Simulación y Optimización

Modelado
Parte V

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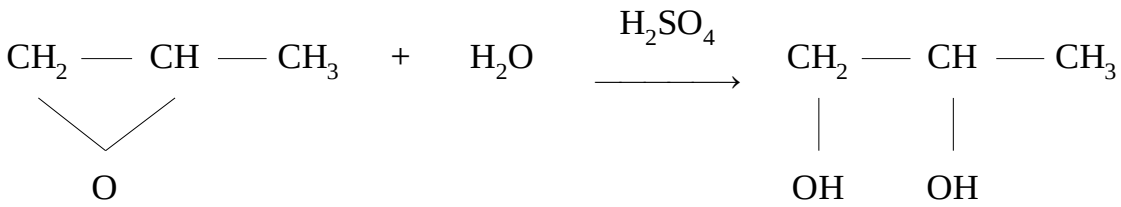
Simulación de un reactor

Reactor productor de propilenglicol

Componentes

- Propileno (A)
- Agua con 0.1 % de H_2SO_4 (B)
- Propilenglicol (C)
- Metanol (M)

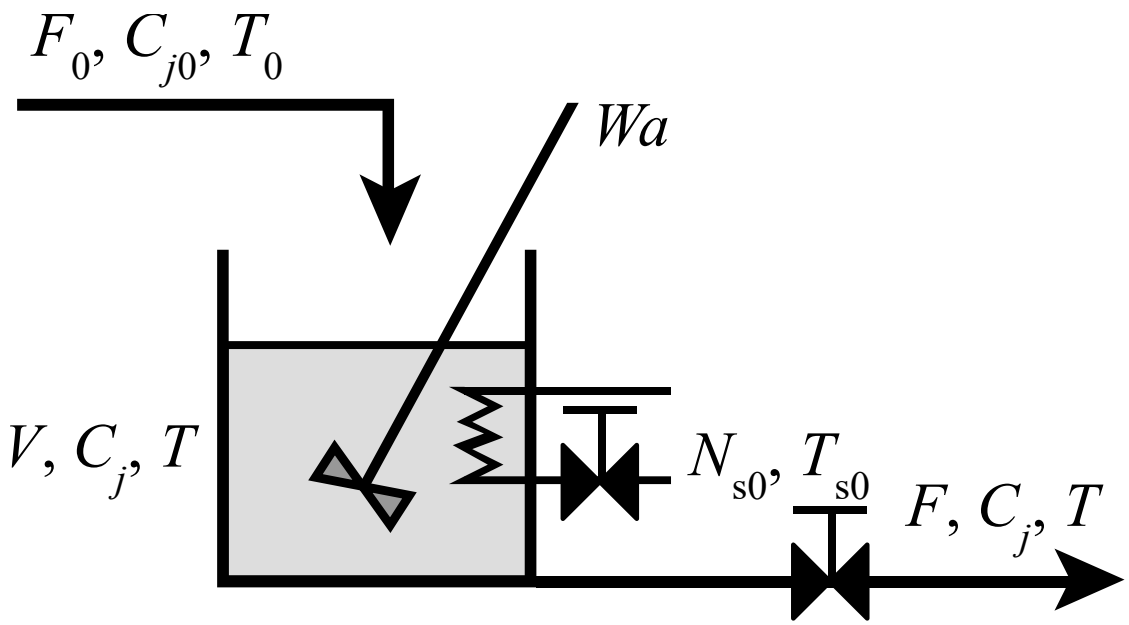
Reacción



Exotérmica

Reactor productor de propilenglicol

- El reactor está apagado.
- *V* es constante.
- Serpentín sumergido.
- Diseñar la puesta en marcha.
- Determinar el estado estacionario.
- Diseñar la parada.
- Analizar la estabilidad.
- Instalar un controlador de *T*.



