Integración IV

Modelado individual de equipos en estado estacionario (III).

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Equipos con reacción química

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

$$\sum_{i=1}^{NC} a_{ij} A_i = 0 \qquad j = 1, 2, \ldots, NR$$

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”

Equipos con reacción química

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

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

$$\sum_{i=1}^{NC} a_{ij} A_i = 0 \qquad j = 1, 2, \ldots, NR$$

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

$$NR = 2$$

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

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

Equipos con reacción química

Para cada una de las NR 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”

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

Equipos con reacción química

Para cada uno de los NC componente:

$$r_i = \sum_{j=1}^{NR} r_{ij} = \sum_{j=1}^{NR} a_{ij} \times r_j$$

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

Generación neta de la especie “i” por unidad de volumen y unidad de tiempo, causada por el conjunto de NR reacciones

Equipos con reacción química

Se pueden definir velocidades netas independientes del volumen del reactor:

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

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

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

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

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:

$$\sum_{j=1}^{NR} \zeta_{ij} = \frac{m_{in} x_{in,i} - m_{out} x_{out,i}}{m_{in} x_{in,i}}$$

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.

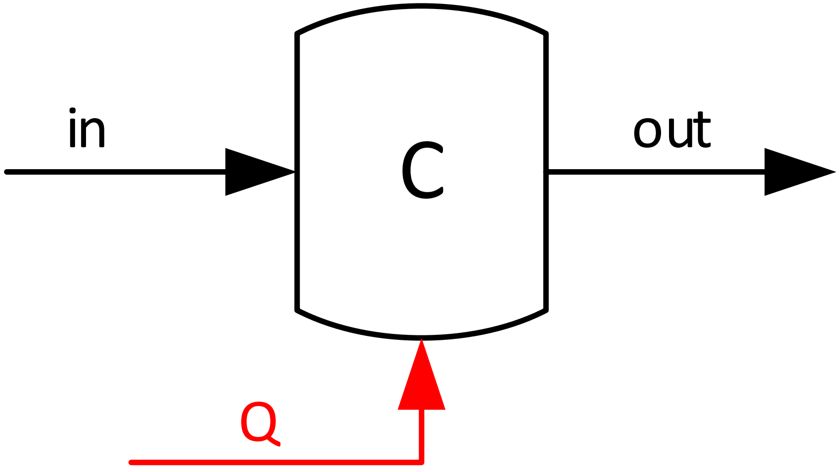
Como se mencionó anteriormente, se cumple la siguiente igualdad para cada reacción:

$$R_i = \sum_{j=1}^{NR} R_{ij} = \sum_{j=1}^{NR} a_{ij} \times R_j$$

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

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

Reactor de conversión fija

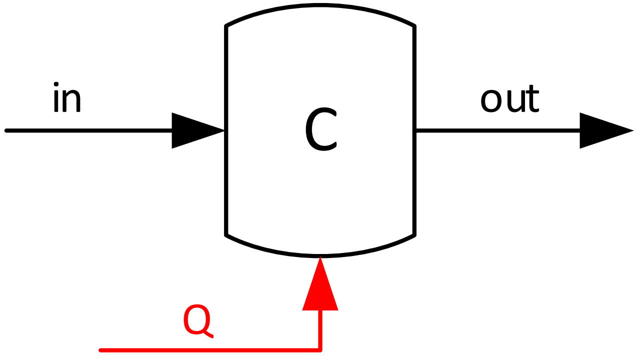


Hipótesis:

- 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 apareceria 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

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

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

m_{in} $x_{in,i}$ $\zeta_{i^* j}$ m_{out} $x_{out,i}$
H_{in} T_{in} P_{in} H_{out} T_{out} P_{out}
Q 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)

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

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

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

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

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

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

H_{out} T_{out} P_{out} Q R_i

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

GL =2

Reactor de conversión fija (adiabático)

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
NR = 1

Asumimos al metano como componente base de la reacción y suponemos una conversión del 100%. Para que esto sea valido se debe alimentar con un exceso de aire suficiente.

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

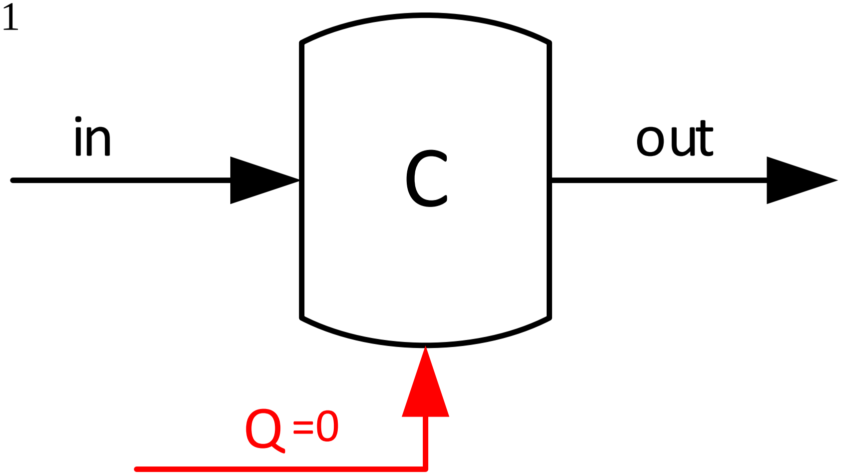
$$x_{in,CH_4} = 0.038$$

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

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

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

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



Combustión de metano con aire (Rx)

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

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

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

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

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

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

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

Combustión de metano con aire (BMxC)

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

$$\downarrow$$

$$\begin{aligned} 3.8 - 3.8 - m_{out}x_{out,CH_4} &= 0 \\ 20.2 - 7.6 - m_{out}x_{out,O_2} &= 0 \\ 76 + 0 - m_{out}x_{out,N_2} &= 0 \\ 0 + 3.8 - m_{out}x_{out,CO_2} &= 0 \\ 0 + 7.6 - m_{out}x_{out,H_2O} &= 0 \end{aligned} \rightarrow \begin{cases} m_{out} = 100 \\ x_{out,CH_4} = 0 \\ x_{out,O_2} = 0.126 \\ x_{out,N_2} = 0.76 \\ x_{out,CO_2} = 0.038 \\ x_{out,H_2O} = 0.076 \end{cases}$$

Combustión de metano con aire (BE)

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

De la librería Raoult Law

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

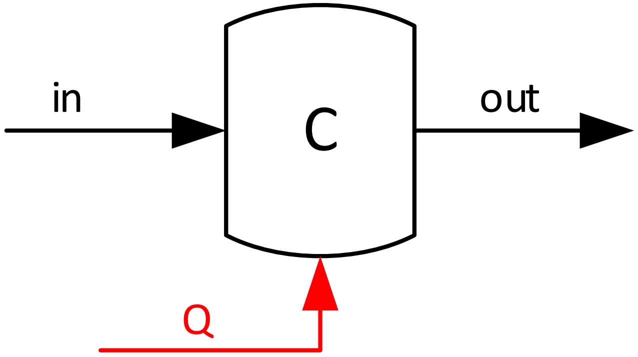
$$H_{out} = 2388.645 \frac{J}{mol}$$

$$T_{out} = 1380.92\, K$$

Obviamente se calcula con la composición de salida

Reactor de conversión fija (flujos x componentes)

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



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

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

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

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

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

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

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

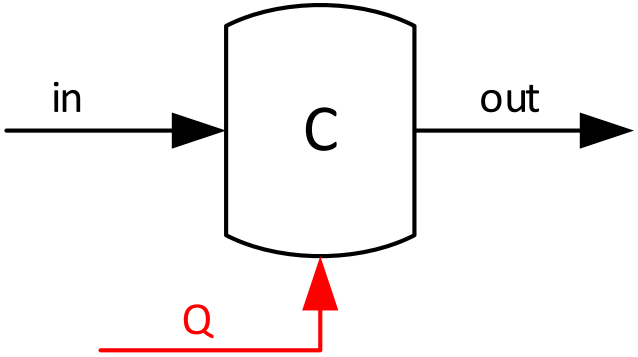
m_{out} $m_{out,i}$ $x_{out,i}$

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

Q R_i

Reactor de conversión fija (flujos x componentes - MS)

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



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

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

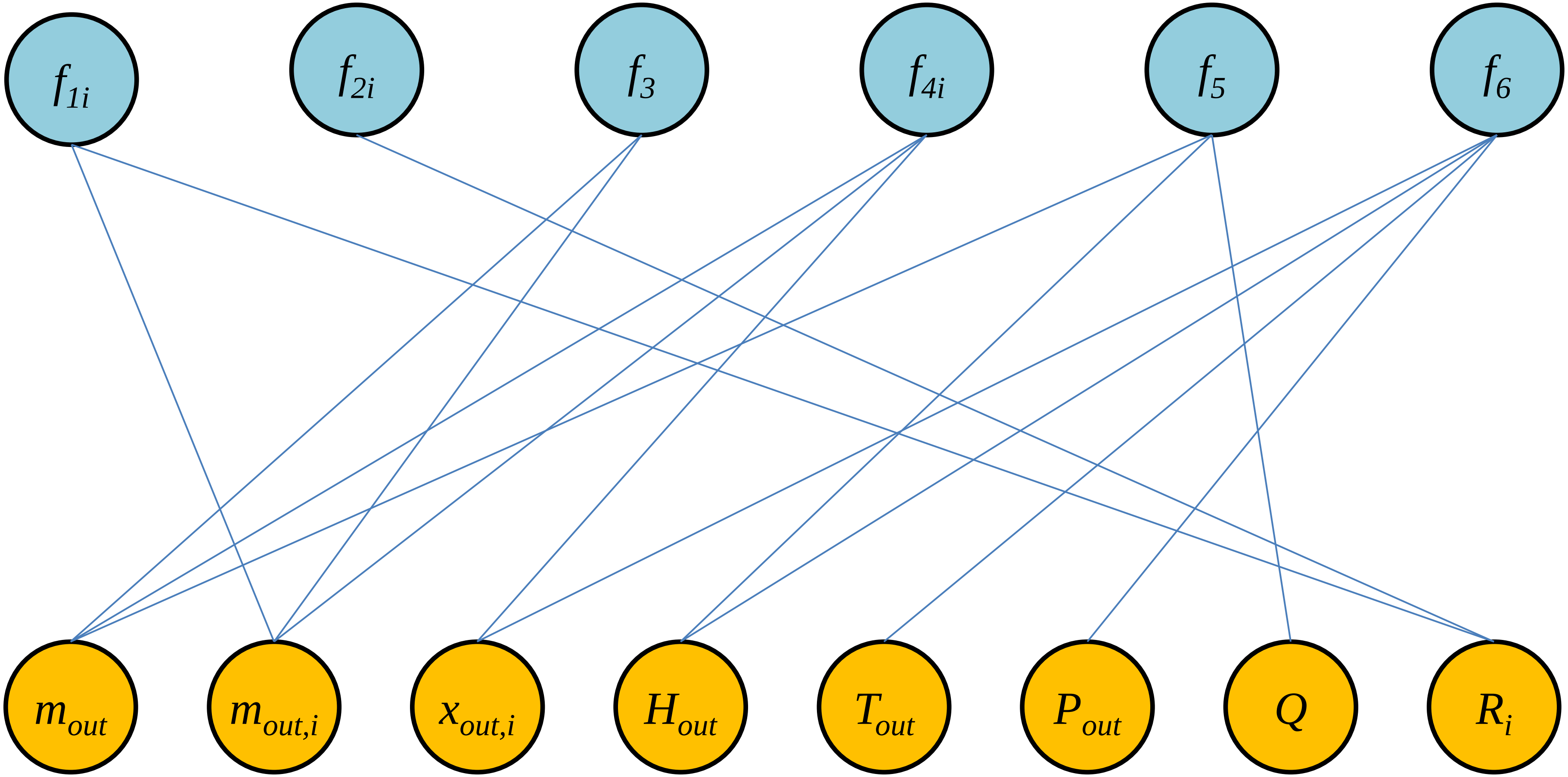
$$H_{out} \quad T_{out} \quad P_{out} \quad Q \quad R_i$$

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

GL =2

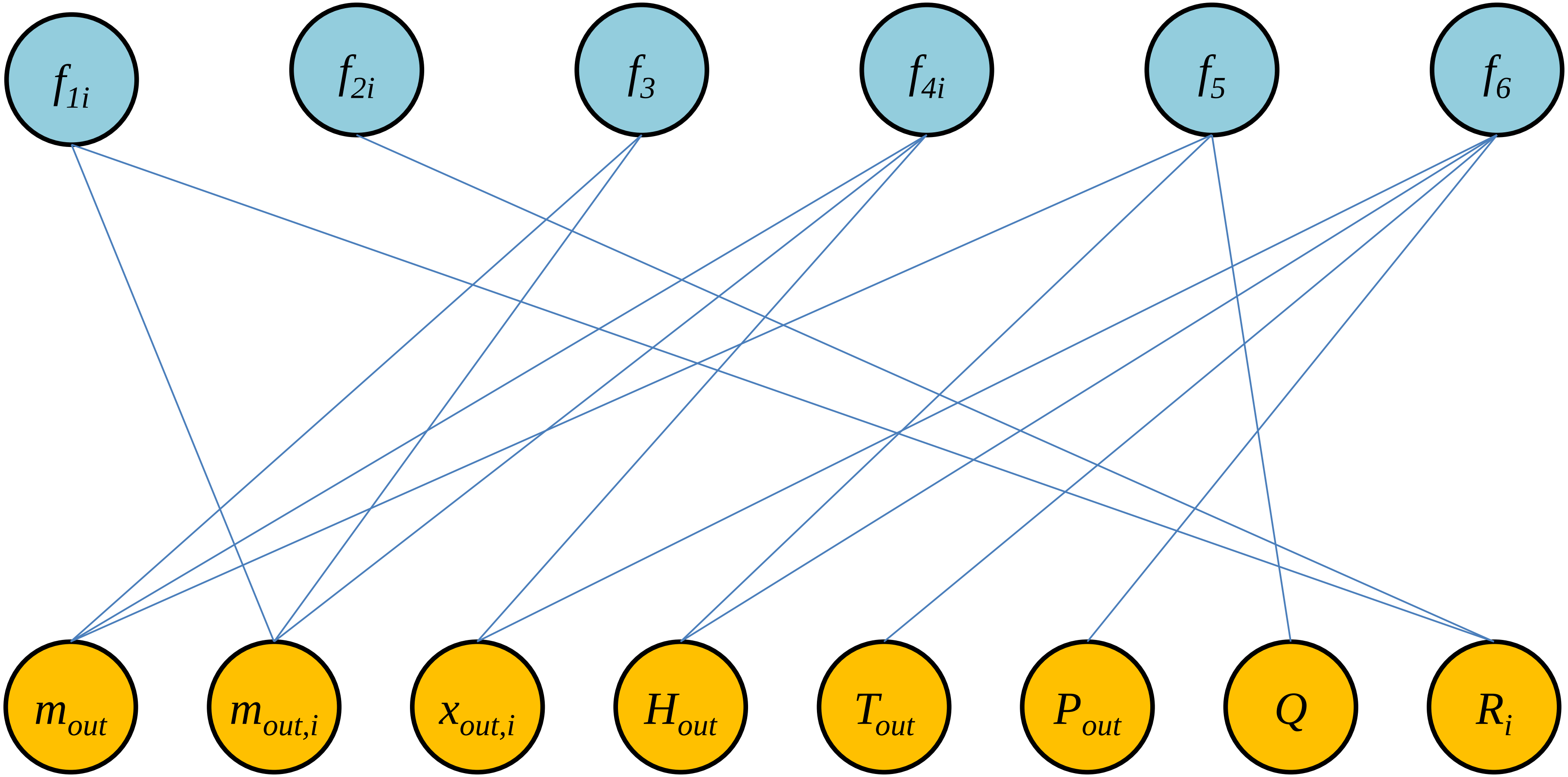
Reactor de conversión fija (flujos x componentes - MS)

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

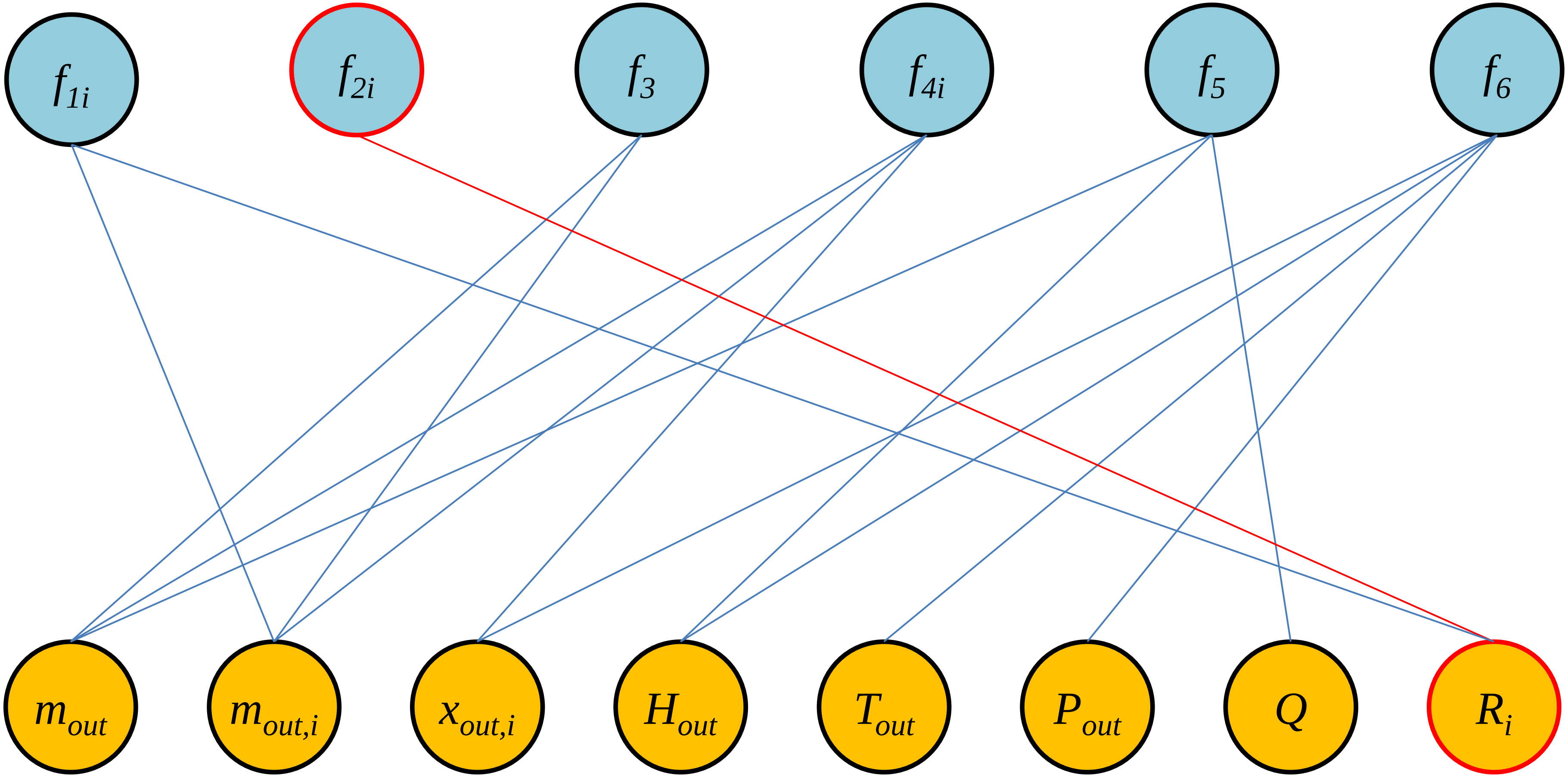


Reactor de conversión fija (flujos x componentes - MS)

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.

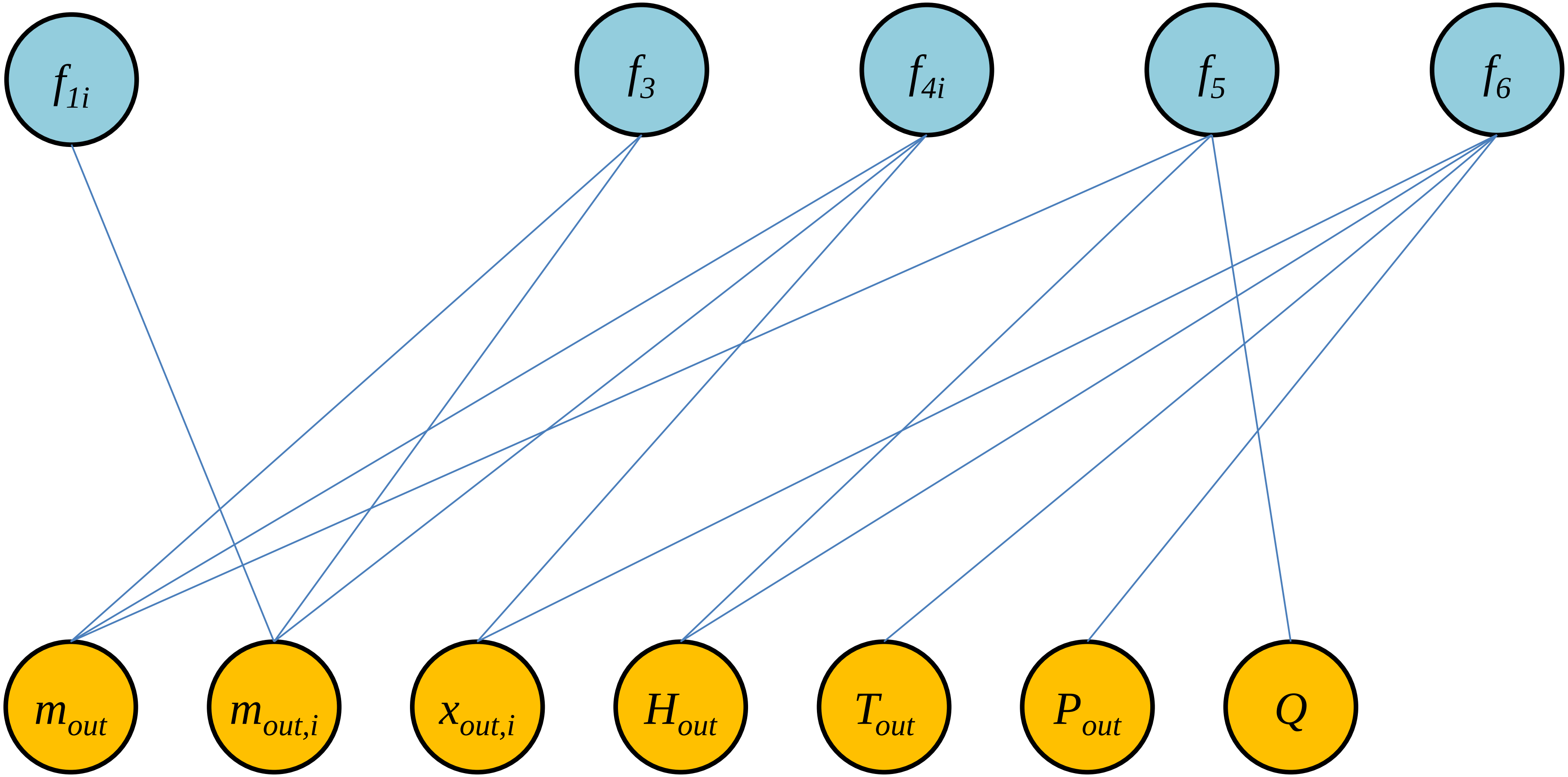


Reactor de conversión fija (flujos x componentes - MS)



Reactor de conversión fija (flujos x componentes - MS)

