Integración IV

Modelado individual de equipos en estado estacionario (III).

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Equipos con reacción química

Un sistema general de N reacciones, en las que intervienen NC componentes puede representarse como:

$$\sum_{i=1}^{NC} a_{ij} A_i = 0 \qquad j = R1, R2, \ldots, RN$$

Donde:

A_i: fórmula molecular de la especie i

a_{ij}: coeficiente estequiométrico de la especie “i” en la reacción “j”

$a_{ij} < 0$: La especie “i” es un reactivo de la reacción “j”

$a_{ij} > 0$: La especie “i” es un producto de la reacción “j”

$a_{ij} = 0$: La especie “i” no interviene en la reacción “j”

Equipos con reacción química

Ejemplo: $$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + 3.5O_2 \rightarrow 2CO_2 + 3H_2O$$

$$\sum_{i=1}^{NC} a_{ij} A_i = 0 \qquad j = R1, R2, \ldots, RN$$

$$i = CH_4,\ O_2,\ CO_2,\ H_2O,\ C_2H_6$$

$$j = R1, R2$$

$$a_{CH_4,R1} = -1 \quad a_{O_2,R1} = -2 \quad a_{CO_2,R1} = 1 \quad a_{H_2O,R1} = 2 \quad a_{C_2H_6,R1} = 0$$

$$a_{CH_4,R2} = 0 \quad a_{O_2,R2} = -3.5 \quad a_{CO_2,R2} = 2 \quad a_{H_2O,R2} = 3 \quad a_{C_2H_6,R2} = -1$$

Equipos con reacción química

Para cada una de las N reacciones:

$r_j \left[\frac{1}{volumen \times tiempo} \right]$ Velocidad de avance de la reacción “j”. Siempre > 0

$r_{ij} \left[\frac{moles\, de\, i}{volumen \times tiempo} \right]$ Generación de la especie “i” por unidad de volumen y unidad de tiempo, causada exclusivamente por el avance de la reacción “j”

$$r_j = \frac{r_{ij}}{a_{ij}} \rightarrow r_j = \frac{r_{1j}}{a_{1j}} = \frac{r_{2j}}{a_{2j}} = \ldots = \frac{r_{NCj}}{a_{NCj}}$$

$$r_{ij} = a_{ij} \times r_j \qquad \forall i, j$$

Equipos con reacción química

Para cada uno de los NC componente:

$$r_i = \sum_{j=R1}^{RN} r_{ij} = \sum_{j=R1}^{RN} a_{ij} \times r_j$$

$$r_i \left[\frac{moles\, de\, i}{volumen \times tiempo} \right]$$

Generación neta de la especie "i" por unidad de volumen y unidad de tiempo, causada por el conjunto de N reacciones

Equipos con reacción química

Se pueden definir velocidades netas independientes del volumen del reactor:

$R_j \left[\frac{1}{tiempo} \right]$ Velocidad de avance de la reacción "j". Siempre > 0

$R_{ij} \left[\frac{moles\, de\, i}{tiempo} \right]$ Generación de la especie "i" por unidad de tiempo, causada exclusivamente por el avance de la reacción "j"

$R_i \left[\frac{moles\, de\, i}{tiempo} \right]$ Generación neta de la especie "i" por unidad de tiempo, causada por el conjunto de NR reacciones

$$R_j = \frac{R_{1j}}{a_{1j}} = \frac{R_{2j}}{a_{2j}} = \ldots = \frac{R_{NCj}}{a_{NCj}} \qquad R_i = \sum_{j=R1}^{RN} R_{ij} = \sum_{j=R1}^{RN} a_{ij} \times R_j$$

Reactor de conversión fija

El reactor de conversión fija es un modelo de reactor simplificado para el que se especifica la conversión de una reacción.

Para reacciones paralelas, se especifican las conversiones del componente i para la reacción j, $\zeta_{i,j}$.

Usando esta definición obtenemos para la conversión general del componente i:

$$\sum_{j=R1}^{RN} \zeta_{ij} = \frac{m_{in} x_{in,i} - m_{out} x_{out,i}}{m_{in} x_{in,i}}$$

Solo se puede definir para compuesto que ingresan al reactor

Entonces, la generación de la especie “i” por unidad de tiempo debido a la reacción j corresponde a:

$$R_{ij} = -\zeta_{ij} m_{in} x_{in,i} \Rightarrow R_j = -\frac{\zeta_{ij}}{a_{ij}} m_{in} x_{in,i}$$

⚠

Cuidado inconsistencias al definir las conversiones

Reactor de conversión fija

Se debe definir la conversión de un solo compuesto por reacción y se lo denomina componente base.

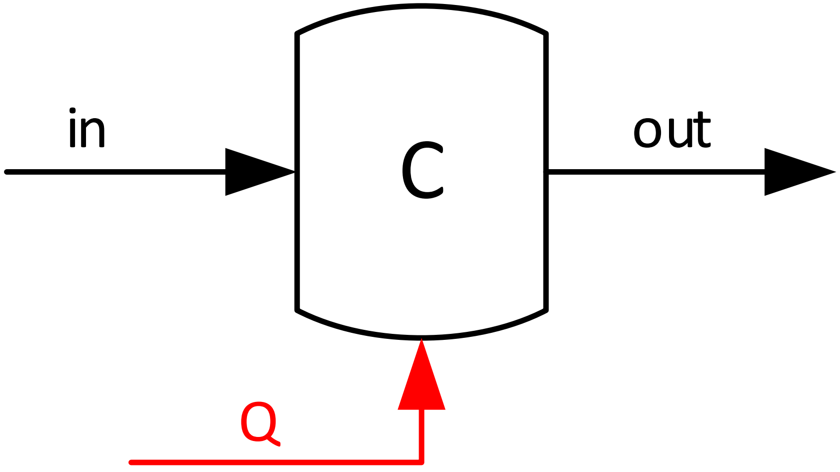
Como se mencionó anteriormente, se cumple la siguiente igualdad para cada reacción:

$$R_i = \sum_{j=R1}^{RN} R_{ij} = \sum_{j=R1}^{RN} a_{ij} \times R_j$$

Si i* es el componente base de la reacción j: $R_j = -\dfrac{\zeta_{i*j}}{a_{i^*j}} m_{in} x_{in,i^*}$

$$R_i = \sum_{j=1}^{NR} -a_{ij} \frac{\zeta_{i^*j}}{a_{i^*j}} m_{in} x_{in,i^*} \qquad \forall i$$

Reactor de conversión fija

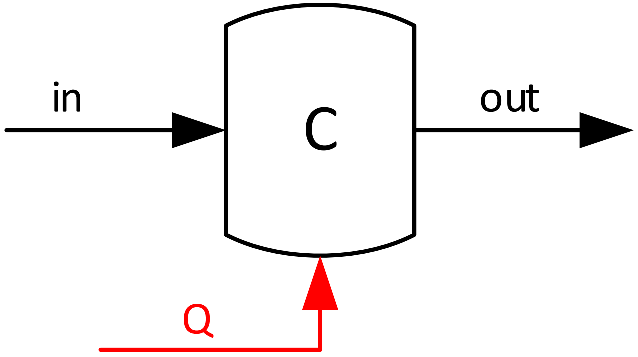


Hipótesis:

- Estado estacionario.
- Se conoce la estequiometría de cada una de las reacciones.
- Se conoce la conversión de un componente por reacción.
- Medio de reacción homogéneo.
- Las entalpías son calculadas tomando como base el calor de formación de cada componente (caso contrario el calor de reacción aparecería en el balance de energía).
- Se toma como positivo el calor que ingresa.

Reactor de conversión fija

$$m_{in} x_{in,i} + R_i - m_{out} x_{out,i} = 0 \qquad \forall i$$



$$R_i = \sum_{j=1}^{NR} -a_{ij} \frac{\zeta_{i^* j}}{a_{i^* j}} m_{in} x_{in,i^*} \qquad \forall i$$

$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

Las entalpías deben incluir el calor de formación!

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \qquad f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$

Reactor de conversión fija

$$m_{in} x_{in,i} + R_i - m_{out} x_{out,i} = 0 \qquad \forall i$$

NC

$$R_i = \sum_{j=1}^{NR} -a_{ij} \frac{\zeta_{i^* j}}{a_{i^* j}} m_{in} x_{in,i^*} \qquad \forall i$$

NC

$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

2

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

1

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \quad f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$

2

5+2NC

Reactor de conversión fija

$$m_{in} x_{in,i} + R_i - m_{out} x_{out,i} = 0 \qquad \forall i$$

$m_{in} \quad x_{in,i} \quad \zeta_{i^* j} \quad m_{out} \quad x_{out,i}$

$$R_i = \sum_{j=1}^{NR} -a_{ij} \frac{\zeta_{i^* j}}{a_{i^* j}} m_{in} x_{in,i^*} \qquad \forall i$$

$H_{in} \quad T_{in} \quad P_{in} \quad H_{out} \quad T_{out} \quad P_{out}$

$Q \quad R_i$

$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

9+3NC+NR

– 5+2NC

4+NC+NR

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \qquad f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$

Reactor de conversión fija (Modular Secuencial)

$$m_{in}x_{in,i} + R_i - m_{out}x_{out,i} = 0 \qquad \forall i$$

$$R_i = \sum_{j=1}^{NR} -a_{ij}\frac{\zeta_{i^*j}}{a_{i^*j}} m_{in}x_{in,i^*} \qquad \forall i$$

$$\cancel{\zeta_{i^*j}} \quad m_{out} \quad x_{out,i}$$

$$H_{out} \quad T_{out} \quad \enclose{circle}{P_{out}} \quad Q \quad R_i$$

$$\sum_{i=1}^{NC} x_{out,i} = 1$$

$$\begin{array}{r} 5+2NC+NR \\ - \qquad\qquad \\ 3+2NC \\ \hline 2+\cancel{NR} \end{array}$$

$$m_{in}H_{in} + Q - m_{out}H_{out} = 0$$

GL =2

$$f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$

Reactor de conversión fija (adiabático o calor dado)

Calculamos generación neta de cada componente.
¡Cuidado! Tienen alcanzan los reactivos sino se obtendrán valores negativos de composición.

Resolvemos el balance de Materia con reacción química.

$$H_{out} = \frac{m_{in} H_{in}}{m_{out}} \rightarrow \text{Si conocemos Q: } H_{out} = \frac{m_{in} H_{in} + Q}{m_{out}}$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0 \rightarrow T_{out}$$

¡Cuidado!
Debemos conocer o encontrar la/s fase/s

Ejemplo: Combustión de metano con aire

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

NC = 4

N = 1

Asumimos al metano como componente base de la reacción y suponemos una conversión del 100%.

$$m_{in} = 100\, mol.seg^{-1}$$

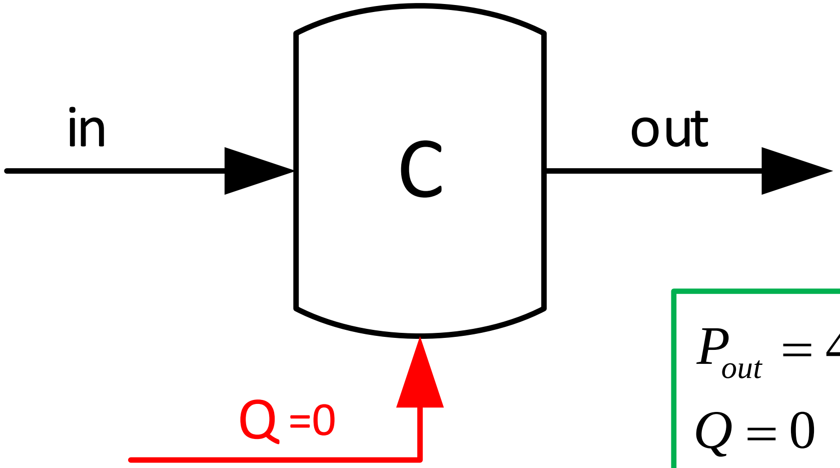
$$x_{in,CH_4} = 0.038$$

$$x_{in,O_2} = 0.202$$

$$x_{in,N_2} = 0.760$$

$$T_{in} = 473.15\, K$$

$$P_{in} = 4\, bar$$



$$P_{out} = 4\, bar$$

$$Q = 0$$

Combustión de metano con aire (Rx)

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$a_{CH_4} = -1 \quad a_{CO_2} = 1 \quad a_{N_2} = 0$$

$$a_{O_2} = -2 \quad a_{H_2O} = 2 \quad \zeta_{CH_4} = 1$$

$$R_i = \sum_{j=1}^{NR} -a_{ij} \frac{\zeta_{i^* j}}{a_{i^* j}} m_{in} x_{in,i^*} \rightarrow R_i = -a_i \frac{\zeta_{CH_4}}{a_{CH_4}} m_{in} x_{in,CH_4}$$

$$R_{CH_4} = -\left(-1\right)\frac{1}{\left(-1\right)}100 \times 0.038 = -3.8 \quad R_{H_2O} = -\left(2\right)\frac{1}{\left(-1\right)}100 \times 0.038 = 7.6$$

$$R_{O_2} = -\left(-2\right)\frac{1}{\left(-1\right)}100 \times 0.038 = -7.6 \quad R_{N_2} = -\left(0\right)\frac{1}{\left(-1\right)}100 \times 0.038 = 0$$

$$R_{CO_2} = -\left(1\right)\frac{1}{\left(-1\right)}100 \times 0.038 = 3.8$$

Combustión de metano con aire (BMxC)

$$m_{in} x_{in,i} + R_i - m_{out} x_{out,i} = 0 \qquad \forall i$$

$$\downarrow$$

$$3.8 - 3.8 - m_{out} x_{out,CH_4} = 0$$

$$20.2 - 7.6 - m_{out} x_{out,O_2} = 0$$

$$76 + 0 - m_{out} x_{out,N_2} = 0$$

$$0 + 3.8 - m_{out} x_{out,CO_2} = 0$$

$$0 + 7.6 - m_{out} x_{out,H_2O} = 0$$

$$x_{out,CH_4} + x_{out,O_2} + x_{out,N_2} + x_{out,CO_2} + x_{out,H_2O} = 1$$

$$\rightarrow \begin{cases} m_{out} = 100 \\ x_{out,CH_4} = 0 \\ x_{out,O_2} = 0.126 \\ x_{out,N_2} = 0.76 \\ x_{out,CO_2} = 0.038 \\ x_{out,H_2O} = 0.076 \end{cases}$$

Combustión de metano con aire (BE)

$$H_{out} = \frac{m_{in} H_{in}}{m_{out}}$$

De la librería Raoult Law

$$H_{out} = \frac{100 \times 2388.645}{100}$$

$$H_{out} = 2388.645 \frac{J}{mol}$$

$$x_{out,CH_4} = 0$$

$$x_{out,O_2} = 0.126$$

$$x_{out,N_2} = 0.76$$

$$x_{out,CO_2} = 0.038$$

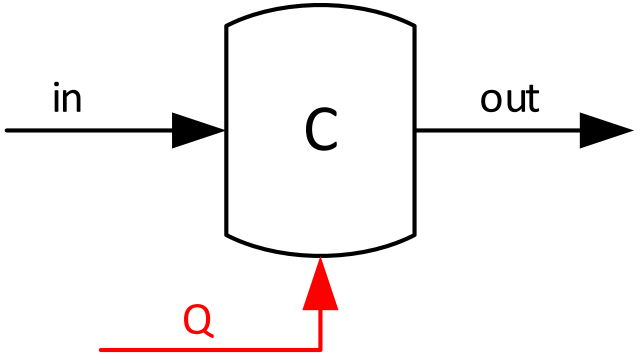
$$x_{out,H_2O} = 0.076$$

$$f\left(T_{out}, \boxed{P_{out}}, \boxed{H_{out}}, \boxed{x_{out}}\right) = 0 \rightarrow T_{out} = 1380.92\,K$$

Fase gaseosa

$$P_{out} = 4\,bar$$

Reactor de conversión fija (flujos x componentes)



$$m_{in,i} + R_i - m_{out,i} = 0 \qquad \forall i$$

$$R_i = \sum_{j=R1}^{RN} -a_{ij} \frac{\zeta_{i^* j}}{a_{i^* j}} m_{in,i^*} \qquad \forall i$$

$$m_{in} = \sum_{i=1}^{NC} m_{in,i} \qquad m_{out} = \sum_{i=1}^{NC} m_{out,i}$$

$$m_{in,i} = m_{in} x_{in,i} \qquad \forall i$$

$$m_{out,i} = m_{out} x_{out,i} \qquad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \qquad f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$

$m_{in} \quad m_{in,i} \quad x_{in,i} \quad \zeta_{i^* j}$

$m_{out} \quad m_{out,i} \quad x_{out,i}$

$H_{in} \quad T_{in} \quad P_{in} \quad H_{out} \quad T_{out} \quad P_{out}$

$Q \quad R_i$

Reactor de conversión fija (flujos x componentes - MS)

$$m_{in,i} + R_i - m_{out,i} = 0 \qquad \forall i$$ ①

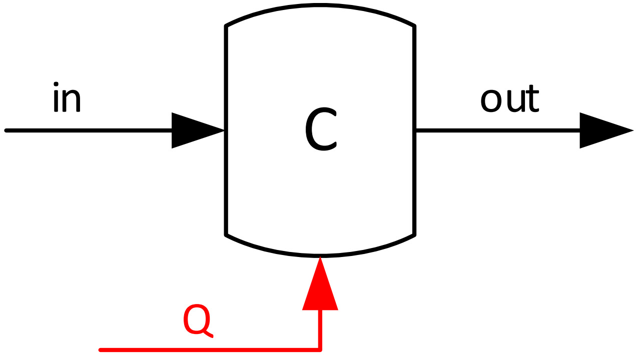
$$R_i = \sum_{j=R1}^{RN} -a_{ij} \frac{\zeta_{i^* j}}{a_{i^* j}} m_{in,i^*} \qquad \forall i$$ ②

$$m_{out} = \sum_{i=1}^{NC} m_{out,i}$$ ③

$$m_{out,i} = m_{out} x_{out,i} \qquad \forall i$$ ④

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$ ⑤

$$f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$ ⑥



$$\zeta_{i^* j} \; m_{out} \; m_{out,i} \; x_{out,i}$$

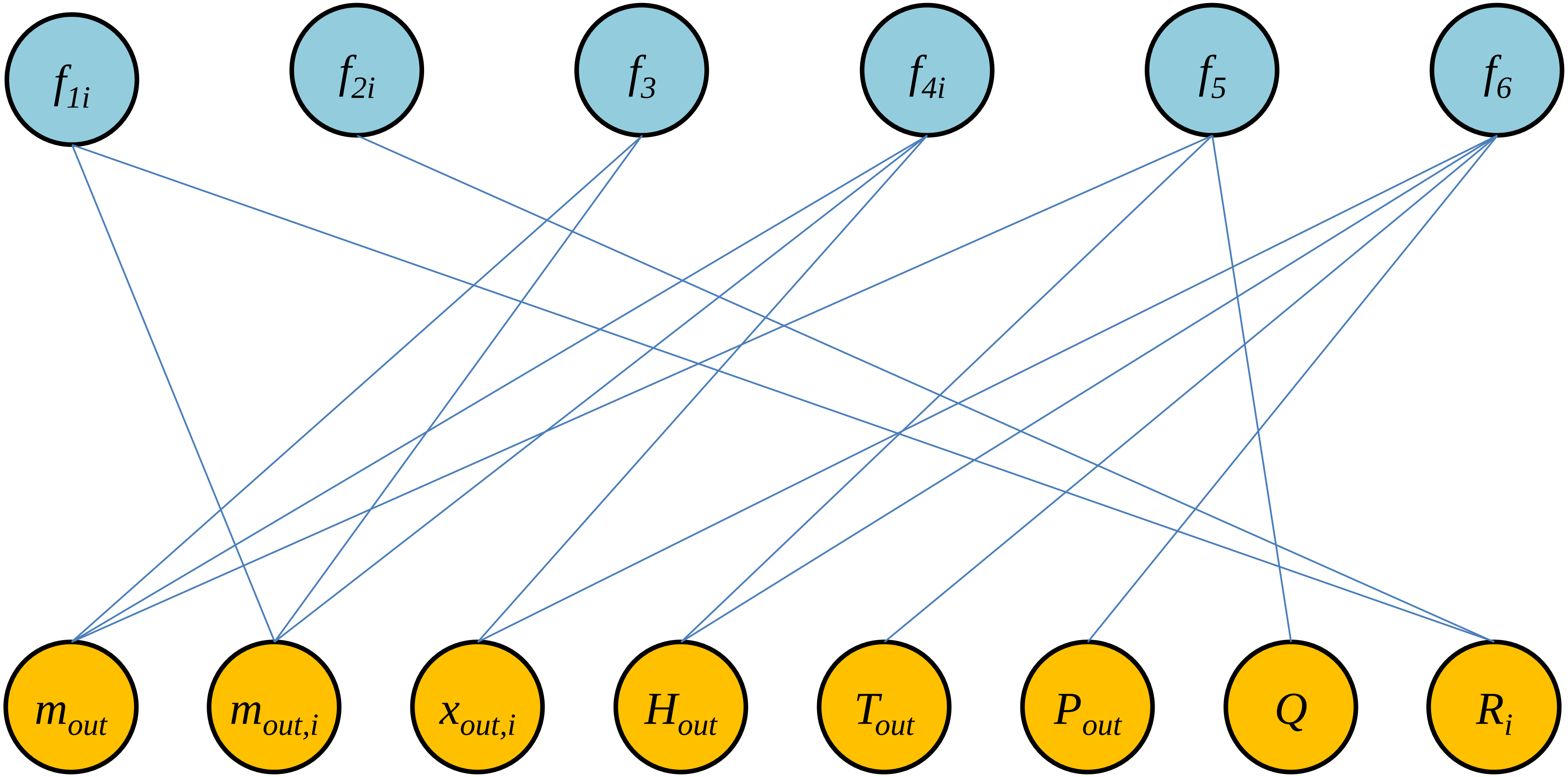
$$H_{out} \; T_{out} \; P_{out} \; Q \; R_i$$

$$\begin{array}{r} 5+3NC+NR \\ -\quad 3+3NC \\ \hline 2+\cancel{NR} \end{array}$$

GL =2

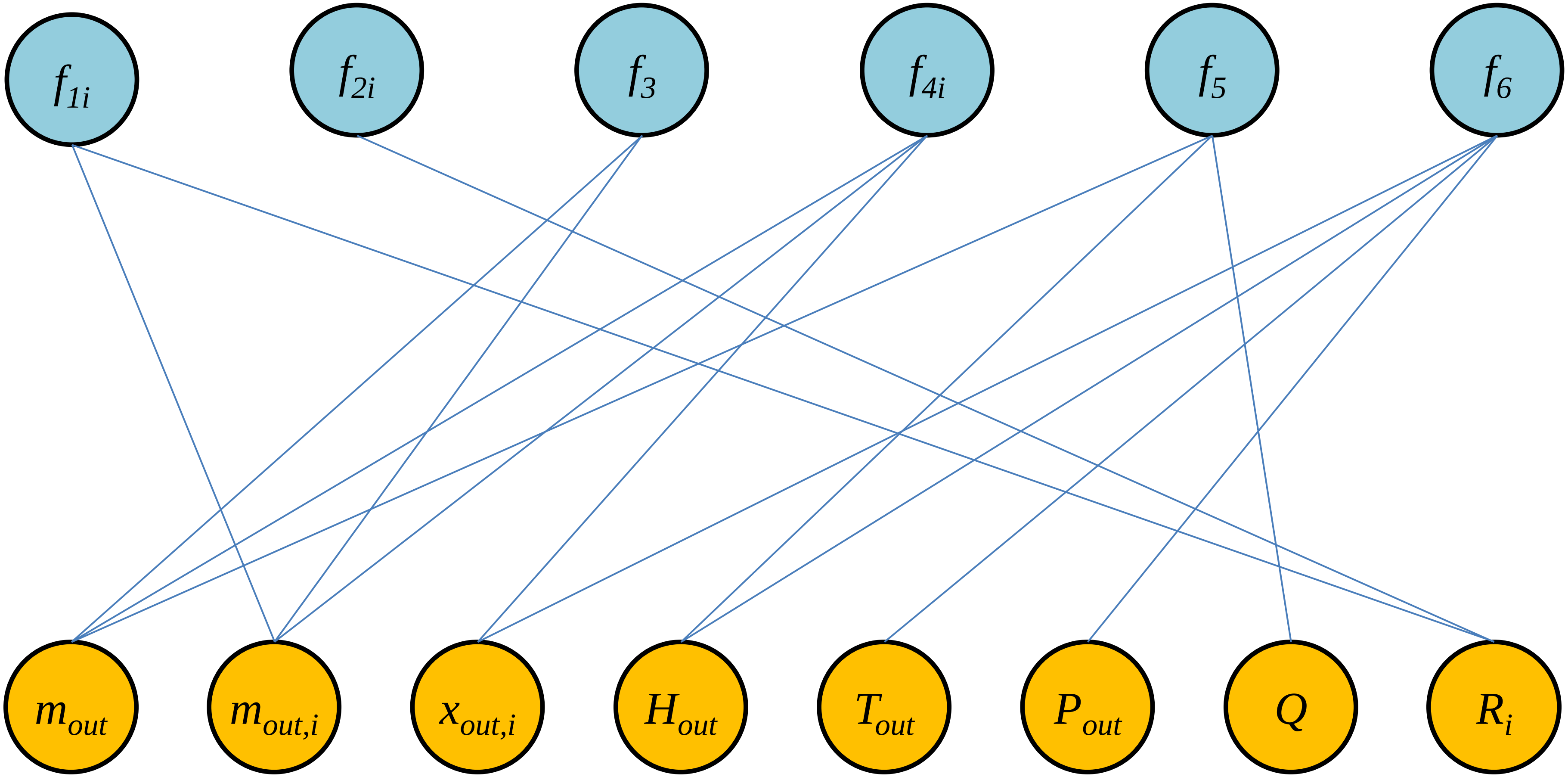
Reactor de conversión fija (flujos x componentes - MS)

Aplicamos el algoritmo de LC&R e imponemos nuestro criterio cuando hay varios opciones para asignar.