Modelo dinámico

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

$$V\frac{dC_B}{dt} = F_0\left(C_{B0} - C_B\right) - V r$$

$$V\frac{dC_C}{dt} = F_0\left(C_{C0} - C_C\right) + V r$$

$$V\frac{dC_M}{dt} = F_0\left(C_{M0} - C_M\right)$$

$$V\,C\,Cp\frac{dT}{dt} = F_0\,C_0\,Cp_0\,(T_0 - T) + V r\,(-\Delta H) - Q$$

Modelo dinámico

$$r = k C_A$$

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

$$Q = UA\,\Delta T_{ml}$$

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

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

$$C = \sum_{j=A,B,C,M} C_j$$

$$Cp = \sum_{j=A,B,C,M} x_j\, Cp_{j0}$$

$$x_j = C_j / C \quad j = A,B,C,M$$

$$C_0 = \sum_{j=A,B,C,M} C_{j0}$$

$$Cp_0 = \sum_{j=A,B,C,M} x_{j0}\, Cp_{j0}$$

$$x_{j0} = C_{j0} / C_0 \quad j = A,B,C,M$$

Modelo dinámico simplificado

Forma normal para Berkeley Madonna

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

$$\frac{dC_B}{dt} = \frac{F_0\left(C_{B0} - C_B\right)}{V} - r$$

$$\frac{dC_C}{dt} = \frac{F_0\left(C_{C0} - C_C\right)}{V} + r$$

$$\frac{dC_M}{dt} = \frac{F_0\left(C_{M0} - C_M\right)}{V}$$

$$\frac{dT}{dt} = \frac{F_0 C_0 Cp_0 (T_0 - T) + V r (-\Delta H) - Q}{V C Cp}$$

Modelo dinámico

Se eliminan k, ΔT_{ml}, x_j y x_{j0}

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

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

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

$$C = \sum_{j=A,B,C,M} C_j$$

$$Cp = \frac{1}{C} \sum_{j=A,B,C,M} C_j Cp_{j0}$$

$$C_0 = \sum_{j=A,B,C,M} C_{j0}$$

$$Cp_0 = \frac{1}{C_0} \sum_{j=A,B,C,M} C_{j0} Cp_{j0}$$

Sistema de ecuaciones

Sistema

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

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

Solución

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

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

Parámetros en sistema inglés

- F_0 = 440.63 ft^3/h
- T_0 = 75 °F
- C_{A0} = 0.1816, C_{B0} = 2.2695, C_{C0} = 0 y C_{M0} = 0.2269 lb-mol/ft^3
- Cp_{A0} = 35, Cp_{B0} = 18, Cp_{C0} = 46 y Cp_{M0} = 19.5 Btu/(lb-mol·°F)
- V = 66.84 ft^3
- ΔH = -36000 Btu/lb-mol
- $\alpha = 16.96 \times 10^{12}\ h^{-1}$
- E = 32400 Btu/lb-mol
- R = 1.987 Btu/(lb-mol·°R)
- N_{s0} = 1000 lb-mol/h
- T_{s0} = 60 °F
- Cp_{s0} = 18 Btu/(lb-mol·°F)
- UA = 16000 Btu/(h·°F)