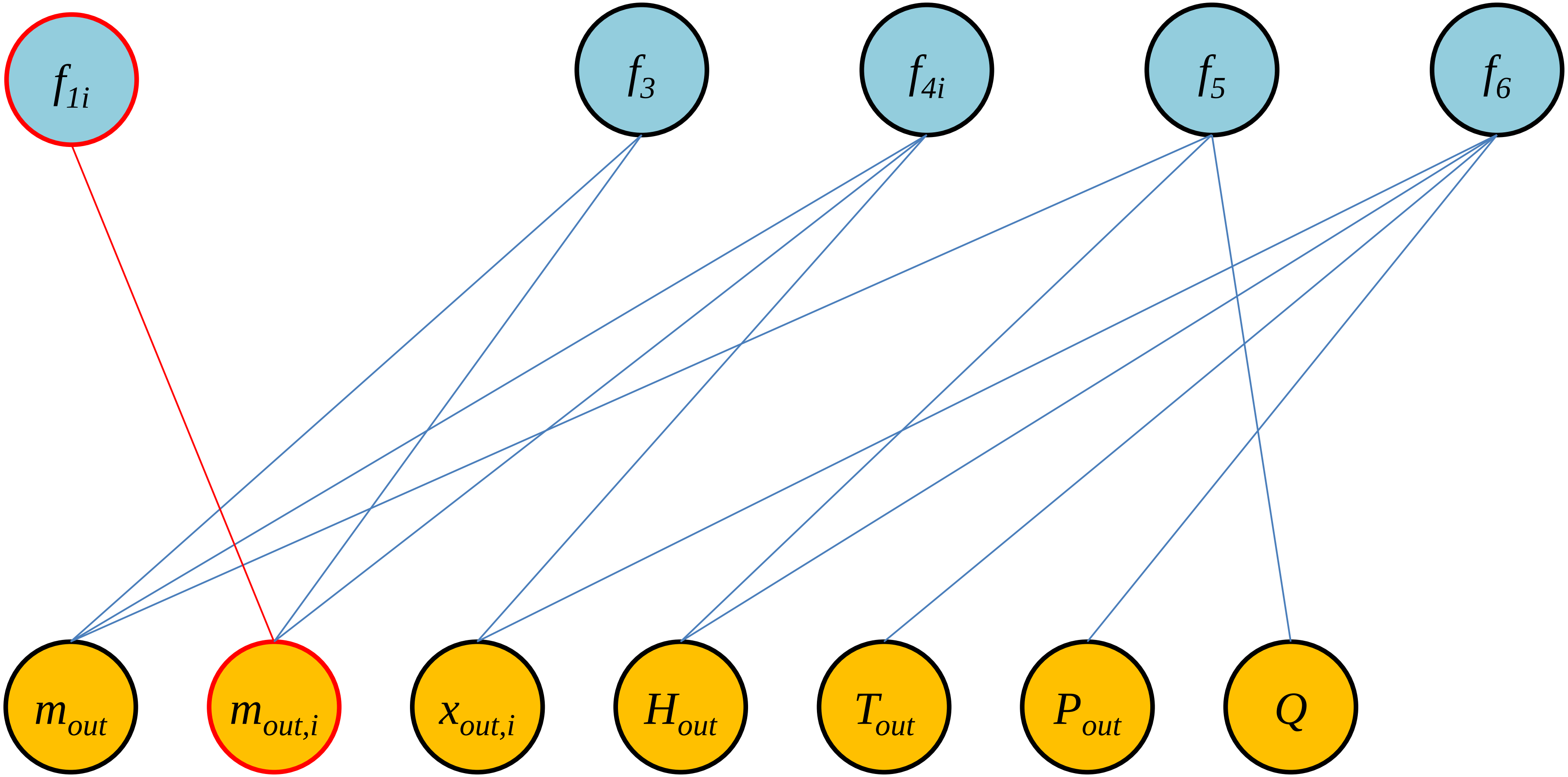
$f_{2,i} \rightarrow R_i$



Reactor de conversión fija (flujos x componentes - MS)

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

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

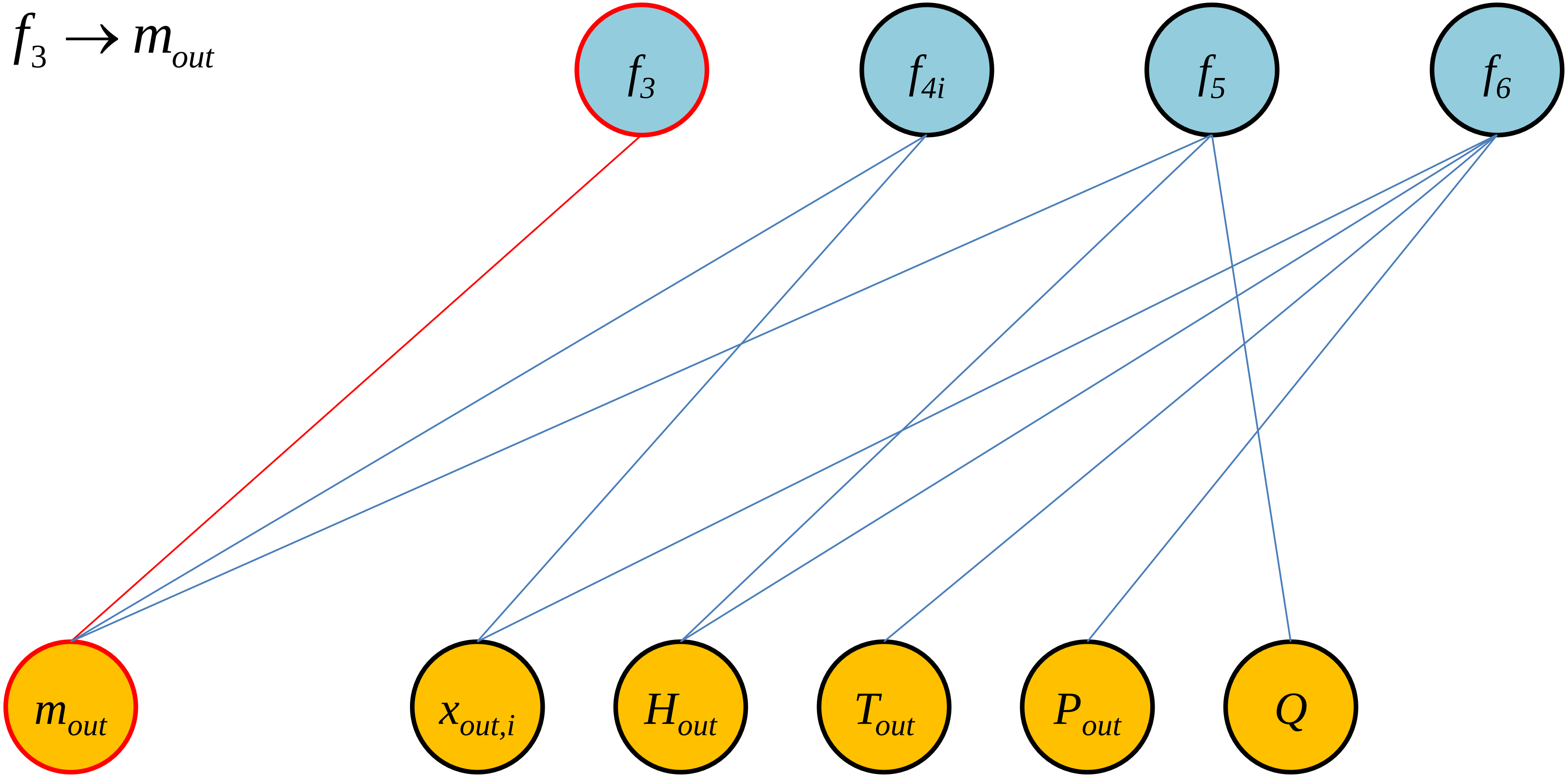


Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

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

$f_3 \rightarrow m_{out}$



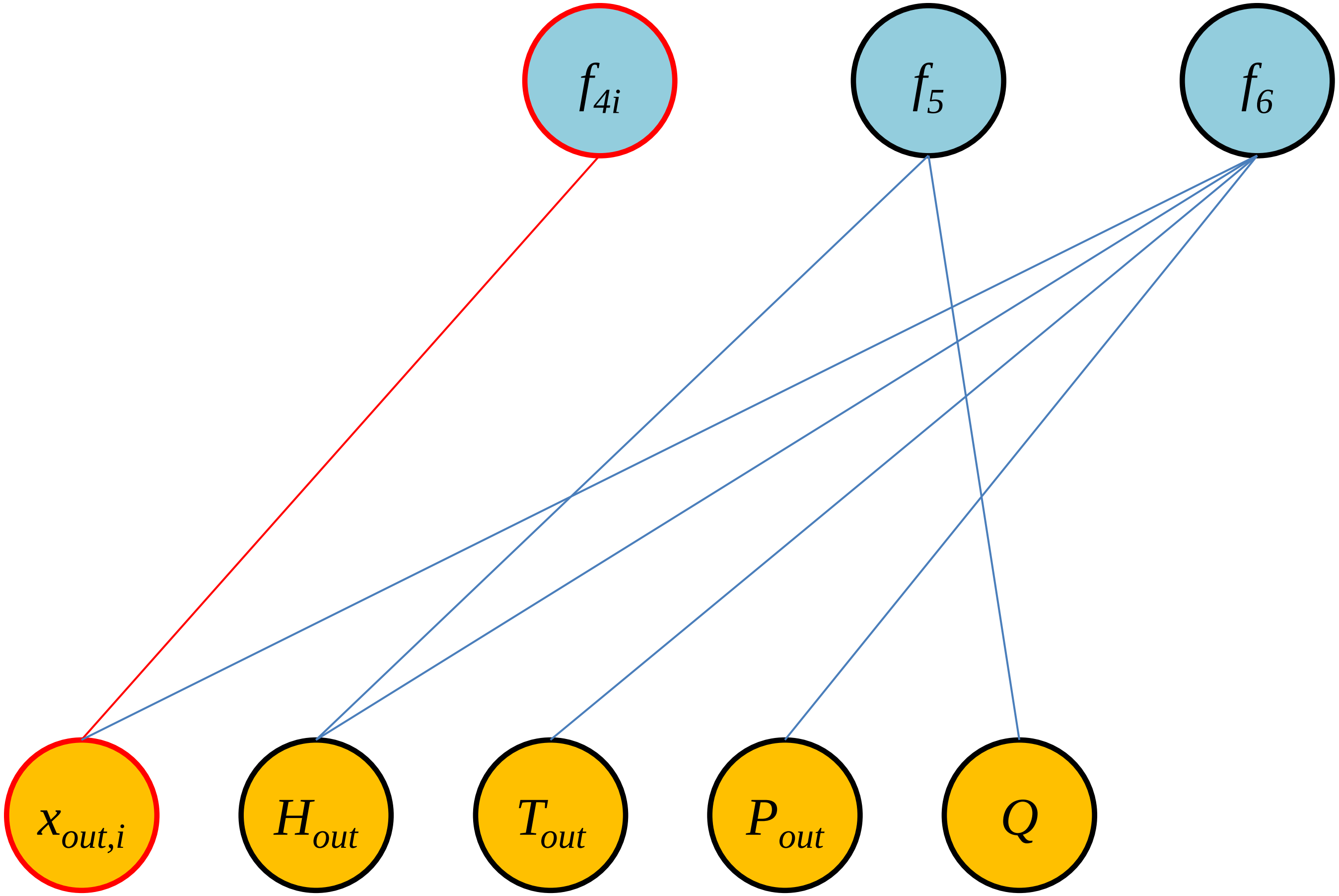
Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

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

$f_3 \rightarrow m_{out}$

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



Reactor de conversión fija (flujos x componentes - MS)

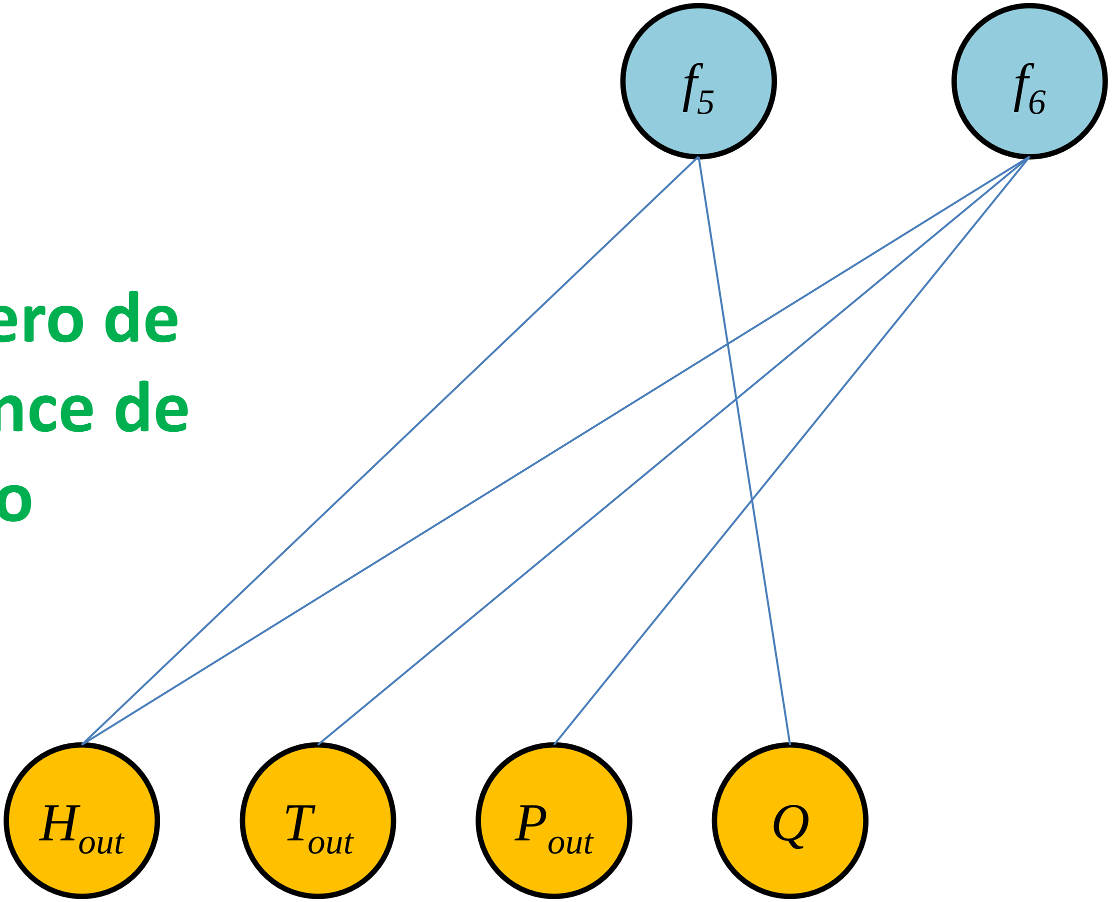
$f_{2,i} \rightarrow R_i$

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

$f_3 \rightarrow m_{out}$

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

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



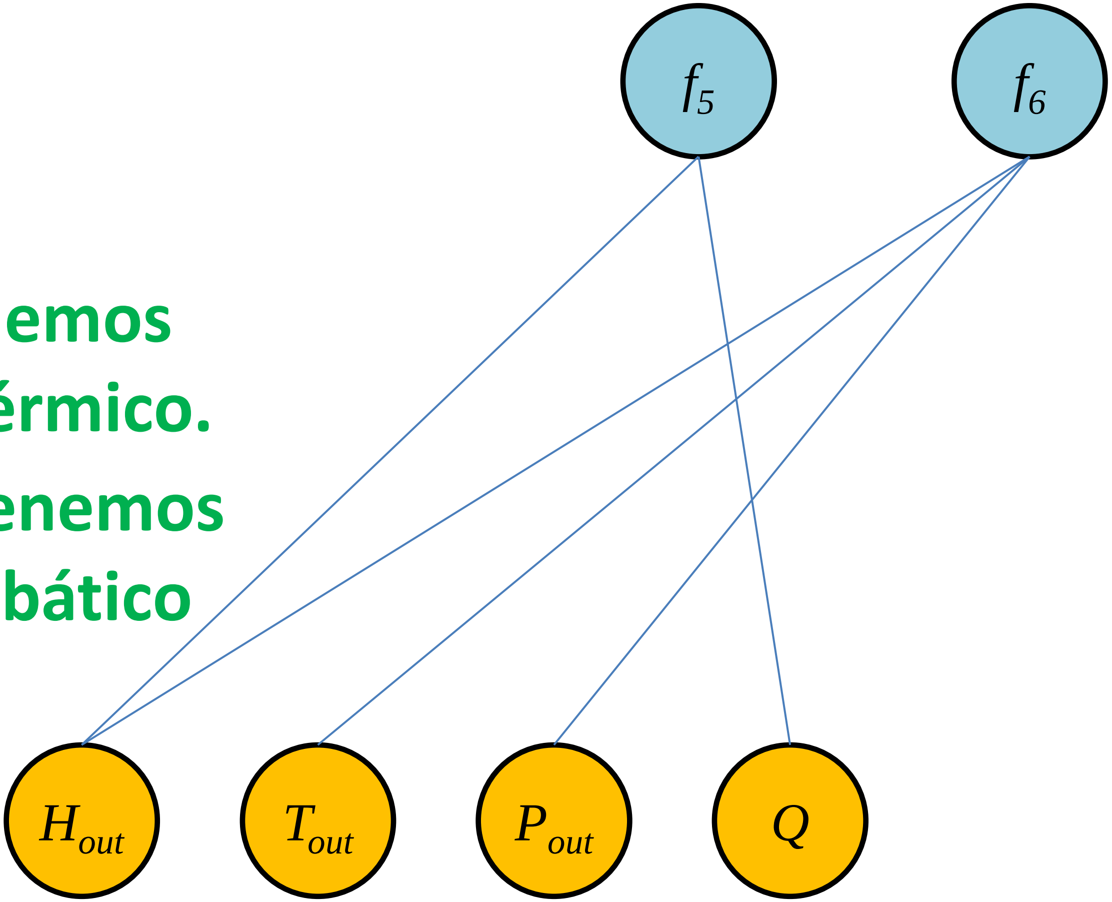
Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

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

$f_3 \rightarrow m_{out}$

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



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)

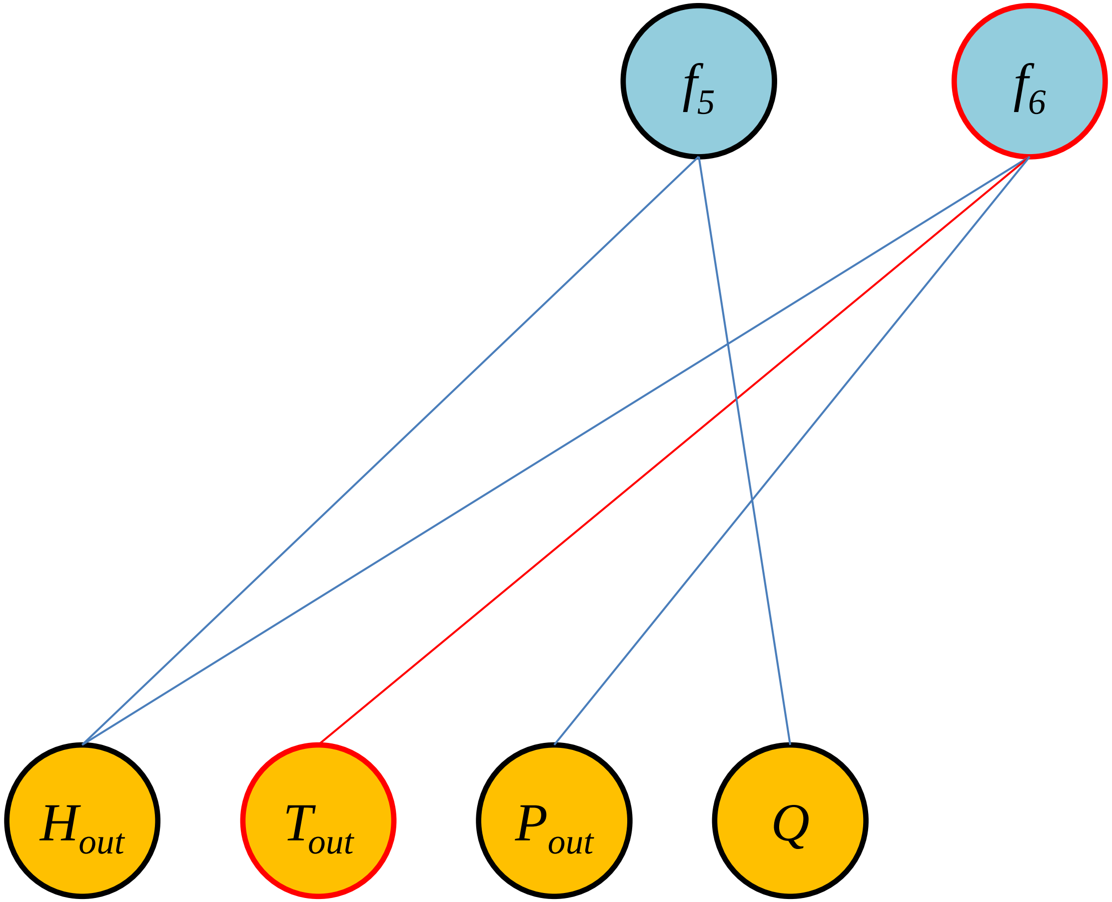
$f_{2,i} \rightarrow R_i$

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

$f_3 \rightarrow m_{out}$

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

$f_6 \rightarrow T_{out}$



Reactor de conversión fija (flujos x componentes - MS)

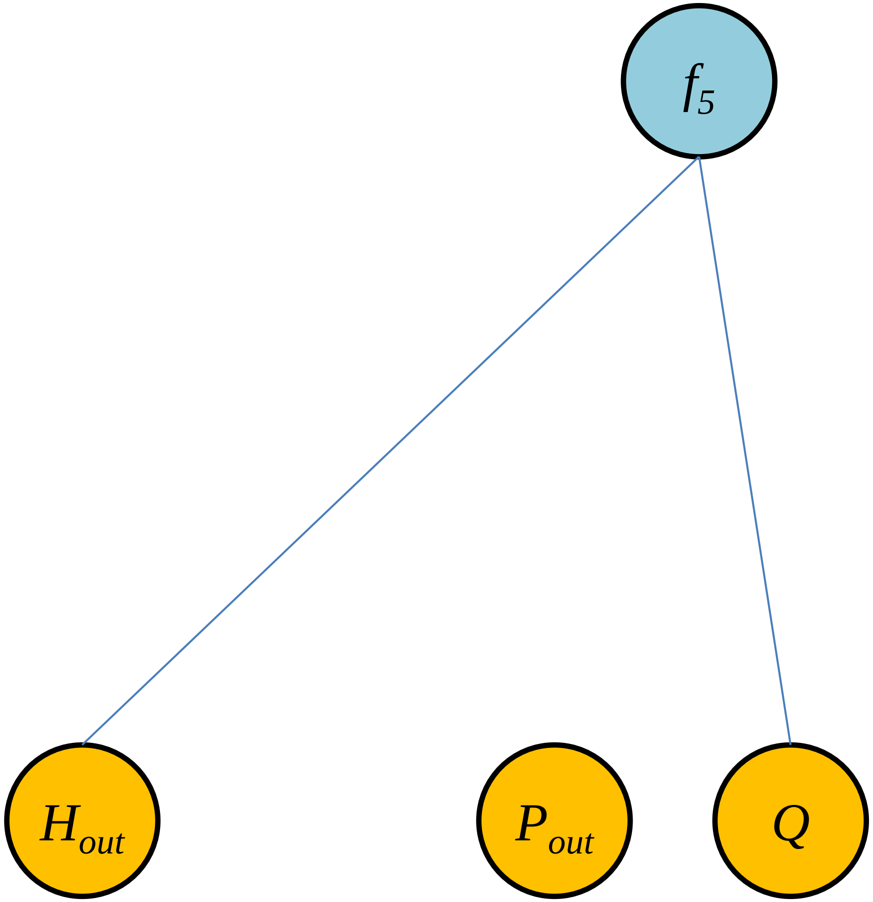
$f_{2,i} \rightarrow R_i$

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

$f_3 \rightarrow m_{out}$

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

$f_6 \rightarrow T_{out}$



Reactor de conversión fija (flujos x componentes - MS)

$f_{2,i} \rightarrow R_i$

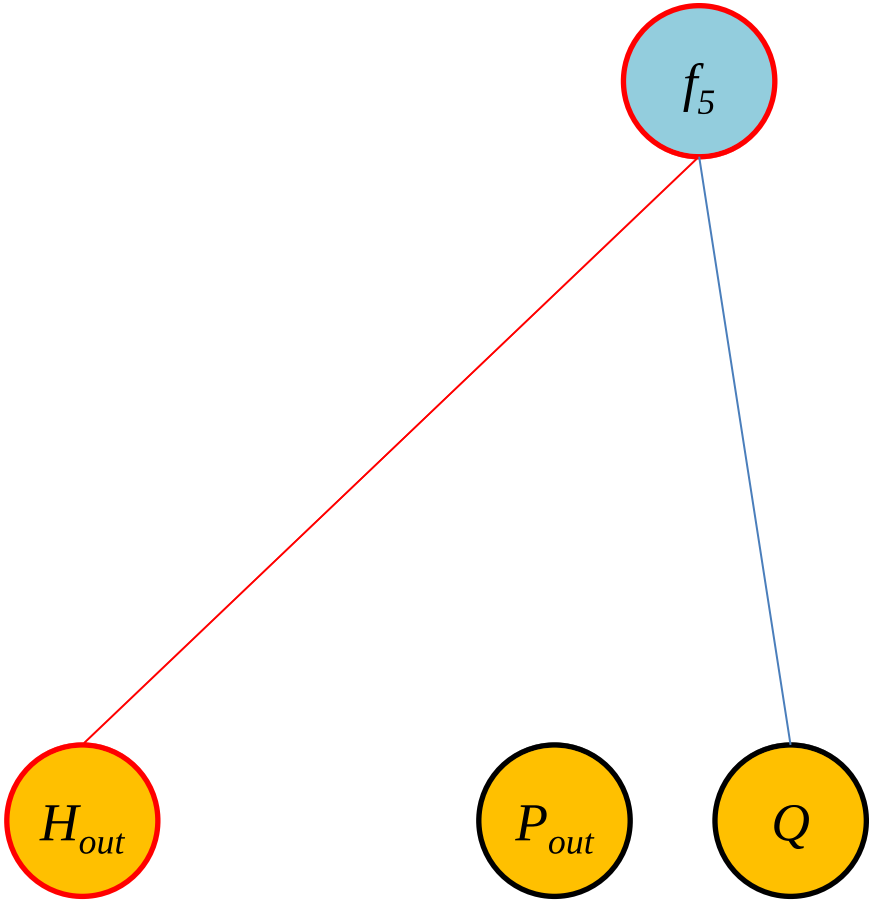
$f_{1,i} \rightarrow m_{out,i}$

$f_3 \rightarrow m_{out}$

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

$f_6 \rightarrow T_{out}$

$f_5 \rightarrow H_{out}$



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.

