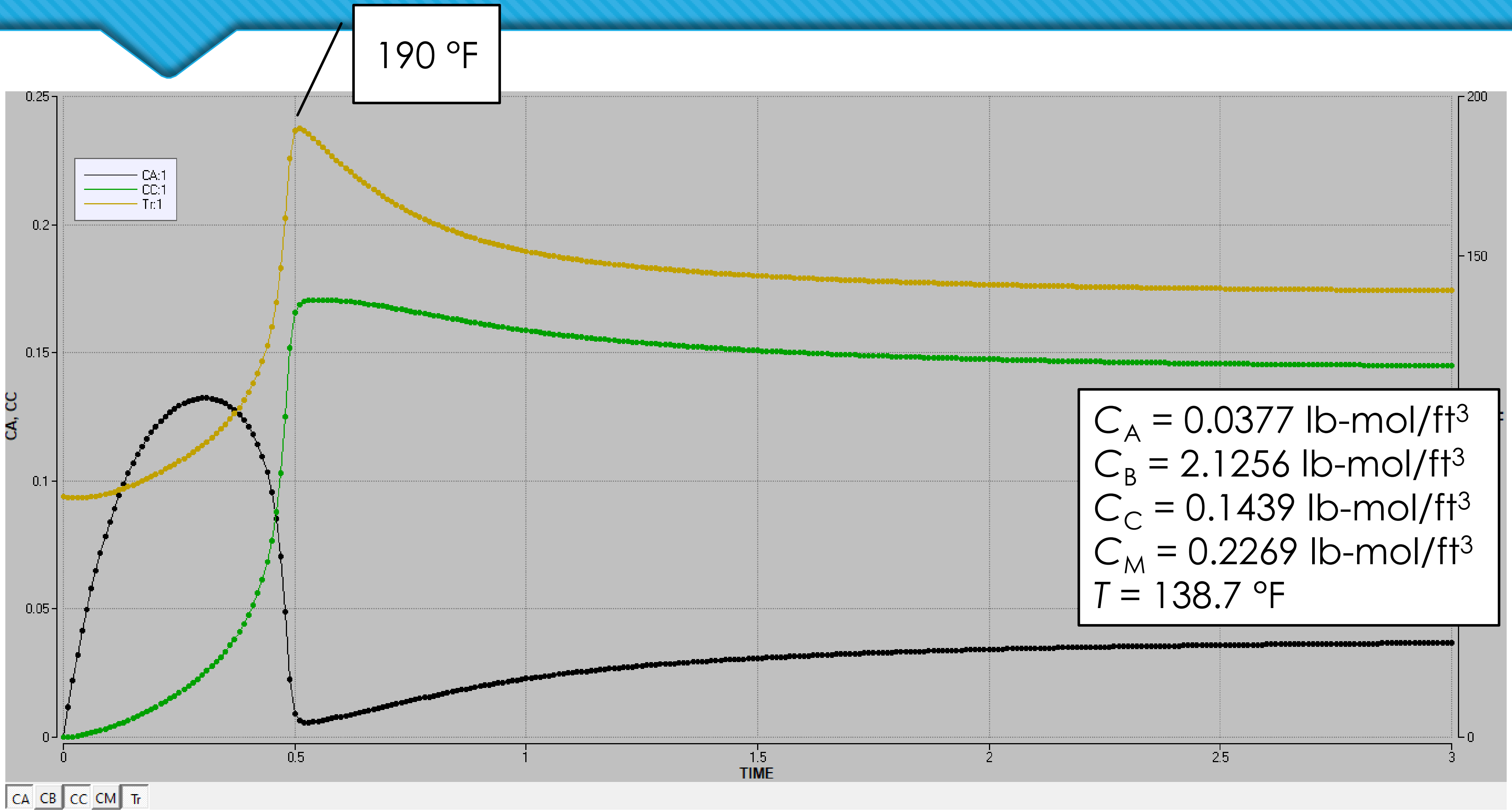
C_A = 0.0377 lb-mol/ft^3
C_B = 2.1256 lb-mol/ft^3
C_C = 0.1439 lb-mol/ft^3
C_M = 0.2269 lb-mol/ft^3
T = 138.7 °F

Puesta en marcha con CT

- Inicialmente, agua a 75° F.
- Serpentín funcionando.

- C_A = 0 lb-mol/ft^3
- C_B = 3.45 lb-mol/ft^3
- C_C = 0 lb-mol/ft^3
- C_M = 0 lb-mol/ft^3
- T = 75 °F
- $Kp = 4.25 \times 10^{-3}$ °F^{-1}
- $x_{min} = 1 \times 10^{-4}$

Puesta en marcha con CT



C_A = 0.0377 lb-mol/ft^3
C_B = 2.1256 lb-mol/ft^3
C_C = 0.1439 lb-mol/ft^3
C_M = 0.2269 lb-mol/ft^3
T = 138.7 °F