Puesta en marcha 1

- 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

Listado en Berkeley Madonna

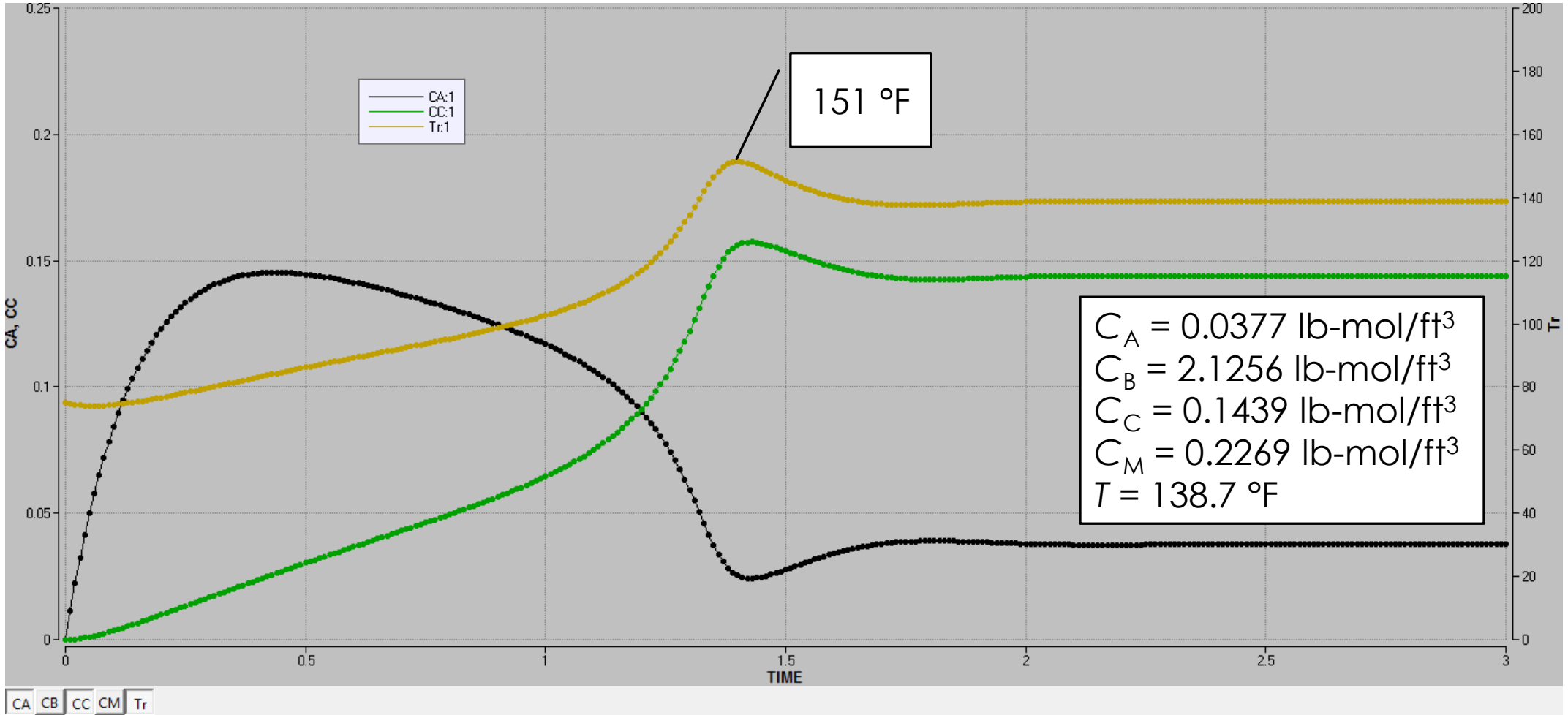
```
{Reactor de propilenglicol
Solución analítica}

METHOD RK4

STARTTIME = 0
STOPTIME = 3
DT = 0.01

; Inicialización
INIT CA = 0
INIT CB = 3.45
INIT CC = 0
INIT CM = 0
INIT Tr = 75

; 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)
```

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

; Solución Analítica
Ts = Ts0+(Tr-Ts0)*(1-EXP(-UA/(Ns0*Cps0)))
Q = Ns0*Cps0*(Ts-Ts0)

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
```

Ver Reactor propilenglicol.mmd