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

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

$$r_i = \sum_{j=1}^{NR} r_{ij} = \sum_{j=1}^{NR} a_{ij} \times r_j \qquad r_i \left[\frac{moles\, de\, i}{volumen \times tiempo} \right]$$

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:

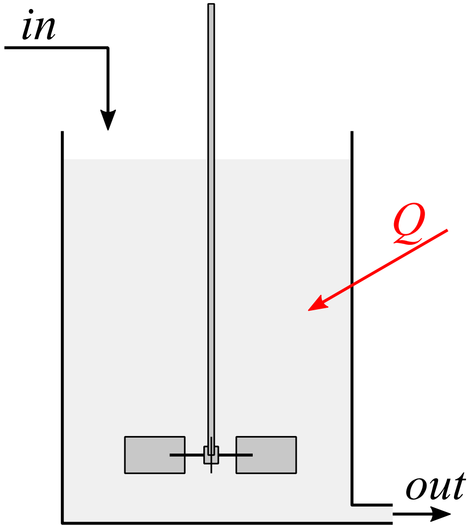
$$r_j = f_j\left(T, C_1, C_2, \ldots, C_{NC}\right) \qquad \forall j$$

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)

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

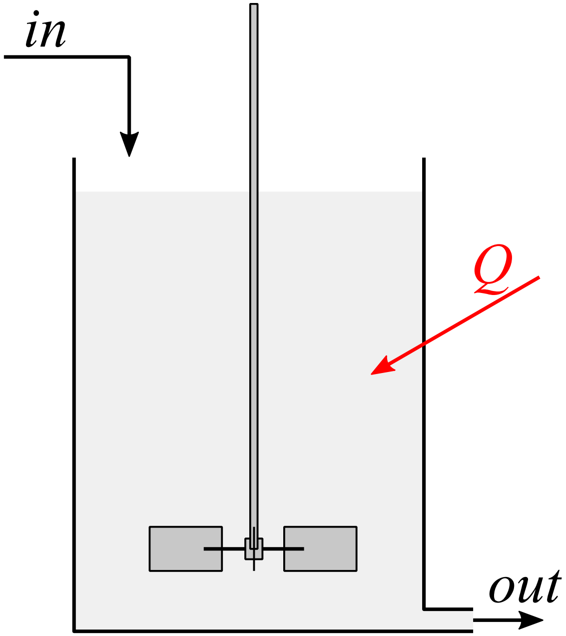
$$r_j = f_j\left(T_{out}, C_{out,1}, C_{out,2}, \ldots, C_{out,NC}\right) \qquad \forall j$$

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

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

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

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



CSTR (Continuously Stirred Tank Reactor)

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

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

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

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

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

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

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

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

CSTR (Continuously Stirred Tank Reactor)

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

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

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

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

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

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

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

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

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

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

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

CSTR (MS)

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

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

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

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

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

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

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

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

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

$$\begin{array}{r} 7+3NC \\ -\quad 4+3NC \\ \hline GL = 3 \end{array}$$

CSTR (adiabático o calor dado)

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

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

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

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

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

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

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

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

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

CSTR (isotérmico)

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

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

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

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

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

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

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

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

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

Reactor CSTR (flujos x componentes - MS)

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

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

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

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

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

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

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

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

7+4NC

–

4+4NC

GL =3

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

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

CSTR - Ejemplo

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

$$r_1\left[\frac{mol}{seg.m^3}\right]=k_1C_{nC4} \qquad k_1=2.94\times10^7\frac{1}{seg}e^{-\frac{65300}{8.314T}}$$

$$r_2\left[\frac{mol}{seg.m^3}\right]=k_2C_{iC4} \qquad k_2=1.176\times10^8\frac{1}{seg}e^{-\frac{72200}{8.314T}}$$

$$r_i=\sum_{j=1}^{NR}a_{ij}f_j\left(T_{out},C_{out}\right)\ \forall i \ \rightarrow r_i=a_{i1}k_1C_{nC4}+a_{i2}k_2C_{iC4} \qquad \forall i$$

$$r_{nC4}=-k_1C_{nC4}+k_2C_{iC4}$$

$$r_{iC4}=k_1C_{nC4}-k_2C_{iC4}$$

$$\boxed{\begin{aligned} r_{nC4}&=-\left(2.94\times10^7e^{-\frac{65300}{8.314T}}\right)C_{nC4}+\left(1.176\times10^8e^{-\frac{72200}{8.314T}}\right)C_{iC4}\\ r_{iC4}&=\left(2.94\times10^7e^{-\frac{65300}{8.314T}}\right)C_{nC4}-\left(1.176\times10^8e^{-\frac{72200}{8.314T}}\right)C_{iC4}\end{aligned}}$$

CSTR - Ejemplo

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

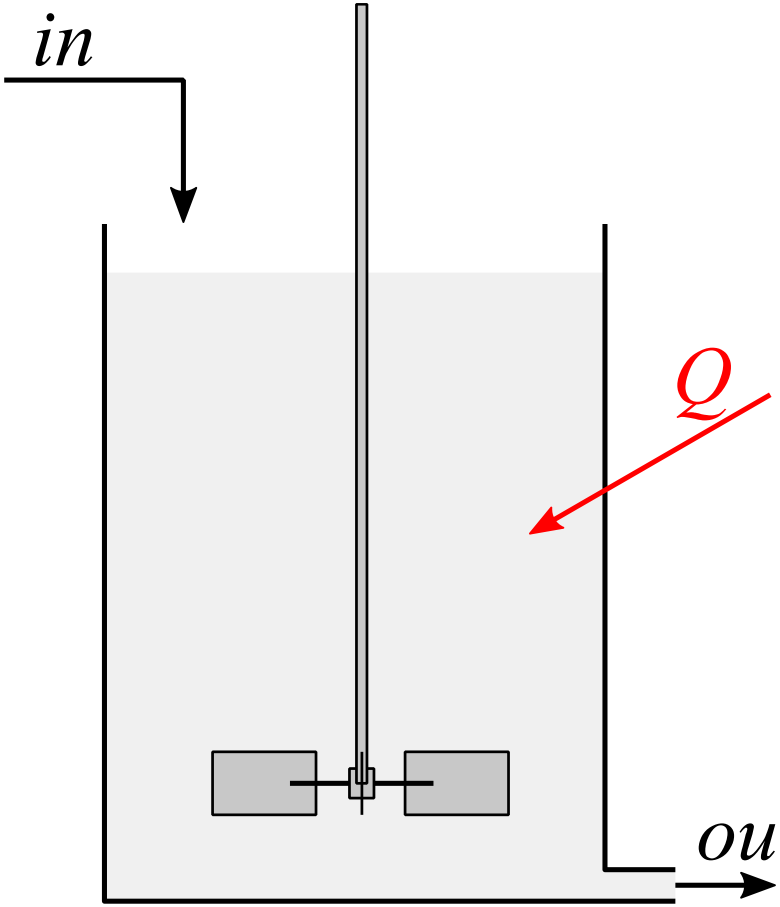
P_{in} : $20\ bar$

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

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

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

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

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

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

$$m_{out,i} = m_{out} x_{out,i}$$

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

$$r_{nC_4} = -\left(2.94\times10^7 e^{-\frac{65300}{8.314T_{out}}}\right) C_{nC_4} + \left(1.176\times10^8 e^{-\frac{72200}{8.314T_{out}}}\right) C_{iC_4}$$

$$r_{iC4} = \left(2.94\times10^7 e^{-\frac{65300}{8.314T_{out}}}\right) C_{nC_4} - \left(1.176\times10^8 e^{-\frac{72200}{8.314T_{out}}}\right) C_{iC_4}$$

$$r_{iC5} = 0$$

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

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

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

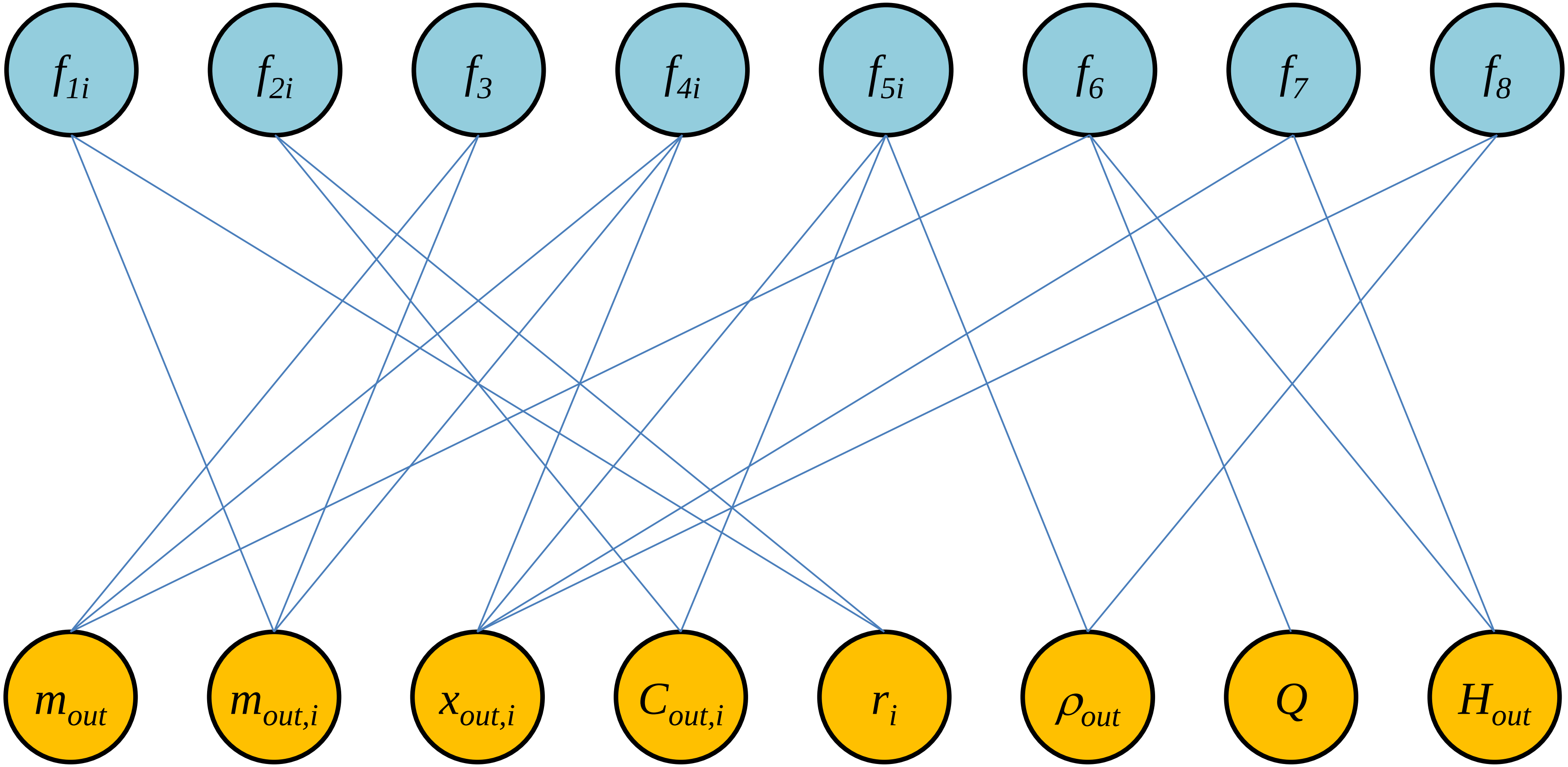
$$m_{in} H_{in} + Q - m_{out} H_{out} = 0$$ ⑥

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

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

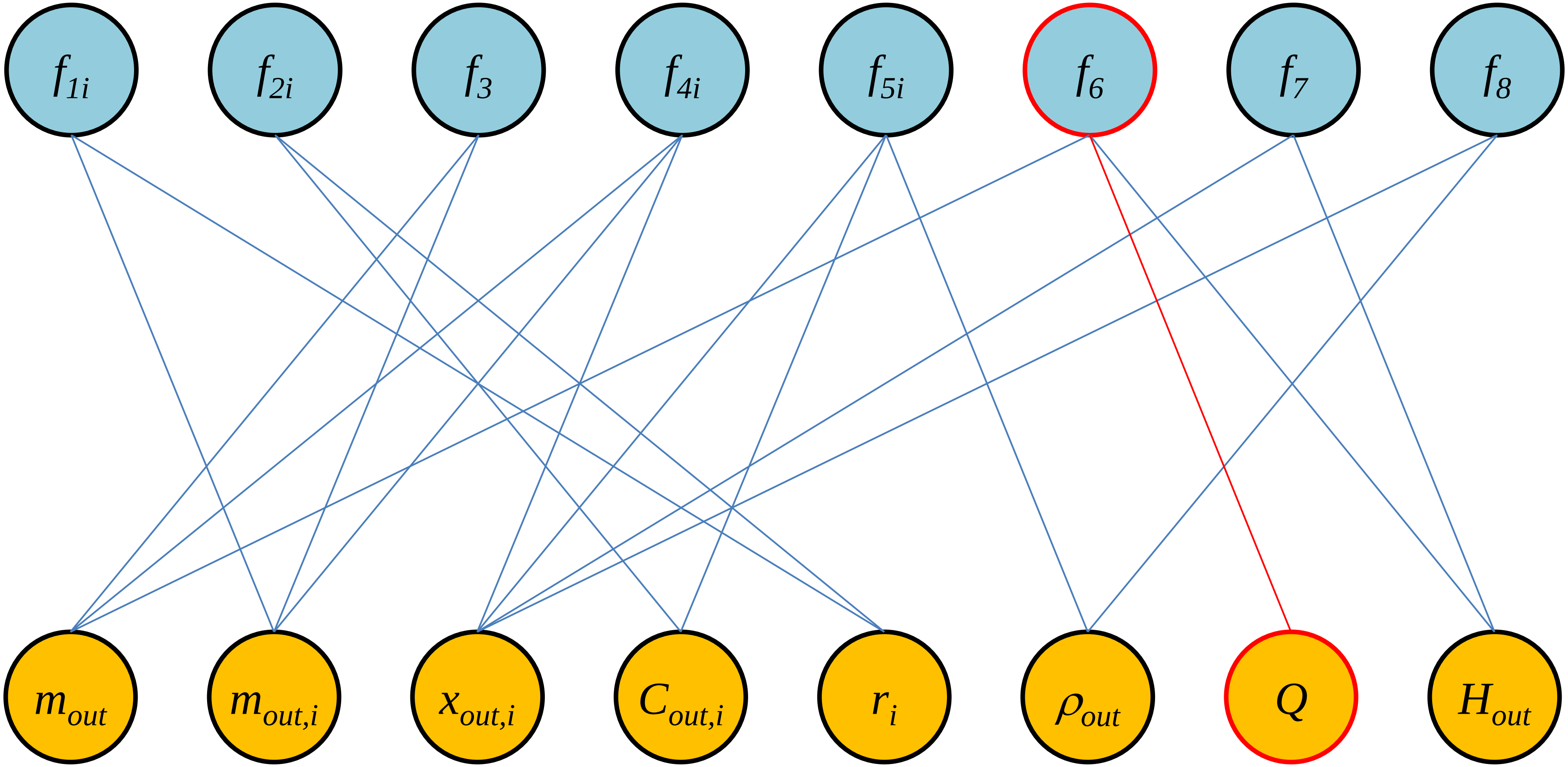
Reactor CSTR (flujos x componentes - MS)

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



Reactor CSTR (flujos x componentes - MS)

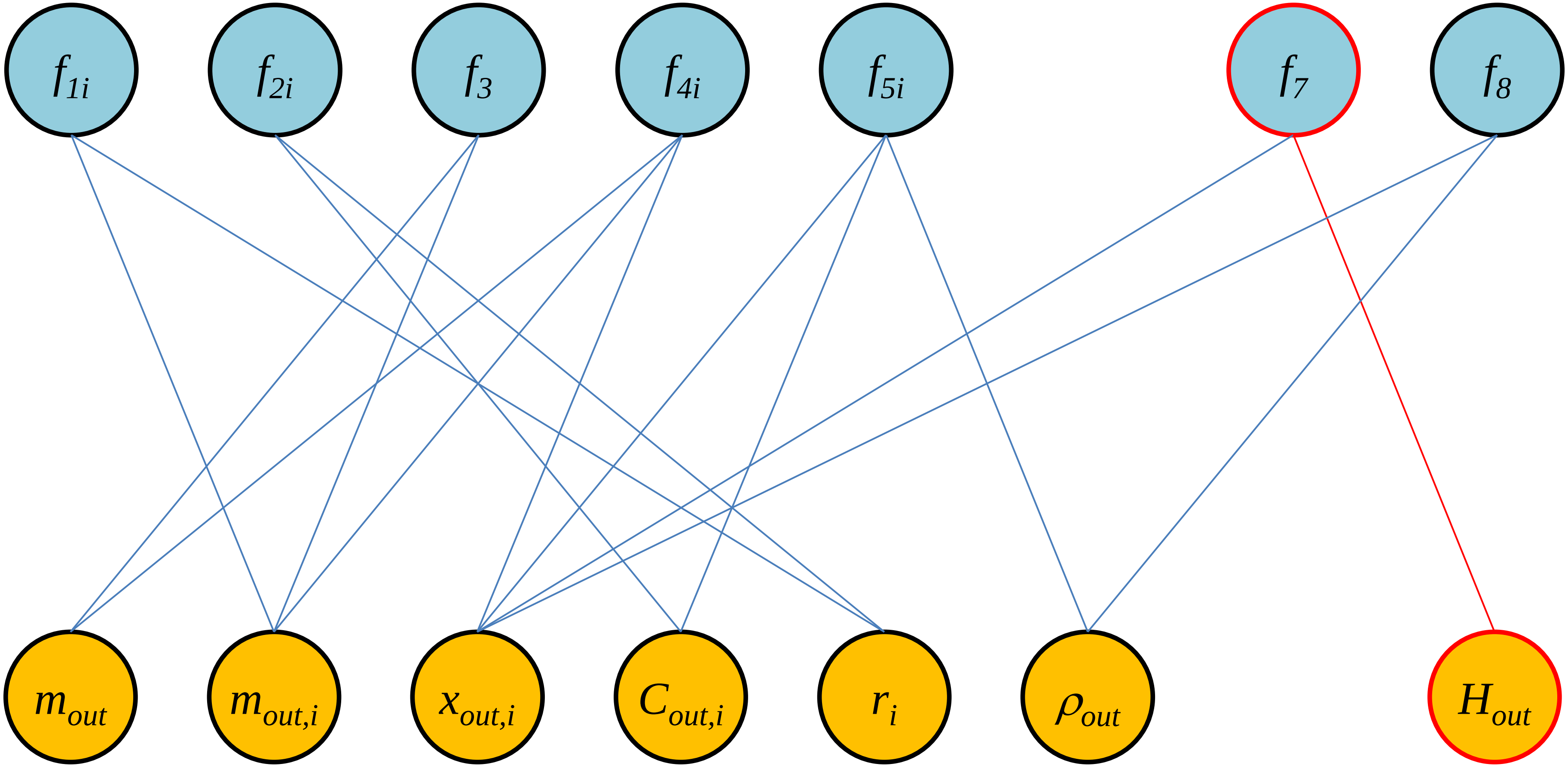
$f_6 \rightarrow Q$



Reactor CSTR (flujos x componentes - MS)

$$f_6 \rightarrow Q$$

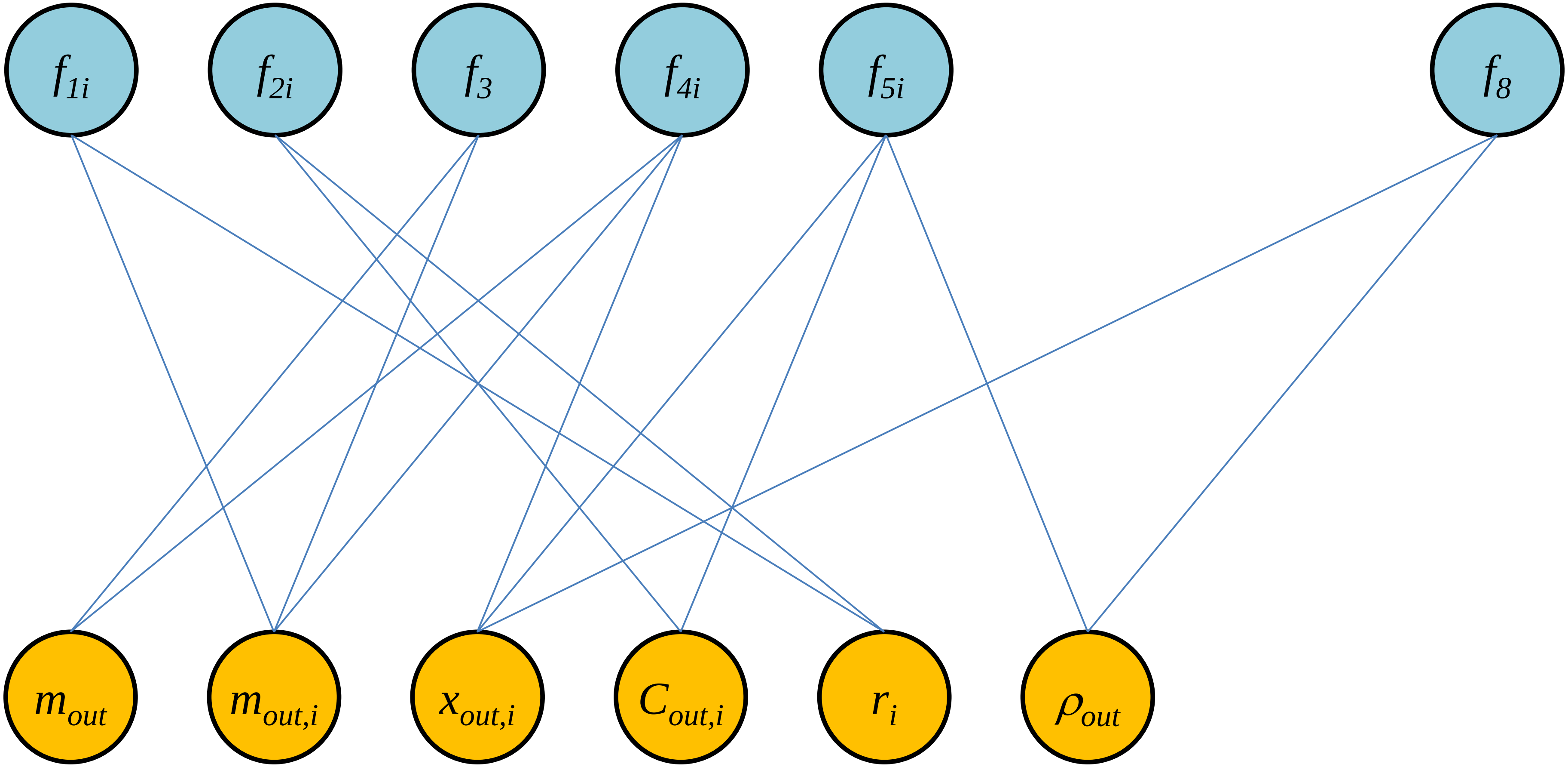
$$f_7 \rightarrow H_{out}$$



Reactor CSTR (flujos x componentes - MS)