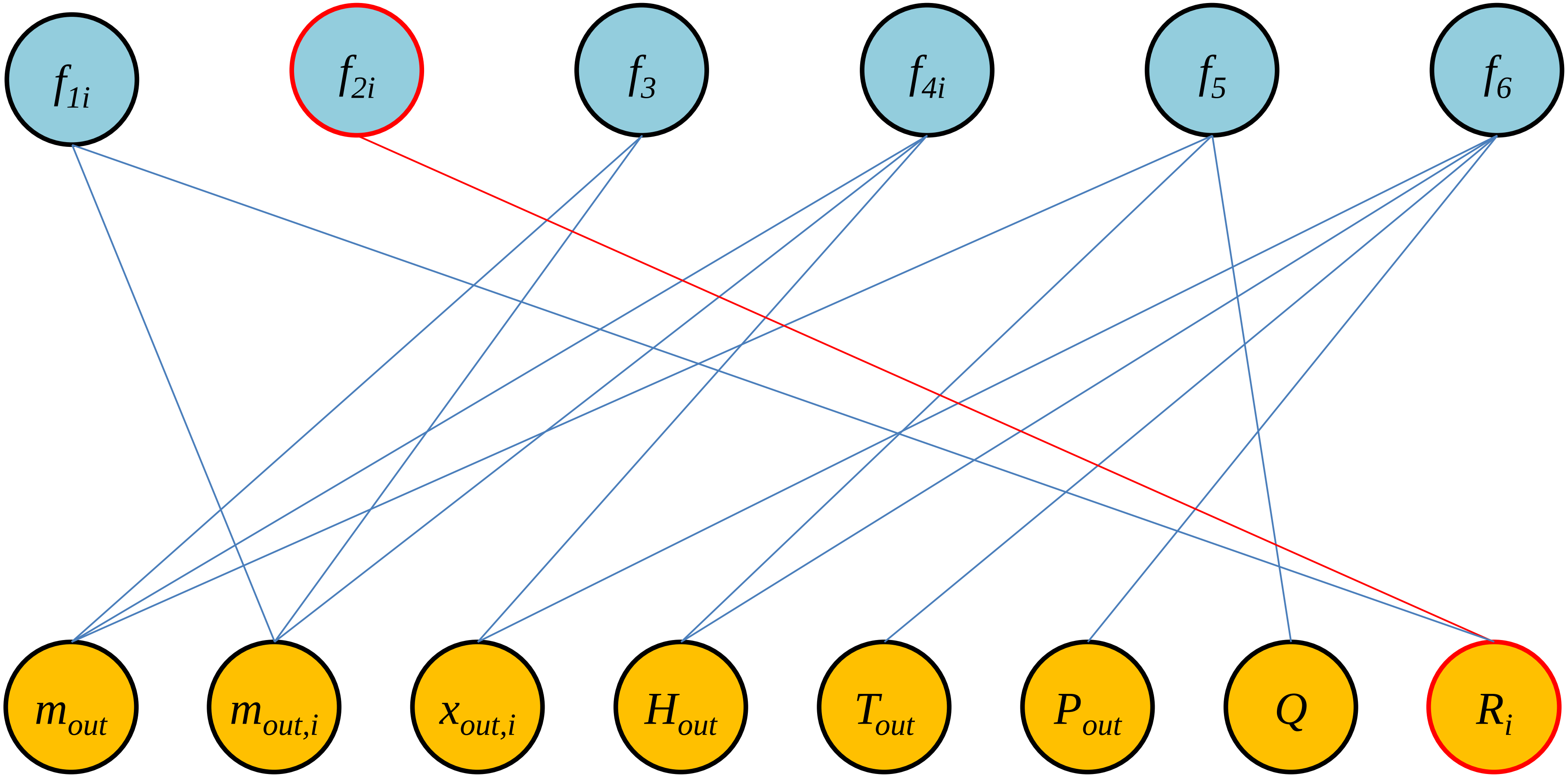


Reactor de conversión fija (flujos x componentes - MS)

Cuidado con las asignaciones, algunos nodos son NC nodos unidos. Es decir una variable con subíndice i deberá ser asignada a un nodo con subíndice i.

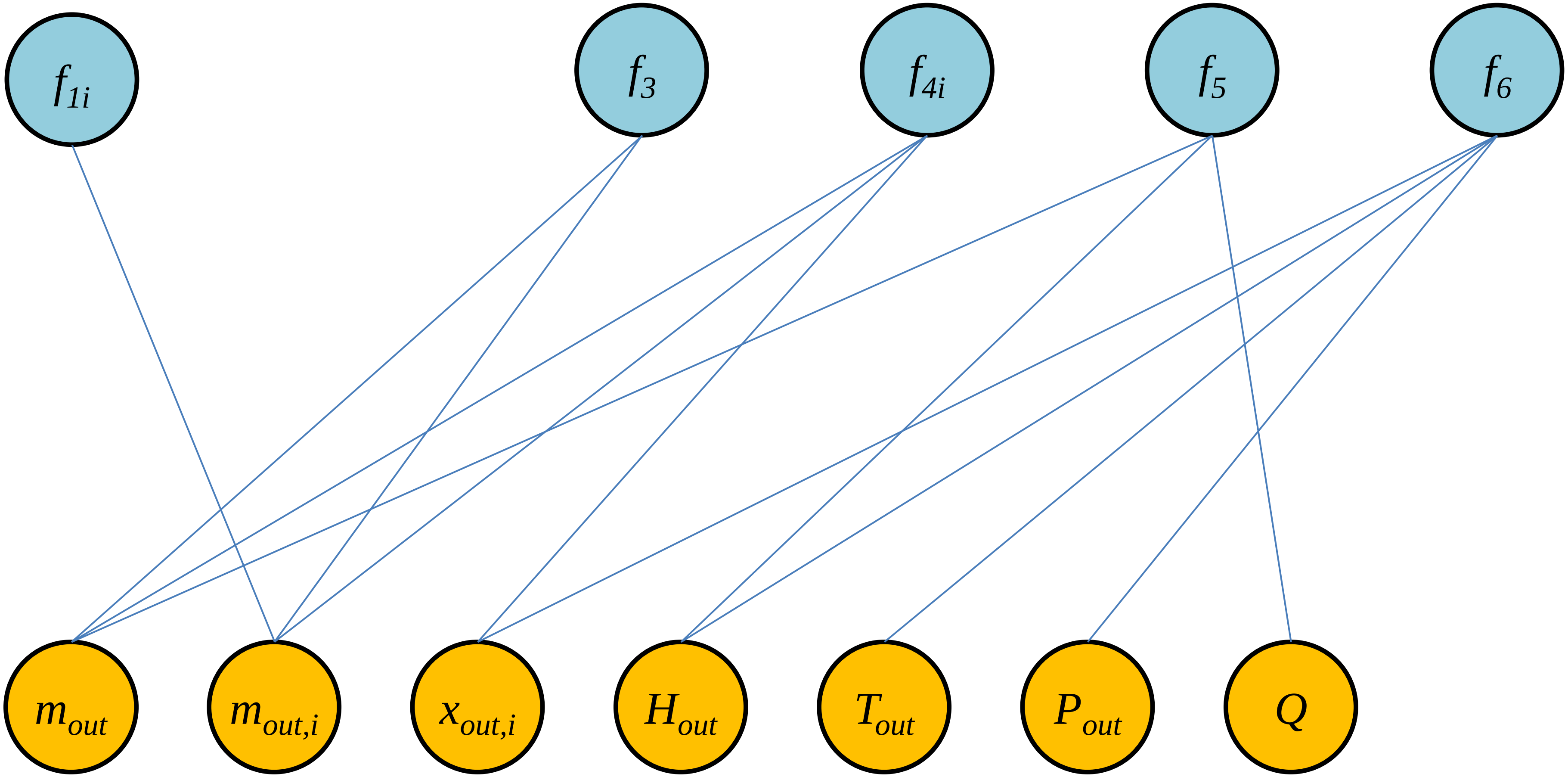


Reactor de conversión fija (flujos x componentes - MS)



Reactor de conversión fija (flujos x componentes - MS)

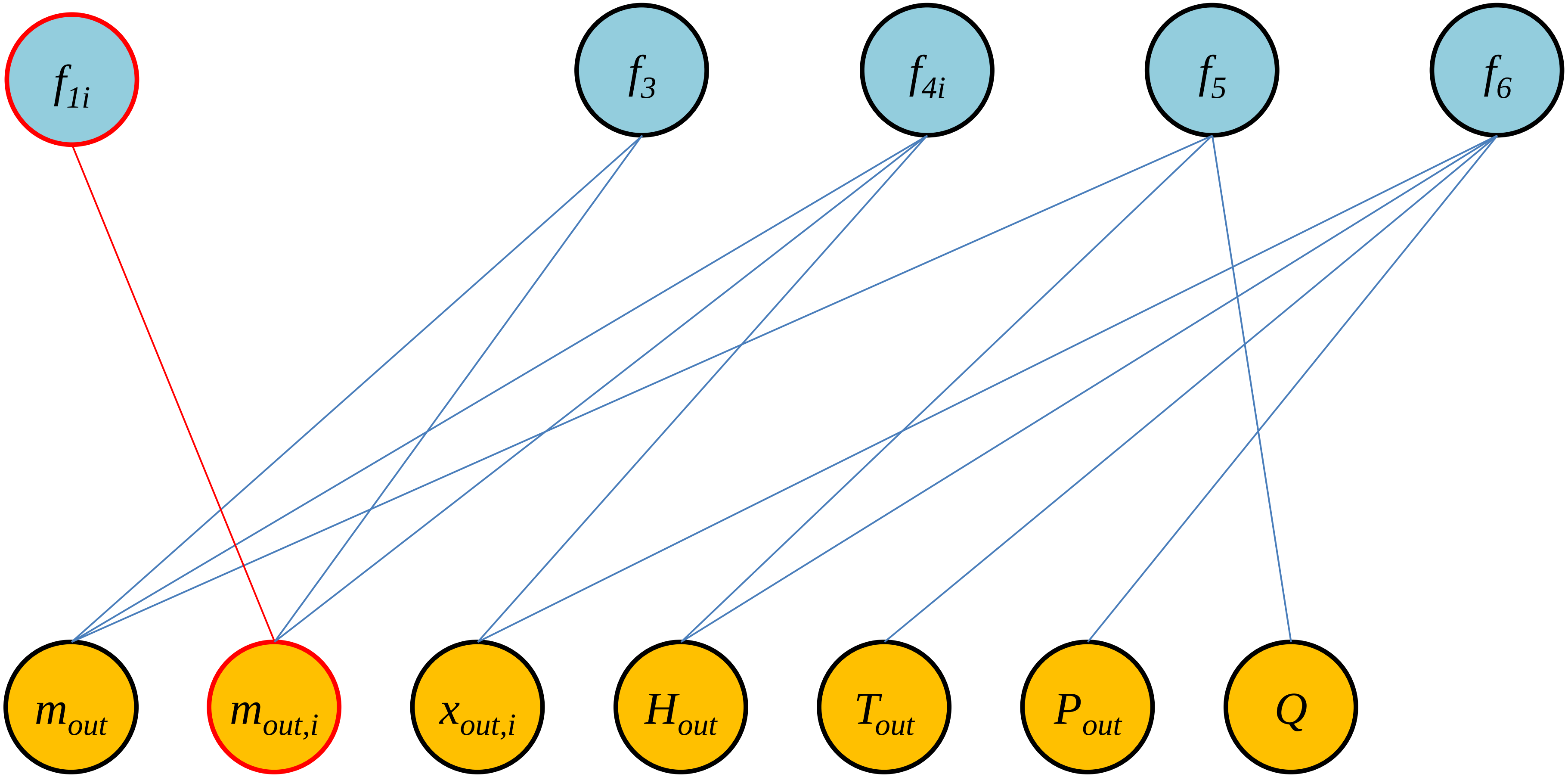
$f_{2,i} \to R_i$



Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

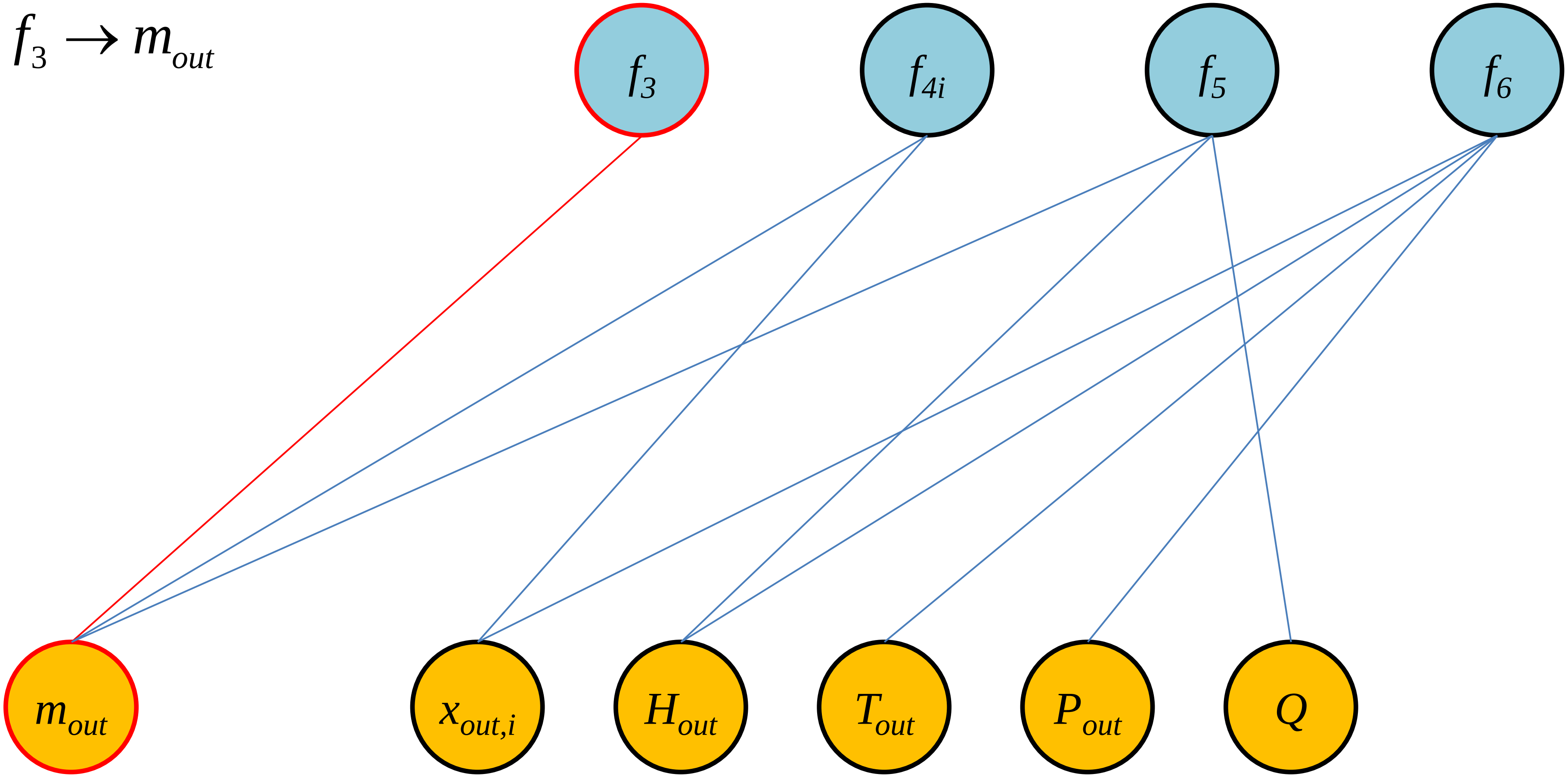


Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$



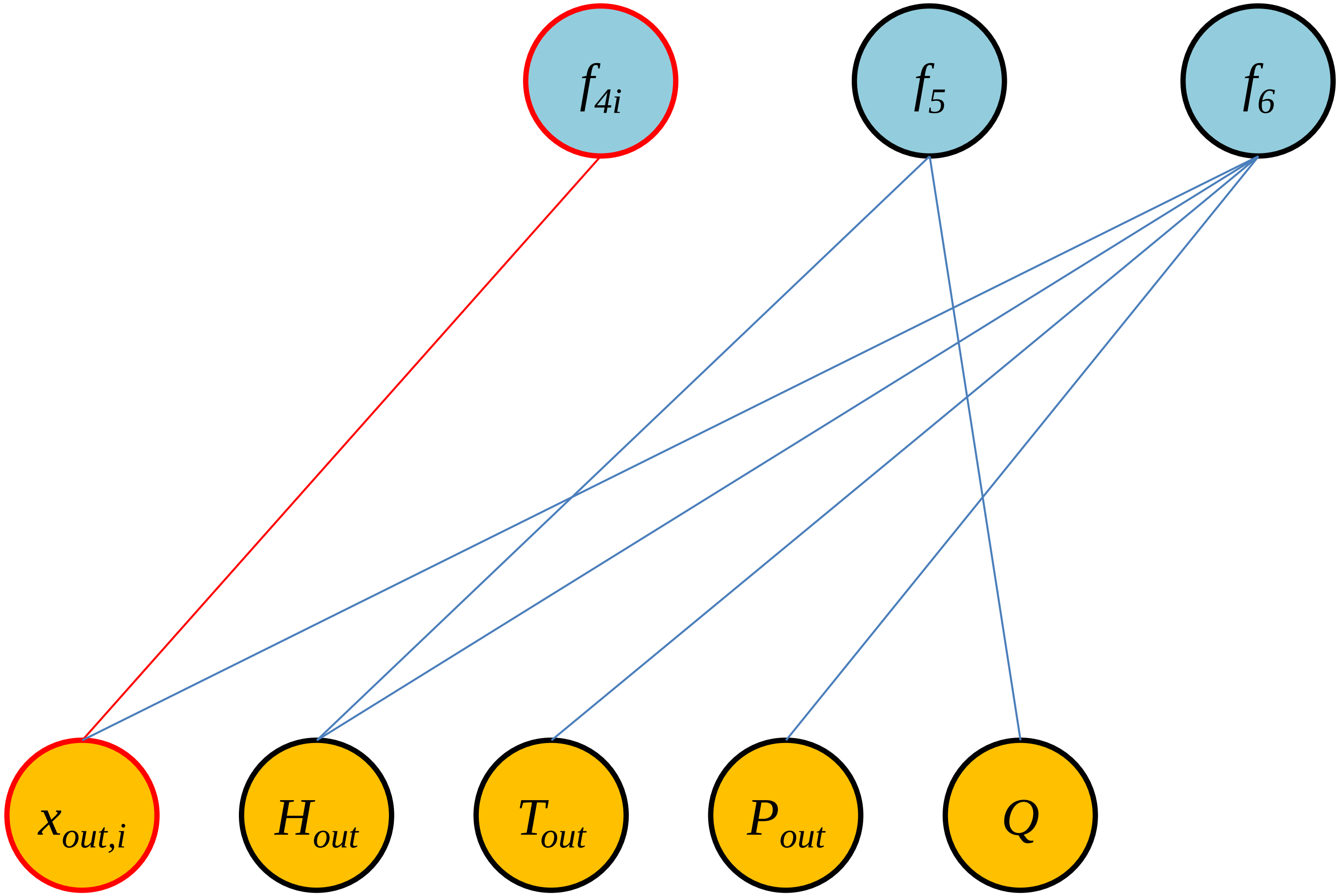
Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

$f_{4,i} \rightarrow x_{out,i}$



Reactor de conversión fija (flujos x componentes - MS)

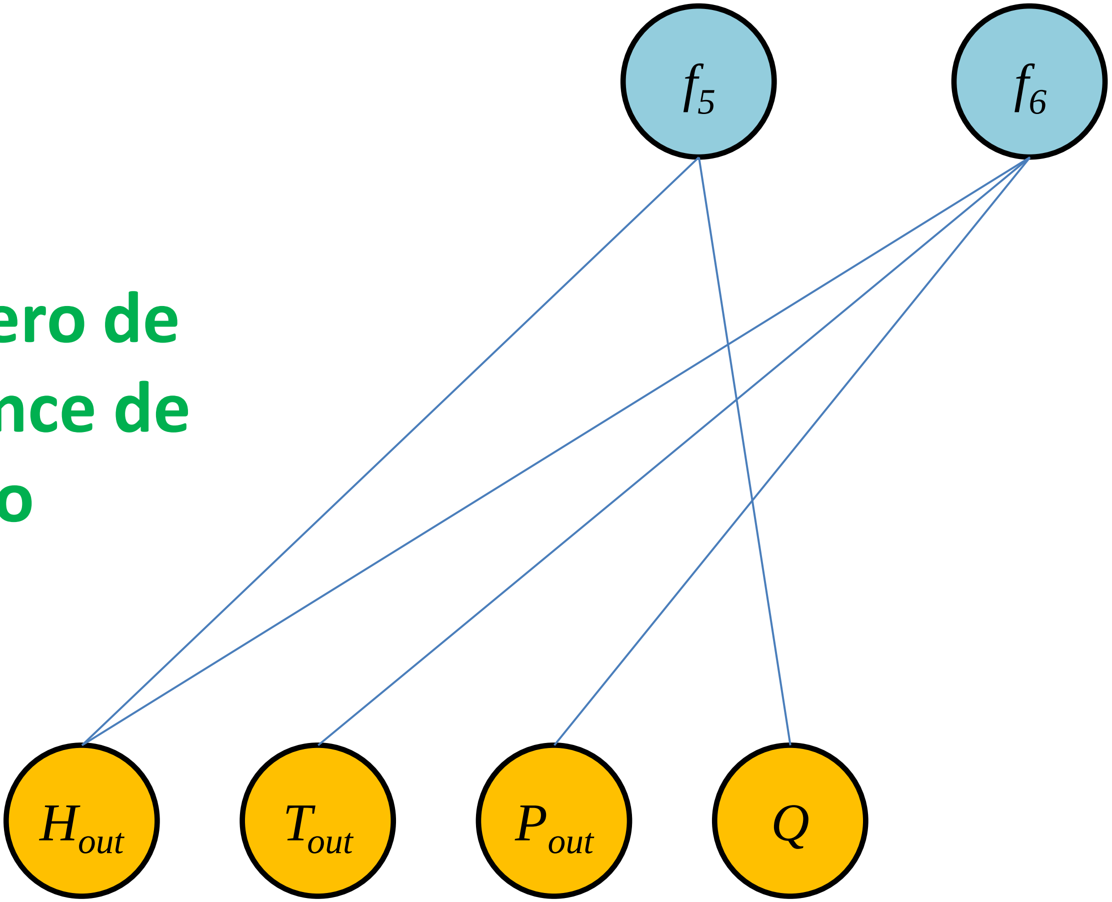
$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

$f_{4,i} \rightarrow x_{out,i}$

Aumentamos el numero de variables pero el balance de masa no es cíclico



Reactor de conversión fija (flujos x componentes - MS)

$$f_{2,i} \rightarrow R_i$$

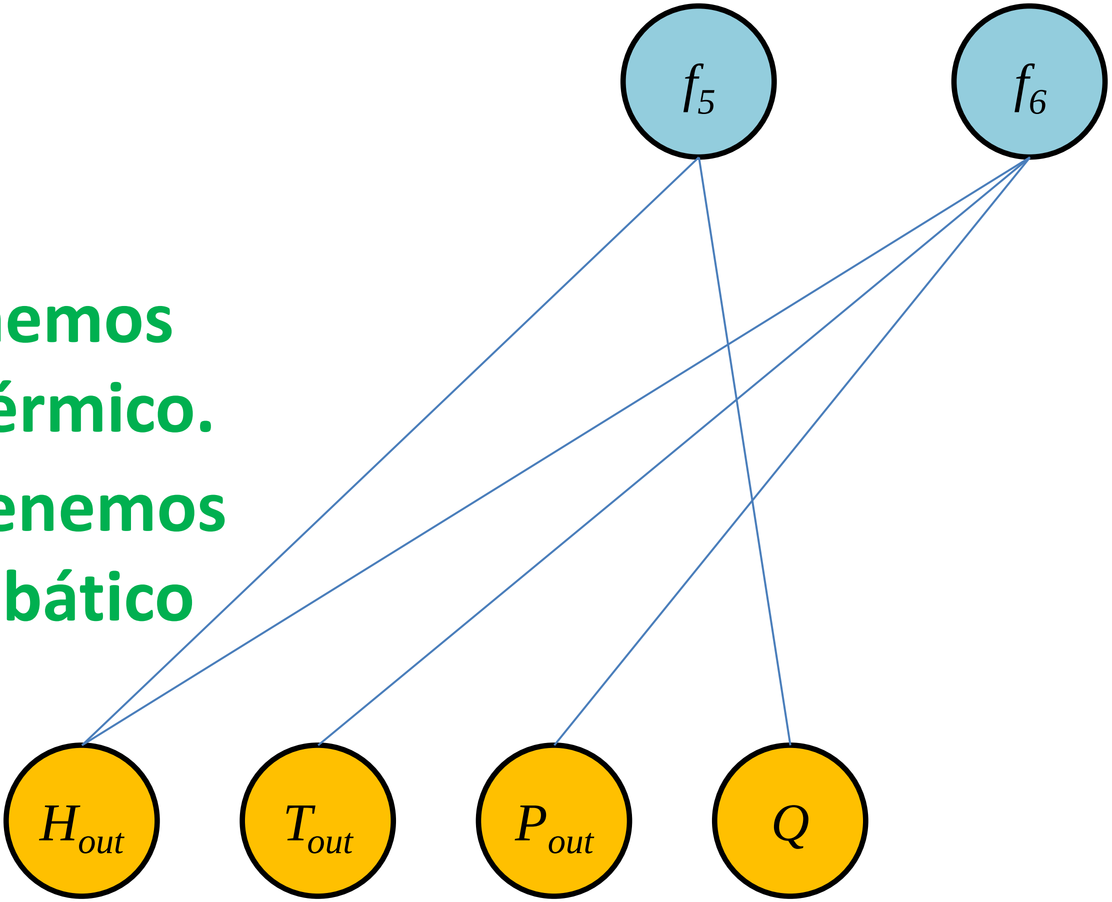
$$f_{1,i} \rightarrow m_{out,i}$$

$$f_3 \rightarrow m_{out}$$

$$f_{4,i} \rightarrow x_{out,i}$$

Si asignamos Q a f_5 tenemos el caso de reactor isotérmico.