```
; Datos
V = 66.84

F0 = 440.63
T0 = 75
CA0 = 0.1816
CB0 = 2.2695
CC0 = 0
CM0 = 0.2269

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

Ns0 = 1000
Ts0 = 60
Cps0 = 18
UA = 16000

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

Puesta en marcha



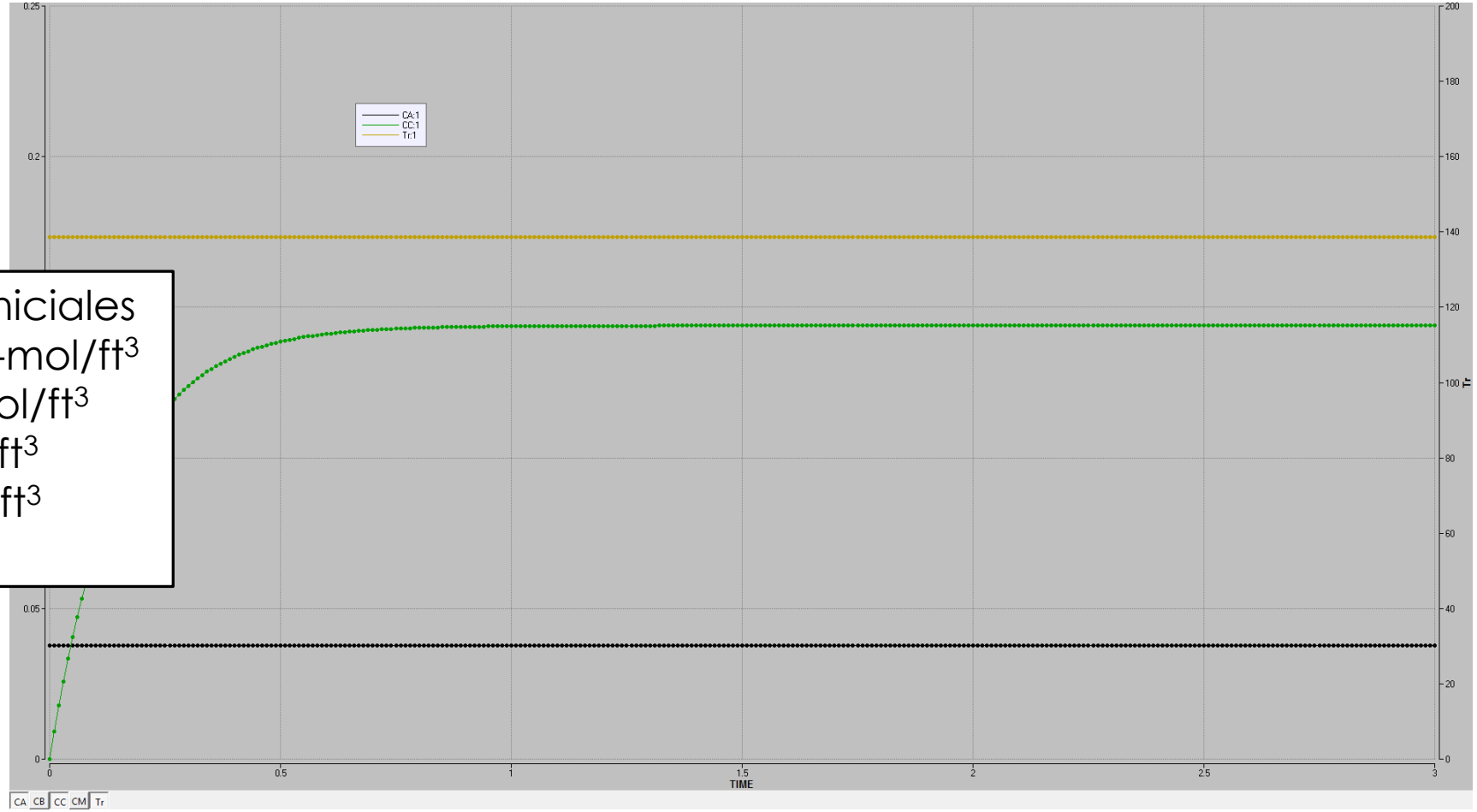
Puesta en marcha 2

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

- C_A = 0.0377 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 = 138.7 °F

Puesta en marcha

Condiciones iniciales
C_A = 0.0377 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 = 138.7 °F