$f_6 \rightarrow Q$

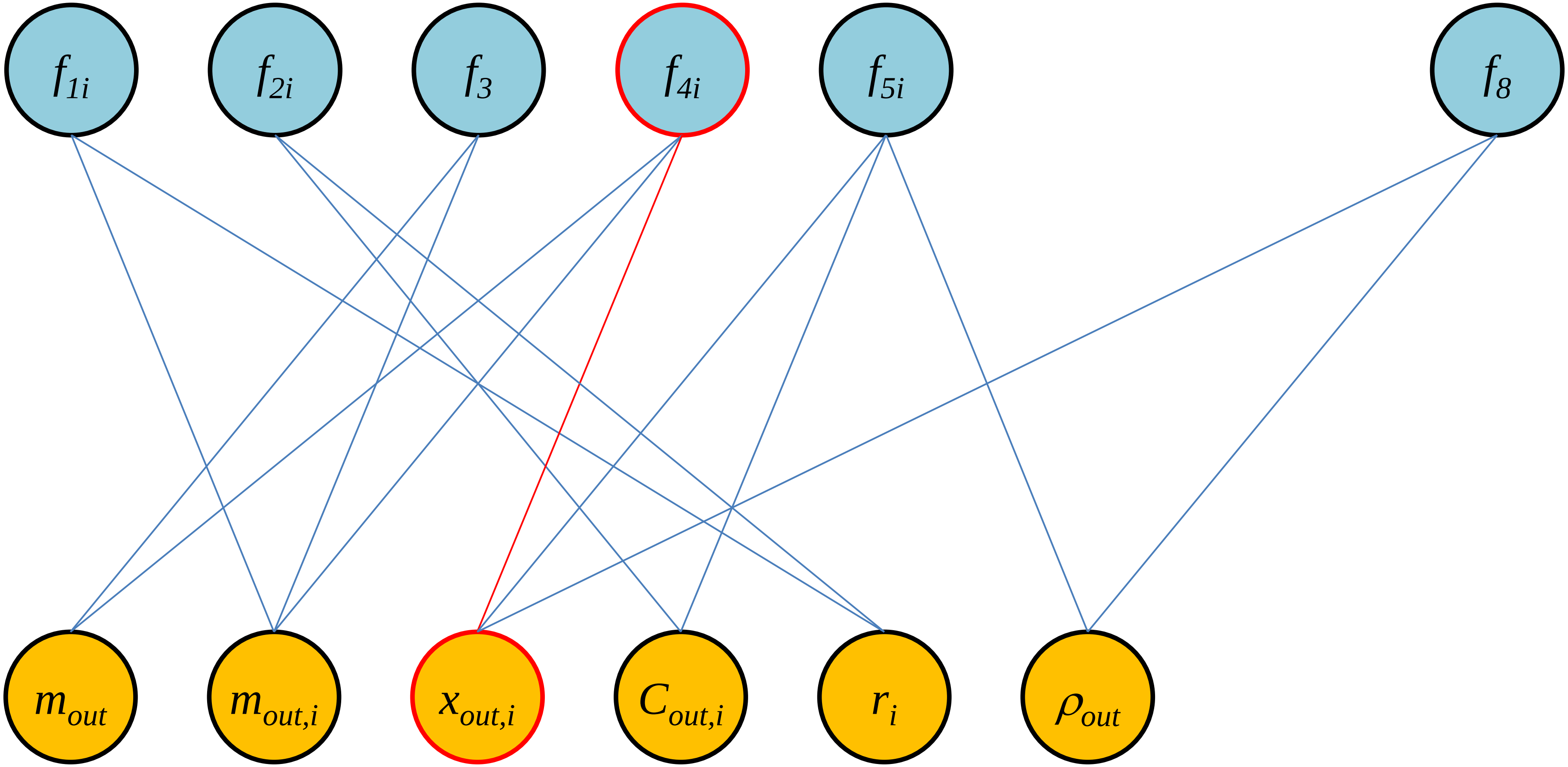
$f_7 \rightarrow H_{out}$



Reactor CSTR (flujos x componentes - MS)

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

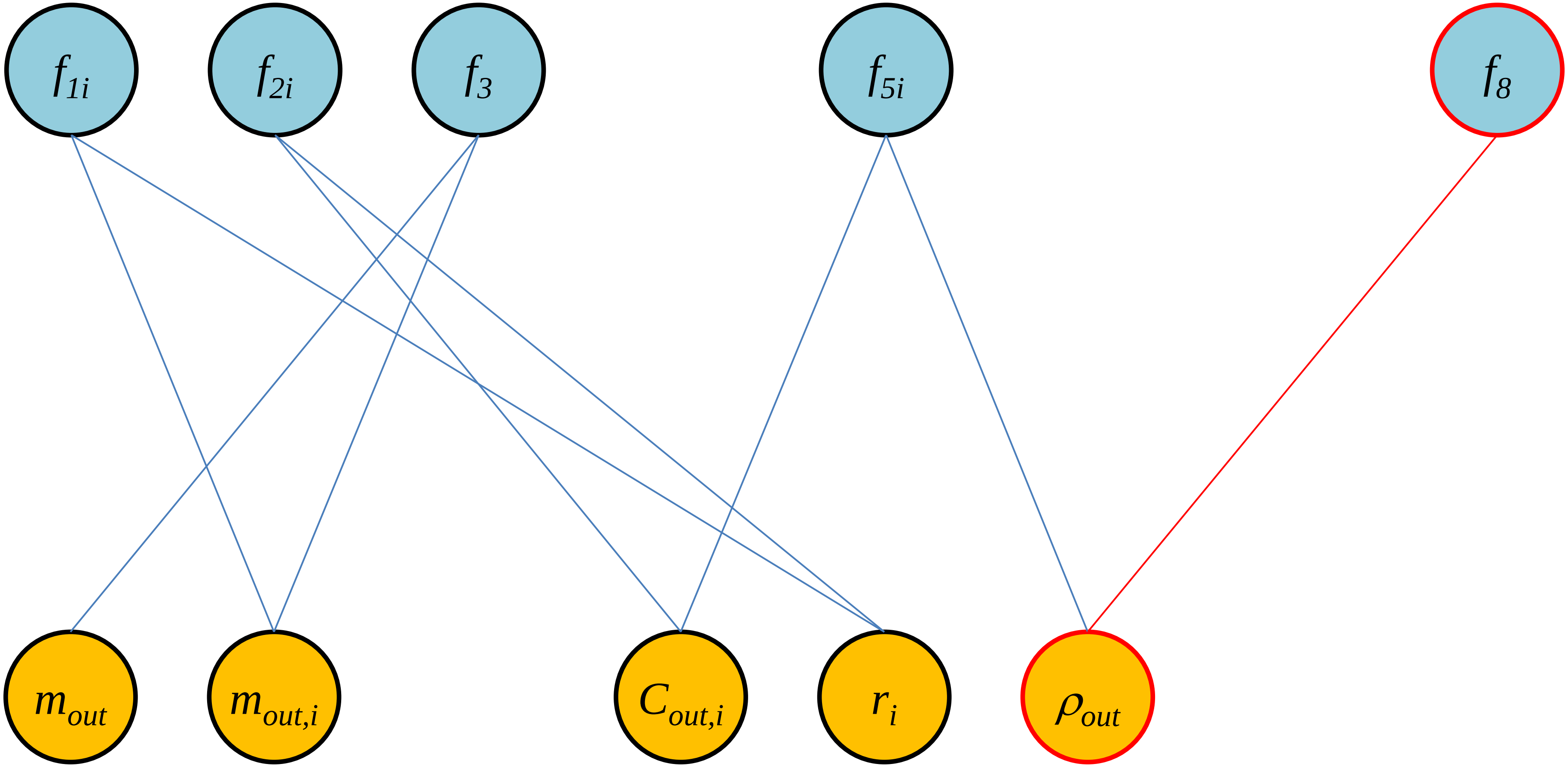
$f_7 \rightarrow H_{out}$



Reactor CSTR (flujos x componentes - MS)

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

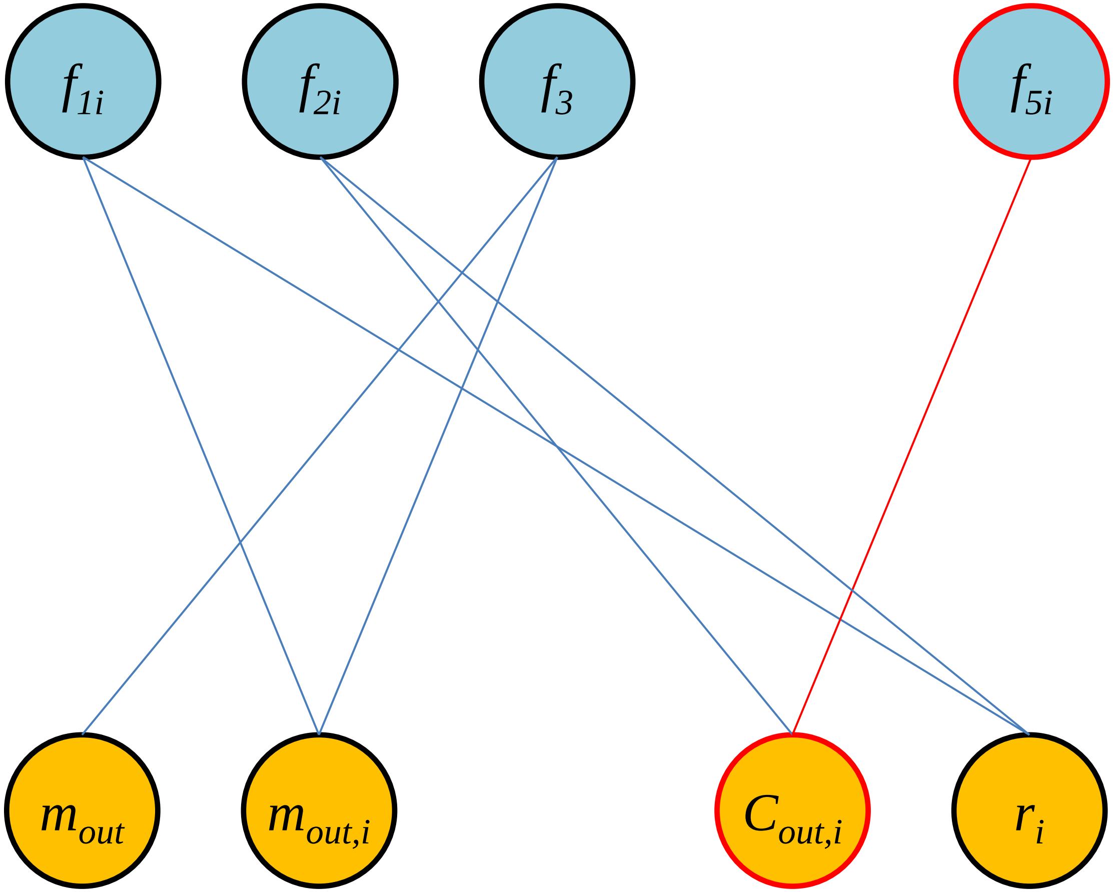
$f_7 \rightarrow H_{out}$ $\quad f_8 \rightarrow \rho_{out}$



Reactor CSTR (flujos x componentes - MS)

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

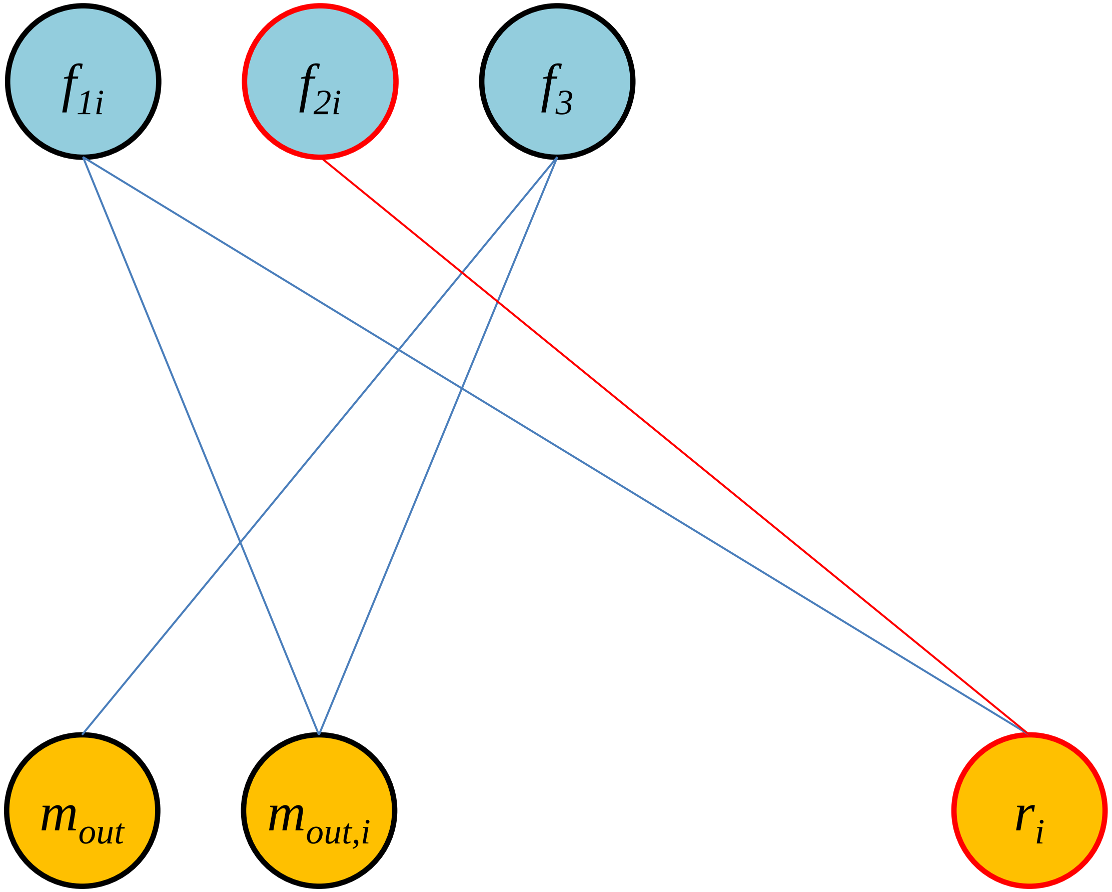
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$



Reactor CSTR (flujos x componentes - MS)

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

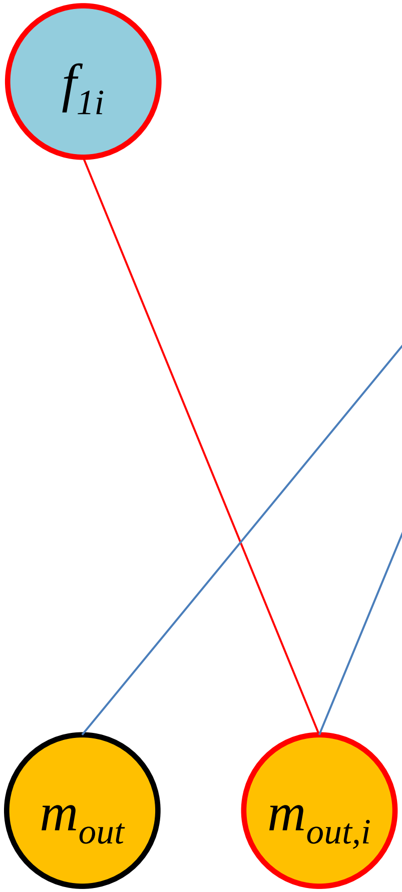
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$



Reactor CSTR (flujos x componentes - MS)

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

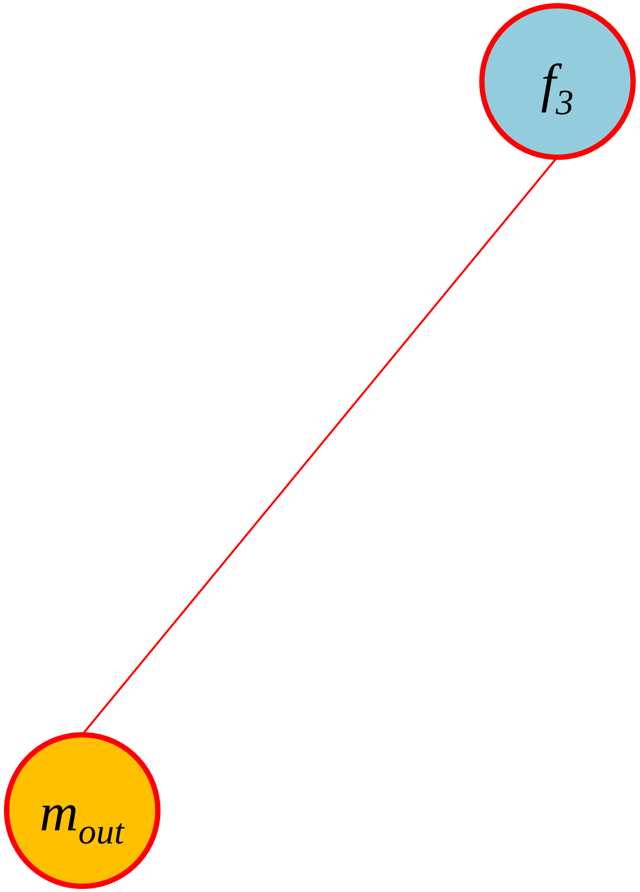
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$



Reactor CSTR (flujos x componentes - MS)

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

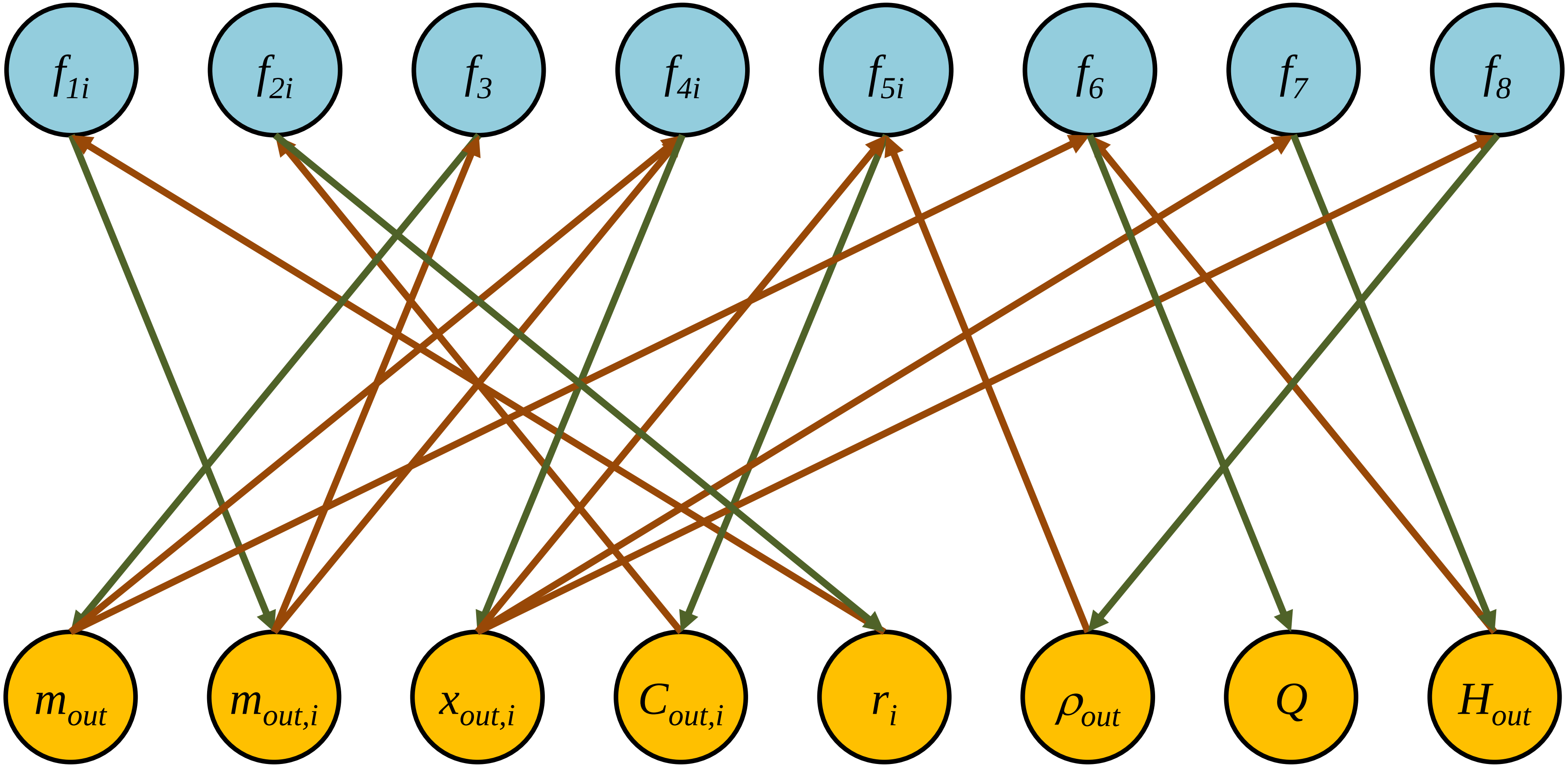
$f_7 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$ $f_3 \rightarrow m_{out}$



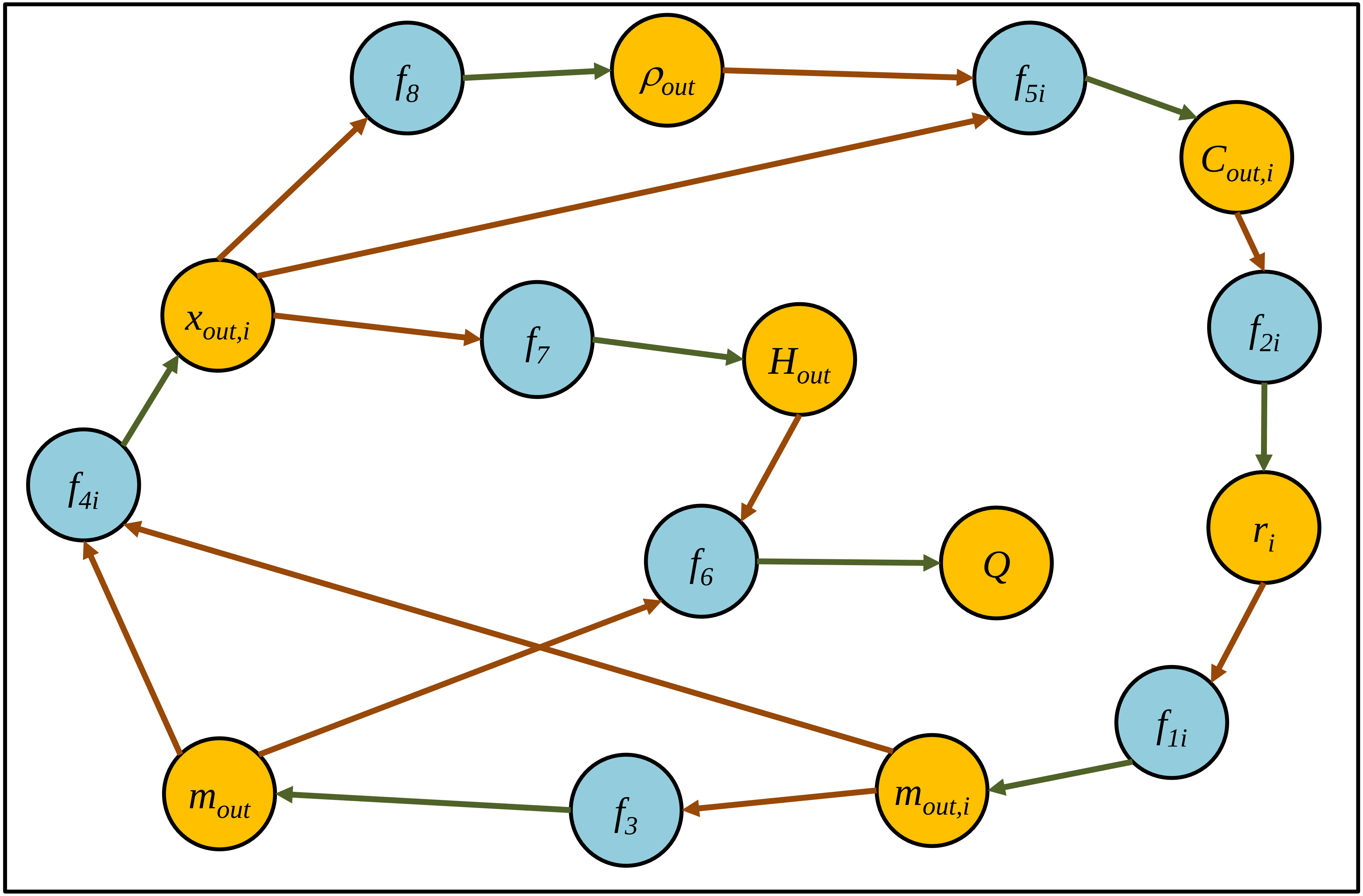
Reactor CSTR (flujos x componentes - MS)