Si asignamos T_{out} a f_6 tenemos el caso de reactor adiabático o calor dado.



Reactor de conversión fija (flujos x componentes - MS)

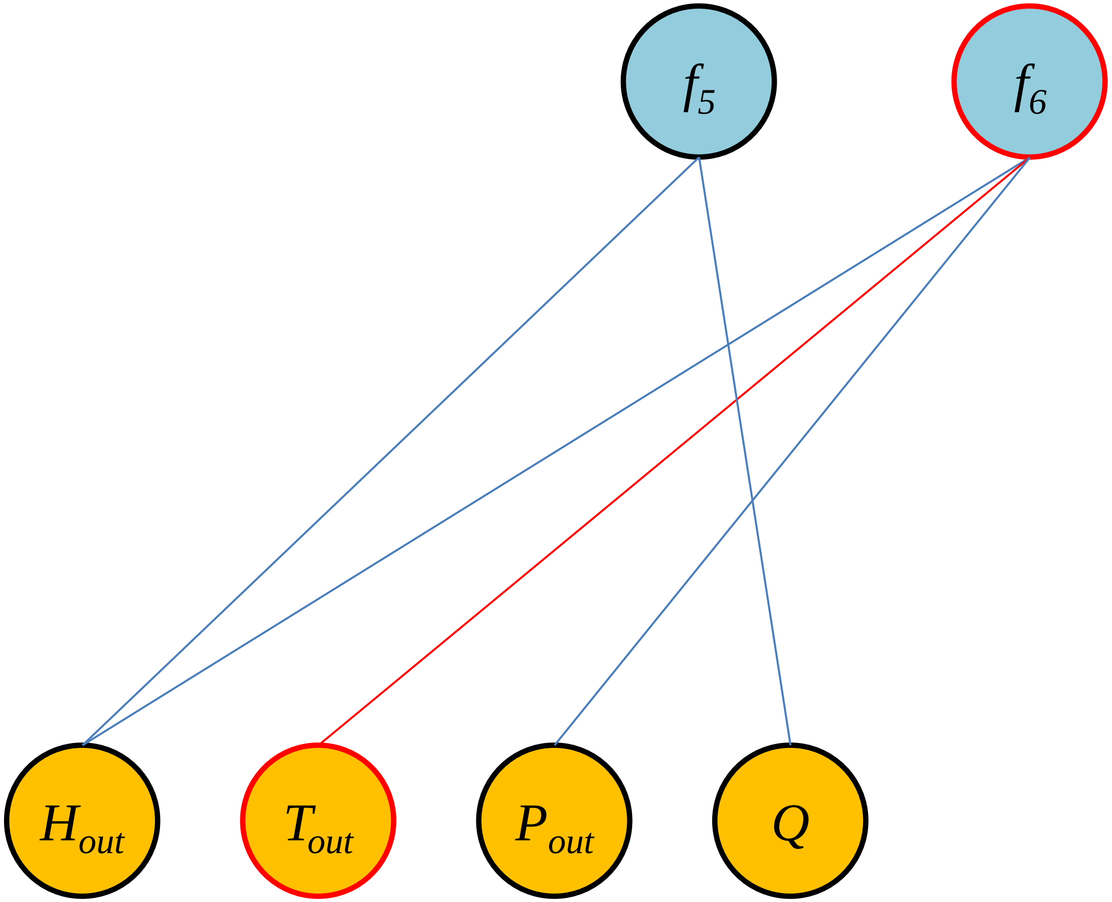
$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

$f_{4,i} \rightarrow x_{out,i}$

$f_6 \rightarrow T_{out}$



Reactor de conversión fija (flujos x componentes - MS)

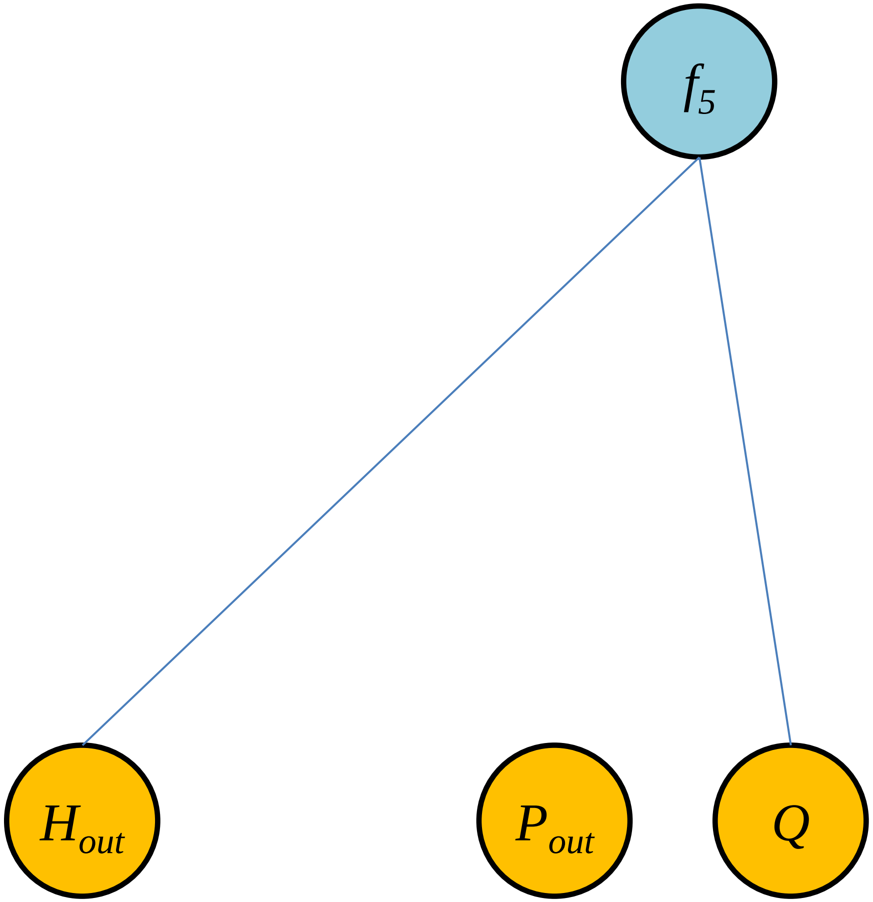
$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

$f_{4,i} \rightarrow x_{out,i}$

$f_6 \rightarrow T_{out}$



Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

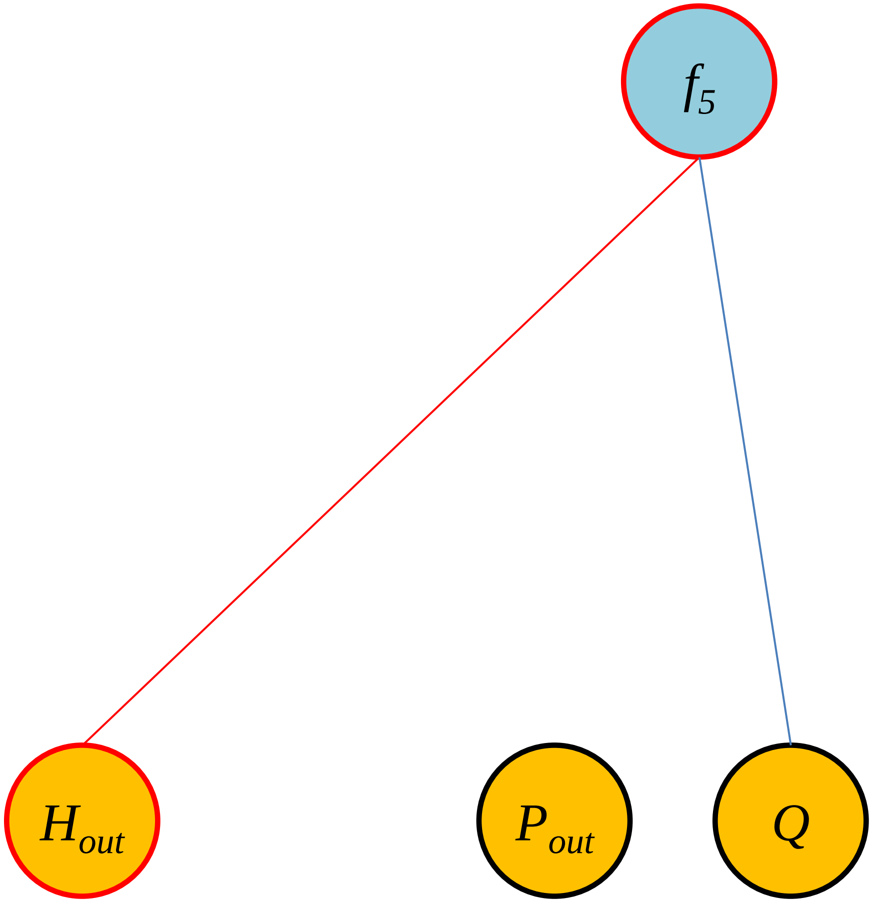
$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

$f_{4,i} \rightarrow x_{out,i}$

$f_6 \rightarrow T_{out}$

$f_5 \rightarrow H_{out}$



Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

$f_{4,i} \rightarrow x_{out,i}$

$f_6 \rightarrow T_{out}$

$f_5 \rightarrow H_{out}$

P_{out}

Q

CSTR (Continuously Stirred Tank Reactor)

El CSTR (Reactor de tanque continuamente agitado o mezcla completa) es un modelo de reactor simplificado en el que se supone que el contenido del reactor es de única fase y está bien mezclado.

- Los balances de materia y energía se plantean suponiendo un medio de reacción completamente homogéneo.
- Se tiene en cuenta las características geométricas del reactor.
- Se consideran las expresiones de velocidad de reacción.

CSTR (Continuously Stirred Tank Reactor)

Como ahora consideramos el volumen del reactor, utilizamos la velocidad de avance de la reacción por unidad de volumen previamente presentadas.

$$r_j \left[\frac{1}{volumen \times tiempo} \right] \qquad r_{ij} \left[\frac{moles\, de\, i}{volumen \times tiempo} \right]$$

$$r_j = \frac{r_{ij}}{a_{ij}} \quad \rightarrow r_j = \frac{r_{1j}}{a_{1j}} = \frac{r_{2j}}{a_{2j}} = \ldots = \frac{r_{NCj}}{a_{NCj}}$$

$$r_i = \sum_{j=R1}^{RN} r_{ij} = \sum_{j=R1}^{RN} a_{ij} \times r_j \qquad r_i \left[\frac{moles\, de\, i}{volumen \times tiempo} \right]$$

CSTR (Continuously Stirred Tank Reactor)

Las velocidades de reacción **por lo general** vienen expresadas como funciones de la temperatura y concentraciones molares de las especies intervinientes:

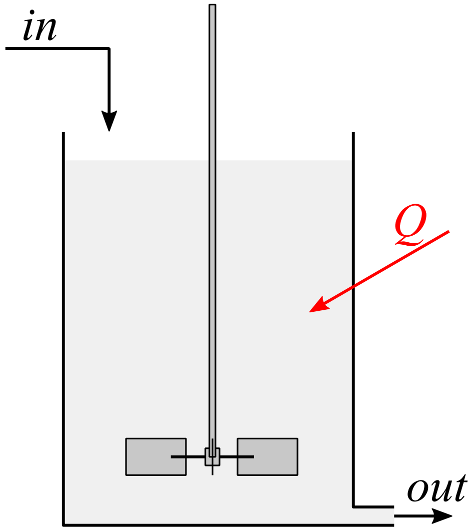
$$r_j = f_j\left(T, C_1, C_2, \ldots, C_{NC}\right) \qquad \forall j$$

Una forma mas generalizada de expresar la velocidad de reacción es:

$$r_j = k_j\left(T\right)\prod_{i=1}^{NC}\left[A_i\right]^{\alpha_{ij}} \qquad \forall j$$

Donde $[A_i]$ se denomina base y α_{ij} orden.
Las bases mas frecuentes son: Concentración, presión parcial, actividad, fugacidad, etc.

CSTR (Continuously Stirred Tank Reactor)



Hipótesis:

- Se conoce la estequiometría de cada una de las reacciones
- Se conocen las expresiones de velocidad de reacción (rj)
- Estado estacionario
- Medio de reacción homogéneo
- Las entalpías están calculadas tomando como base el calor de formación de cada componente.
- Se considera que el medio de reacción intercambia calor con una corriente energética.

CSTR (Continuously Stirred Tank Reactor)

$$m_{in} x_{in,i} + r_i V - m_{out} x_{out,i} = 0 \qquad \forall i$$

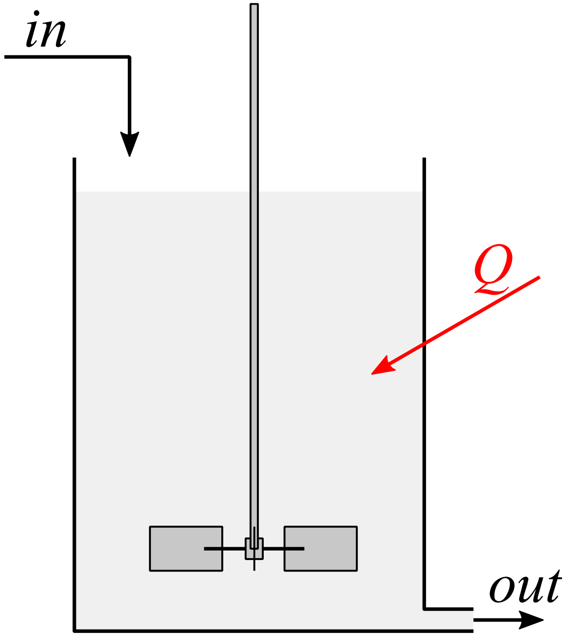
$$r_j = f_j\left(T_{out}, C_{out,1}, C_{out,2}, \ldots, C_{out,NC}\right) \qquad \forall j$$

$$r_i = \sum_{j=1}^{NR} a_{ij} r_j \qquad \forall i$$

$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

$$C_{out,i} = \rho_{out} x_{out,i} \qquad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$



CSTR (Continuously Stirred Tank Reactor)

$$m_{in} x_{in,i} + r_i V - m_{out} x_{out,i} = 0 \qquad \forall i$$

$$r_j = f_j \left(T_{out}, C_{out,1}, C_{out,2}, \ldots, C_{out,NC} \right) \qquad \forall j$$

$$r_i = \sum_{j=1}^{NR} a_{ij} r_j \qquad \forall i$$

$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

$$C_{out,i} = \rho_{out} x_{out,i} \qquad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f \left(T_{out}, P_{out}, H_{out}, x_{out} \right) = 0$$

$$f \left(T_{in}, P_{in}, H_{in}, x_{in} \right) = 0$$

$$f \left(T_{out}, P_{out}, \rho_{out}, x_{out} \right) = 0$$

CSTR (Continuously Stirred Tank Reactor)

$$m_{in}x_{in,i} + r_iV - m_{out}x_{out,i} = 0 \qquad \forall i$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j\left(T_{out}, C_{out}\right) \ \forall i$$

$$m_{in} \ \ x_{in,i} \ \ r_i \ \ V \ \ m_{out} \ \ x_{out,i}$$

$$H_{in} \ \ T_{in} \ \ P_{in} \ \ H_{out} \ \ T_{out} \ \ P_{out}$$

$$Q \ \ C_{out,i} \ \ \rho_{out}$$

$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

$$C_{out,i} = \rho_{out}x_{out,i} \qquad \forall i$$

$$m_{in}H_{in} + Q - m_{out}H_{out} = 0$$

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0$$

$$f\left(T_{out}, P_{out}, \rho_{out}, x_{out}\right) = 0$$

CSTR (MS)

$$m_{in} x_{in,i} + r_i V - m_{out} x_{out,i} = 0 \qquad \forall i$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j \left(T_{out}, C_{out} \right) \ \forall i$$

$$\sum_{i=1}^{NC} x_{out,i} = 1$$

$$C_{out,i} = \rho_{out} x_{out,i} \qquad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out} \right) = 0 \quad f\left(T_{out}, P_{out}, \rho_{out}, x_{out} \right) = 0$$

r_i V m_{out} $x_{out,i}$

H_{out} T_{out} P_{out}

Q $C_{out,i}$ ρ_{out}

7+3NC

–

4+3NC

GL =3

CSTR (adiabático o calor dado)

$$m_{in} x_{in,i} + r_i V - m_{out} x_{out,i} = 0 \qquad \forall i$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j \left(T_{out}, C_{out} \right) \ \forall i$$

$$\sum_{i=1}^{NC} x_{out,i} = 1$$

$$C_{out,i} = \rho_{out} x_{out,i} \qquad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out} \right) = 0 \quad f\left(T_{out}, P_{out}, \rho_{out}, x_{out} \right) = 0$$

$$r_i \ \enclose{circle}{V} \ m_{out} \ \ x_{out,i}$$

$$H_{out} \ \ T_{out} \ \ \enclose{circle}{P_{out}}$$

$$\enclose{circle}{Q} \ C_{out,i} \ \ \rho_{out}$$

CSTR (isotérmico)

$$m_{in} x_{in,i} + r_i V - m_{out} x_{out,i} = 0 \qquad \forall i$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j \left(T_{out}, C_{out} \right) \ \forall i$$

$$\sum_{i=1}^{NC} x_{out,i} = 1$$

$$C_{out,i} = \rho_{out} x_{out,i} \qquad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out} \right) = 0 \quad f\left(T_{out}, P_{out}, \rho_{out}, x_{out} \right) = 0$$

$$r_i \ \boxed{V} \ m_{out} \ \ x_{out,i}$$

$$H_{out} \ \boxed{T_{out}} \ \boxed{P_{out}}$$

$$Q \ \ C_{out,i} \ \ \rho_{out}$$

Reactor CSTR (flujos x componentes - MS)

$$m_{in,i} + r_i V - m_{out,i} = 0 \quad \forall i$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j \left(T_{out}, C_{out} \right) \; \forall i$$

$$m_{out} = \sum_{i=1}^{NC} m_{out,i}$$

$$m_{out,i} = m_{out} x_{out,i} \quad \forall i$$

$$C_{out,i} = \rho_{out} x_{out,i} \quad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out} \right) = 0 \quad f\left(T_{out}, P_{out}, \rho_{out}, x_{out} \right) = 0$$

$r_i \; V \; m_{out} \; m_{out,i} \; x_{out,i}$

$H_{out} \; T_{out} \; P_{out}$

$Q \; C_{out,i} \; \rho_{out}$

7+4NC

–

4+4NC

GL =3

CSTR - Ejemplo

$$n-C_4H_{10} \underset{k_2}{\overset{k_1}{\rightleftarrows}} i-C_4H_{10}$$

$$r_{R1}\left[\frac{mol}{seg.m^3}\right]=k_1C_{nC4} \quad k_1=2.94\times10^7\frac{1}{seg}e^{-\frac{65300}{8.314T}}$$

$$r_{R2}\left[\frac{mol}{seg.m^3}\right]=k_2C_{iC4} \quad k_2=1.176\times10^8\frac{1}{seg}e^{-\frac{72200}{8.314T}}$$

$$r_i=\sum_{j=1}^{NR}a_{ij}f_j\left(T_{out},C_{out}\right)\ \forall i \ \rightarrow r_i=a_{iR1}k_1C_{nC4}+a_{iR2}k_2C_{iC4} \quad \forall i$$

$$r_{nC4}=-k_1C_{nC4}+k_2C_{iC4} \quad k_1=2.94\times10^7\frac{1}{seg}e^{-\frac{65300}{8.314T}}$$

$$r_{iC4}=k_1C_{nC4}-k_2C_{iC4} \quad k_2=1.176\times10^8\frac{1}{seg}e^{-\frac{72200}{8.314T}}$$

CSTR - Ejemplo

m_{in} : $45.27\, mol.seg^{-1}$

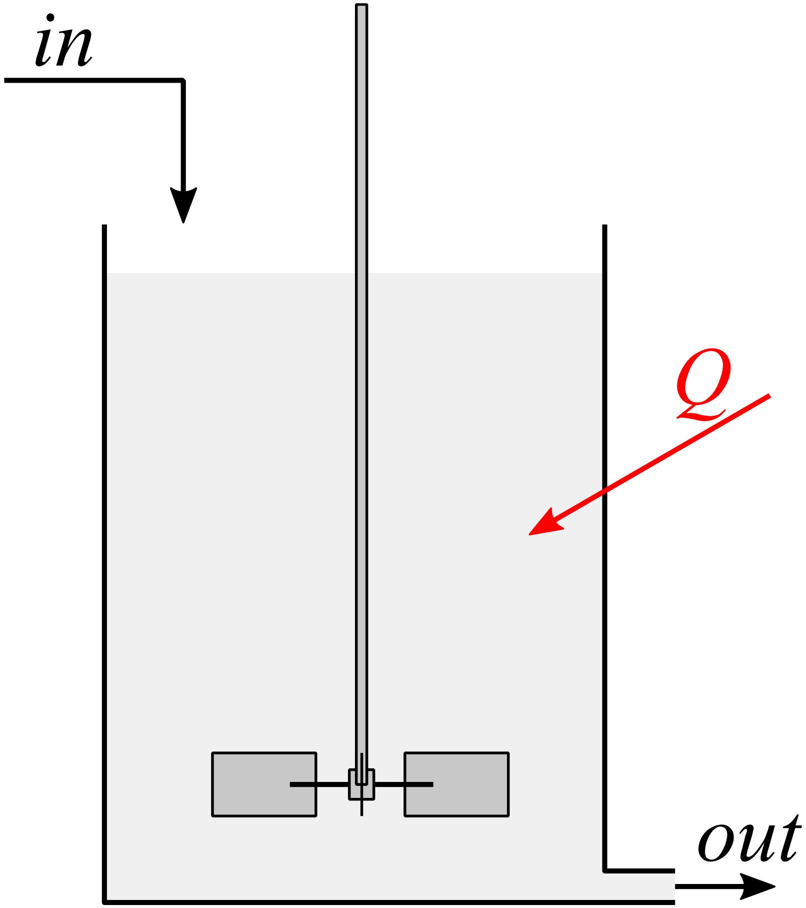
P_{in} : $20\ bar$

T_{in} : $330\, K$

$x_{in,nC_4H_{10}}$: 0.9

$x_{in,iC_5H_{12}}$: 0.1

$x_{in,iC_4H_{10}}$: 0



P_{out} : $20\ bar$

T_{out} : $350\, K$

$V = 3\ m^3$

CSTR - Ejemplo

$$m_{in,i} + r_i V - m_{out,i} = 0 \quad \forall i$$

$$r_i \quad m_{out} \quad m_{out,i} \quad x_{out,i}$$

$$H_{out} \quad Q \quad C_{out,i} \quad \rho_{out}$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j\left(T_{out}, C_{out}\right) \quad \forall i$$

$$r_{nC4} = -k_1 C_{nC4} + k_2 C_{iC4}$$

$$r_{iC4} = k_1 C_{nC4} - k_2 C_{iC4}$$

$$k_1 = 2.94 \times 10^7 \frac{1}{seg} e^{-\frac{65300}{8.314T}}$$

$$k_2 = 1.176 \times 10^8 \frac{1}{seg} e^{-\frac{72200}{8.314T}}$$

$$m_{out} = \sum_{i=1}^{NC} m_{out,i}$$

$$m_{out,i} = m_{out} x_{out,i} \quad \forall i$$

$$C_{out,i} = \rho_{out} x_{out,i} \quad \forall i$$

$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$

$$f\left(T_{out}, P_{out}, H_{out}, x_{out}\right) = 0 \qquad f\left(T_{out}, P_{out}, \rho_{out}, x_{out}\right) = 0$$