Parada 1

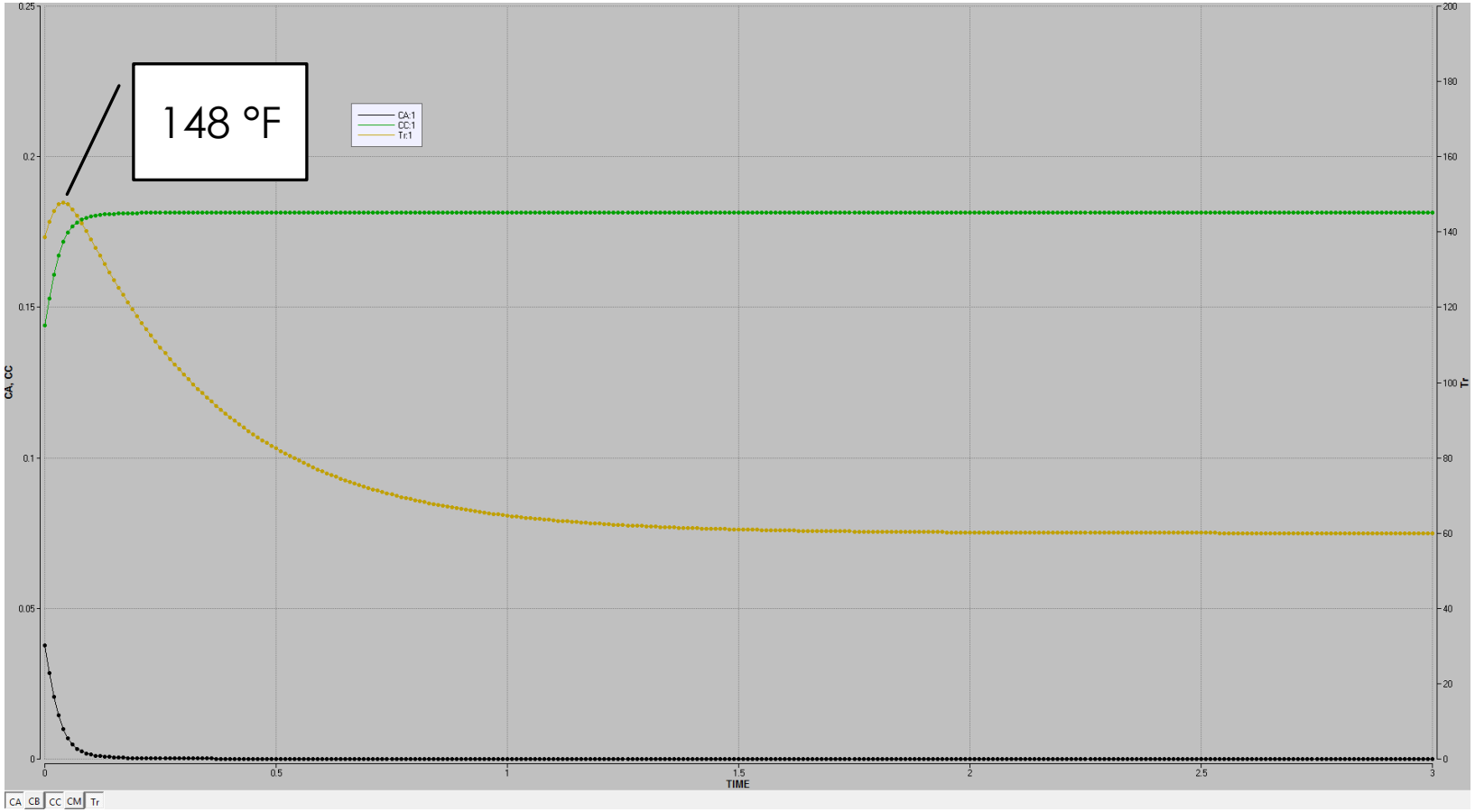
Estado de régimen

- 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

Parada

- F_0 = 0 ft^3/h

Parada 1


148 °F
CA:1
CC:1
Tr:1
CA, CC
Tr
TIME
0.25
0.2
0.15
0.1
0.05
0
200
180
160
140
120
100
80
60
40
20
0
0.5
1
1.5
2
2.5
3
CA CB CC CM Tr