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

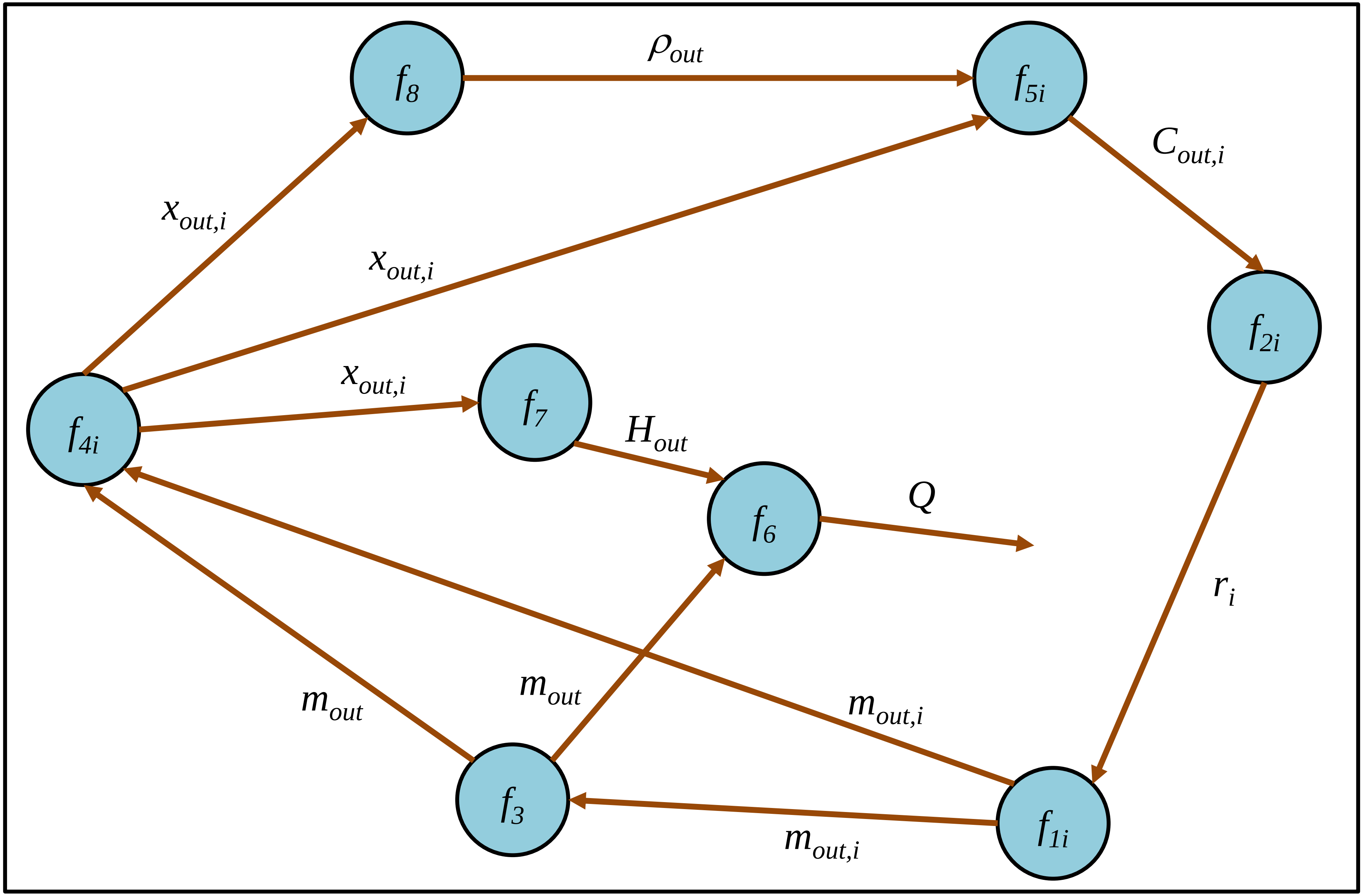
$f_7 \rightarrow H_{out}$ $\quad f_8 \rightarrow \rho_{out}$ $\quad f_{2i} \rightarrow r_i$ $\quad f_3 \rightarrow m_{out}$



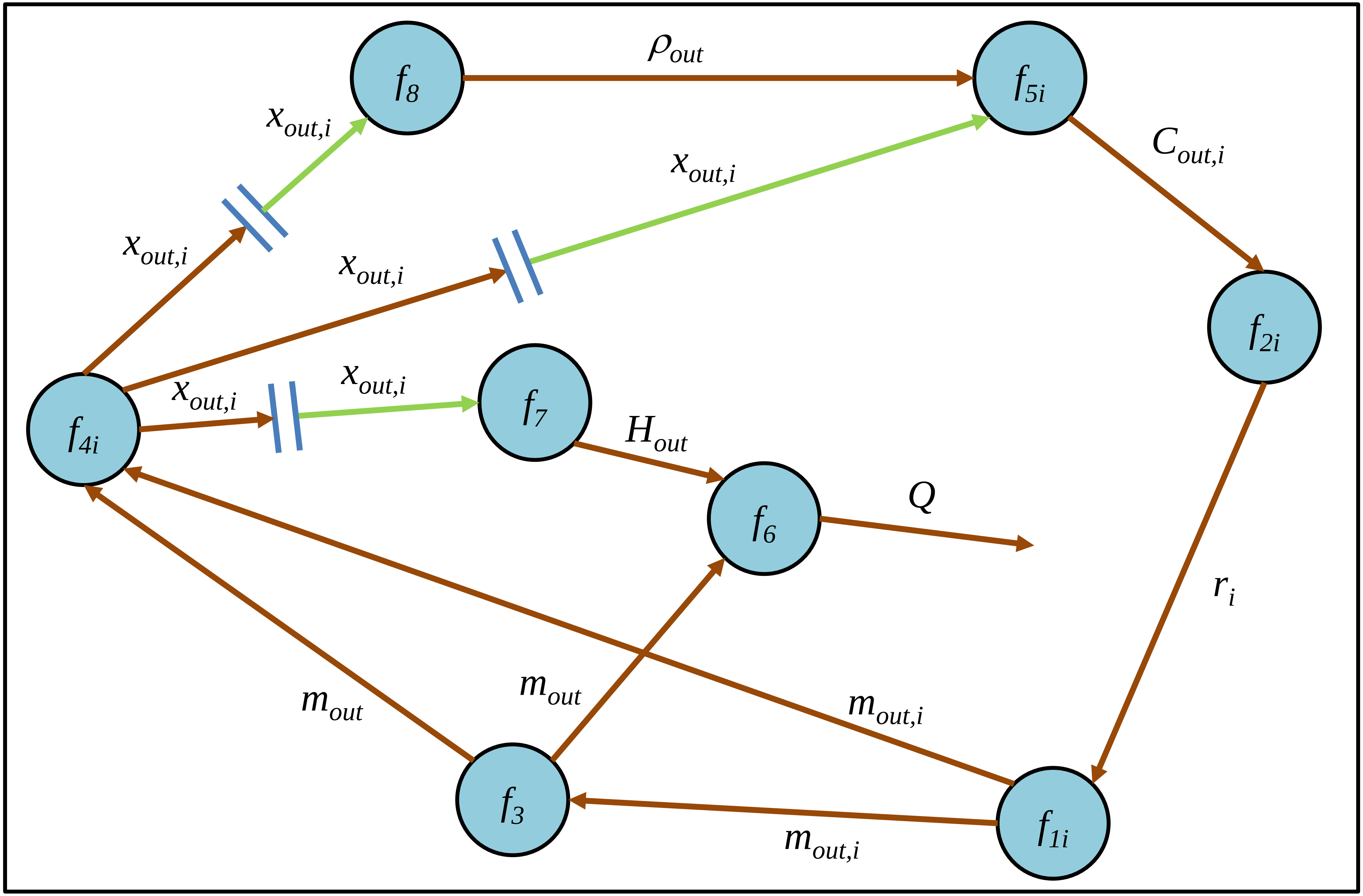
Reactor CSTR (flujos x componentes - MS)



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} : $330\,K$

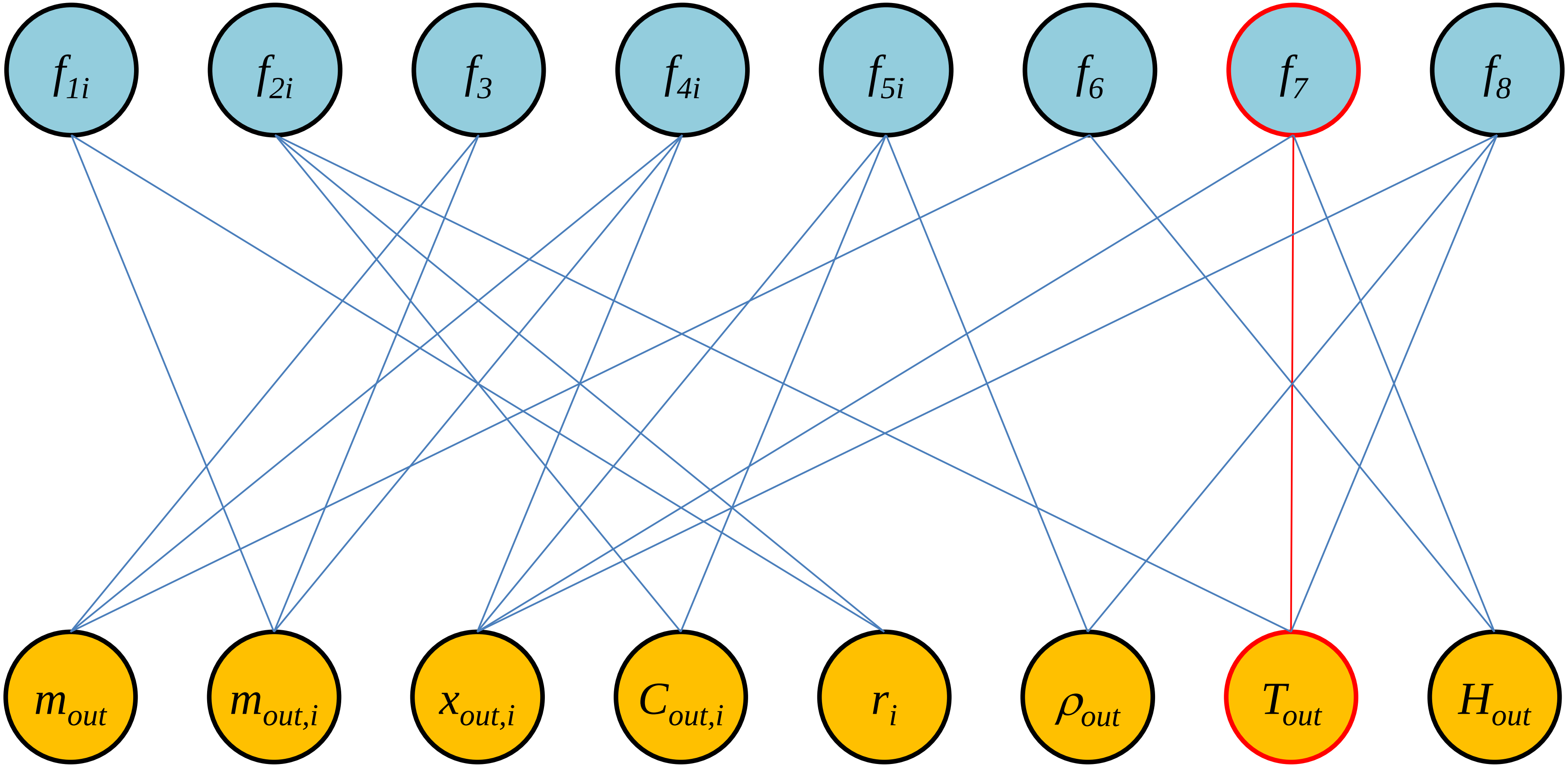
P_{out} : $20\ bar$

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

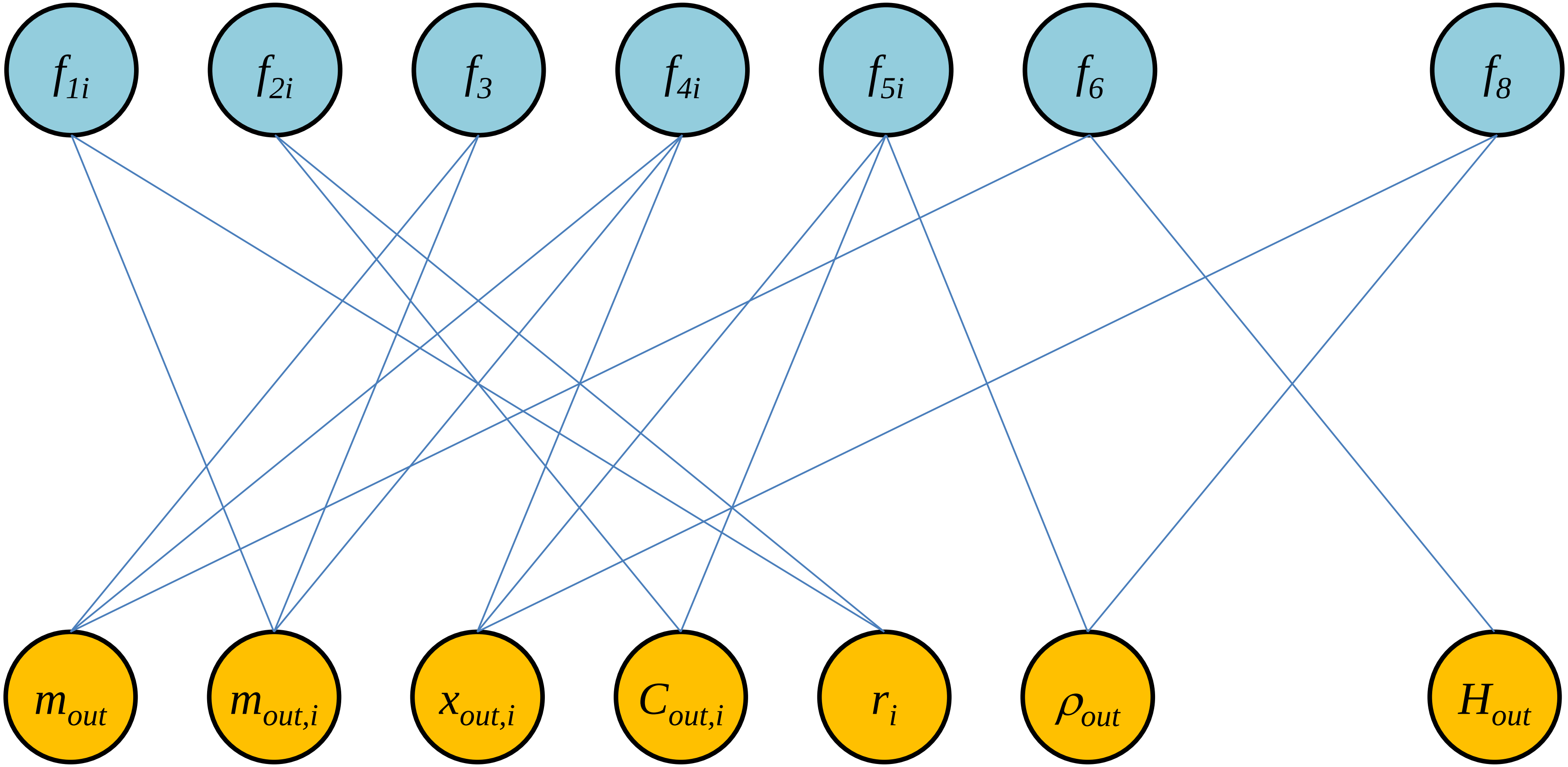
Reactor de conversión fija (flujos x componentes - MS)

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



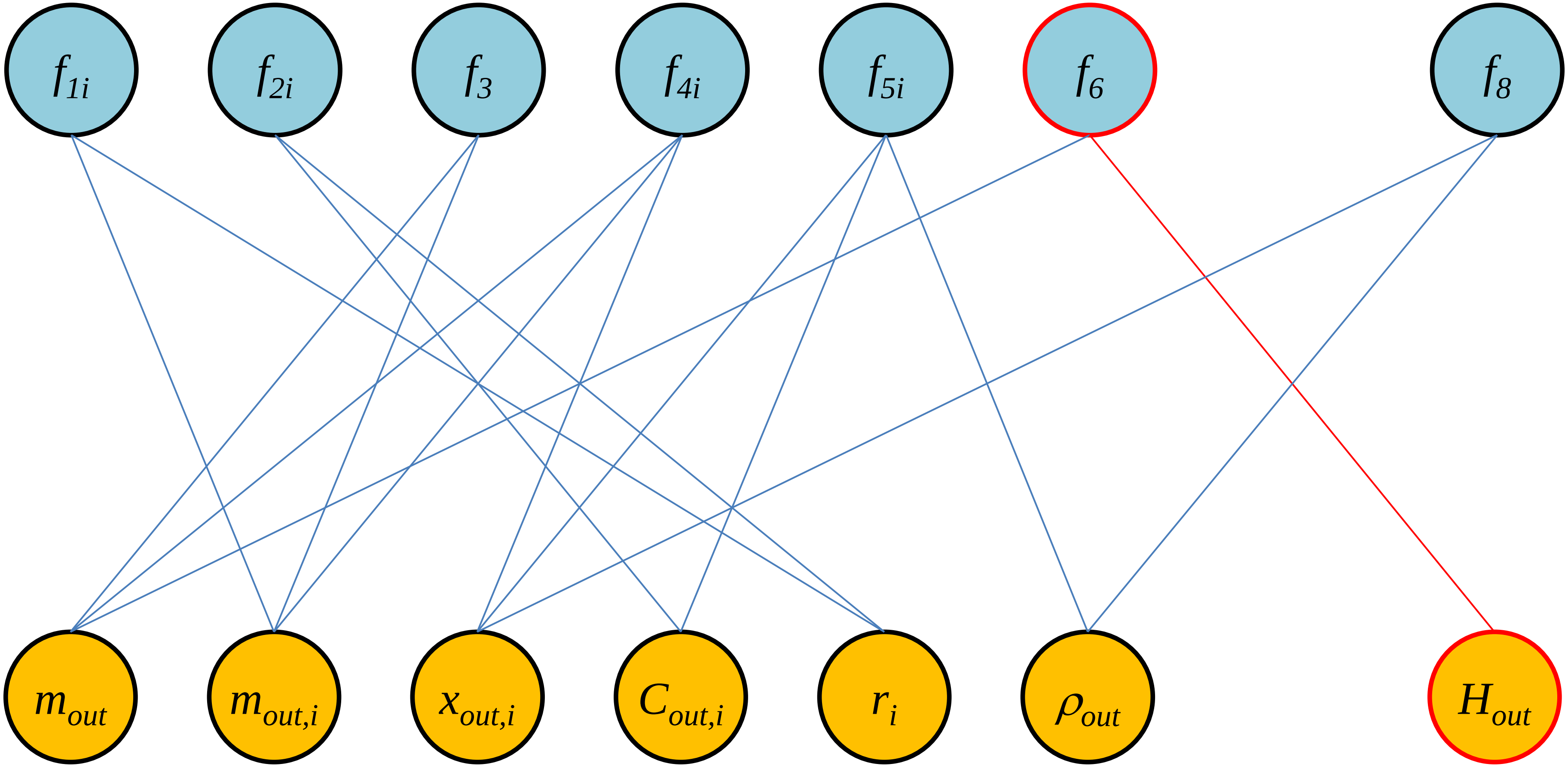
Reactor de conversión fija (flujos x componentes - MS)

$f_7 \rightarrow T_{out}$



Reactor de conversión fija (flujos x componentes - MS)

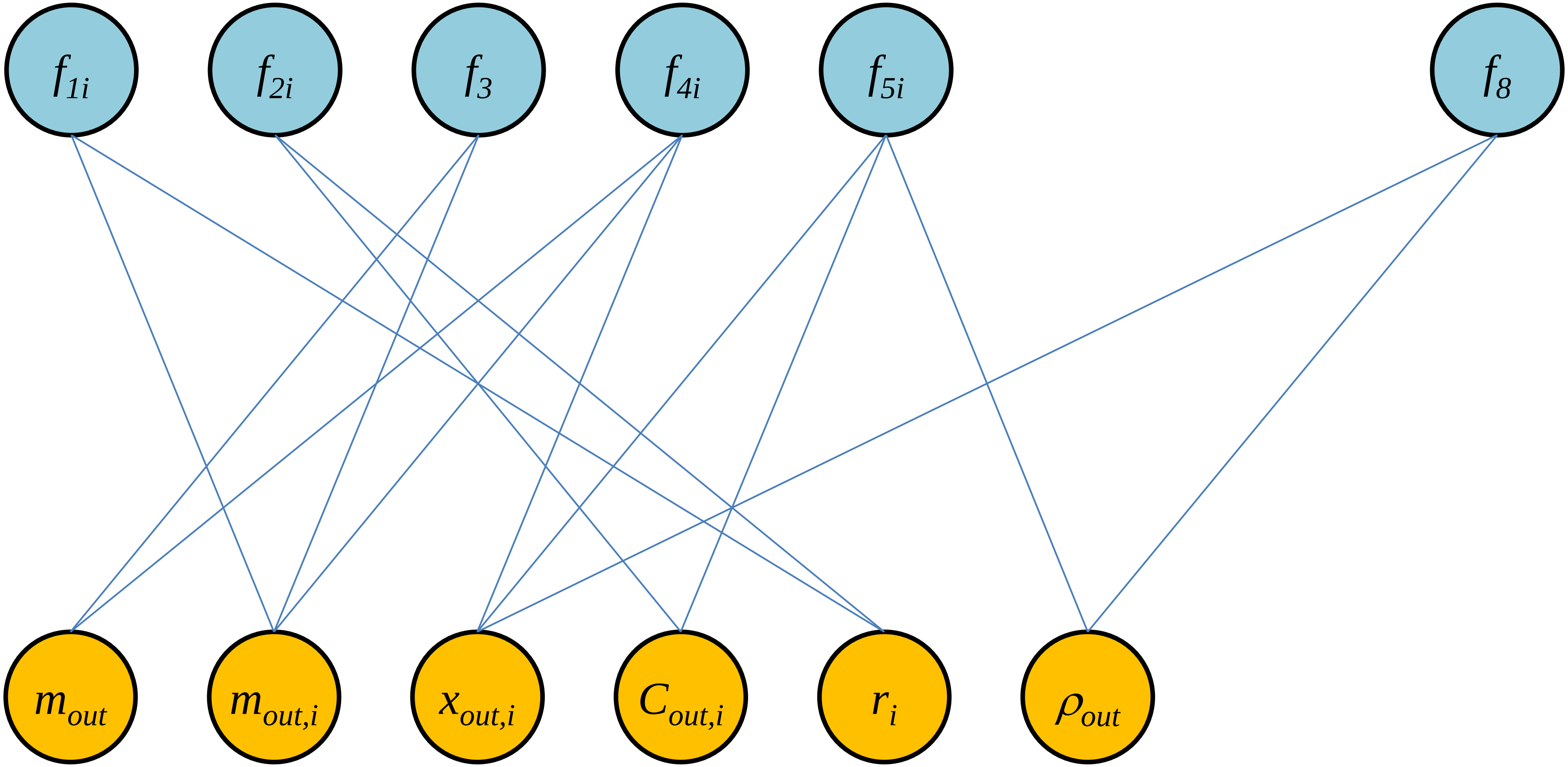
$f_7 \rightarrow T_{out}$



Reactor de conversión fija (flujos x componentes - MS)