CSTR - Ejemplo

$$m_{in,i} + r_i V - m_{out,i} = 0 \quad \forall i$$ ①

$$r_i \quad m_{out} \quad m_{out,i} \quad x_{out,i}$$

$$H_{out} \quad Q \quad C_{out,i} \quad \rho_{out}$$

$$r_i = \sum_{j=1}^{NR} a_{ij} f_j \left(T_{out}, C_{out} \right) \quad \forall i$$ ②

$$m_{out} = \sum_{i=1}^{NC} m_{out,i}$$ ③

$$m_{out,i} = m_{out} x_{out,i} \quad \forall i$$ ④

$$C_{out,i} = \rho_{out} x_{out,i} \quad \forall i$$ ⑤

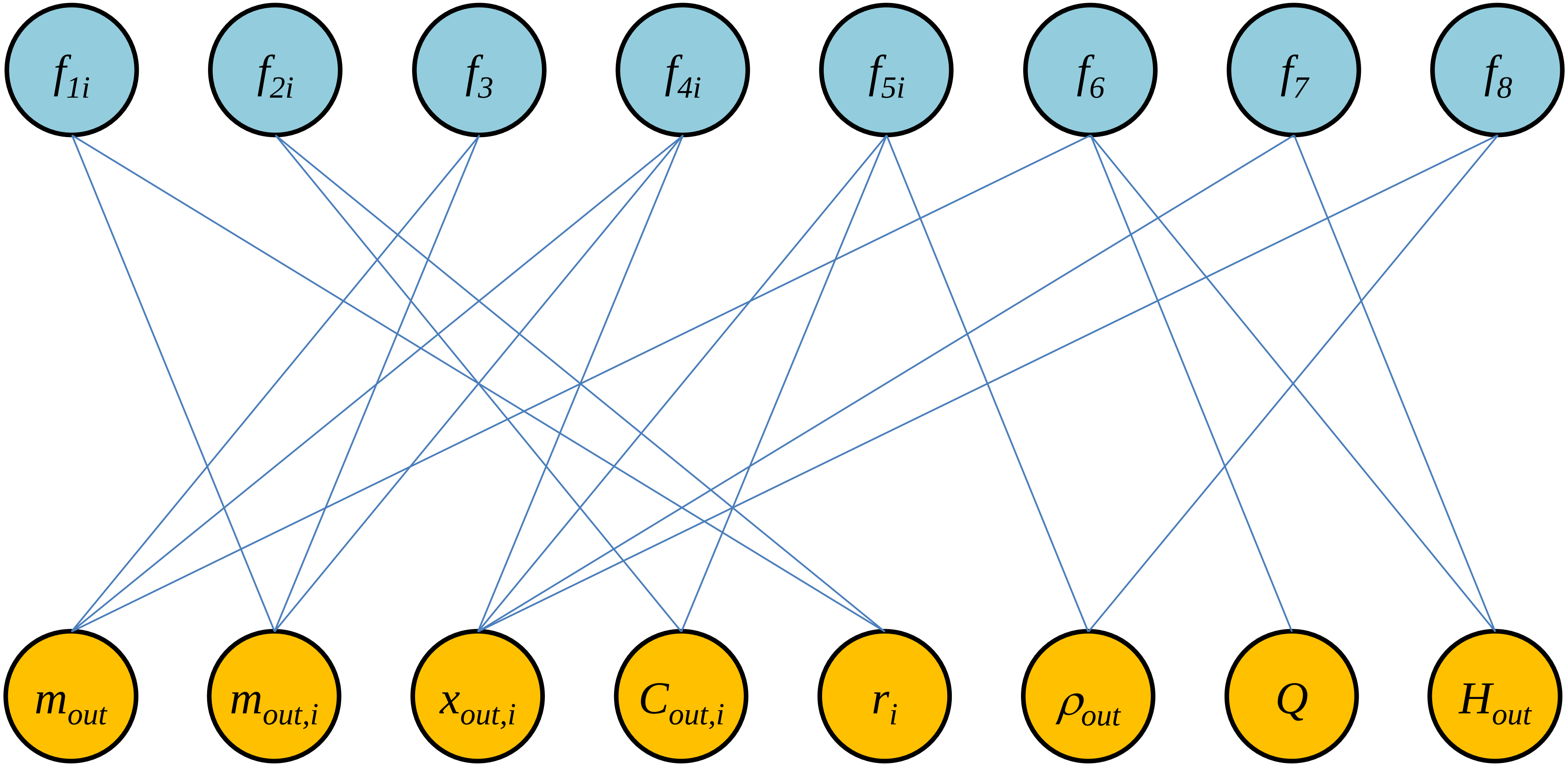
$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$ ⑥

$$f\left(T_{out}, P_{out}, H_{out}, x_{out} \right) = 0$$ ⑦

$$f\left(T_{out}, P_{out}, \rho_{out}, x_{out} \right) = 0$$ ⑧

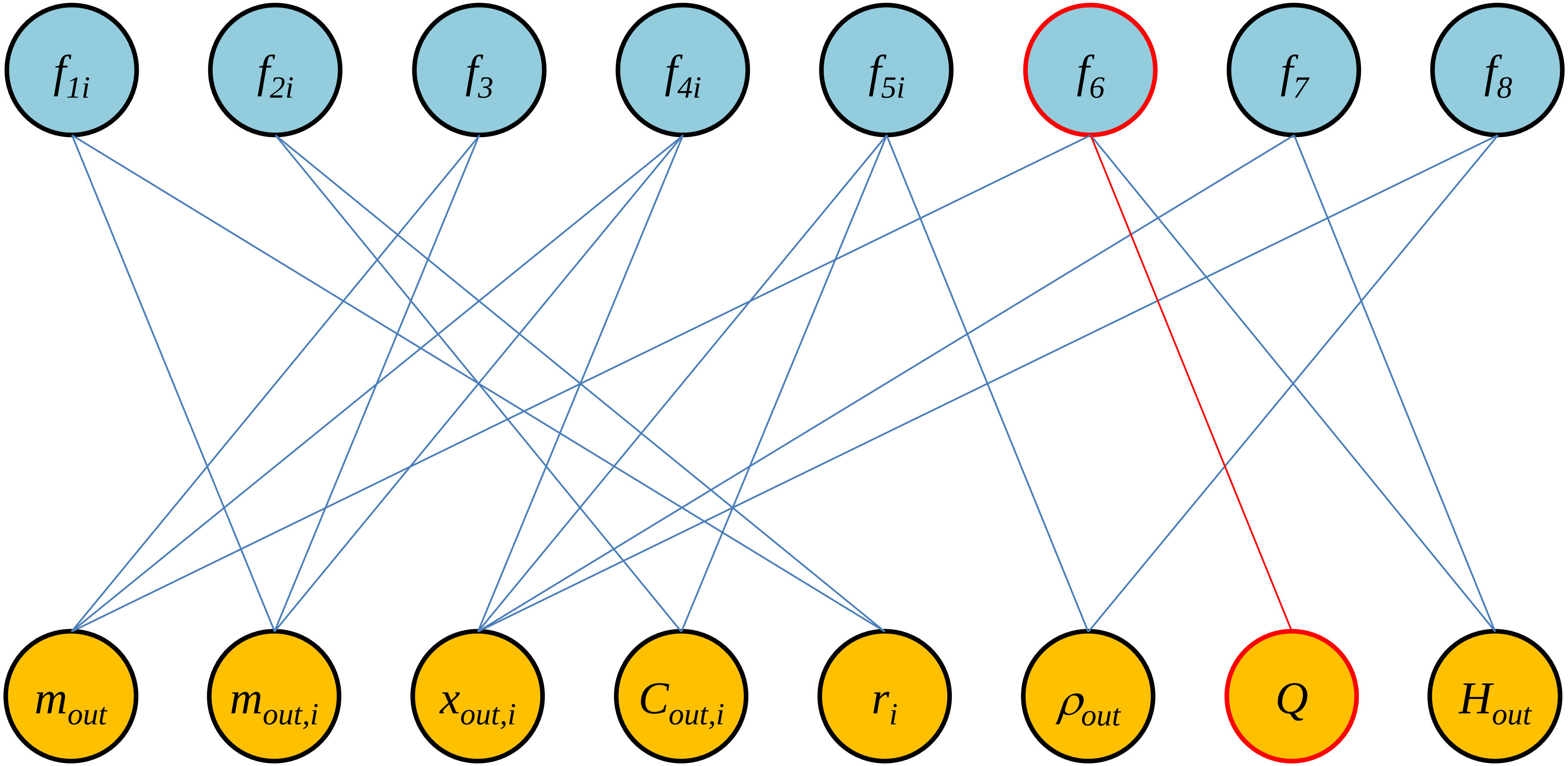
Reactor CSTR (flujos x componentes - MS)

Aplicamos el algoritmo de LC&R e imponemos nuestro criterio cuando hay varios opciones para asignar.



Reactor CSTR (flujos x componentes - MS)

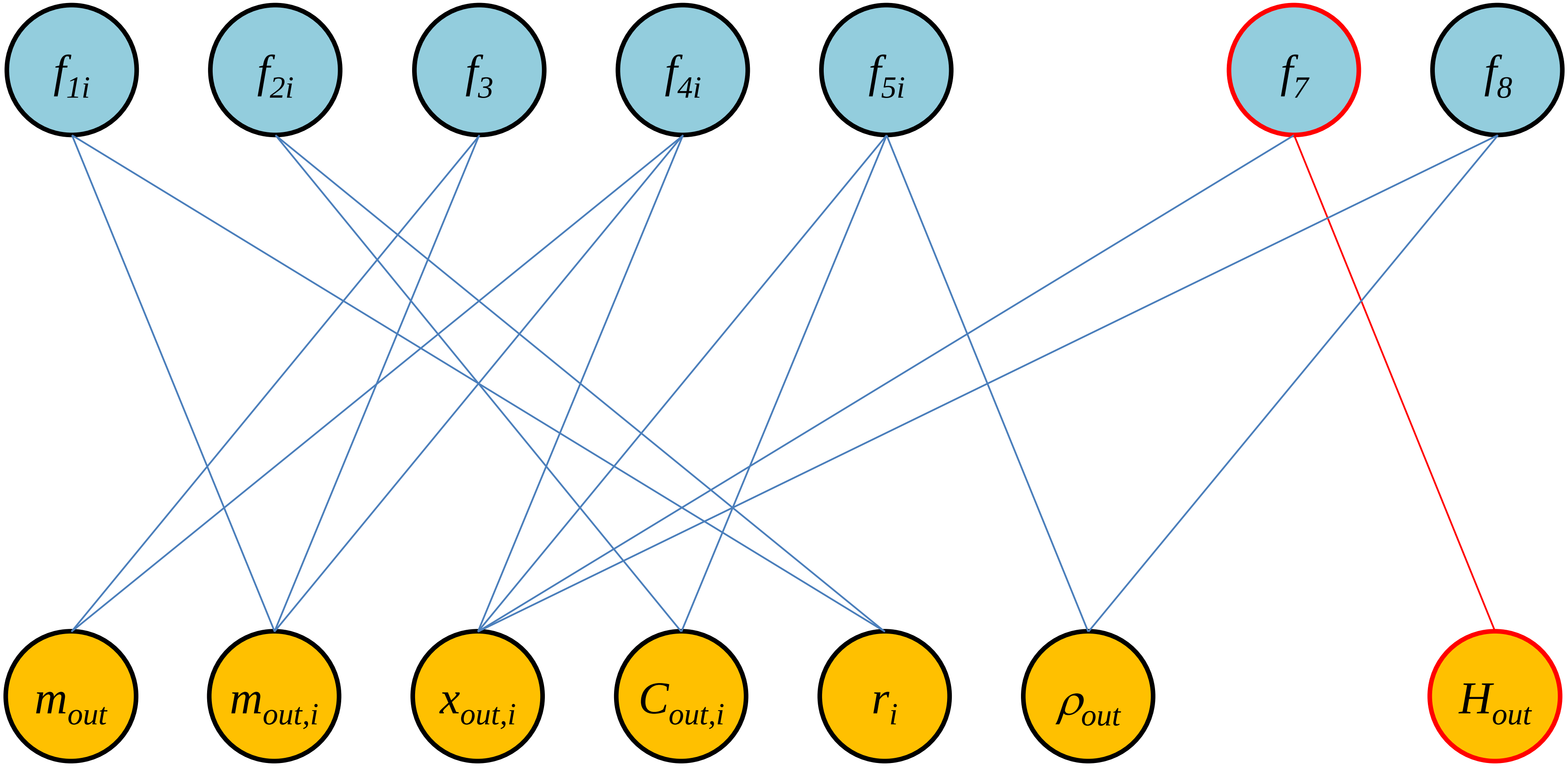
$f_6 \rightarrow Q$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$

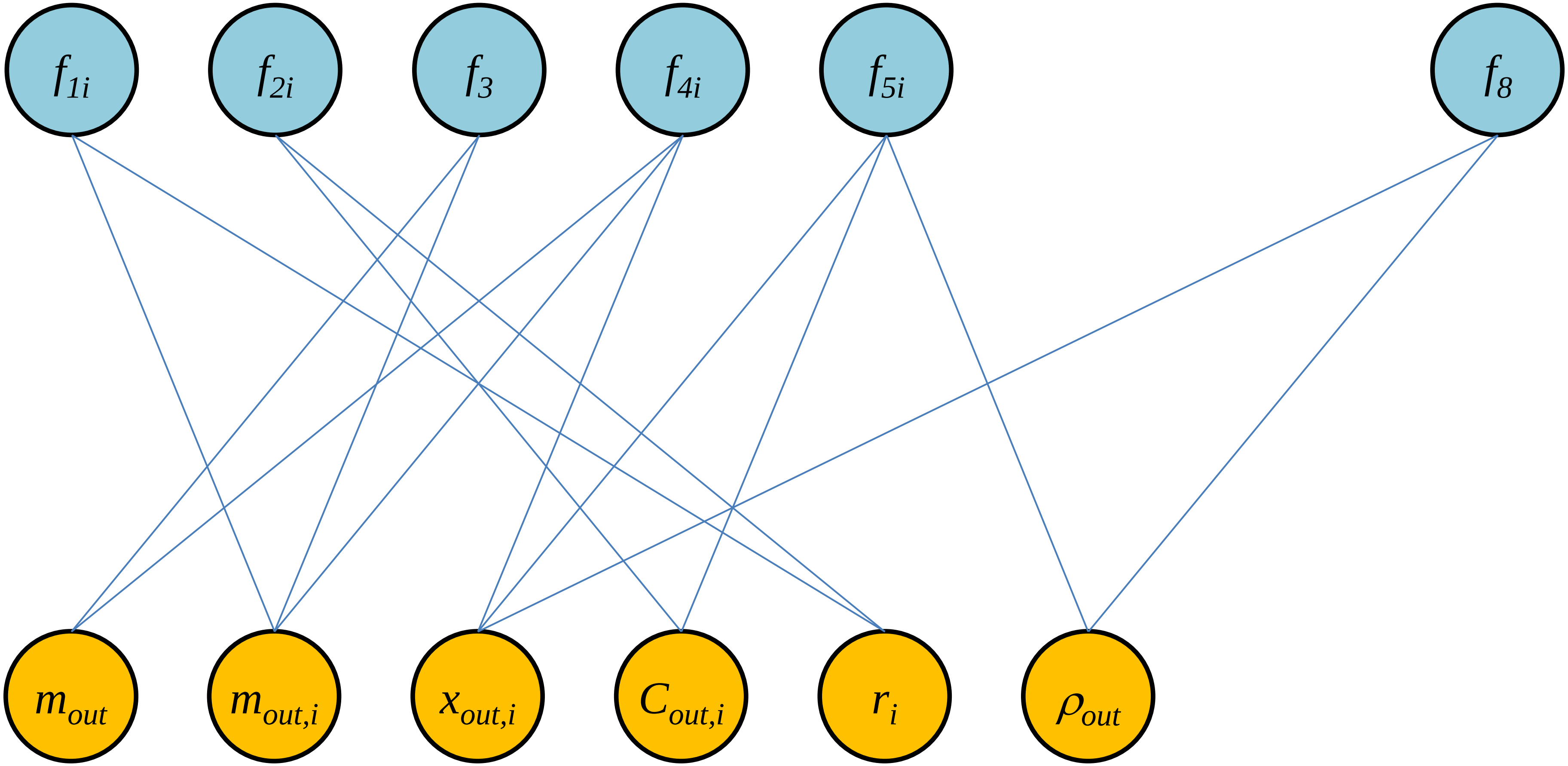
$f_7 \rightarrow H_{out}$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$

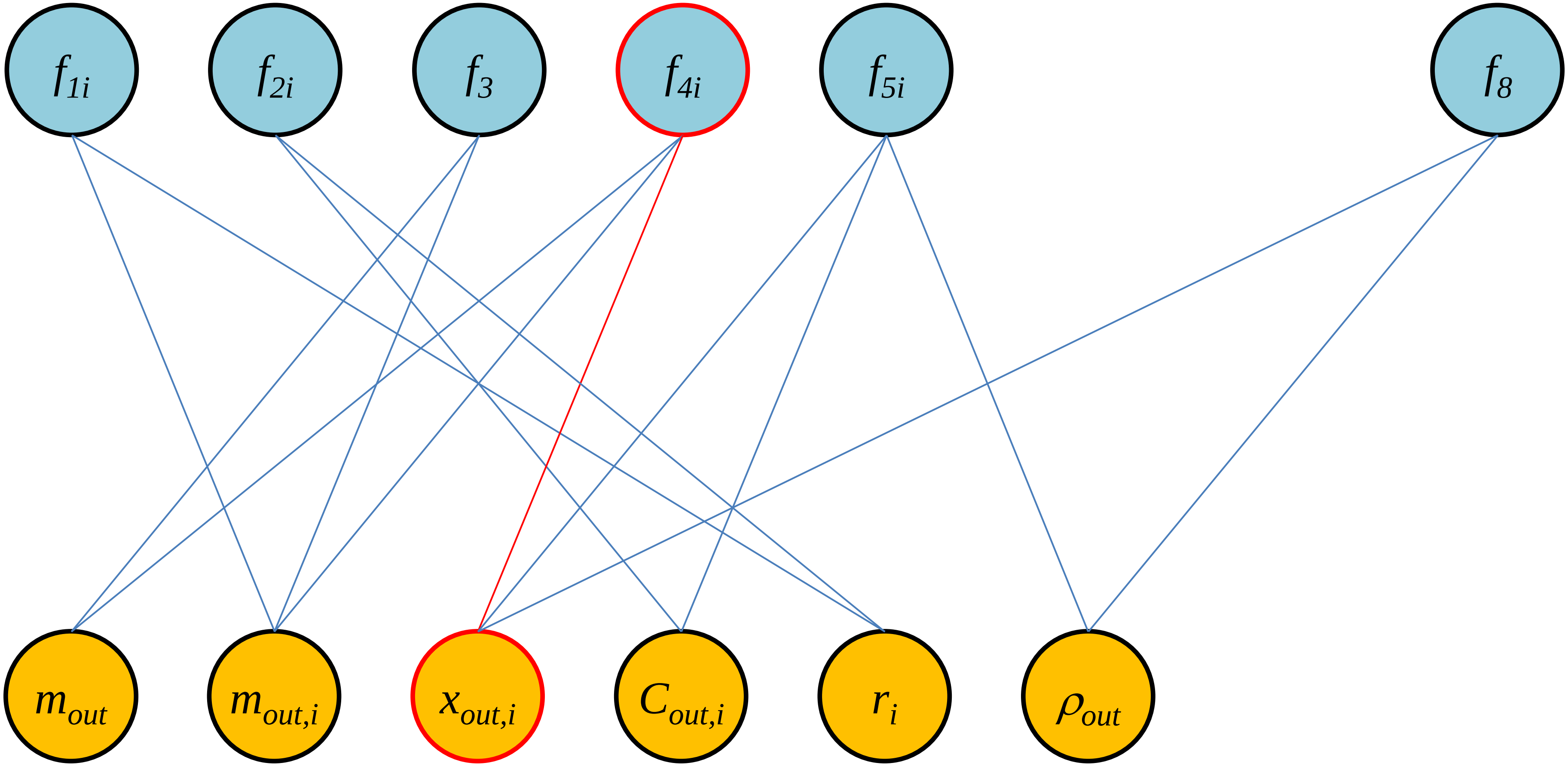
$f_7 \rightarrow H_{out}$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $\qquad$ $f_{4i} \rightarrow x_{out,i}$

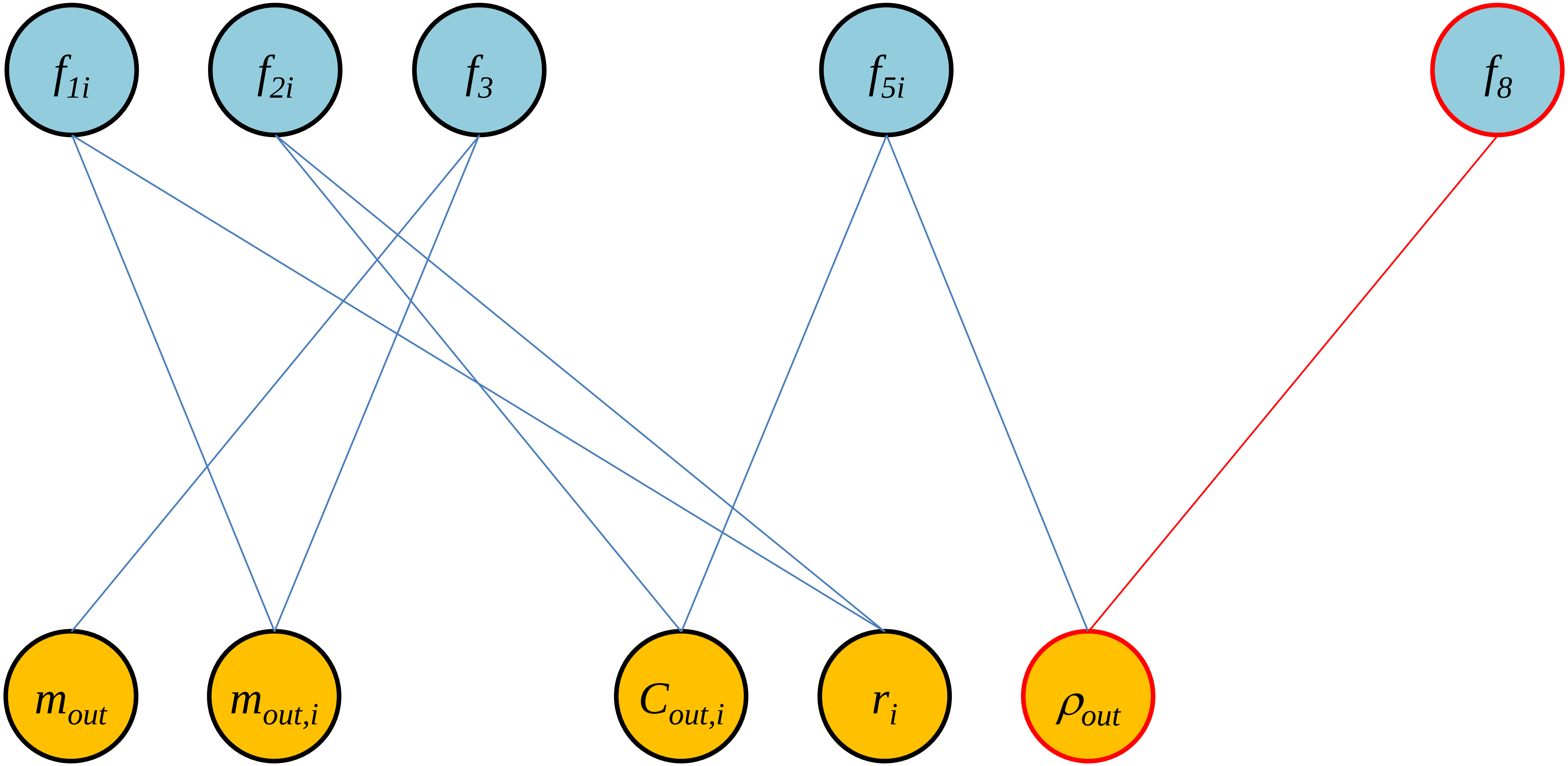
$f_7 \rightarrow H_{out}$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $f_{4i} \rightarrow x_{out,i}$