Parada 2

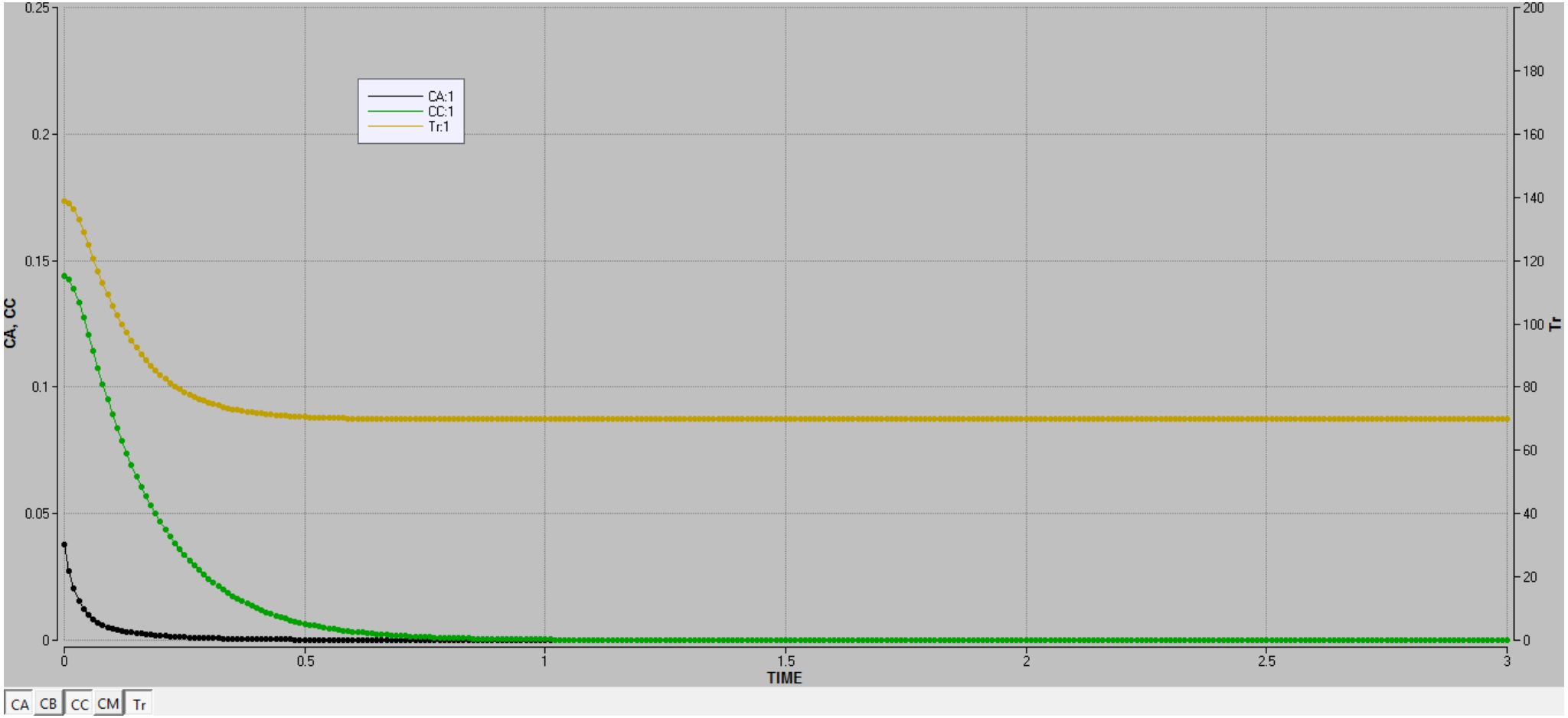
Estado de régimen

- 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

Parada

- C_{A0} = 0 lb-mol/ft^3

Parada 2


CA:1
CC:1
Tr:1
CA, CC
Tr
TIME
0.25
0.2
0.15
0.1
0.05
0
200
180
160
140
120
100
80
60
40
20
0
0
0.5
1
1.5
2
2.5
3
CA
CB
CC
CM
Tr