$f_7 \rightarrow T_{out}$

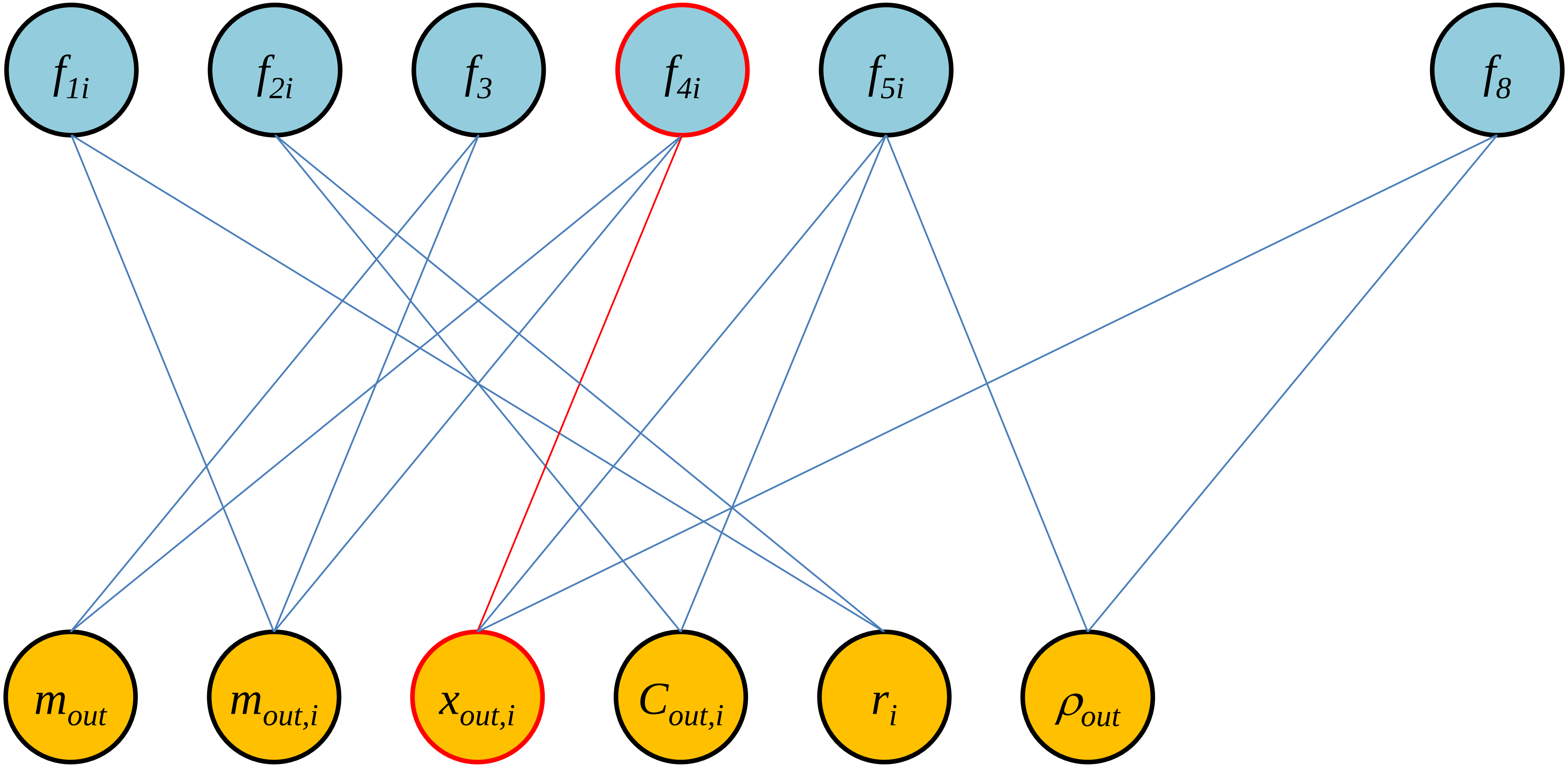
$f_6 \rightarrow H_{out}$



Reactor de conversión fija (flujos x componentes - MS)

$f_7 \rightarrow T_{out}$

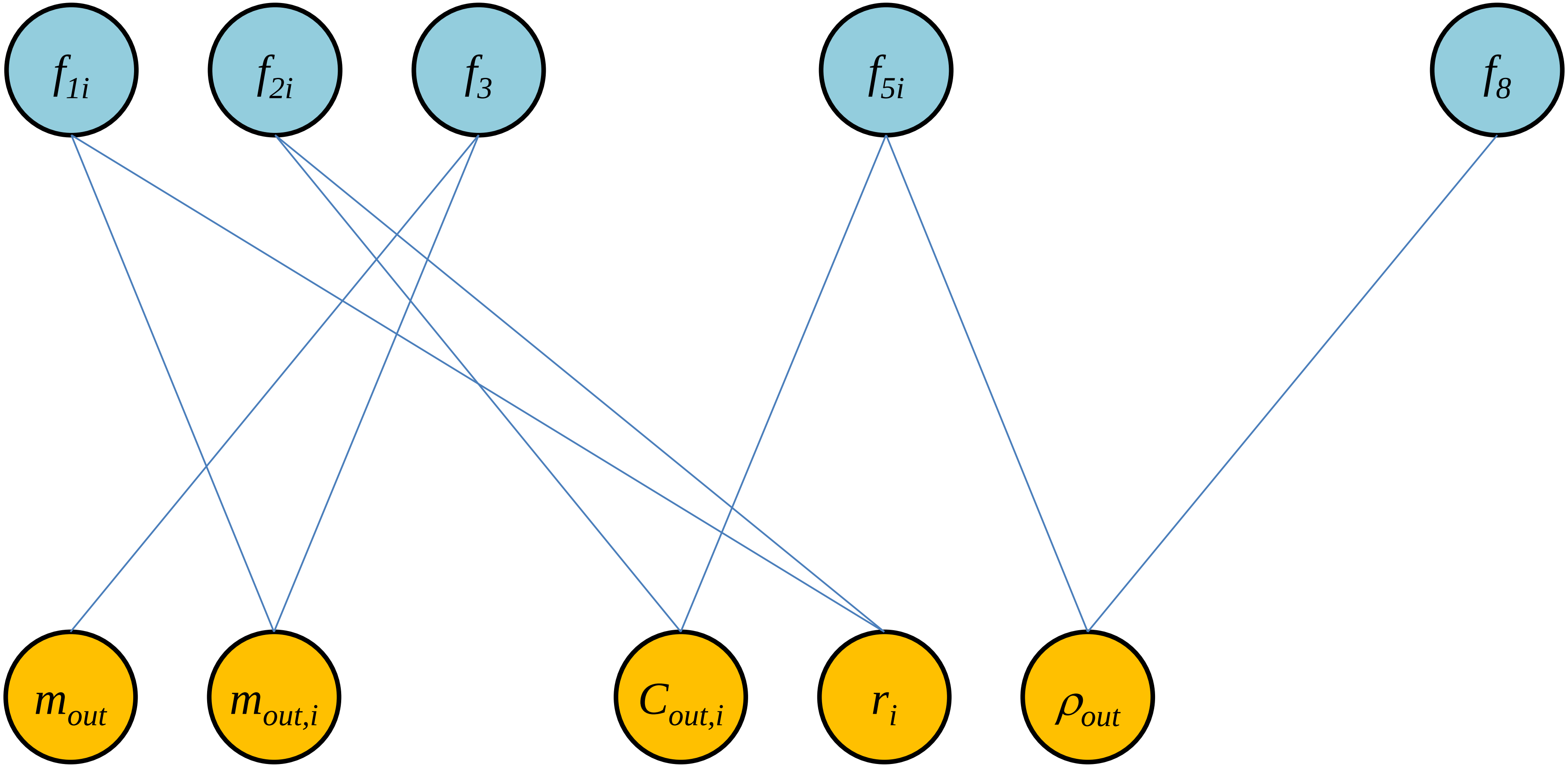
$f_6 \rightarrow H_{out}$



Reactor de conversión fija (flujos x componentes - MS)

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

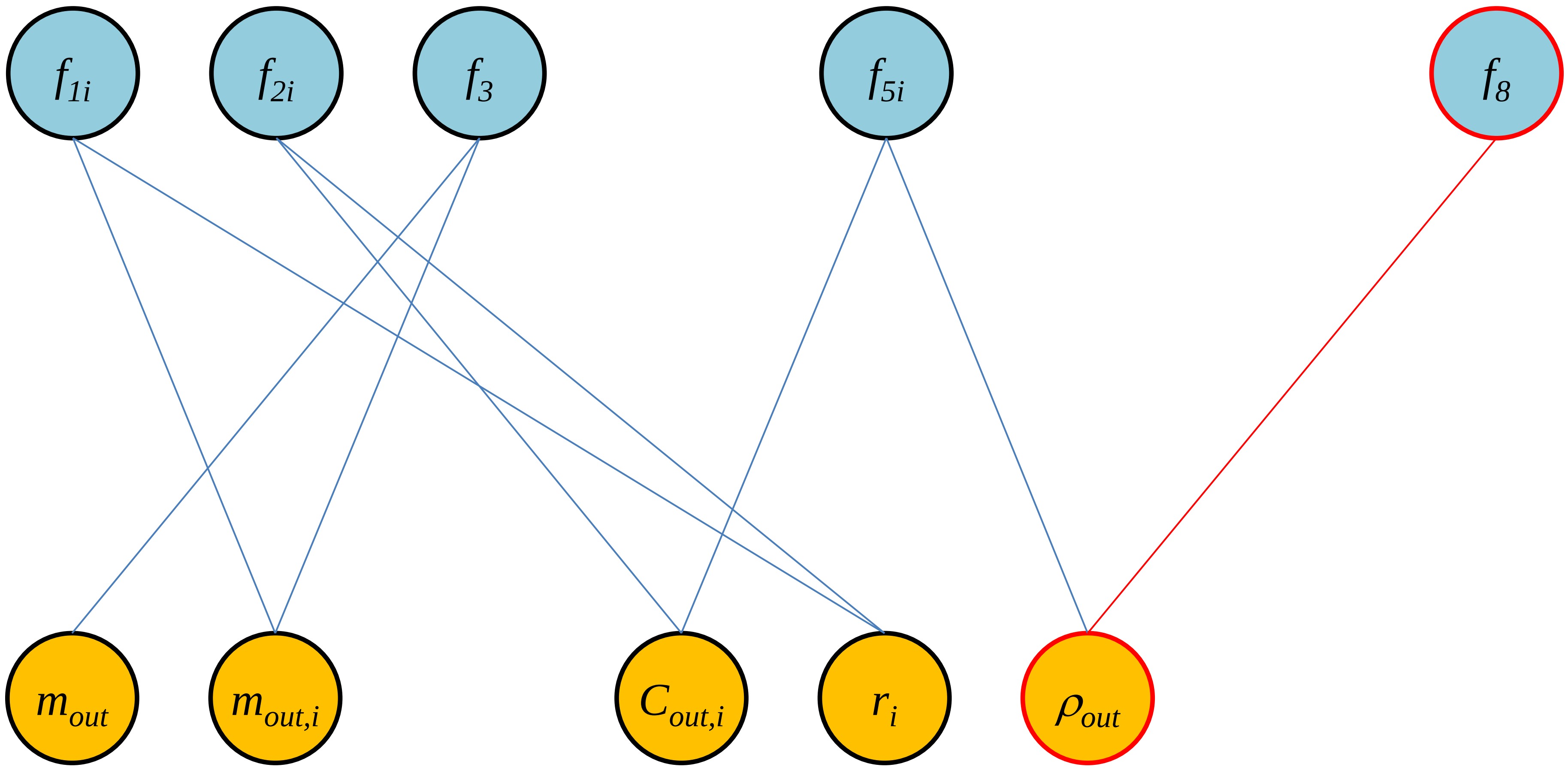
$f_6 \rightarrow H_{out}$



Reactor de conversión fija (flujos x componentes - MS)

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

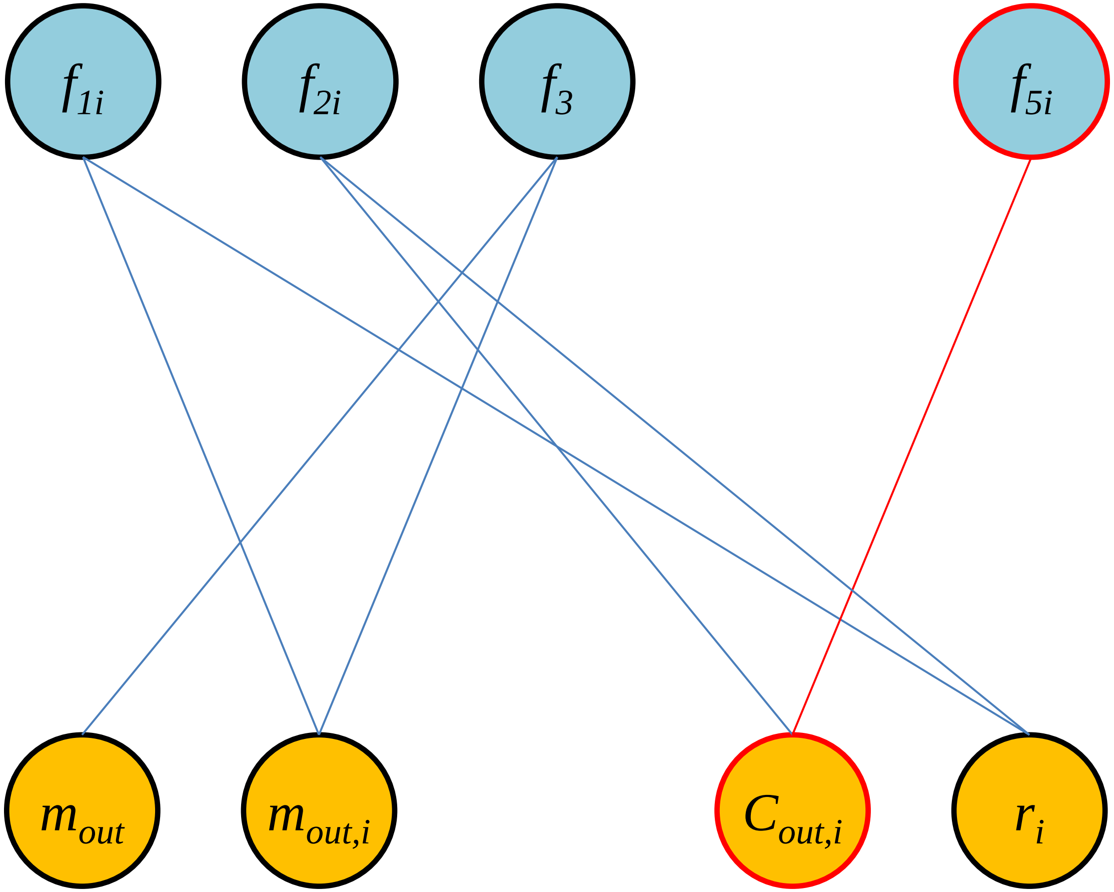
$f_6 \rightarrow H_{out}$ $\quad f_8 \rightarrow \rho_{out}$



Reactor de conversión fija (flujos x componentes - MS)

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

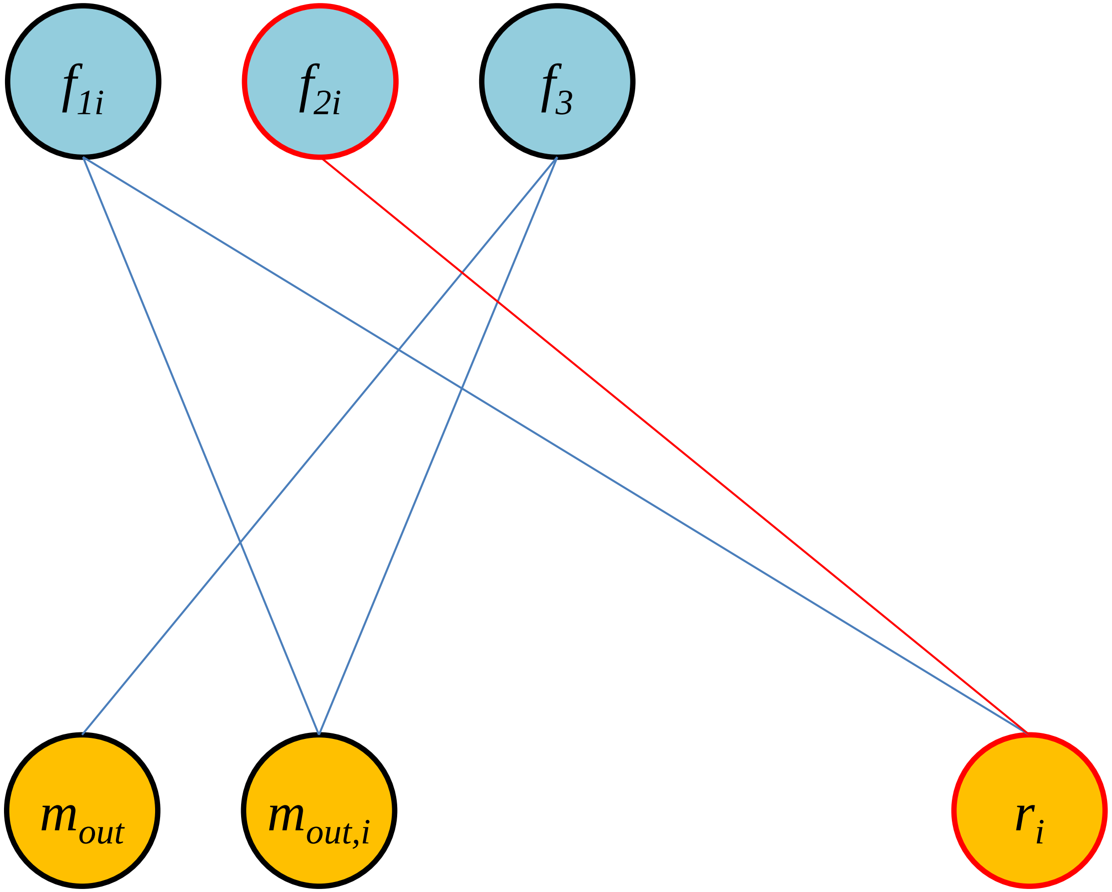
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$



Reactor de conversión fija (flujos x componentes - MS)

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

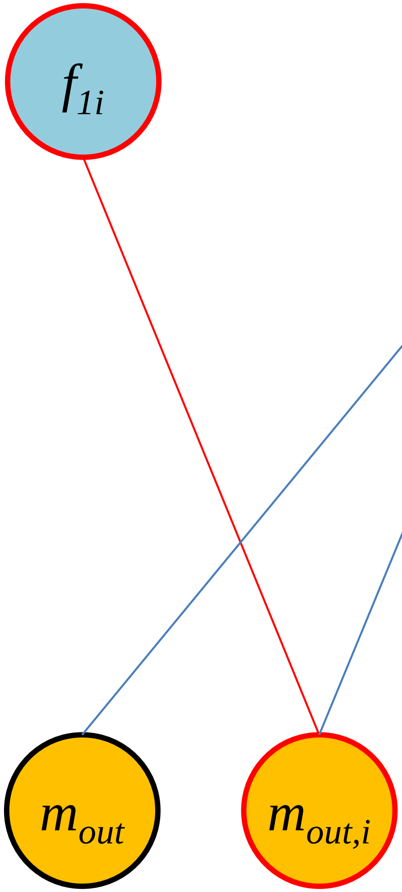
$f_6 \rightarrow H_{out}$ $\quad f_8 \rightarrow \rho_{out}$ $\quad f_{2i} \rightarrow r_i$



Reactor de conversión fija (flujos x componentes - MS)

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

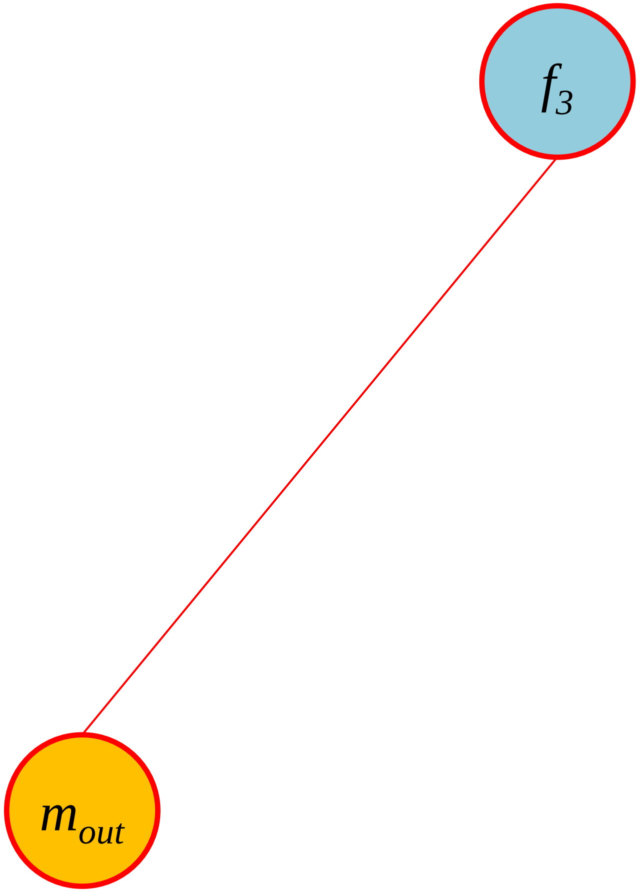
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$



Reactor de conversión fija (flujos x componentes - MS)

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

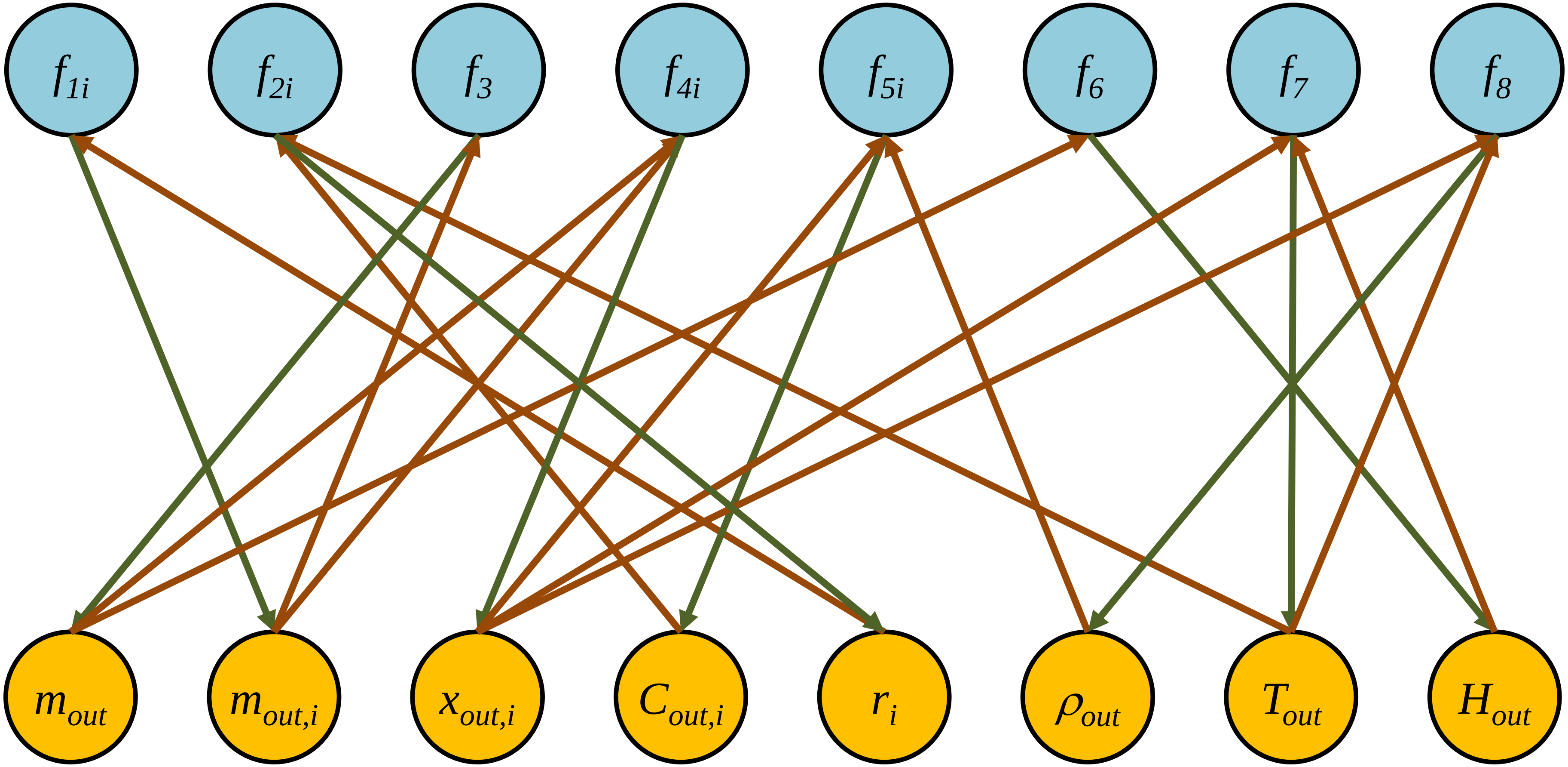
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$ $f_3 \rightarrow m_{out}$