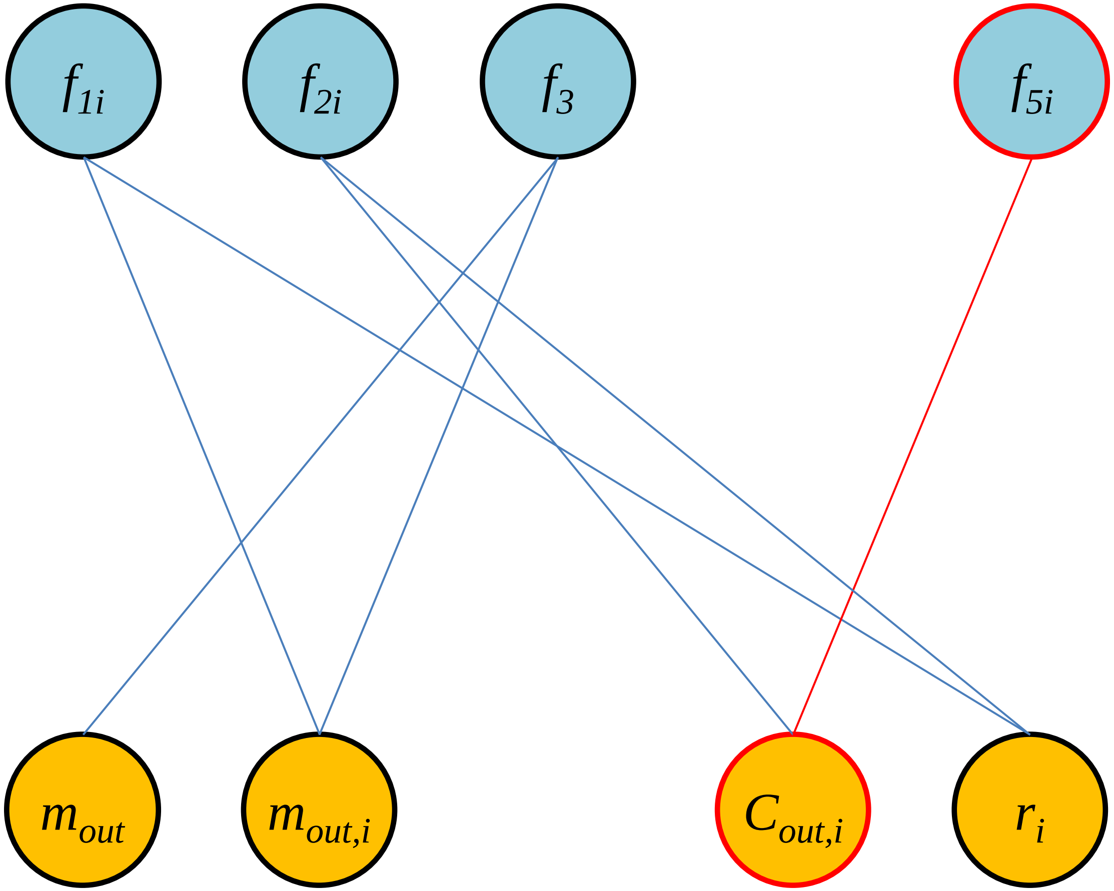
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $f_{4i} \rightarrow x_{out,i}$ $f_{5i} \rightarrow C_{out,i}$

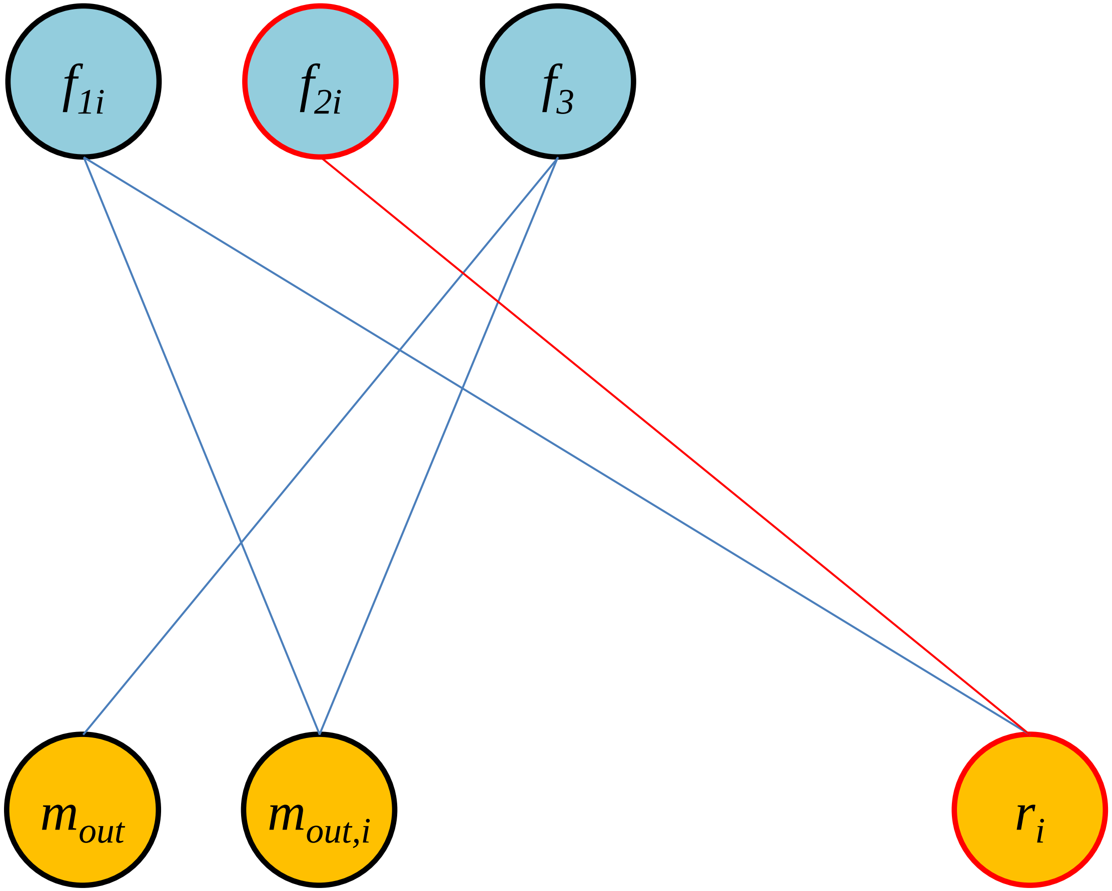
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $f_{4i} \rightarrow x_{out,i}$ $f_{5i} \rightarrow C_{out,i}$

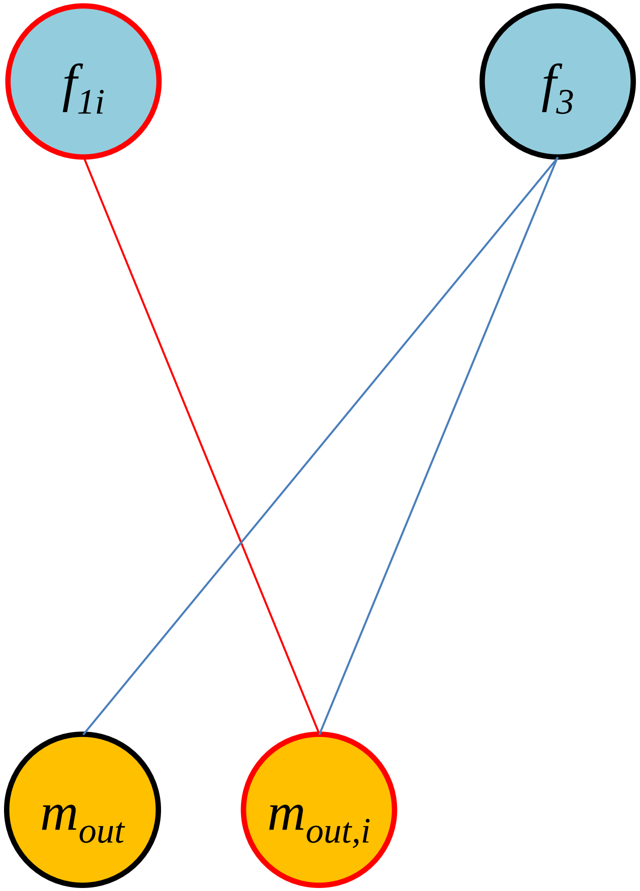
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $f_{4i} \rightarrow x_{out,i}$ $f_{5i} \rightarrow C_{out,i}$ $f_{1i} \rightarrow m_{out,i}$

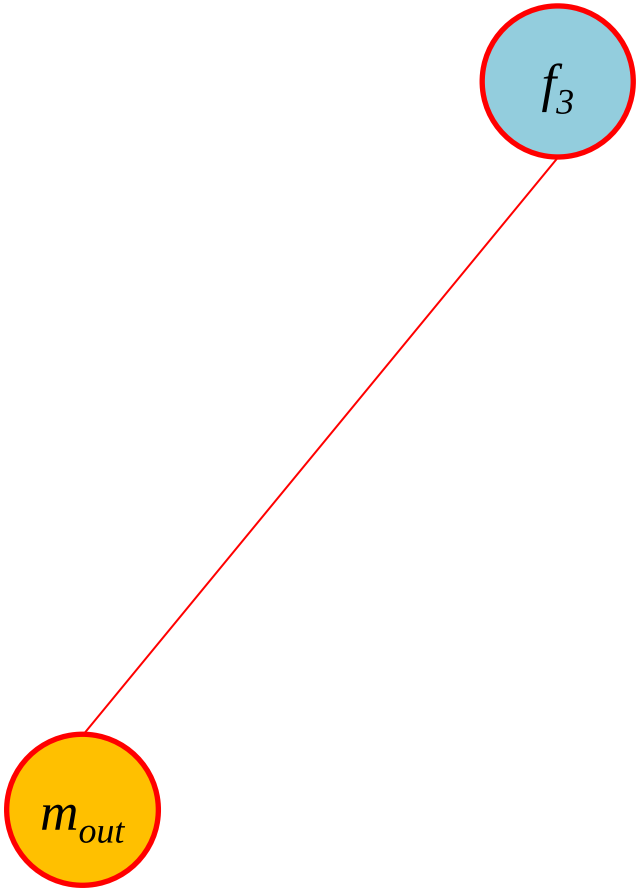
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $f_{4i} \rightarrow x_{out,i}$ $f_{5i} \rightarrow C_{out,i}$ $f_{1i} \rightarrow m_{out,i}$

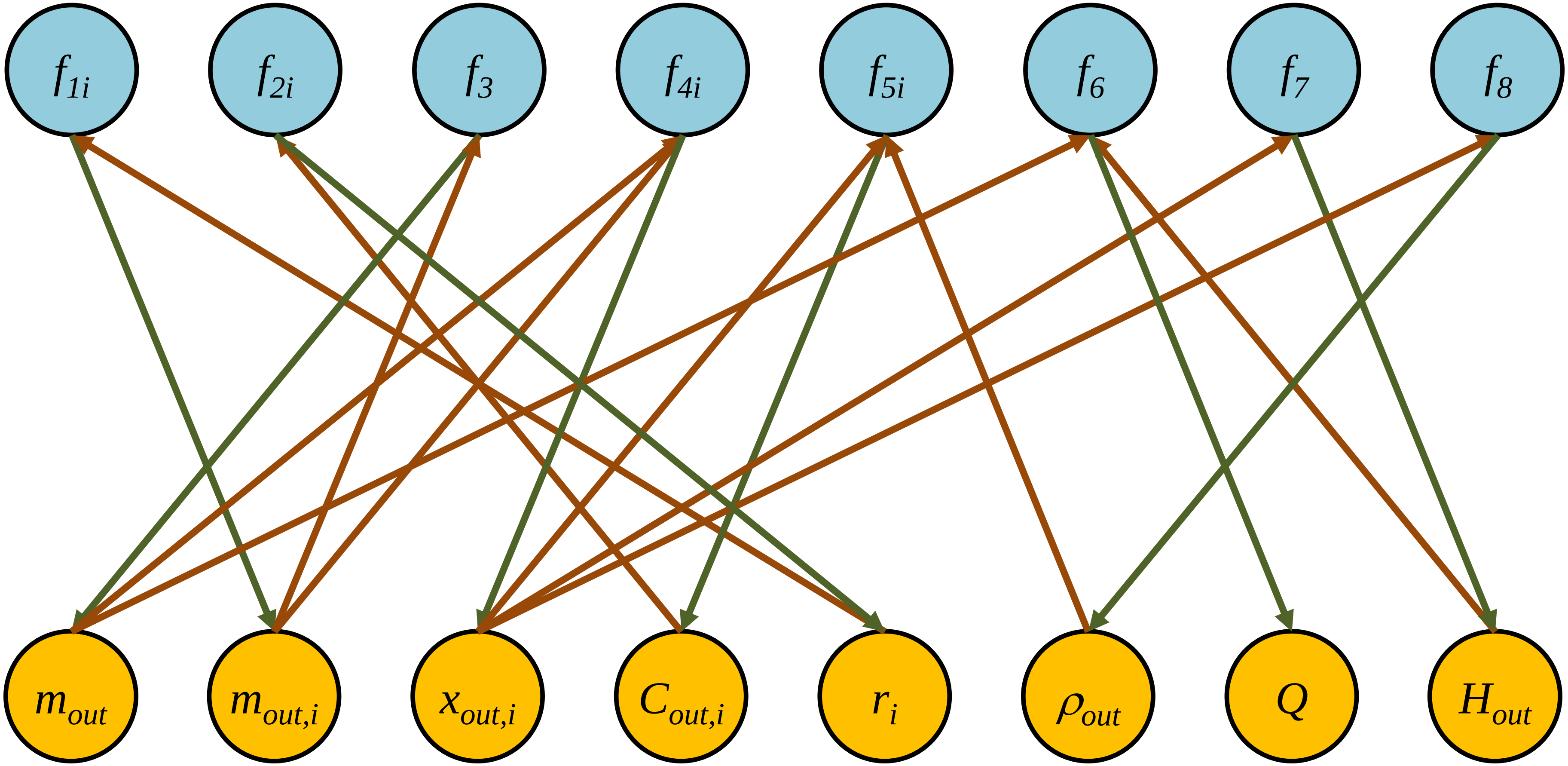
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$ $f_3 \rightarrow m_{out}$



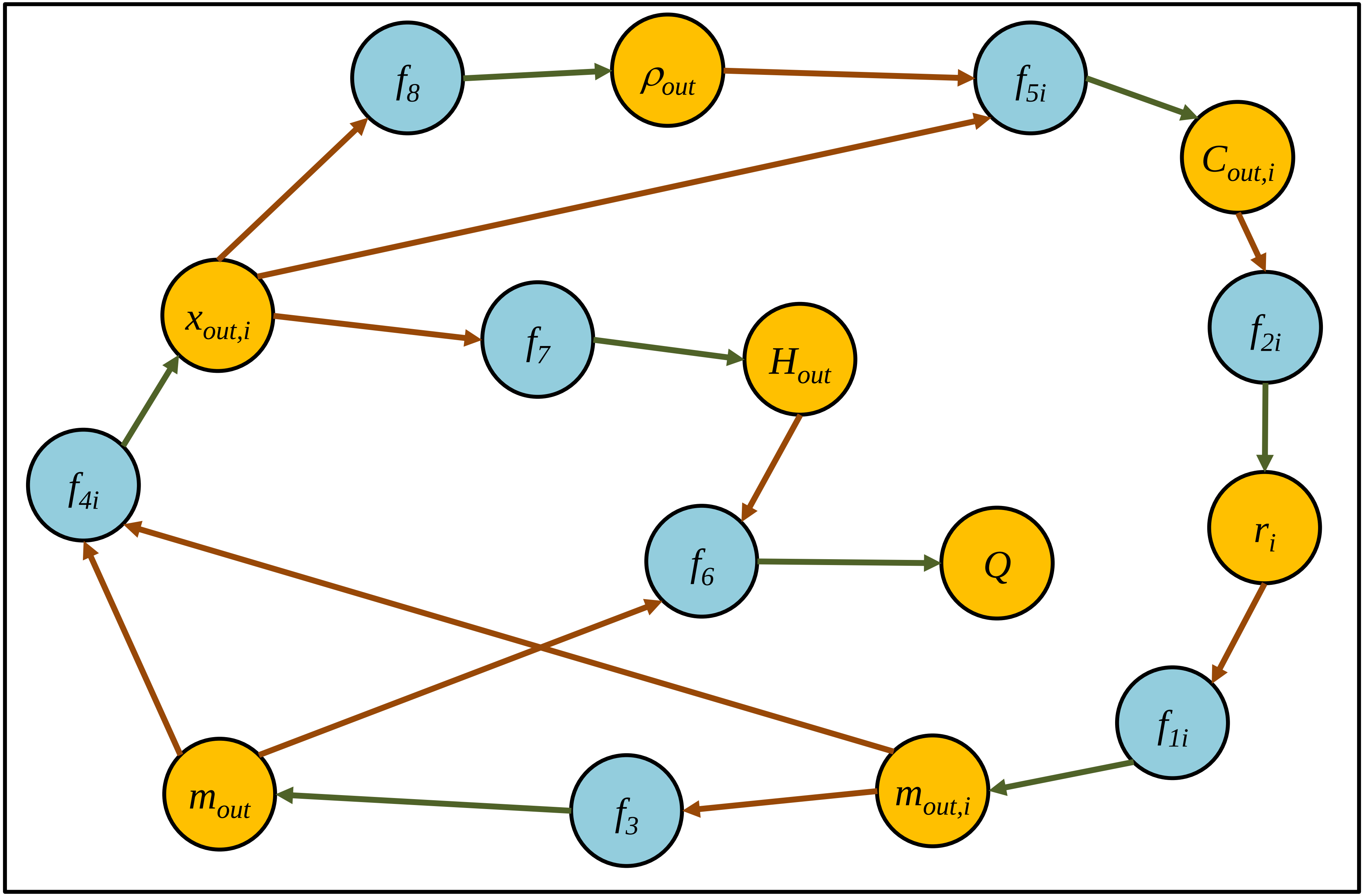
Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$ $\quad f_{4i} \rightarrow x_{out,i}$ $\quad f_{5i} \rightarrow C_{out,i}$ $\quad f_{1i} \rightarrow m_{out,i}$

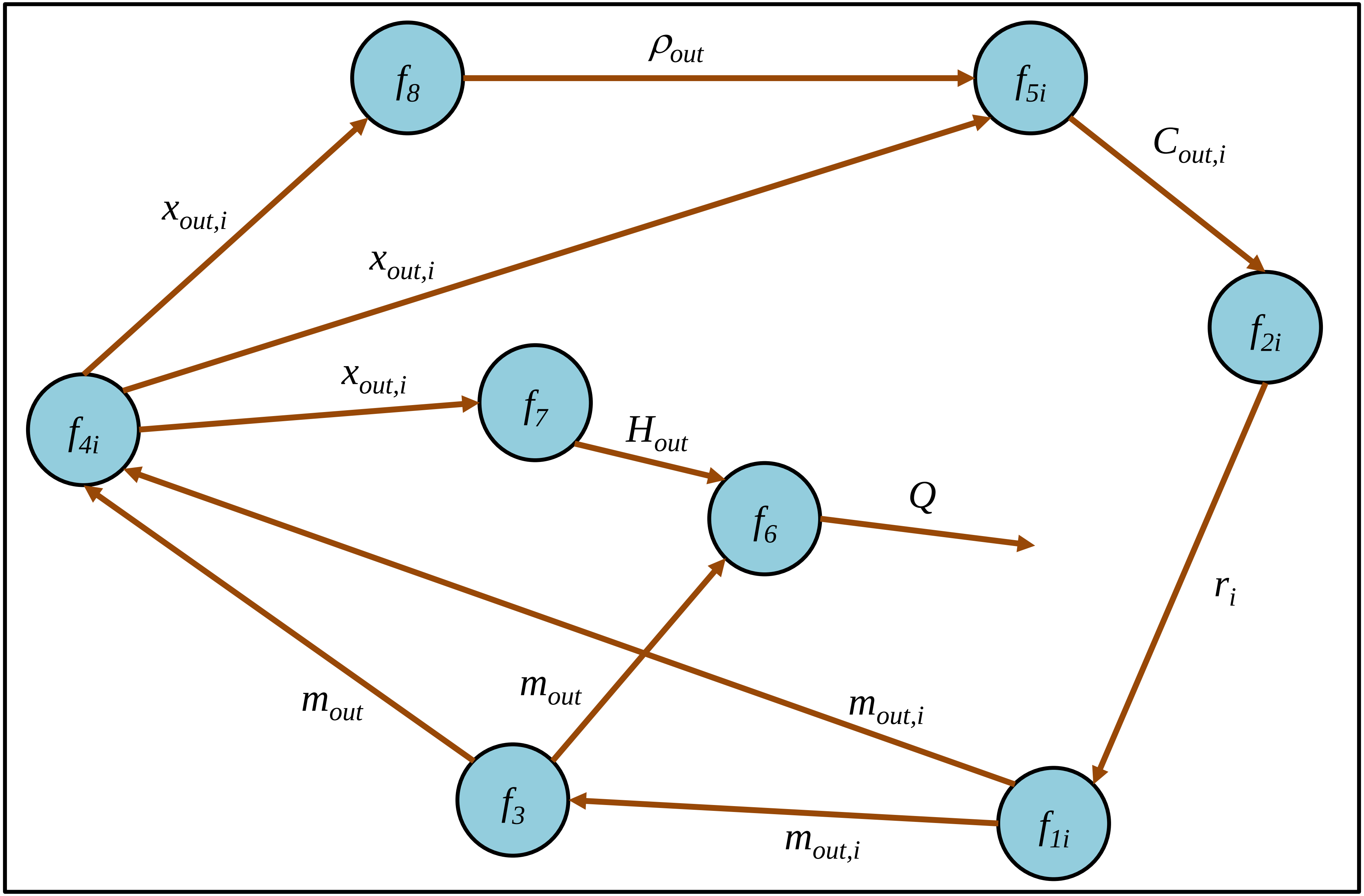
$f_7 \rightarrow H_{out}$ $\quad f_8 \rightarrow \rho_{out}$ $\quad f_{2i} \rightarrow r_i$ $\quad f_3 \rightarrow m_{out}$



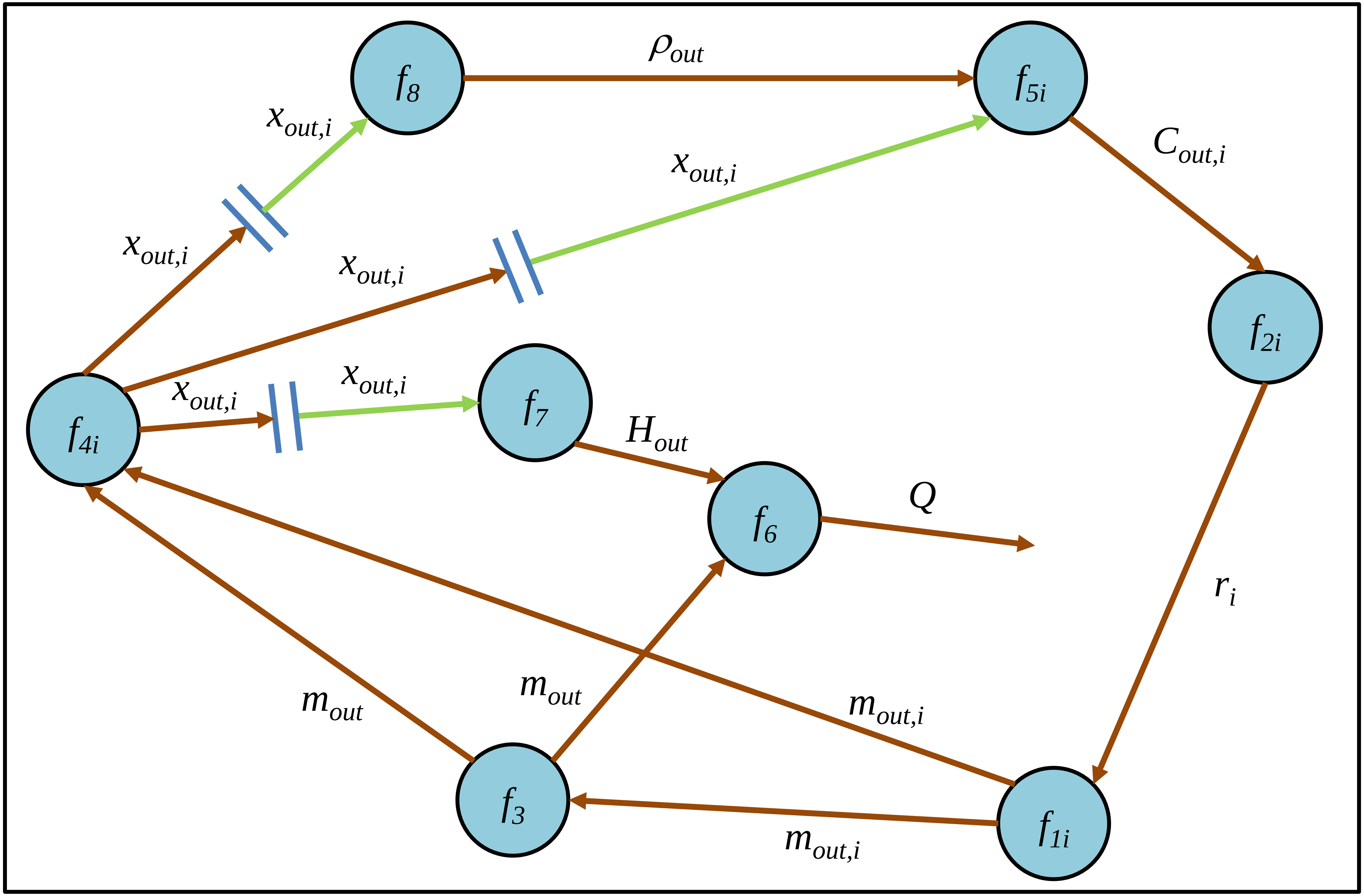
Reactor CSTR (flujos x componentes - MS)



Reactor CSTR (flujos x componentes - MS)



Reactor CSTR (flujos x componentes - MS)