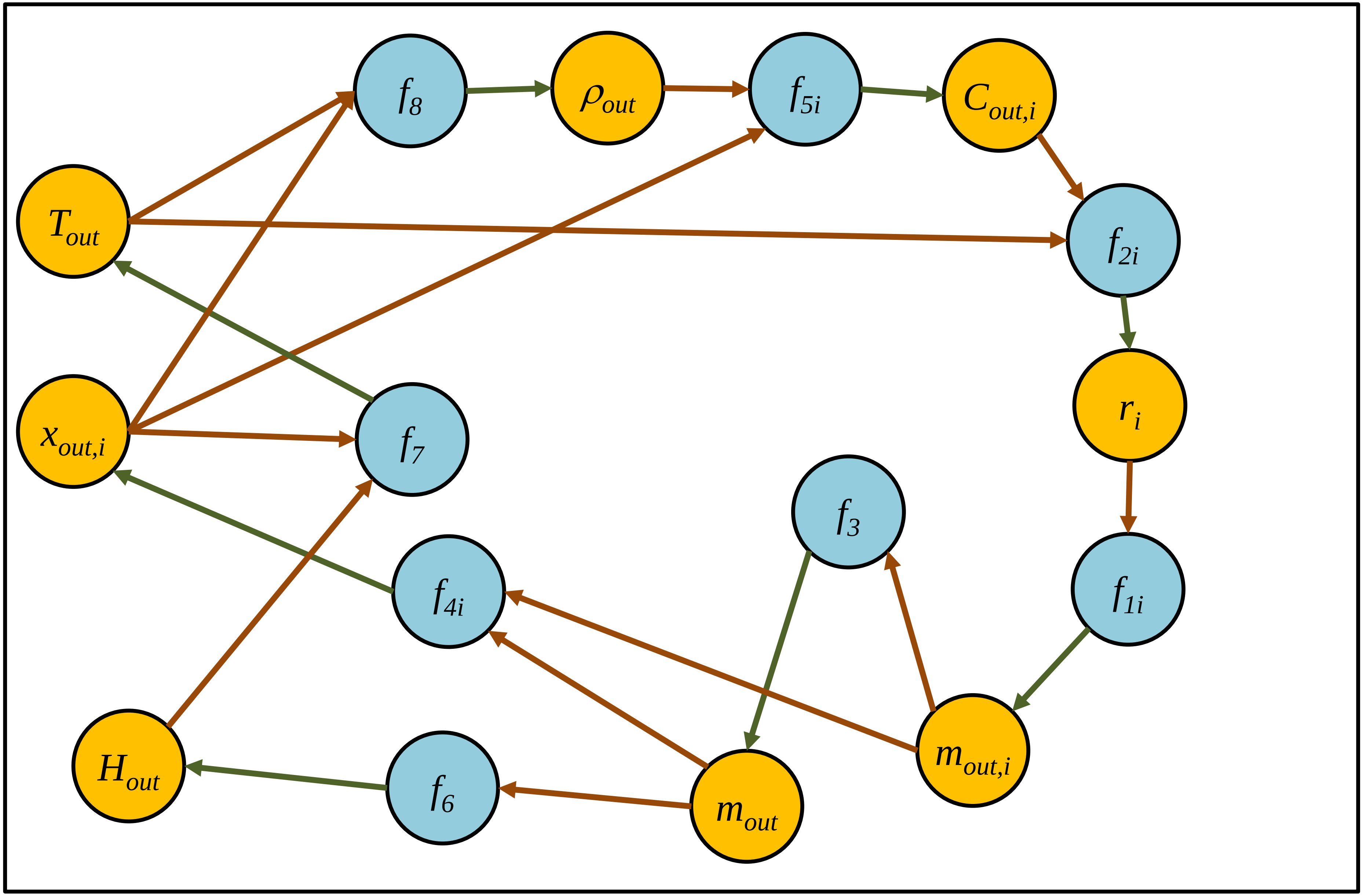
Reactor de conversión fija (flujos x componentes - MS)

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

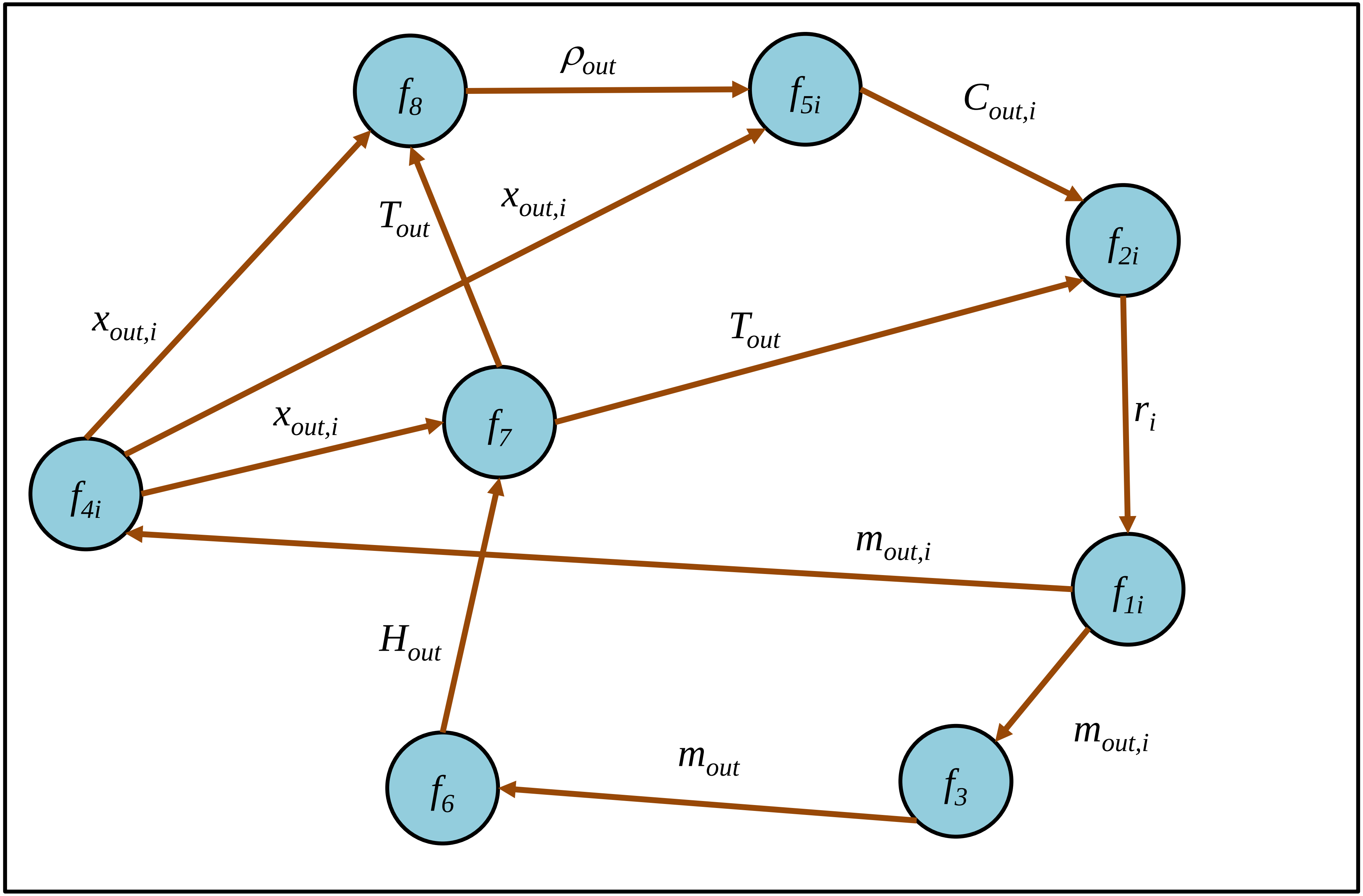
$f_6 \rightarrow H_{out}$ $f_8 \rightarrow \rho_{out}$ $f_{2i} \rightarrow r_i$ $f_3 \rightarrow m_{out}$



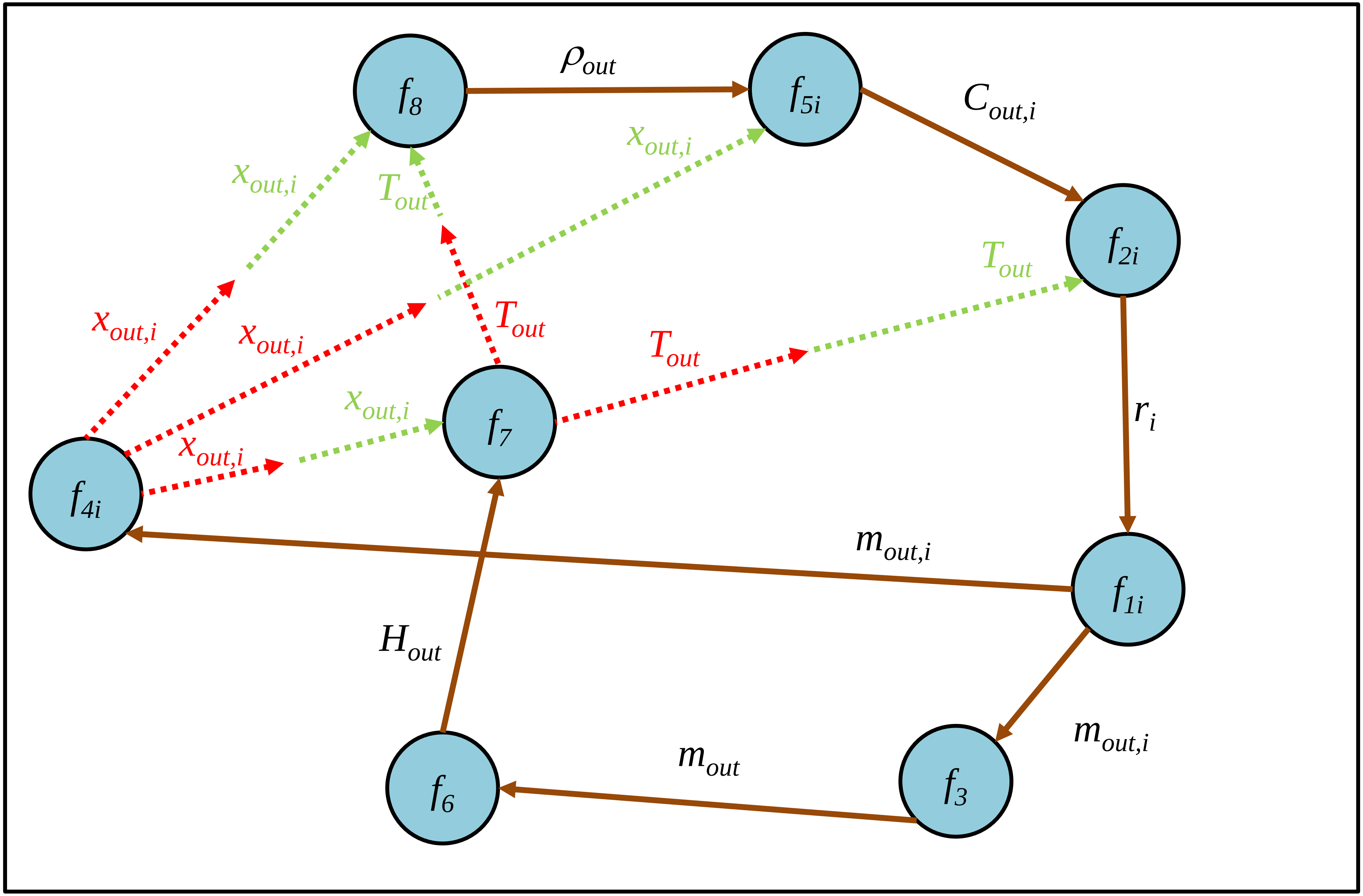
Reactor de conversión fija (flujos x componentes - MS)



Reactor de conversión fija (flujos x componentes - MS)



Reactor de conversión fija (flujos x componentes - MS)



CSTR – Ejercicio propuesto

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

$P_{in}:\quad 20\ bar$

$T_{in}:\quad 330\, K$

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

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

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

$H_{in} = -145725.677$

$V = 3\ m^3$

$Q:0$

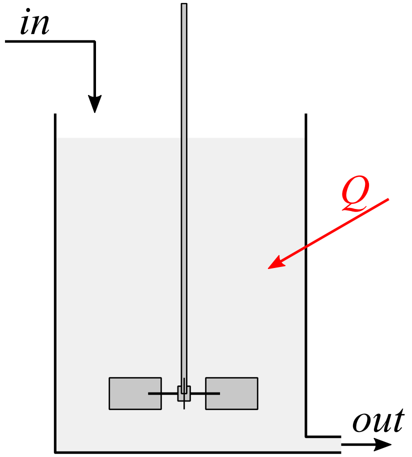
$P_{out}:20\ bar$

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

CSTR – Utilizando caudales

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



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

$$q_{in} \rho_{in} + V \sum_{i=1}^{NC} r_i - q_{out} \rho_{out} = 0$$

$$q_{in} \tilde{H}_{in} + Q - q_{out} \tilde{H}_{out} = 0$$

$$f\left(T_{in}, P_{in}, \tilde{H}_{in}, C_{in} \right) = 0$$

$$f\left(T_{out}, P_{out}, \tilde{H}_{out}, C_{out} \right) = 0$$

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

$$f\left(T_{in}, P_{in}, \rho_{in}, C_{in} \right) = 0$$

$q_{in} \;\; C_{in,i} \;\; r_i \;\; V \;\; q_{out} \;\; C_{out,i}$

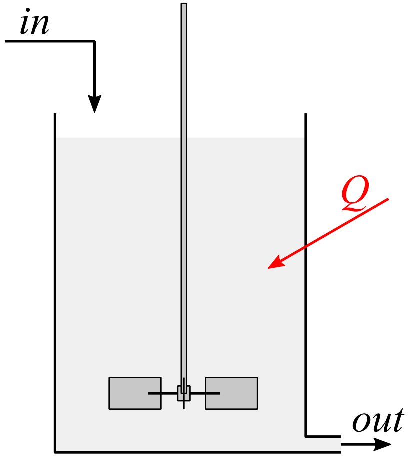
$\tilde{H}_{in} \;\; T_{in} \;\; P_{in} \;\; \tilde{H}_{out} \;\; T_{out} \;\; P_{out} \;\; Q$

$\rho_{in} \;\; \rho_{out}$

Debemos calcular las entalpías en unidades consistentes (por unidad de volumen)

CSTR – Utilizando caudales (MS)

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



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

$$q_{in} \rho_{in} + V \sum_{i=1}^{NC} r_i - q_{out} \rho_{out} = 0$$

$$r_i \quad V \quad q_{out} \quad C_{out,i}$$

$$\tilde{H}_{out} \quad T_{out} \quad P_{out} \quad \rho_{out} \quad Q$$

$$q_{in} \tilde{H}_{in} + Q - q_{out} \tilde{H}_{out} = 0$$

$$f \left(T_{out}, P_{out}, \tilde{H}_{out}, C_{out} \right) = 0$$

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

CSTR – Utilizando caudales (MS)

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

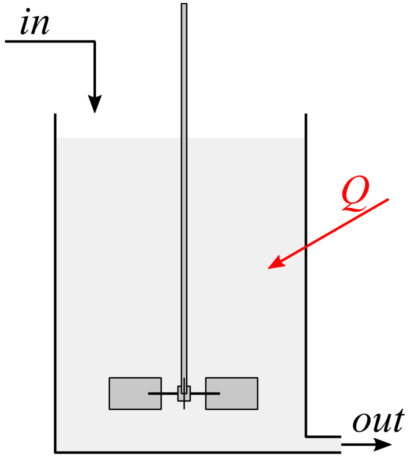
$$r_i = \sum_{j=1}^{NR} a_{ij}\, f\left(T_{out}, C_{out}\right) \quad \forall i$$

$$q_{in}\rho_{in} + V\sum_{i=1}^{NC} r_i - q_{out}\rho_{out} = 0$$

$$q_{in}\tilde{H}_{in} + Q - q_{out}\tilde{H}_{out} = 0$$

$$f\left(T_{out}, P_{out}, \tilde{H}_{out}, C_{out}\right) = 0$$

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



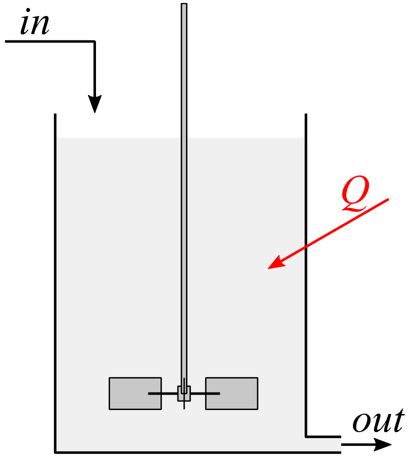
$r_i \;\; V \;\; q_{out} \;\; C_{out,i}$

$\tilde{H}_{out} \;\; T_{out} \;\; P_{out} \;\; \rho_{out} \;\; Q$

$$\begin{array}{rr} & 7+2NC \\ - & 4+2NC \\ \hline & GL=3 \end{array}$$

CSTR – Utilizando caudales (adiabático o calor dado)

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



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

$$q_{in}\tilde{H}_{in} + Q - q_{out}\tilde{H}_{out} = 0$$

$$r_i \enclose{circle}{V} q_{out} \quad C_{out,i}$$

$$q_{in}\rho_{in} + V\sum_{i=1}^{NC} r_i - q_{out}\rho_{out} = 0$$

$$\tilde{H}_{out} \quad T_{out} \quad \enclose{circle}{P_{out}} \; \rho_{out} \enclose{circle}{Q}$$

$$f\left(T_{out}, P_{out}, \tilde{H}_{out}, C_{out}\right) = 0$$

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

CSTR – Utilizando caudales (isotérmico)

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

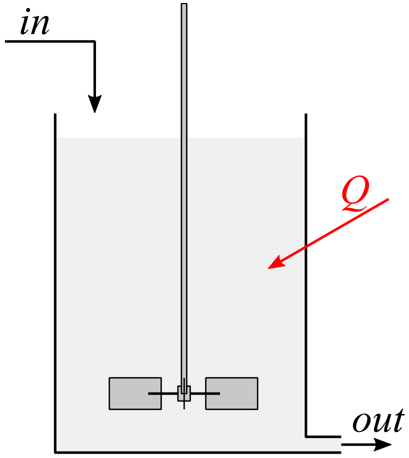
$$r_i = \sum_{j=1}^{NR} a_{ij} f\left(T_{out}, C_{out}\right) \quad \forall i$$

$$q_{in} \tilde{H}_{in} + Q - q_{out} \tilde{H}_{out} = 0$$

$$q_{in} \rho_{in} + V \sum_{i=1}^{NC} r_i - q_{out} \rho_{out} = 0$$

$$f\left(T_{out}, P_{out}, \tilde{H}_{out}, C_{out}\right) = 0$$

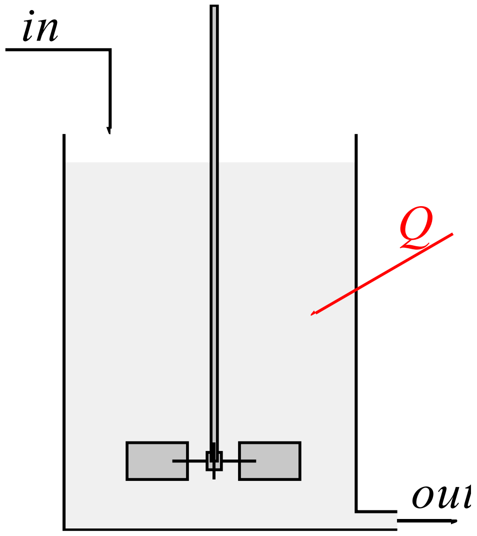
$$f\left(T_{out}, P_{out}, \rho_{out}, C_{out}\right) = 0$$



$$r_i \quad \boxed{V} \quad q_{out} \quad C_{out,i}$$

$$\tilde{H}_{out} \quad \boxed{T_{out}} \quad \boxed{P_{out}} \quad \rho_{out} \quad Q$$

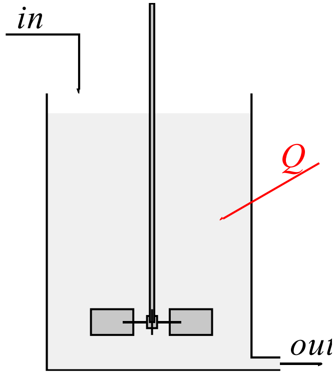
Tanque de almacenamiento de una entrada y salida gravitatoria por orificio



Hipótesis:

- Estado estacionario
- Tanque mezcla completa
- No hay reacciones químicas
- No hay cambios de fase
- Tanque cilíndrico de base circular (área: A_T)
- Orificio de salida (área: A_o)

Tanque de almacenamiento de una entrada y salida gravitatoria por orificio



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

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

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

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

Bernoulli en la superficie y salida:

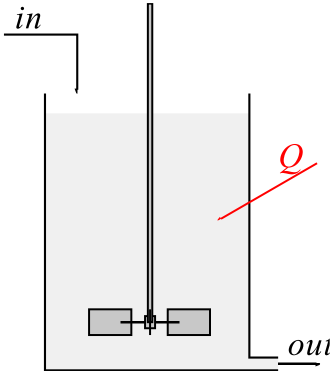
$$\cancel{\frac{v_h^{2} \rho_{out}}{2}} + \cancel{P_h} + \rho_{out} g h = \frac{v_o^{2} \rho_{out}}{2} + \cancel{P_o} + \cancel{\rho_{out} g h_o}$$

$v_h = 0$ $\qquad$ $P_h = P_s$ $\qquad$ $h_o = 0$

$$\rho_{out} g h = \frac{v_o^{2} \rho_{out}}{2} \rightarrow v_o = \sqrt{2gh}$$

$$m_{out} = \rho_{out} A_o v_o \rightarrow m_{out} = \rho_{out} A_o \sqrt{2gh}$$

Tanque de almacenamiento de una entrada y salida gravitatoria por orificio



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

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

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

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

$$m_{out} = \rho_{out} A_s \sqrt{2gh}$$

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

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

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

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

Tanque de almacenamiento de una entrada y salida gravitatoria por orificio (MS)

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

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

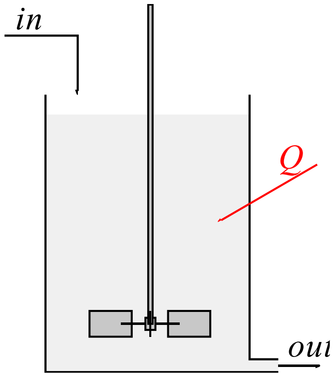
$$m_{out,i} = m_{out} x_{out,i} \qquad \forall i$$

$$m_{out} = \rho_{out} A_s \sqrt{2gh}$$

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

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

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



$$m_{out} \quad T_{out} \quad \boxed{P_{out}} \quad H_{out} \quad \boxed{Q}$$

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

7+2NC

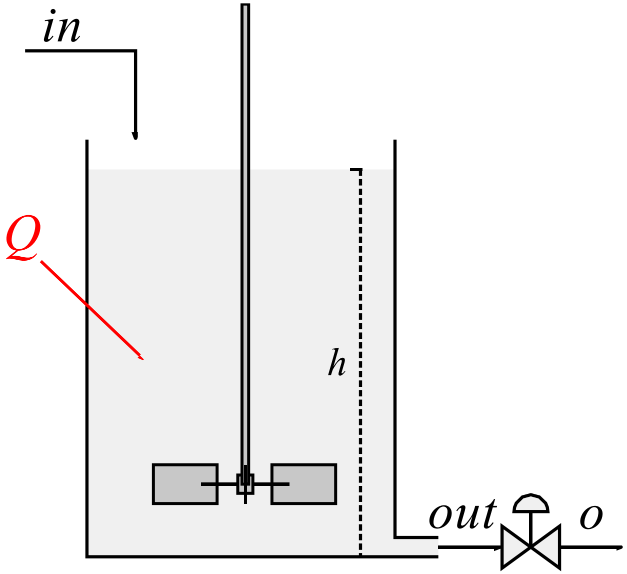
–

5+2NC

GL =2

Proponer secuencias de resolución y variables a especificar aplicando los algoritmos vistos en clase