CSTR – Ejercicio propuesto

m_{in} : $45.27\, mol.seg^{-1}$

P_{in} : $20\ bar$

T_{in} : $330\, K$

$x_{in,nC_4H_{10}}$: 0.9

$x_{in,iC_5H_{12}}$: 0.1

$x_{in,iC_4H_{10}}$: 0

$$H_{in} = -145725.677$$

$$V = 3\ m^3$$

T_{out} : $330\, K$

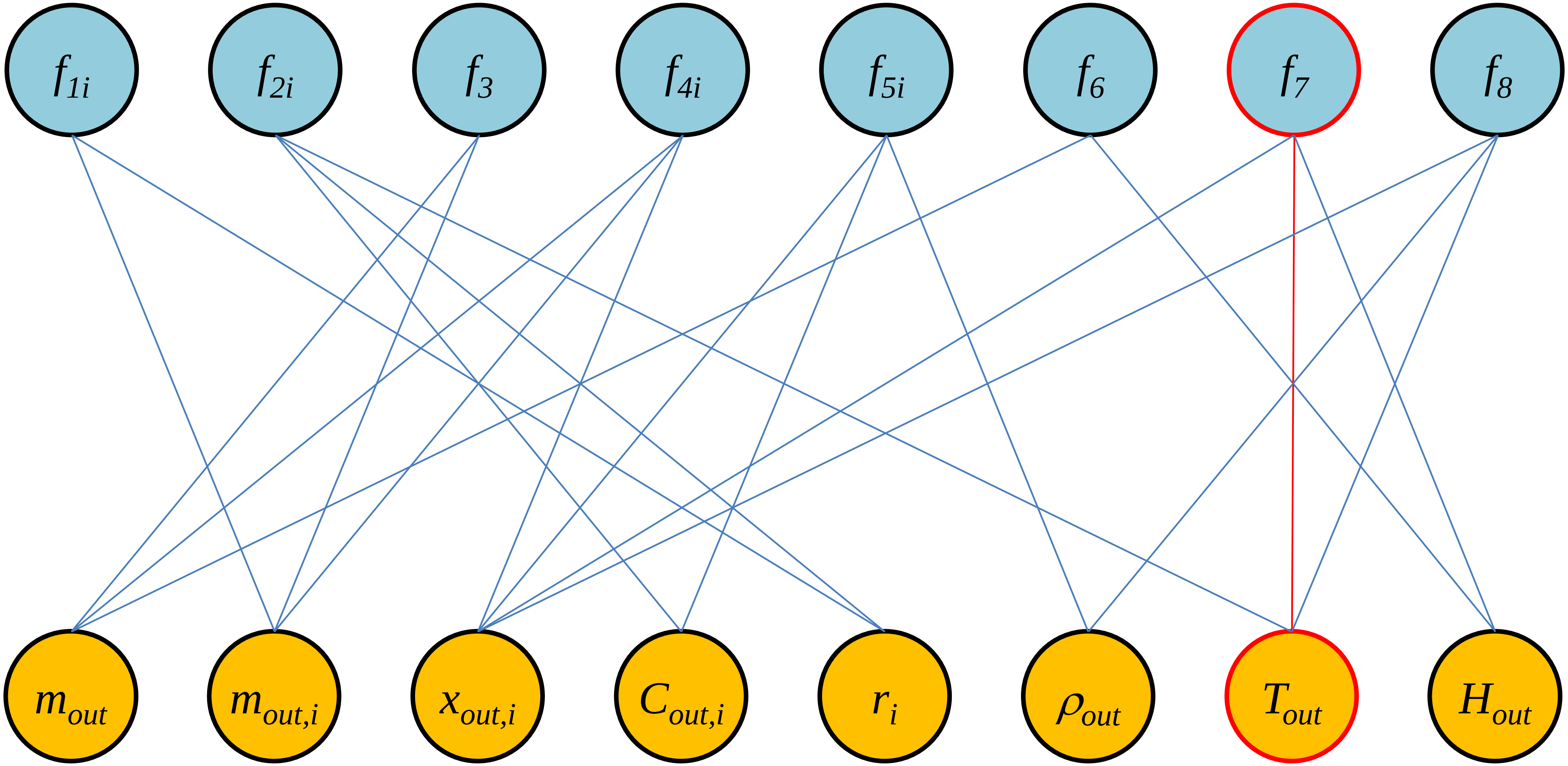
P_{out} : $20\ bar$

ID	Nombre
5	N-butane
8	Isopentane
4	Isobutane

alpha	N-butane	Isopentane	Isobutane
N-butane	0	0.0015	-0.0004
Isopentane	0.0015	0	0.00107
Isobutane	-0.0004	0.00107	0

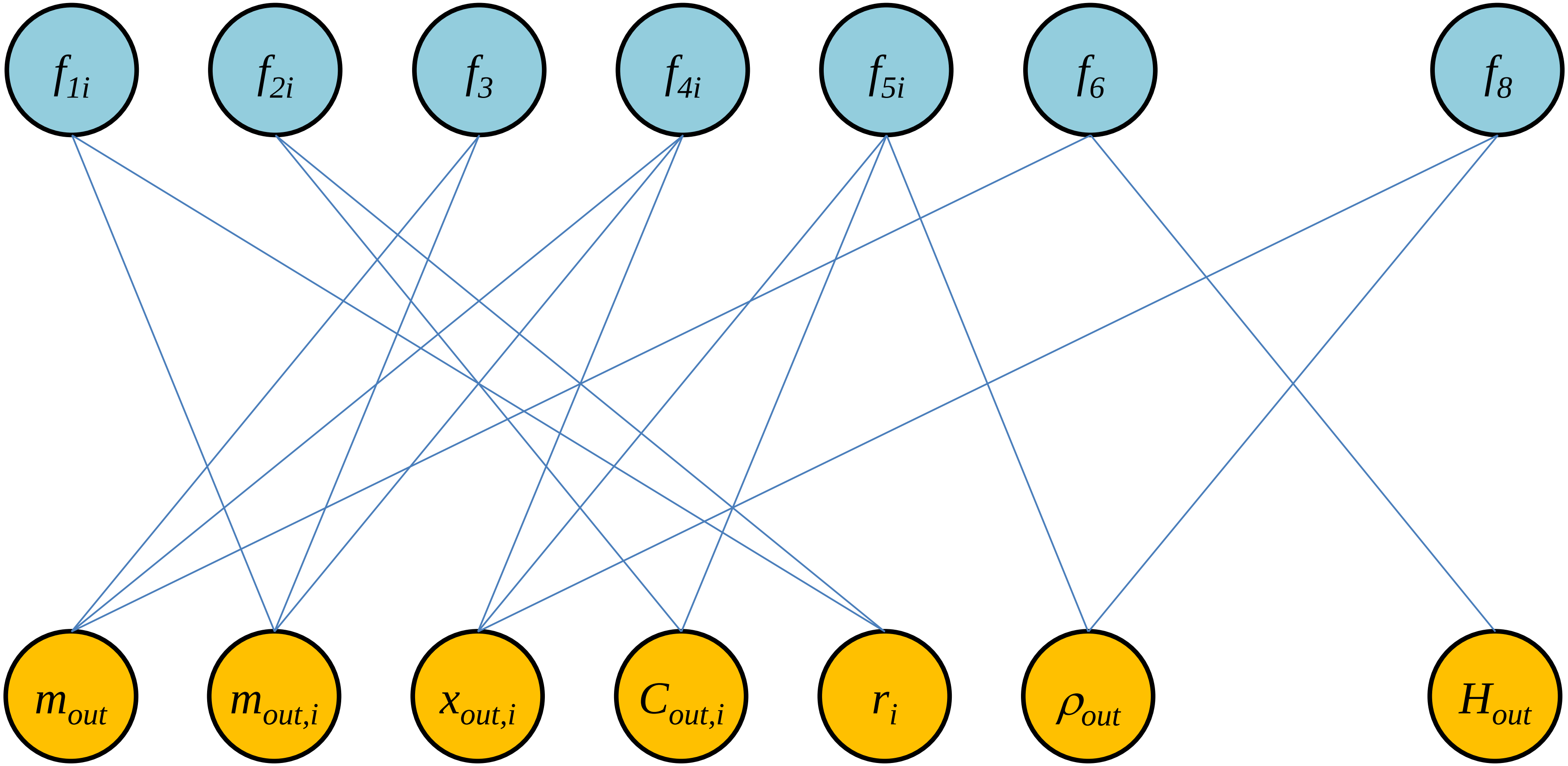
Reactor CSTR (P, Q y V conocidos)

A simple vista se observa que es una secuencia cíclica. Elegimos como corriente de corte a la Temperatura de salida.



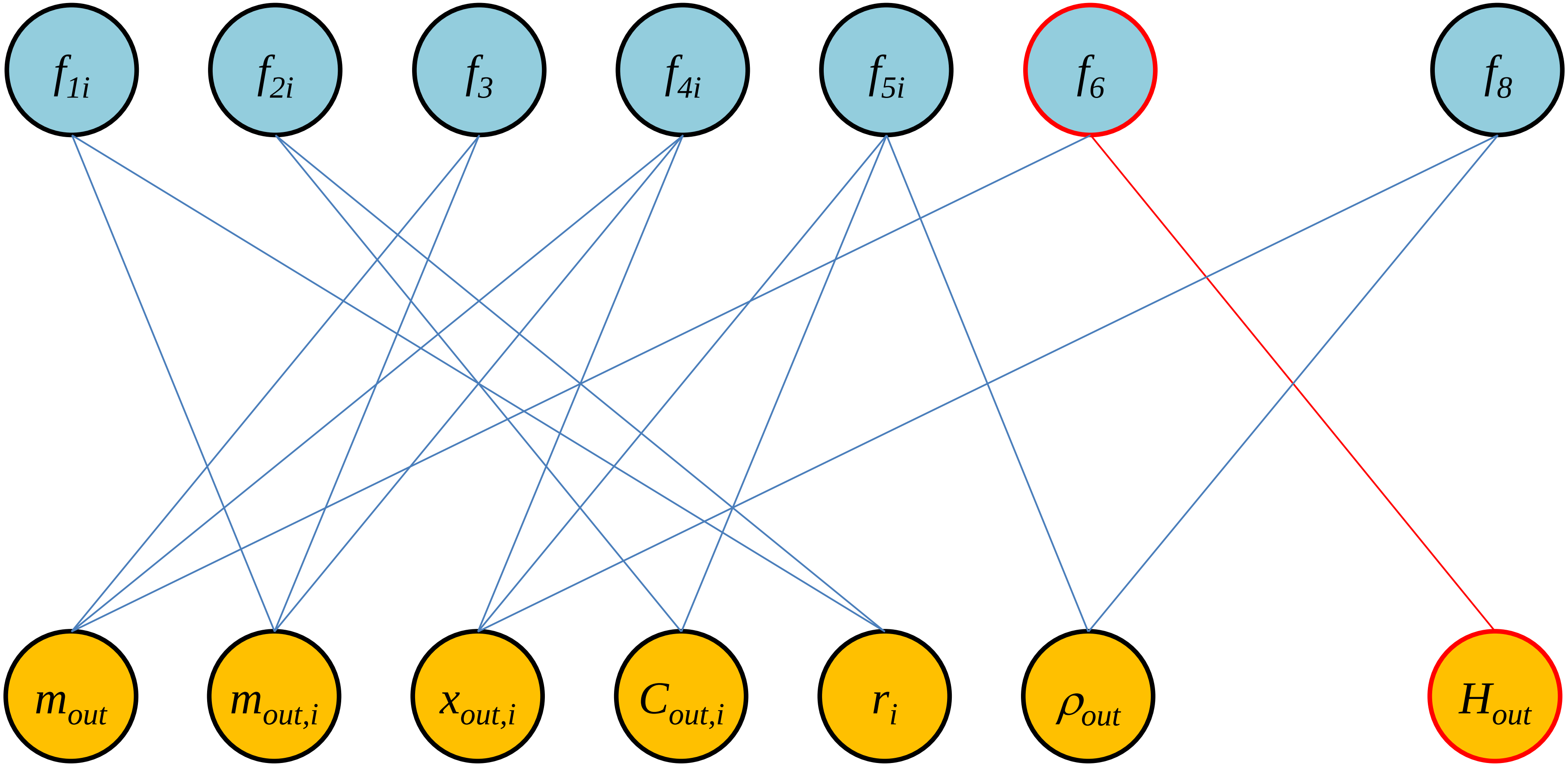
Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$



Reactor CSTR (P, Q y V conocidos)

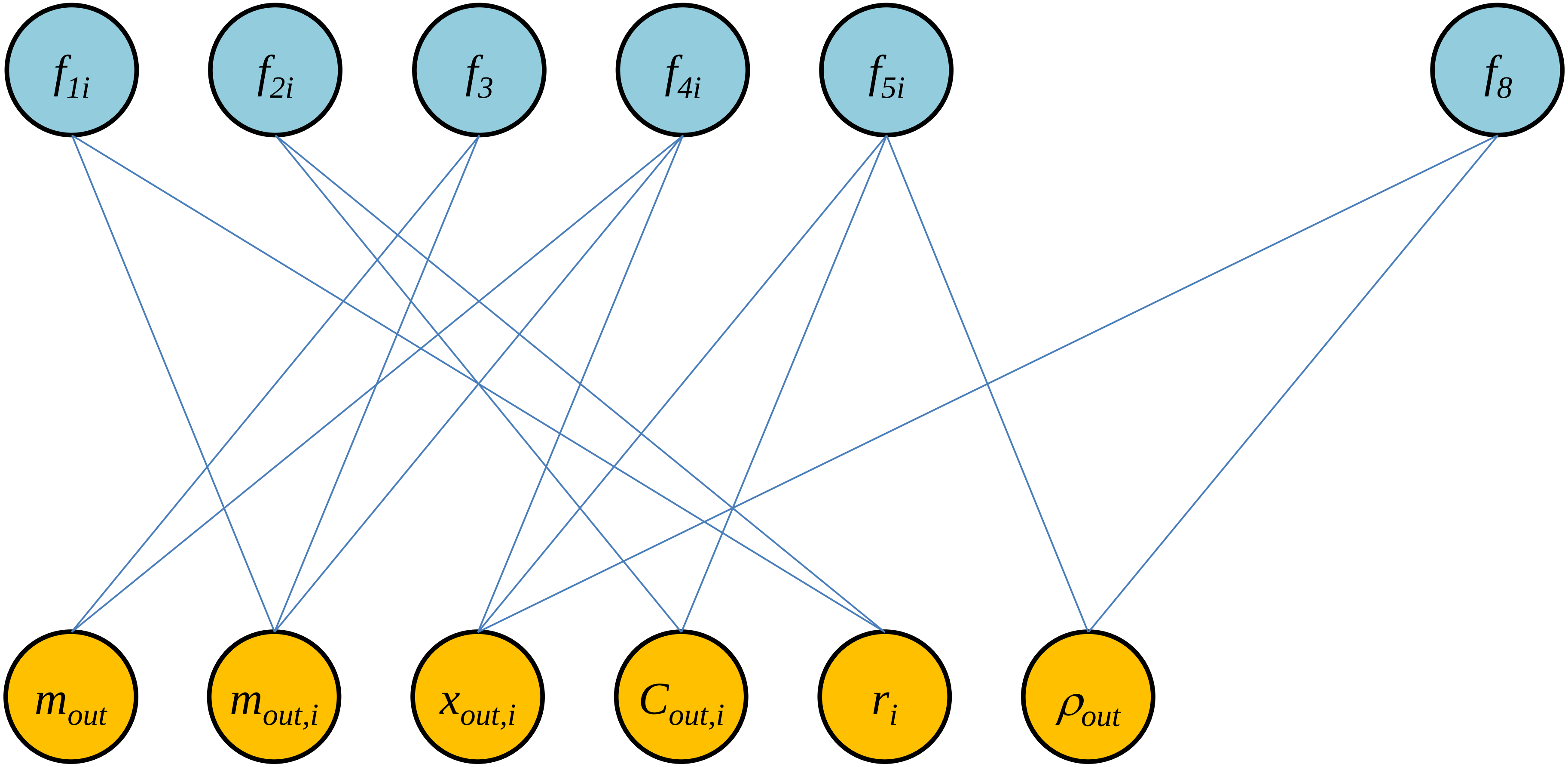
$f_7 \rightarrow T_{out}$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$

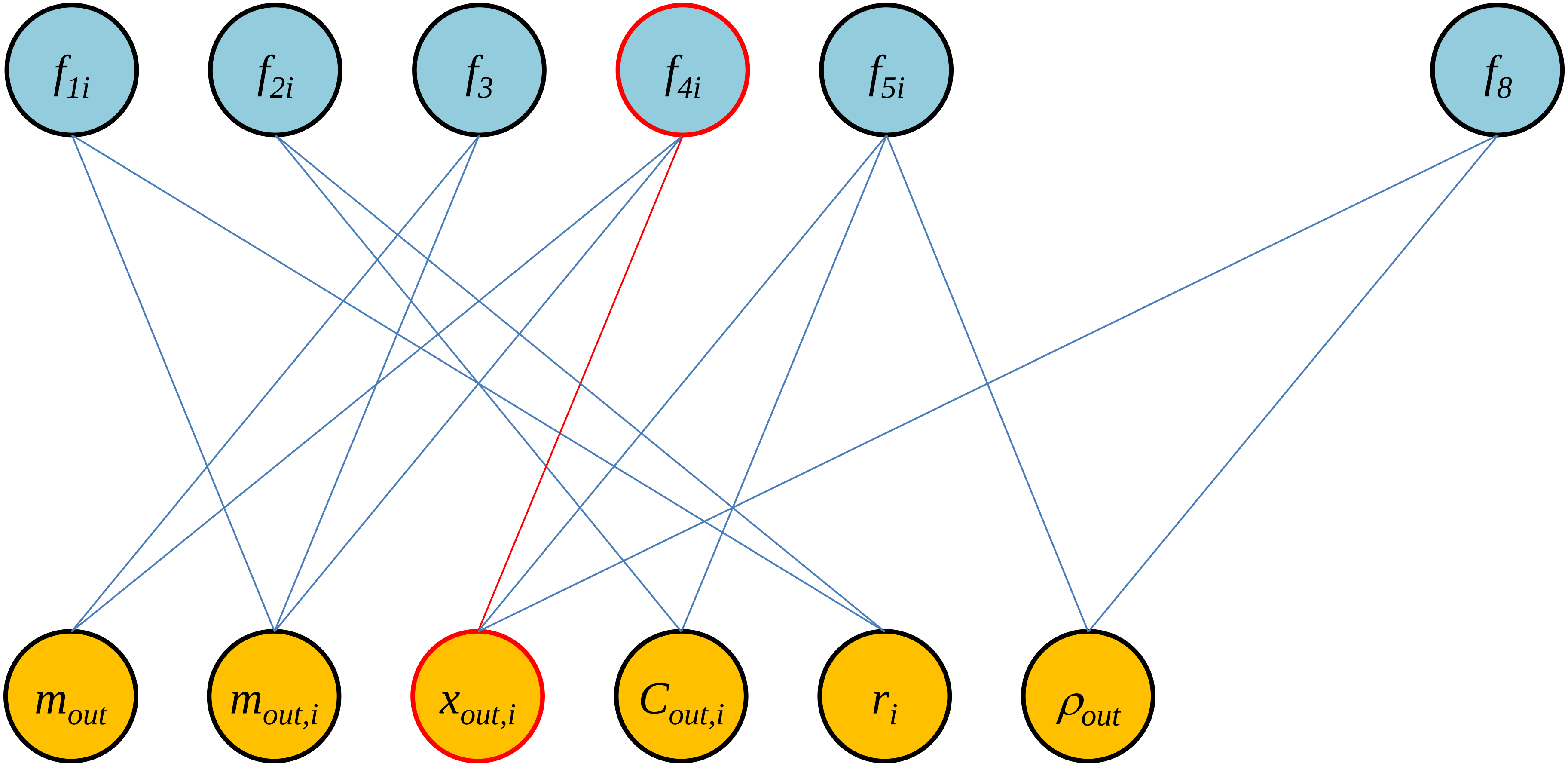
$f_6 \rightarrow H_{out}$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$

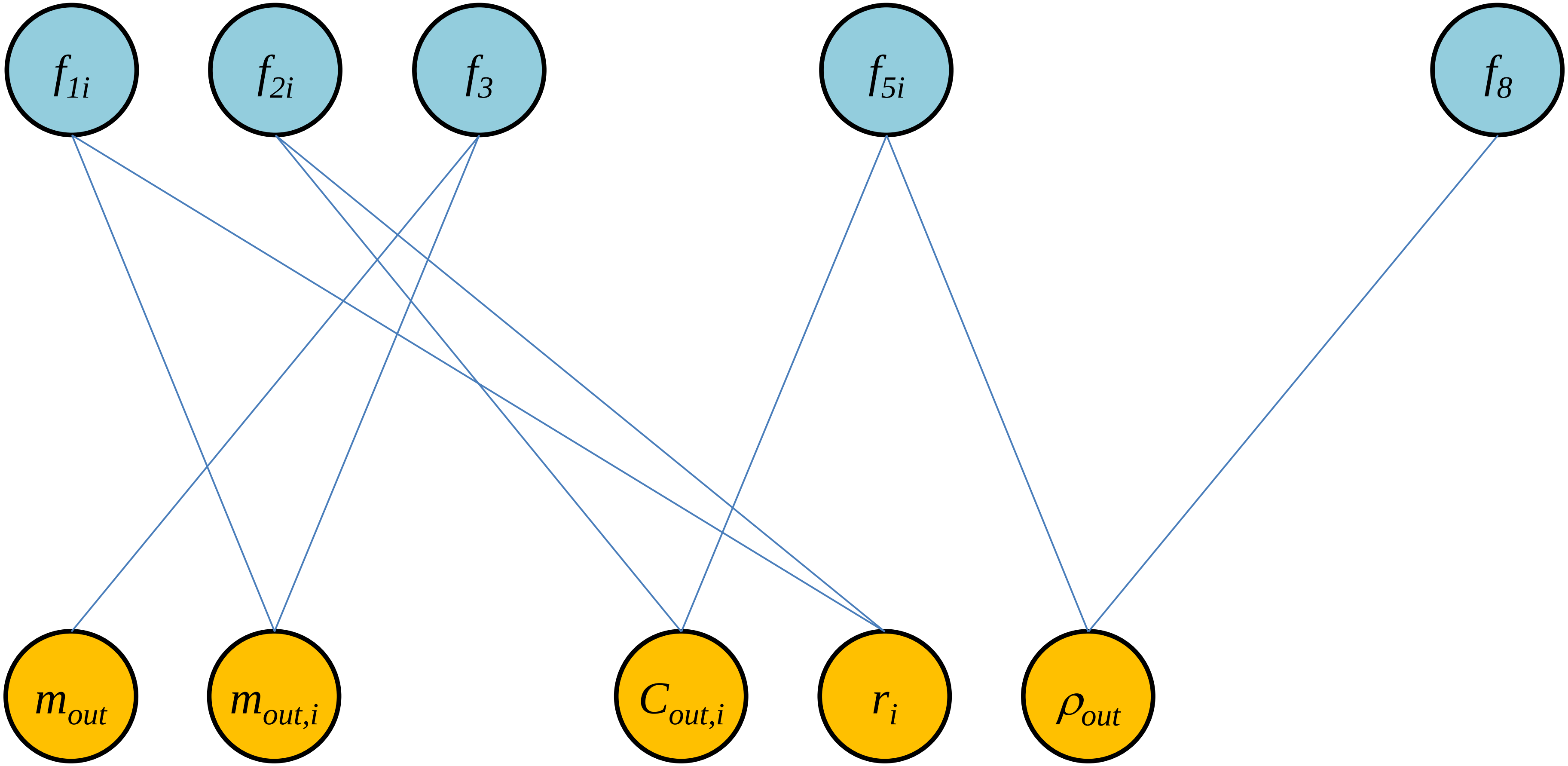
$f_6 \rightarrow H_{out}$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$ $f_{4i} \rightarrow x_{4i}$

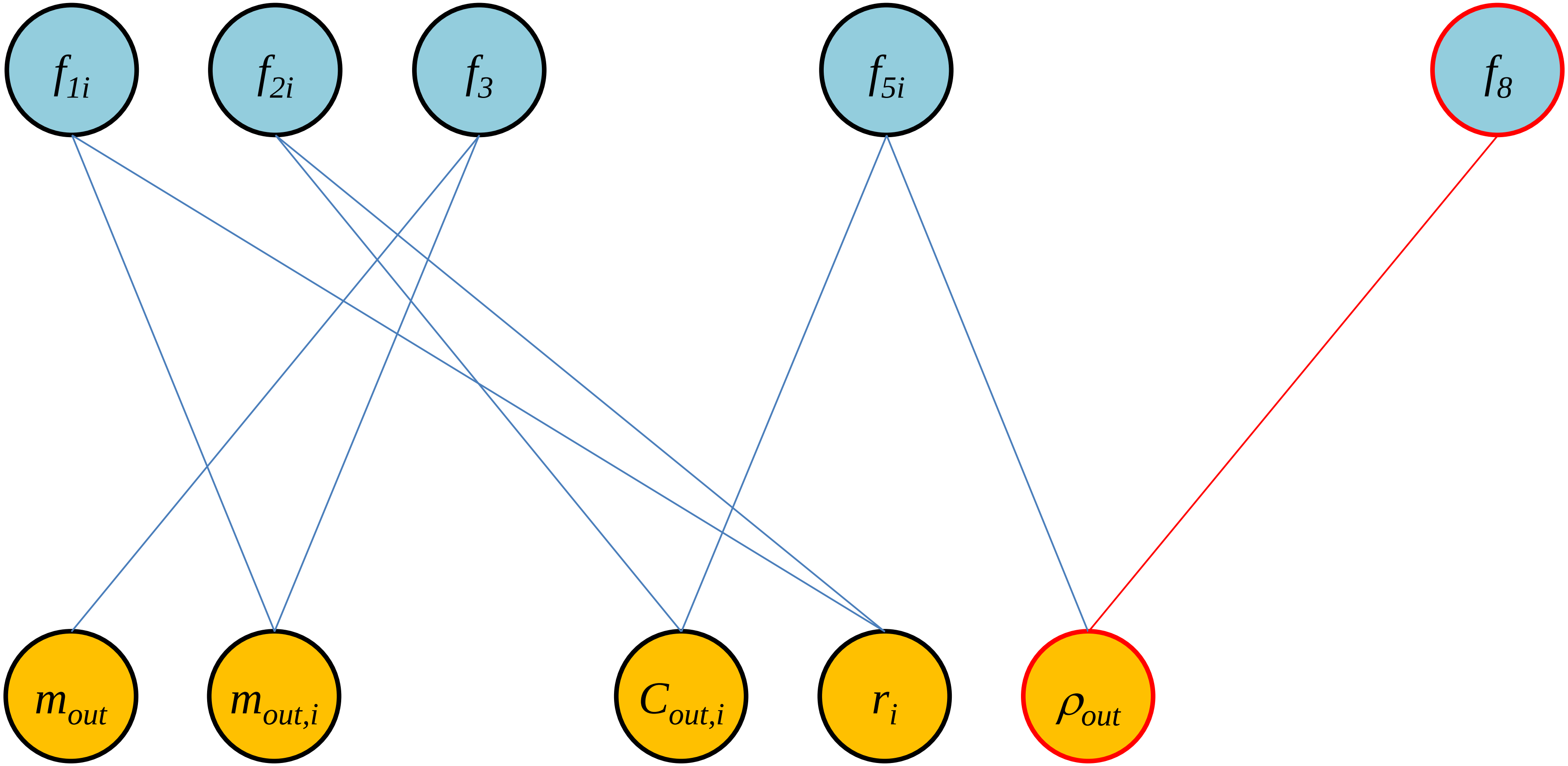
$f_6 \rightarrow H_{out}$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$ $f_{4i} \rightarrow x_{4i}$

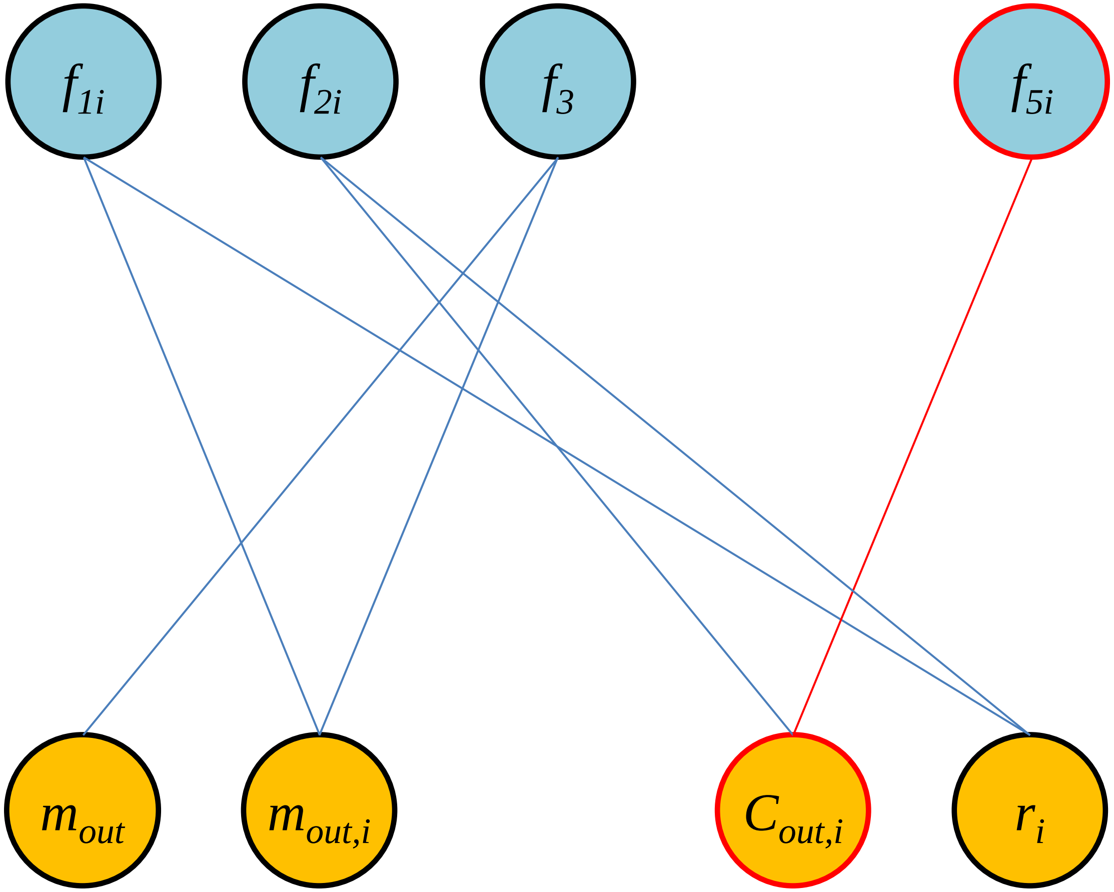
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$ $f_{4i} \rightarrow x_{4i}$ $f_{5i} \rightarrow C_{out,i}$

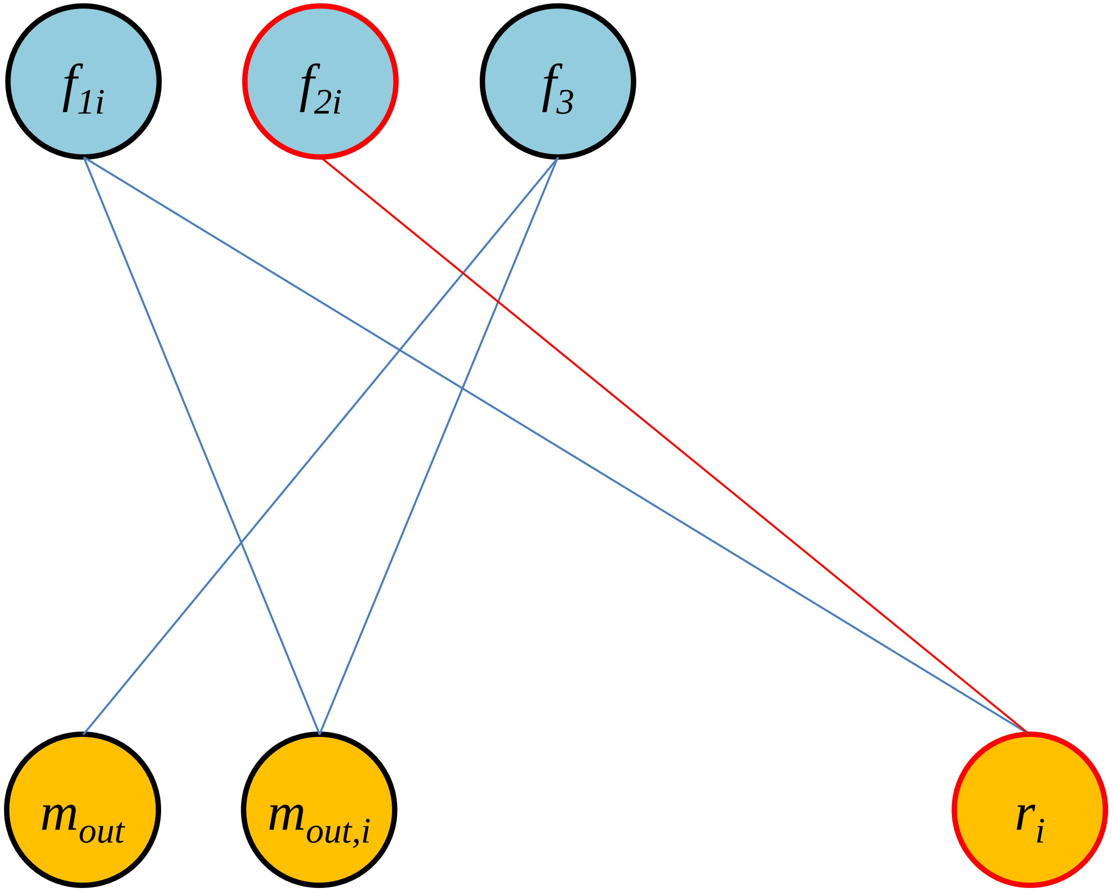
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$ $f_{4i} \rightarrow x_{4i}$ $f_{5i} \rightarrow C_{out,i}$

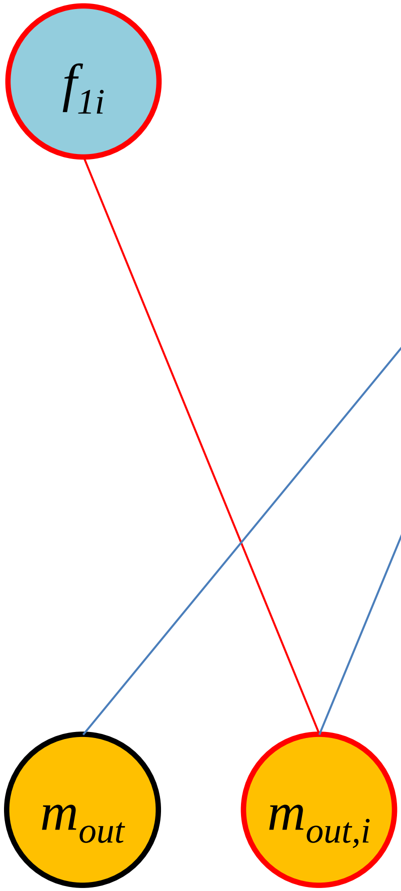
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$



Reactor CSTR (P, Q y V conocidos)

$f_7 \to T_{out}$ $f_{4i} \to x_{4i}$ $f_{5i} \to C_{out,i}$ $f_{1i} \to m_{out,i}$

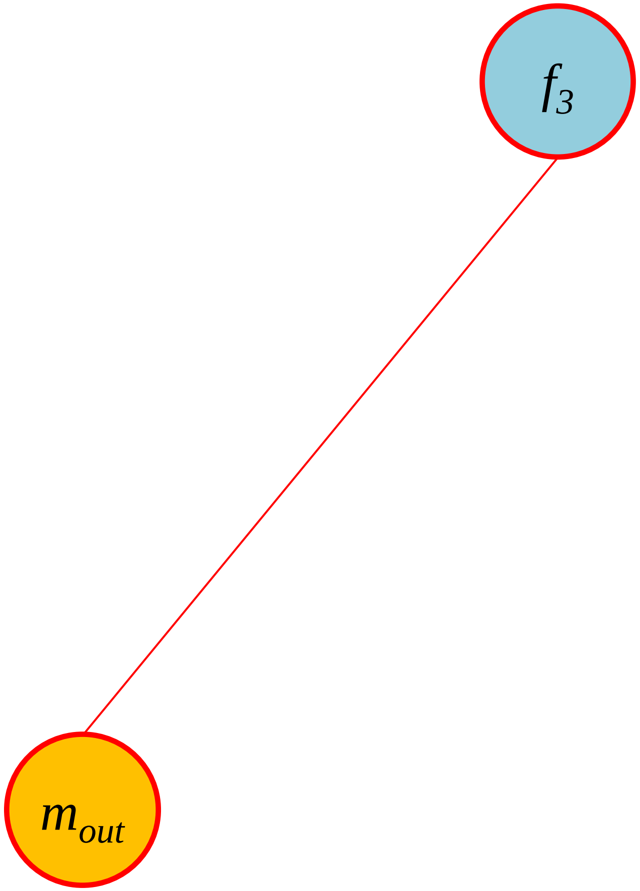
$f_6 \to H_{out}$ $f_8 \to \rho_{out}$ $f_{2i} \to r_i$



Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$ $f_{4i} \rightarrow x_{4i}$ $f_{5i} \rightarrow C_{out,i}$ $f_{1i} \rightarrow m_{out,i}$

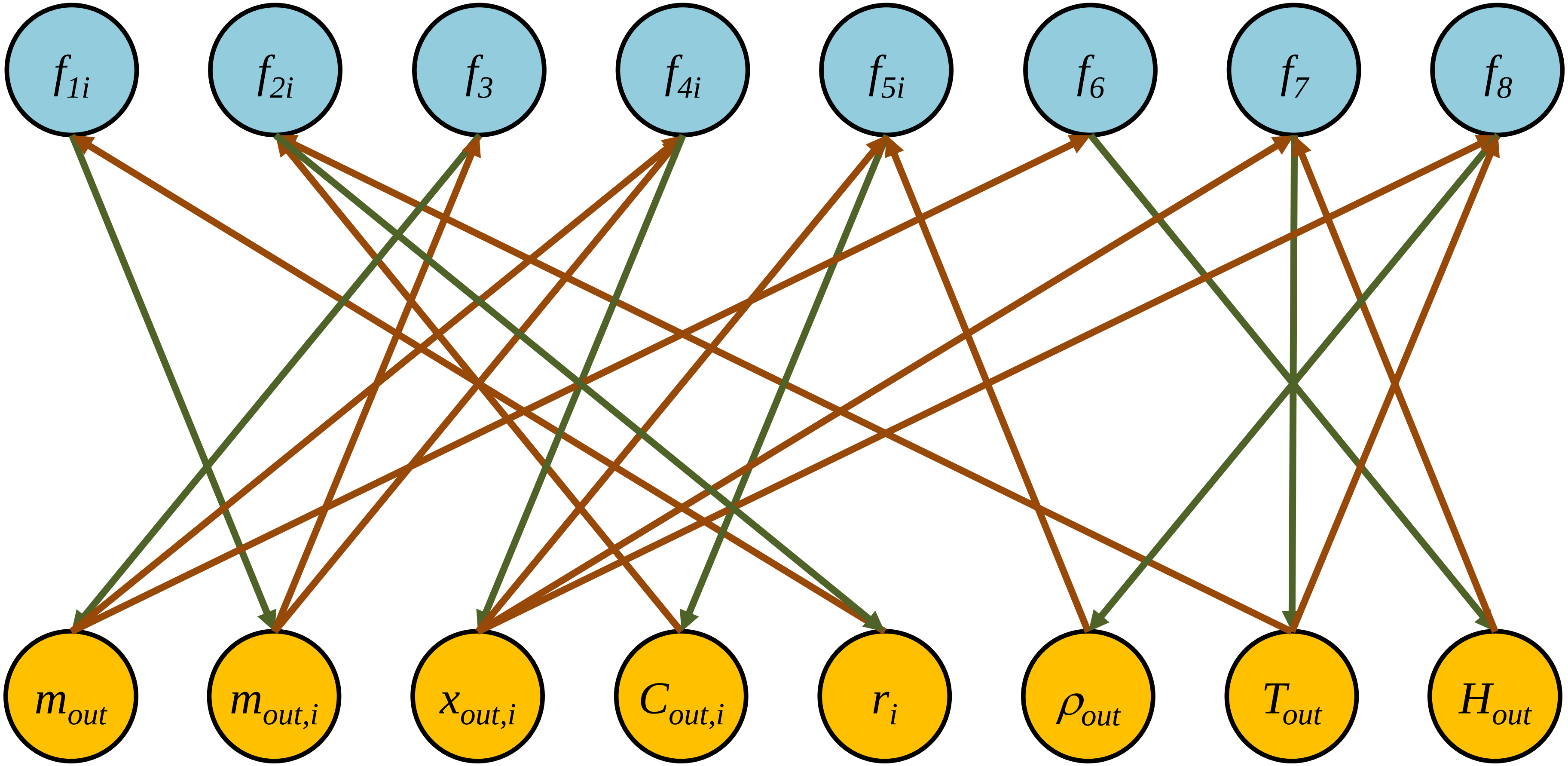
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$ $f_3 \rightarrow m_{out}$



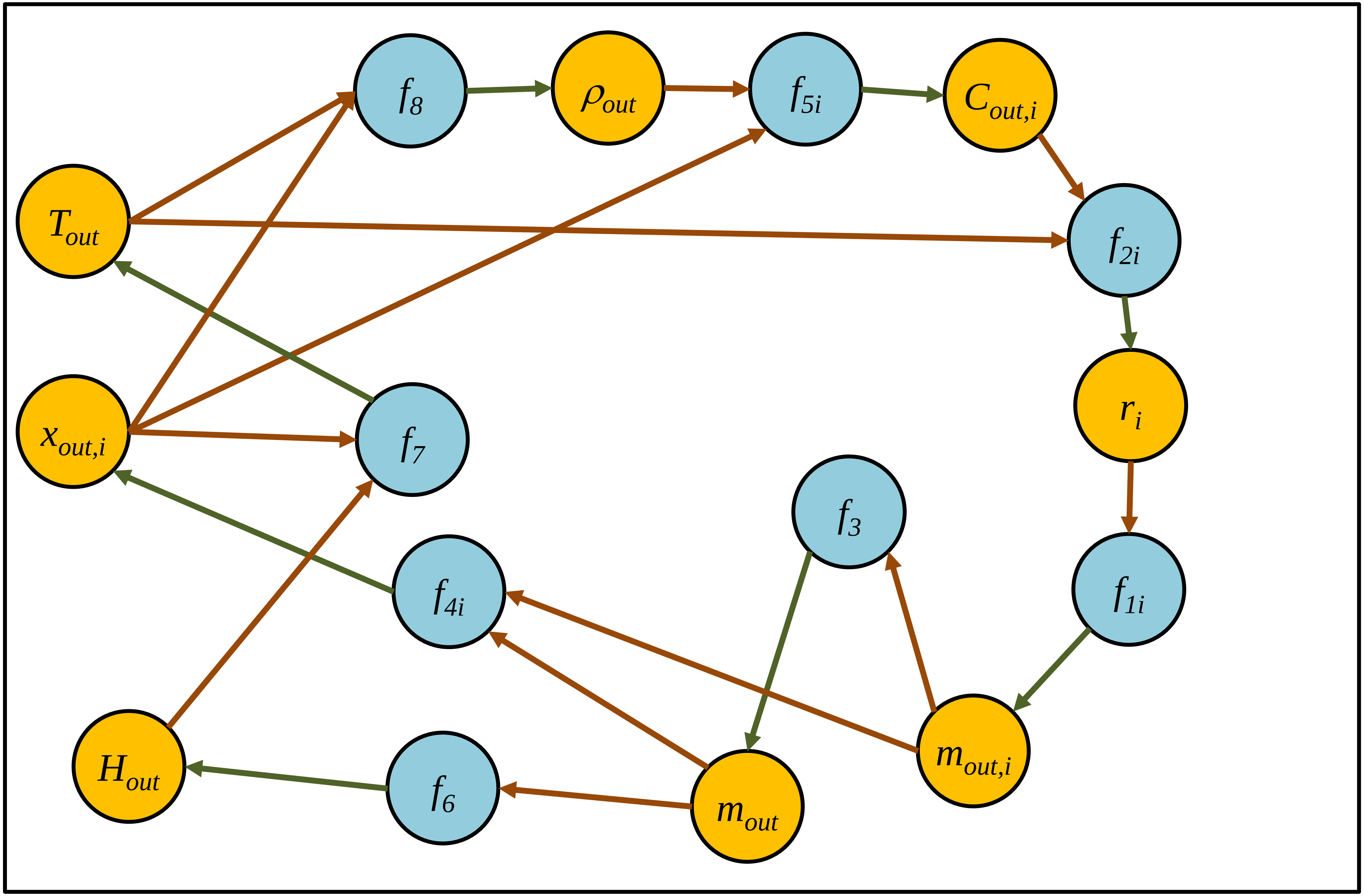
Reactor CSTR (P, Q y V conocidos)

$f_7 \rightarrow T_{out}$ $\quad$ $f_{4i} \rightarrow x_{4i}$ $\quad$ $f_{5i} \rightarrow C_{out,i}$ $\quad$ $f_{1i} \rightarrow m_{out,i}$

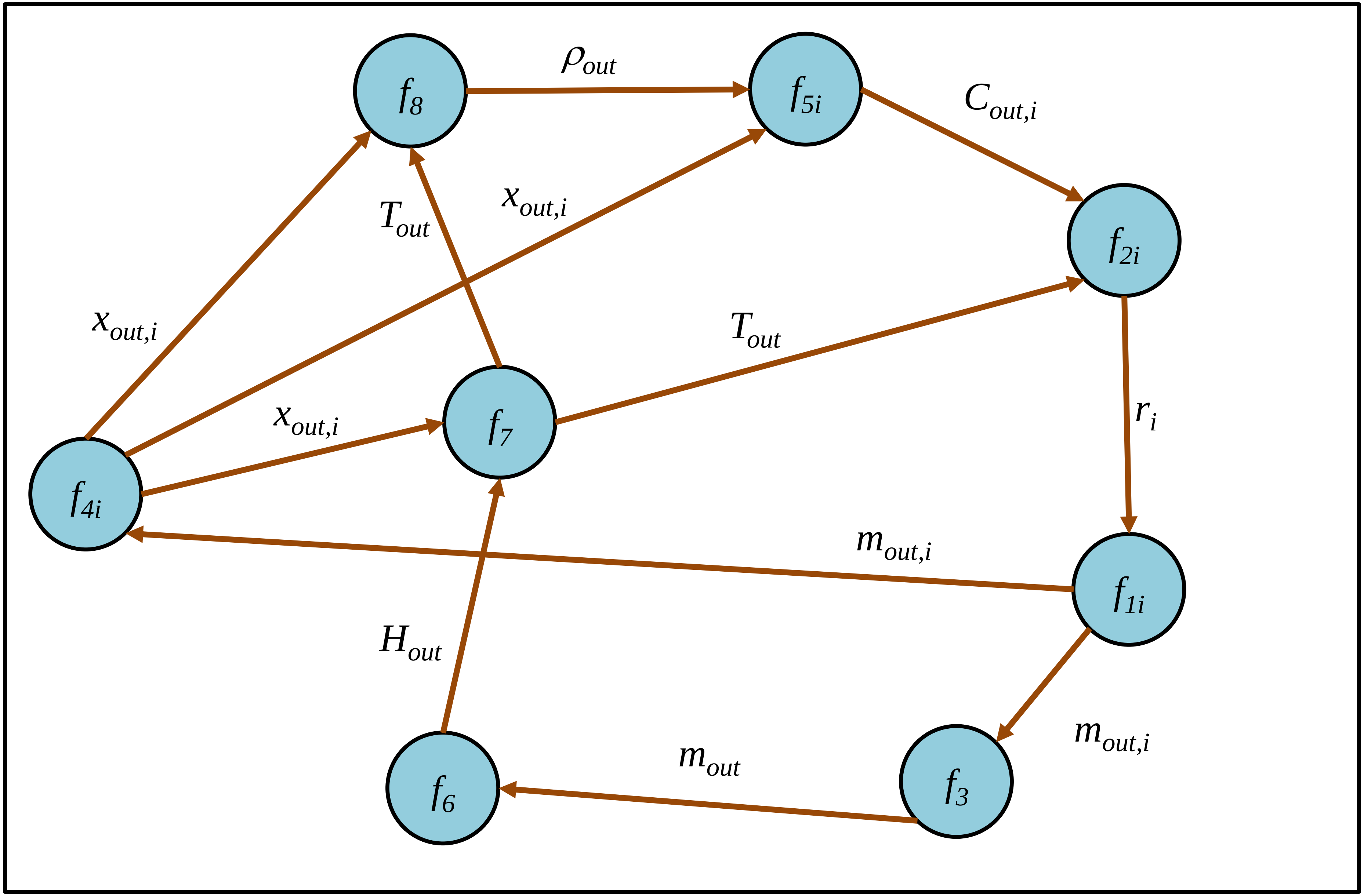
$f_6 \rightarrow H_{out}$ $\quad$ $f_8 \rightarrow \rho_{out}$ $\quad$ $f_{2i} \rightarrow r_i$ $\quad$ $f_3 \rightarrow m_{out}$



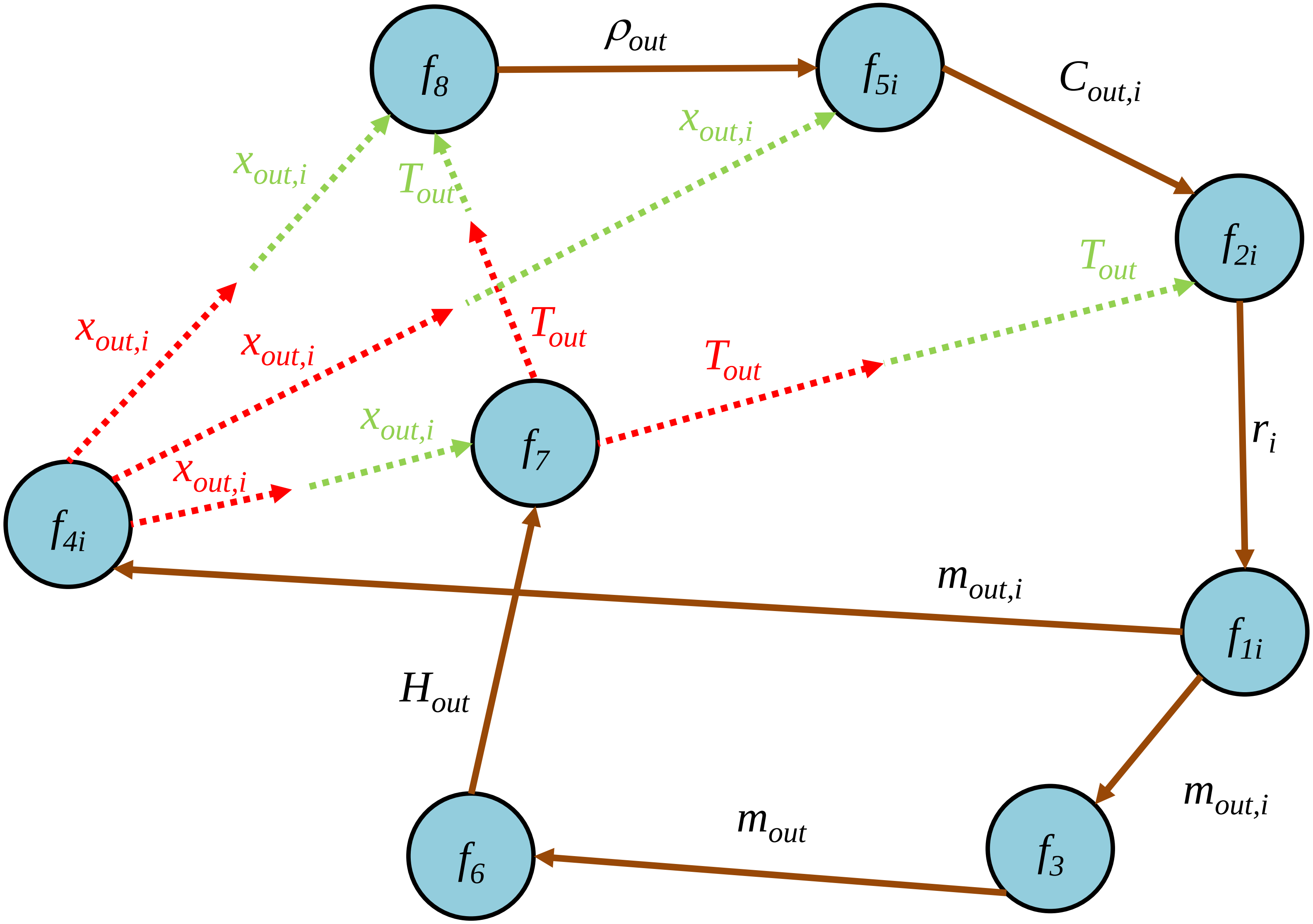
Reactor CSTR (P, Q y V conocidos)



Reactor CSTR (P, Q y V conocidos)



Reactor CSTR (P, Q y V conocidos)



CSTR – Ejercicio propuesto

m_{in} : $45.27\, mol.seg^{-1}$

P_{in} : $20\ bar$

T_{in} : $330\, K$

$x_{in,nC_4H_{10}}$: 0.9

$x_{in,iC_5H_{12}}$: 0.1

$x_{in,iC_4H_{10}}$: 0

$$H_{in} = -145725.677$$

$$V = 3\ m^3$$

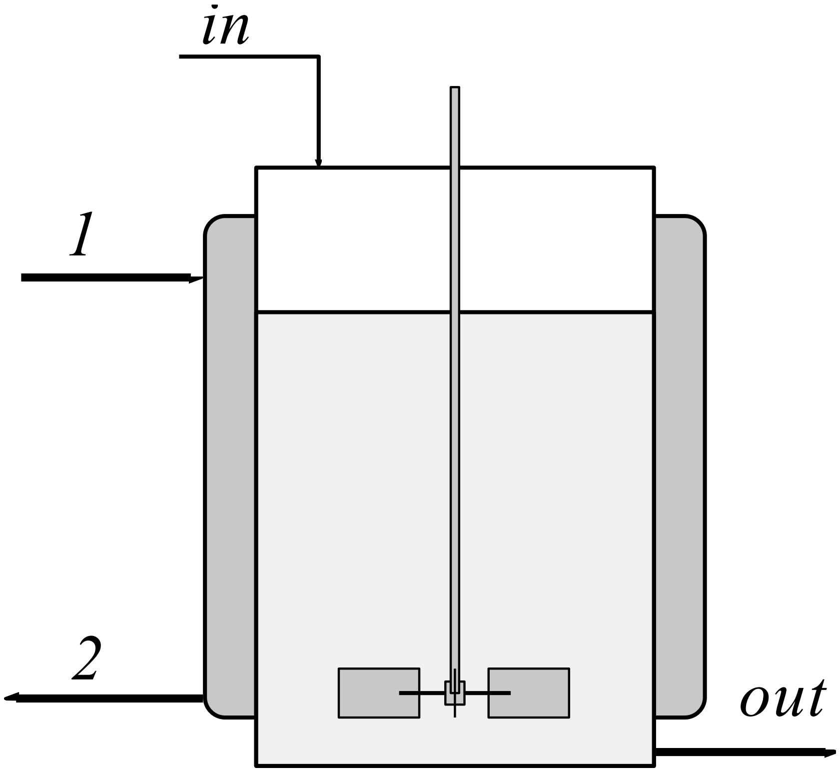
$$Q : 0$$

P_{out} : $20\ bar$

ID	**Nombre**
5	N-butane
8	Isopentane
4	Isobutane

alpha	**N-butane**	**Isopentane**	**Isobutane**
N-butane	0	0.0015	-0.0004
Isopentane	0.0015	0	0.00107
Isobutane	-0.0004	0.00107	0

Ejemplo: Reactor CSTR refrigerado



$$A \leftrightarrow B + C$$

$$r_D = k_D \times C_A$$

$$r_I = k_I \times C_B \times C_C$$

$$r_A = -k_D C_A + k_I C_B C_C$$

$$r_B = k_D C_A - k_I C_B C_C$$

$$r_C = k_D C_A - k_I C_B C_C$$

Ejemplo

Hipótesis:

- Reacción reversible exotérmica en fase homogénea.
- Reactor Mezcla completa.
- Camisa de refrigeración mezcla completa.
- Los coeficientes cinéticos son conocidos ya que son función de la temperatura (funcional tipo Arrhenius).
- Evaporación del líquido despreciable.
- UA es dato
- Tanque cilíndrico de área A_T.
- Caída de presión a través de la camisa nula
- Fluido de la camisa compuesto puro.

Reactor CSTR

$$m_{in,i} + r_i V - m_i = 0 \qquad i = A, B, C$$

$$r_A = -k_D C_A + k_I C_B C_C \qquad r_B = k_D C_A - k_I C_B C_C \qquad r_C = k_D C_A - k_I C_B C_C$$

$$m_{in,i} = m_{in} x_{in,i} \quad i = A, B, C \qquad m_i = m x_i \qquad i = A, B, C$$

$$C_i = \rho x_i \qquad \forall i$$

$$m_{in} = \sum_{i=1}^{NC} m_{in,i} \qquad m = \sum_{i=1}^{NC} m_i$$

La reacción es exotérmica, buscamos que el calor sea positivo

$$m_{in} H_{in} - Q - mH = 0$$

$$f\left(T, P, H, x\right) = 0$$

$$f\left(T, P, \rho, x\right) = 0 \qquad k_D = A_D e^{\frac{-E_D}{RT}} \quad k_I = A_D e^{\frac{-E_I}{RT}}$$

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0$$

Utilizamos el calor de formación como entalpia de de referencia

Reactor CSTR (MS)

$$m_{in,i} + r_i V - m_i = 0 \qquad i = A, B, C$$

$$r_A = -k_D C_A + k_I C_B C_C \qquad r_B = k_D C_A - k_I C_B C_C \qquad r_C = k_D C_A - k_I C_B C_C$$

$$m_i = m x_i \qquad i = A, B, C$$

Variables: 20

Ecuaciones: 18

$$C_i = \rho x_i \qquad \forall i$$

$$m = \sum_{i=1}^{NC} m_i$$

$$r_i \quad V \quad m \quad m_i \quad x_i$$

$$H \quad T \quad \cancel{P} \quad k_D \quad k_I$$

$$Q \quad C_i \quad \rho$$

$$m_{in} H_{in} - Q - mH = 0$$

$$f\left(T, P, H, x\right) = 0$$

$$f\left(T, P, \rho, x\right) = 0 \qquad k_D = A_D e^{\frac{-E_D}{RT}} \qquad k_I = A_D e^{\frac{-E_I}{RT}}$$

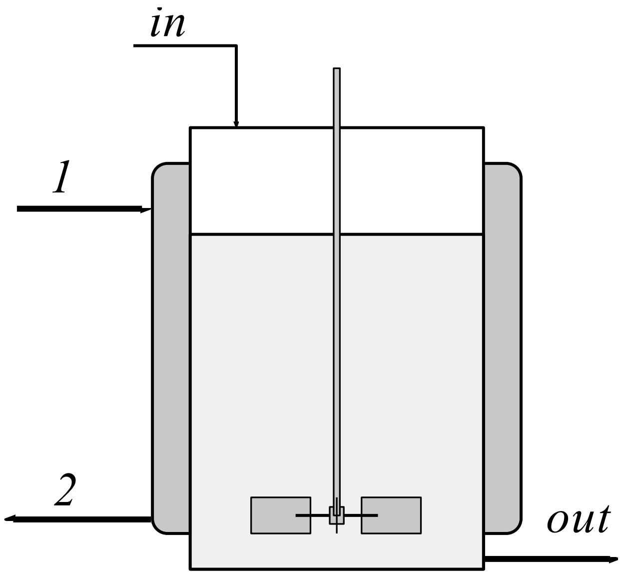
Camisa de enfriamiento

$$m_1 - m_2 = 0$$

$$f\left(T_1, P_1, H_1\right) = 0$$

$$f\left(T_2, P_2, H_2\right) = 0$$

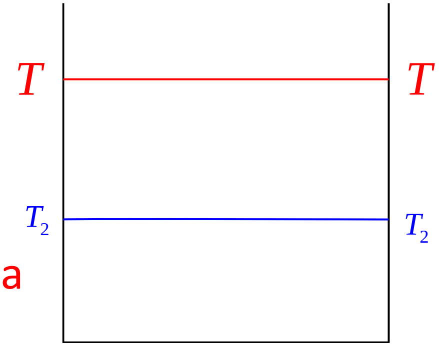
$$m_1 H_1 + Q - m_2 H_2 = 0$$



$$Q = UA\Delta t_c$$

$$\Delta t_c = T - T_2$$

Camisa mezcla completa



Camisa de enfriamiento (MS)

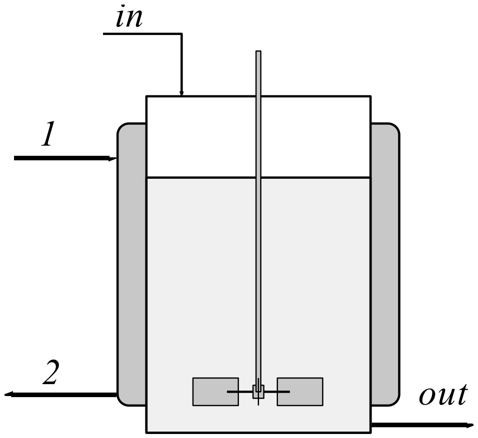
$$m_1 - m_2 = 0$$

$$f\left(T_2, P_2, H_2\right) = 0$$

$$m_1 H_1 + Q - m_2 H_2 = 0$$

$$Q = UA\Delta t_c$$

$$\Delta t_c = T - T_2$$



$$m_2 \quad T_2 \quad H_2 \quad \overset{P_1}{\cancel{P_2}} \quad \Delta t_c$$

Variables: 4

Ecuaciones: 5

Cuidado, faltan Q y T que las contabilizamos en el reactor

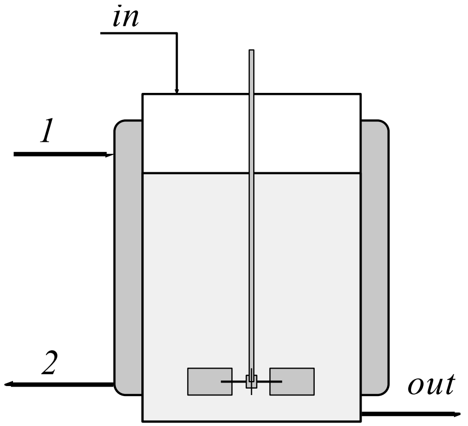
Reactor CSTR refrigerado(MS)

r_i $\boxed{V}$ m m_i x_i

H T k_D k_I

Q C_i ρ

m_2 T_2 H_2 Δt_c



Variables: 20

Ecuaciones: 18

Variables: 4

Ecuaciones: 5

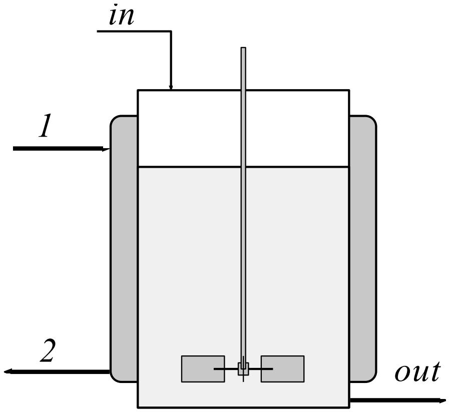
Variables: 24

Ecuaciones: 23

GL: 1

Reactor CSTR refrigerado (Estrategia de resolución)

Propongo: T^*



Resuelvo el reactor CSTR isotérmico a la temperatura propuesta.

Calculamos la temperatura de salida de la camisa:

$$H_2 = \frac{m_1 H_1 + Q^*}{m_2} \qquad f\left(T_2, P_2, H_2\right) = 0 \rightarrow T_2$$

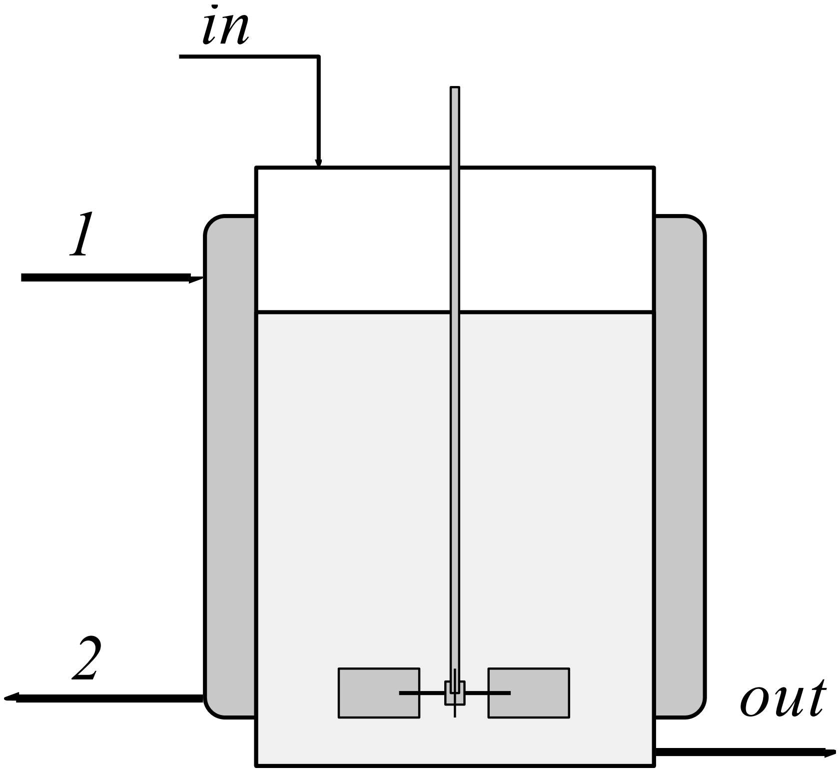
Chequemos la ecuación de transferencia de calor:

$$\Delta t_c = T^* - T_2$$

$$Q = UA\Delta t_c$$

$$¿Q = Q^*? \begin{cases} si: \text{ Terminamos} \\ no: \text{Proponemos } T^* = \dfrac{Q^*}{(UA)} + T_2 \end{cases}$$

Ejercicio: Reactor CSTR calefaccionado



$$A \rightarrow 2B$$

$$r_D = k_D \times C_A$$

Reactor CSTR calefaccionado

Hipótesis:

- Reacción endotérmica en fase homogénea.
- La reacción ocurre en una solución acuosa.
- Reactor Mezcla completa.
- Se calefacciona con vapor saturado de agua.
- Los coeficientes cinéticos son conocidos ya que son función de la temperatura (funcional tipo Arrhenius).
- Evaporación del líquido despreciable.
- Presión en el cuerpo de vapor del reactor es conocida.
- La condensación del vapor saturado es total.
- Caída de presión a través de la camisa nula.

Reactor CSTR

$$m_{in,i} + r_i V - m_i = 0 \qquad i = A, B, C$$

C: agua

$$r_A = -k_D C_A \quad r_B = 2k_D C_A \quad r_C = 0$$

$$m_{in,i} = m_{in} x_{in,i} \quad i = A, B, C \qquad m_i = m x_i \qquad i = A, B, C$$

$$\mathrm{m_{in}} = \sum_{i=1}^{NC} m_{in,i} \qquad m = \sum_{i=1}^{NC} m_i$$

$$C_i = \rho x_i \qquad \forall i$$

$$m_{in} H_{in} + Q - mH = 0$$

$$f\left(T, P, H, x\right) = 0$$

$$f\left(T, P, \rho, x\right) = 0$$

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \qquad k_D = A_D e^{\frac{-E_D}{RT}}$$

Reactor CSTR (MS)

$$m_{in,i} + r_i V - m_i = 0 \qquad i = A, B, C$$

$$r_A = -k_D C_A \quad r_B = 2k_D C_A \quad r_C = 0$$

$$m_i = m x_i \qquad i = A, B, C$$

$$C_i = \rho x_i \qquad \forall i$$

$$m = \sum_{i=1}^{NC} m_i$$

$$m_{in} H_{in} + Q - mH = 0$$

$$f\left(T, P, H, x\right) = 0$$

$$f\left(T, P, \rho, x\right) = 0$$

$$k_D = A_D e^{\frac{-E_D}{RT}}$$

Reactor CSTR

$$m_{in,A} - k_D C_A V - m_A = 0$$

$$m_{in,B} + 2k_D C_A V - m_B = 0$$

$$m_{in,C} - m_C = 0$$

$$m_i = m x_i \qquad i = A, B, C$$

$$C_i = \rho x_i \qquad i = A, B, C$$

$$m = \sum_{i=1}^{NC} m_i$$

$$m_{in} H_{in} + Q - mH = 0$$

$$f\left(T, P, H, x\right) = 0$$

$$f\left(T, P, \rho, x\right) = 0 \qquad k_D = A_D e^{\frac{-E_D}{RT}}$$

Variables: 16

Ecuaciones: 14

$$V \quad m \quad m_i \quad x_i$$

$$H \quad T \quad \cancel{P} \quad k_D$$

$$Q \quad C_i \quad \rho$$

Camisa de calefacción

$$m_1 - m_2 = 0$$

$$f\left(T_1, P_1, H_1\right) = 0$$

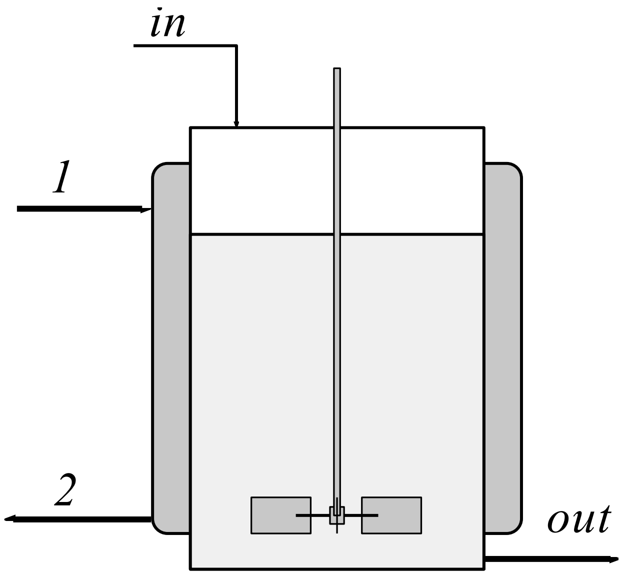
$$m_1 H_1 + Q - m_2 H_2 = 0$$

$$f\left(T_2, P_2, H_2\right) = 0$$

¡Cuidado!
La salida es líquido saturado
θ=0

$$T_2 = FLASH\left(P_2, \theta\right)$$

$$H_2 = FLASH\left(P_2, \theta\right)$$



Camisa de calefacción (MS)

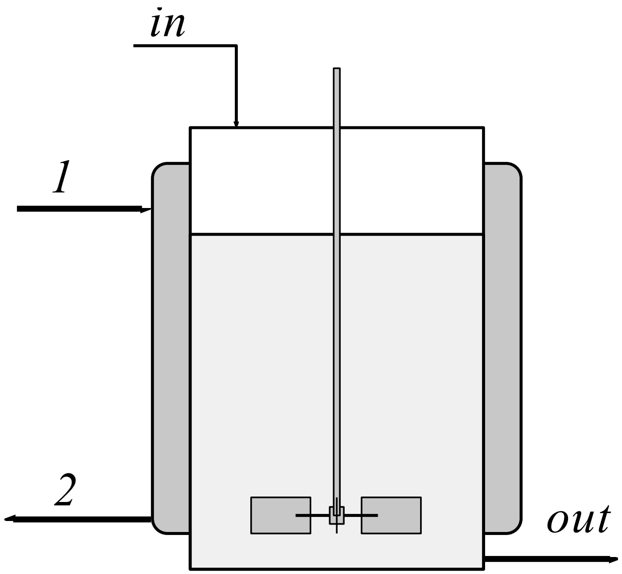
$$m_1 - m_2 = 0$$

$$m_1 H_1 + Q - m_2 H_2 = 0$$

$$T_2 = FLASH\left(P_2, \theta_2\right)$$

$$H_2 = FLASH\left(P_2, \theta_2\right)$$

$$Q = m_1 \lambda_{vap}$$ Variante simplificada



$$m_2 \quad T_2 \quad \cancel{P_2} \quad H_2 \quad \cancel{\theta_2}$$

Variables: 3

Ecuaciones: 4

Reactor CSTR calefaccionado (MS)

$V \; m \; m_i \; x_i$

$H \; T \; k_D$

$Q \; C_i \; \rho$

$m_2 \; T_2 \; H_2$

Variables: 16

Ecuaciones: 14

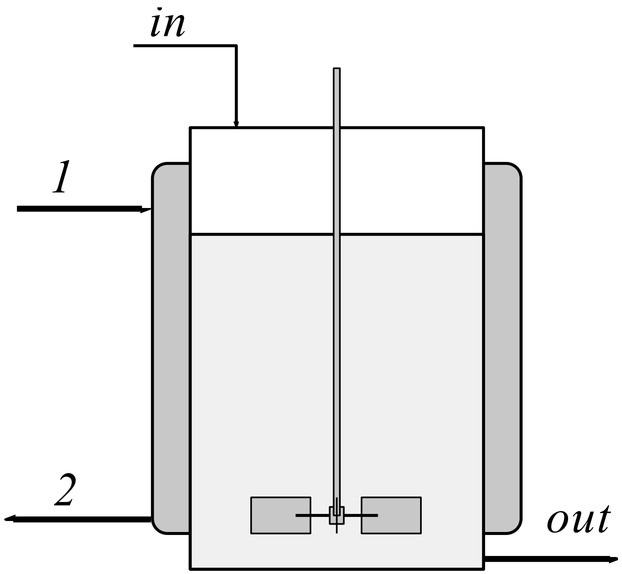
Variables: 3

Ecuaciones: 4

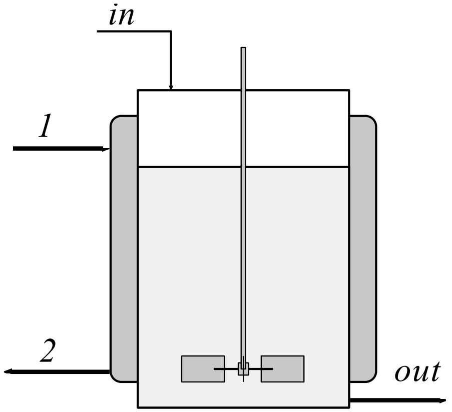
Variables: 19

Ecuaciones: 18

GL: 1



Reactor CSTR calefaccionado (estrategia de resolución)



Obtenemos Q de la camisa:

$$T_2 = FLASH\left(P_2, \theta_2\right)$$

$$H_2 = FLASH\left(P_2, \theta_2\right)$$

$$m_2 = m_1$$

$$Q = m_2 H_2 - m_1 H_1$$

Resuelvo el reactor CSTR adiabático a calor dado Q.

Reactor CSTR calefaccionado (estrategia simplificada)

Calculo Q de la camisa: $Q = m_1 \lambda_{vap}$

Resuelvo el reactor CSTR adiabático a calor dado Q.