Tanque de almacenamiento de una entrada y salida gravitatoria por válvula



Hipótesis:

- Estado estacionario
- Tanque mezcla completa
- No hay reacciones químicas
- No hay cambios de fase
- Tanque cilíndrico de base circular (área: A_T)
- Válvula de salida conocida

Modelos simples de válvulas

$$q = C_v \sqrt{\frac{\Delta P}{\rho}}$$

$q \rightarrow$ Caudal volumetrico que atravieza la válvula $\left[m^3/seg \right]$

$\Delta P \rightarrow$ Diferencia de presión a traves de la válvula $\left[Pa \right]$

$\rho \rightarrow$ Densidad del fluido $\left[kg/m^3 \right]$

$C_v \rightarrow$ Coeficiente caracteristico de la válvula $\left[m^2 \right]$

- Ecuación valida para líquidos
- Con baja variación de presión puede utilizarse en gases
- El predominio histórico de los fabricantes de válvulas en Estados Unidos ha llevado a que las características de las válvulas se den a menudo en unidades estadounidenses. Para gases suele utilizarse la misma ecuación pero con la gravedad especifica referenciada al aire y el caudal expresado de forma estándar.

$$q^* = C_v^* \sqrt{\frac{\Delta P^*}{G}}$$

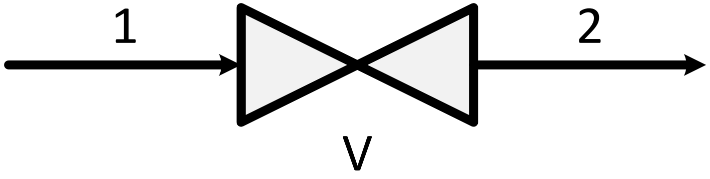
$q^* \rightarrow$ Caudal volumetrico que atravieza la válvula $\left[US\ gpm \right]$

$\Delta P^* \rightarrow$ Diferencia de presión a traves de la válvula $\left[psi \right]$

$G \rightarrow$ Gravedad específica del fluido $\rho / \rho_{60^\circ F}^{agua}$ $\left[adim \right]$

$C_v^* \rightarrow$ Capacidad de la valvula para agua a 60 ºF $\left[US\ gpm/\sqrt{psi} \right]$

Modelo de una Válvula



$$m_1 x_{1,i} - m_2 x_{2,i} = 0 \qquad \forall i$$

$$\sum_i x_{1,i} = 1$$

$$\sum_i x_{2,i} = 1$$

$$H_1 = H_2$$

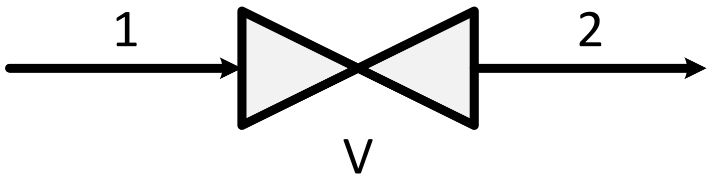
$$f\left(T_1, P_1, x_1, H_1\right) = 0$$

$$f\left(T_2, P_2, x_2, H_2\right) = 0$$

$$q_1 = C_v \sqrt{\frac{\Delta P}{\rho_1}} \rightarrow m_1 = \rho_1 C_v \sqrt{\frac{\Delta P}{\tilde{\rho}_1}} \qquad f\left(T_1, P_1, x_1, \rho_1\right) = 0$$

Modelo de una Válvula (MS)

$$m_1 x_{1,i} - m_2 x_{2,i} = 0 \qquad \forall i$$



$$\sum_i x_{2,i} = 1$$

$$H_1 = H_2$$

$$m_2 \quad x_{2,i} \quad T_2 \quad P_2 \quad H_2$$

$$f\left(T_2, P_2, x_2, H_2\right) = 0$$

$$m_1 = \rho_1 C_v \sqrt{\frac{P_1 - P_2}{\tilde{\rho}_1}}$$

4+NC

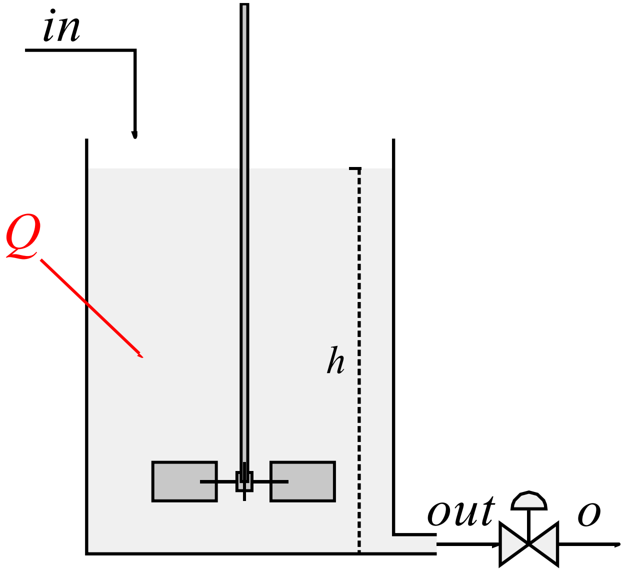
−

4+NC

GL =0

Tanque de almacenamiento de una entrada y salida gravitatoria por válvula

$$q_{out} = C_v \sqrt{\frac{\Delta P}{\tilde{\rho}_{out}}}$$



$$\Delta P = P_{out} - P_o$$

$$q_{out} = C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

Presión de descarga

$$m_{out} = \rho_{out} q_{out} \rightarrow m_{out} = \rho_{out} C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

$$P_{out} = P_s + \tilde{\rho}_{out} g h$$

Presión en la superficie

Tanque de almacenamiento de una entrada y salida gravitatoria por válvula

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

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

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

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

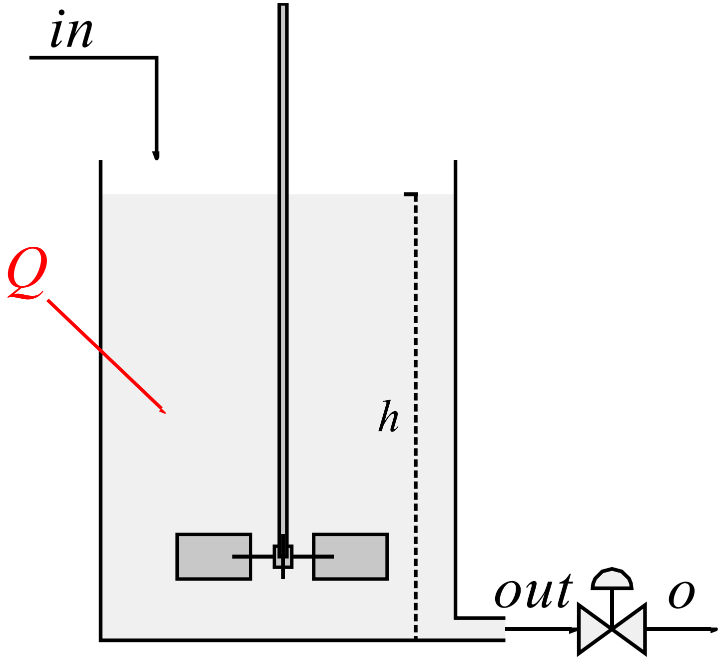
$$m_{out} = \rho_{out} C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

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

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

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

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \qquad P_{out} = P_s + \tilde{\rho}_{out} g h$$



Tanque de almacenamiento de una entrada y salida gravitatoria por válvula (MS)

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

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

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

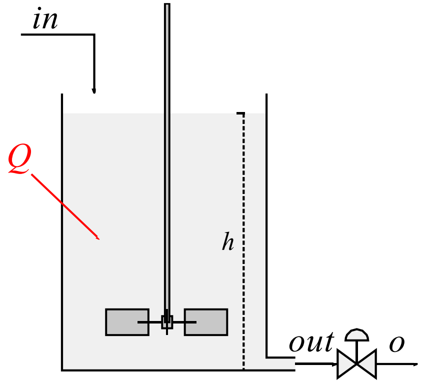
$$m_{out} = \rho_{out} C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

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

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

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

$$P_{out} = P_s + \tilde{\rho}_{out} g h$$



$$m_{out} \quad T_{out} \quad P_{out} \quad H_{out} \quad \boxed{Q}$$

$$\rho_{out} \quad h \quad x_{out,i} \quad m_{out,i} \quad \boxed{P_o}$$

$$\boxed{P_S}$$

9+2NC

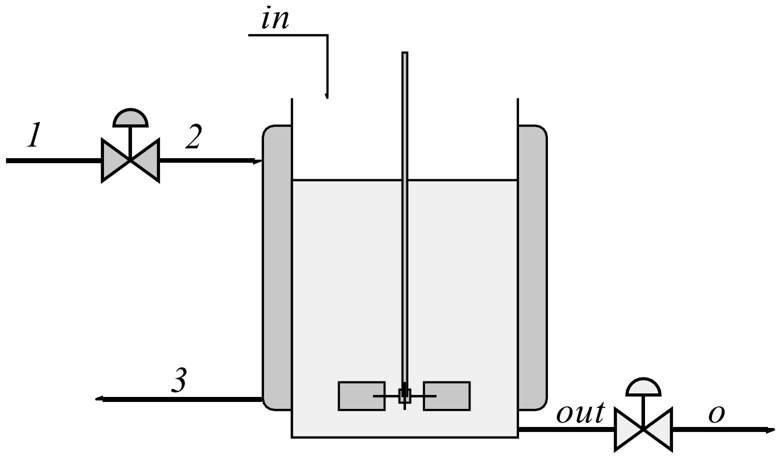
−

6+2NC

GL =3

Proponer secuencias de resolución y variables a especificar aplicando los algoritmos vistos en clase

Tanque de almacenamiento de una entrada y salida gravitatoria por válvula con camisa de enfriamiento



Hipótesis:

- Estado estacionario
- Tanque y camisa de enfriamiento mezcla completa
- No hay reacciones químicas
- No hay cambios de fase
- Tanque cilíndrico de base circular (área: A_T)
- Válvulas conocidas

Balances del lado del tanque

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

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

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

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

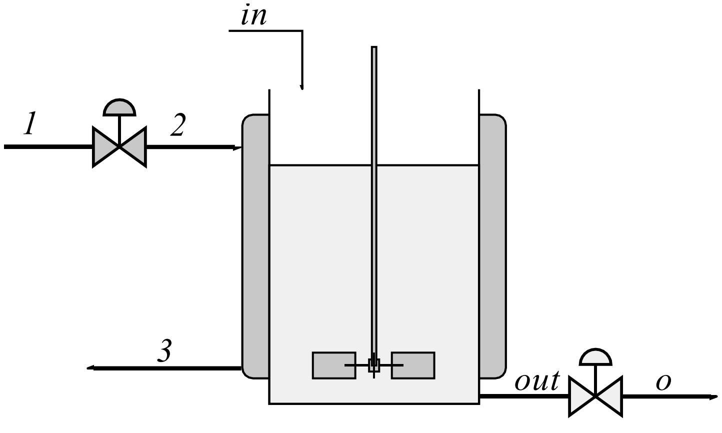
$$m_{out} = \rho_{out} C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

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

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

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

$$f\left(T_{in}, P_{in}, H_{in}, x_{in}\right) = 0 \qquad P_{out} = P_s + \tilde{\rho}_{out} g h$$



Del lado del tanque no cambia nada

Balances del lado de la camisa

$$m_{1,i} - m_{2,i} = 0 \qquad \forall i$$

$$m_{1,i} = m_1 x_{1,i} \qquad \forall i$$

$$m_{2,i} = m_2 x_{2,i} \qquad \forall i$$

$$m_1 = \sum_{i=1}^{NC} m_{1,i} \qquad m_2 = \sum_{i=1}^{NC} m_{2,i}$$

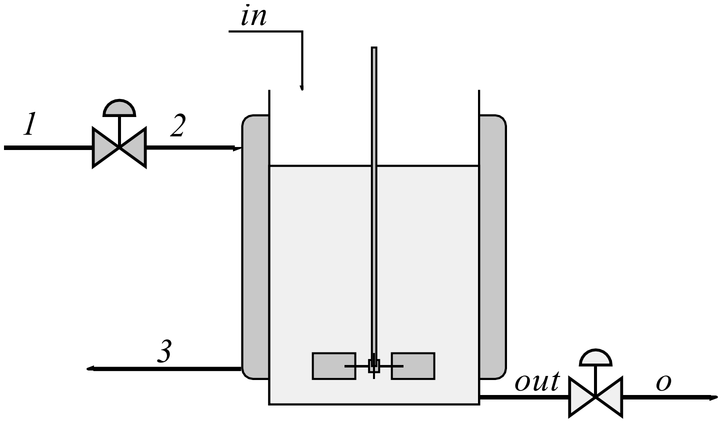
$$H_1 = H_2$$

$$f\left(T_1, P_1, H_1, x_1\right) = 0$$

$$f\left(T_2, P_2, H_2, x_2\right) = 0$$

$$m_1 = \rho_1 C_v \sqrt{\frac{P_1 - P_2}{\tilde{\rho}_1}}$$

$$f\left(T_1, P_1, x_1, \rho_1\right) = 0$$



$$m_{2,i} - m_{3,i} = 0 \qquad \forall i$$

$$m_{3,i} = m_3 x_{3,i} \qquad \forall i$$

$$m_2 = \sum_{i=1}^{NC} m_{3,i}$$

El calor es opuesto al que cede o pierde el tanque

$$m_2 H_2 \boxed{-Q} - m_3 H_3 = 0$$

$$f\left(T_3, P_3, H_3, x_3\right) = 0$$

Tanque de almacenamiento de una entrada y salida gravitatoria por válvula con camisa de enfriamiento (MS)

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

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

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

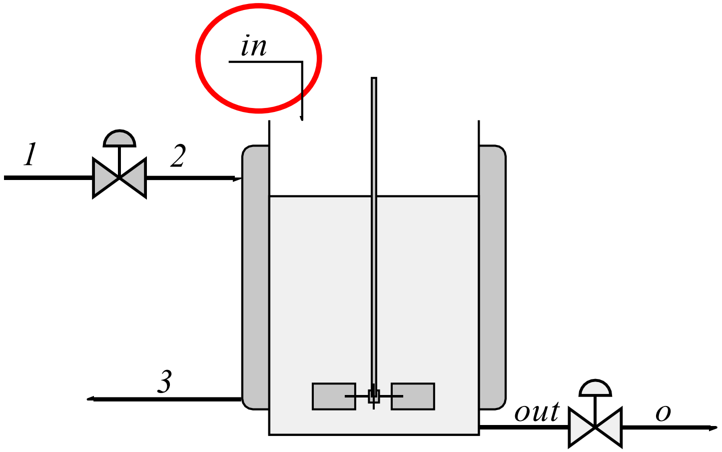
$$m_{out} = \rho_{out} C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

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

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

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

$$P_{out} = P_s + \tilde{\rho}_{out} g h$$



Ecuaciones:
6+2NC

Tanque de almacenamiento de una entrada y salida gravitatoria por válvula con camisa de enfriamiento (MS)

$$m_{1,i} - m_{2,i} = 0 \qquad \forall i$$

$$m_{2,i} = m_2 x_{2,i} \qquad \forall i$$

$$m_2 = \sum_{i=1}^{NC} m_{2,i}$$

$$H_1 = H_2$$

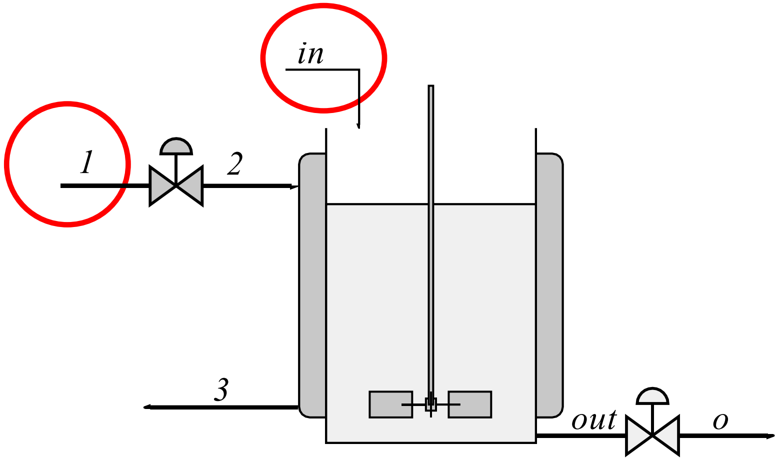
$$f\left(T_2, P_2, H_2, x_2\right) = 0$$

$$m_1 = \rho_1 C_v \sqrt{\frac{P_1 - P_2}{\tilde{\rho}_1}}$$

$$m_{2,i} - m_{3,i} = 0 \qquad \forall i$$

$$m_{3,i} = m_3 x_{3,i} \qquad \forall i$$

$$m_2 = \sum_{i=1}^{NC} m_{3,i}$$



Ecuaciones: 7+4NC

$$m_2 H_2 - Q - m_3 H_3 = 0$$

$$f\left(T_3, P_3, H_3, x_3\right) = 0$$

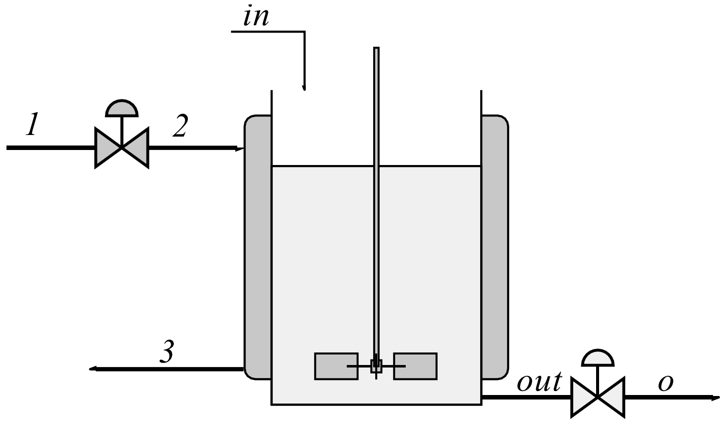
Tanque de almacenamiento de una entrada y salida gravitatoria por válvula con camisa de enfriamiento (MS)

$$m_{out} \quad T_{out} \quad P_{out} \quad H_{out} \quad Q$$

$$\rho_{out} \quad h \quad x_{out,i} \quad m_{out,i} \quad P_o \quad P_s$$

$$m_2 \quad m_{2,i} \quad x_{2,i} \quad T_2 \quad H_2 \quad P_2$$

$$m_3 \quad m_{3,i} \quad x_{3,i} \quad T_3 \quad H_3 \quad P_3$$



Variables: 17+6NC

Ecuaciones: 13+6NC

GL: 4

Se puede relacionar P_3 con P_2 y reducir un grado de libertad

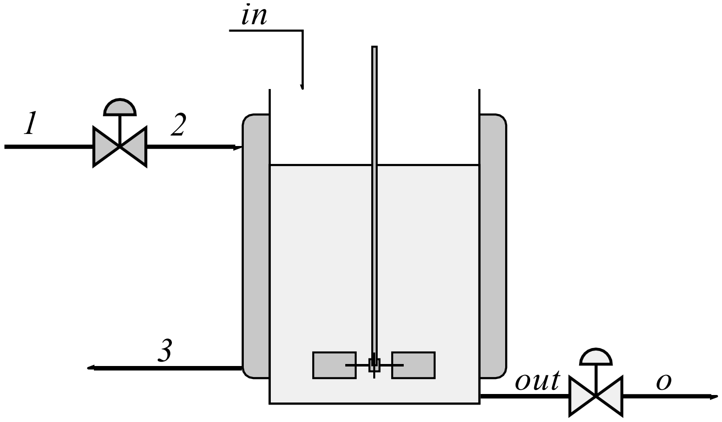
Tanque de almacenamiento de una entrada y salida gravitatoria por válvula con camisa de enfriamiento (MS)

$$m_{out} \quad T_{out} \quad P_{out} \quad H_{out} \quad Q$$

$$\rho_{out} \quad h \quad x_{out,i} \quad m_{out,i} \enclose{circle}{P_o} \enclose{circle}{P_s}$$

$$m_2 \quad m_{2,i} \quad x_{2,i} \quad T_2 \quad H_2 \quad P_2$$

$$m_3 \quad m_{3,i} \quad x_{3,i} \enclose{circle}{T_3} H_3 \enclose{circle}{P_3}$$

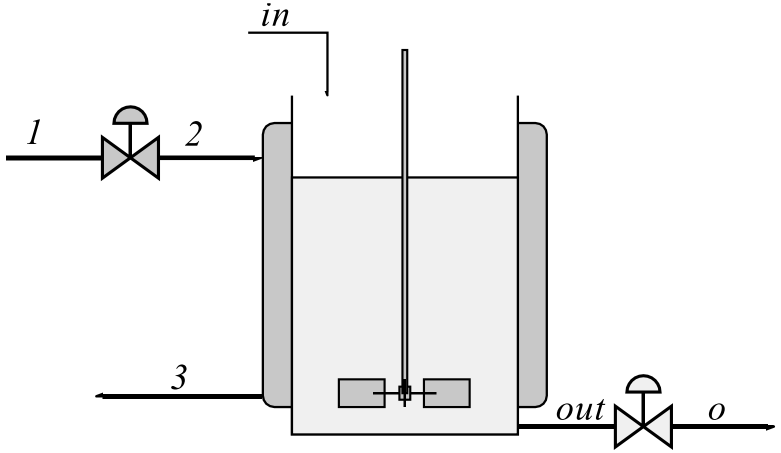


Variables: 17+6NC

Ecuaciones: 13+6NC

GL: 4

Reactor de una entrada y salida gravitatoria por válvula con camisa de enfriamiento



Hipótesis:

- Estado estacionario
- Tanque y camisa de enfriamiento mezcla completa
- Se conoce la cinética de las reacciones químicas
- No hay cambios de fase
- Tanque cilíndrico de base circular (área: A_T)
- Válvulas conocidas

Reactor de una entrada y salida gravitatoria por válvula con camisa de enfriamiento

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

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

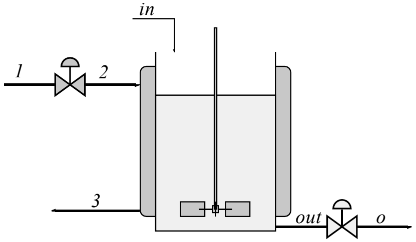
$$\sum_{i=1}^{NC} x_{in,i} = 1 \qquad \sum_{i=1}^{NC} x_{out,i} = 1$$

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

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

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

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



Solo se debe agregar la válvula y relacionar el volumen del reactor con su altura.

$$V = A_T h$$

$$m_{out} = \rho_{out} C_v \sqrt{\frac{P_{out} - P_o}{\tilde{\rho}_{out}}}$$

$$P_{out} = P_s + \tilde{\rho}_{out} g h$$

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

Reactor de una entrada y salida gravitatoria por válvula con camisa de enfriamiento (MS)

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

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

$$\sum_{i=1}^{NC}x_{out,i}=1 \qquad C_{out,i}=\rho_{out}x_{out,i}\ \forall i$$

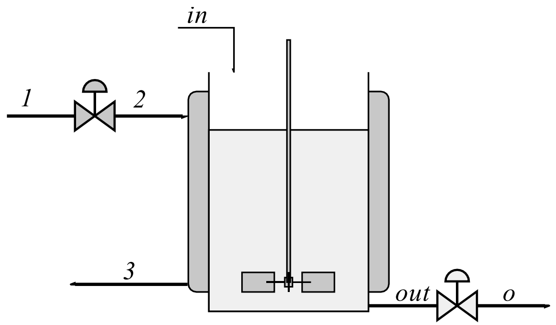
$$m_{in}H_{in}+Q-m_{out}H_{out}=0$$

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

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

$$P_{out}=P_s+\tilde{\rho}_{out}gh$$

$$V=A_Th \qquad m_{out}=\rho_{out}C_v\sqrt{\frac{P_{out}-P_o}{\tilde{\rho}_{out}}}$$



Ecuaciones: 7+3NC

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

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

$$Q \quad C_{out,i} \quad \rho_{out} \quad P_s \quad P_o$$

Variables: 10+3NC

Balances del lado de la camisa para el reactor

$$m_{1,i} - m_{2,i} = 0 \qquad \forall i$$

$$m_{1,i} = m_1 x_{1,i} \qquad \forall i$$

$$m_{2,i} = m_2 x_{2,i} \qquad \forall i$$

$$m_1 = \sum_{i=1}^{NC} m_{1,i} \qquad m_2 = \sum_{i=1}^{NC} m_{2,i}$$

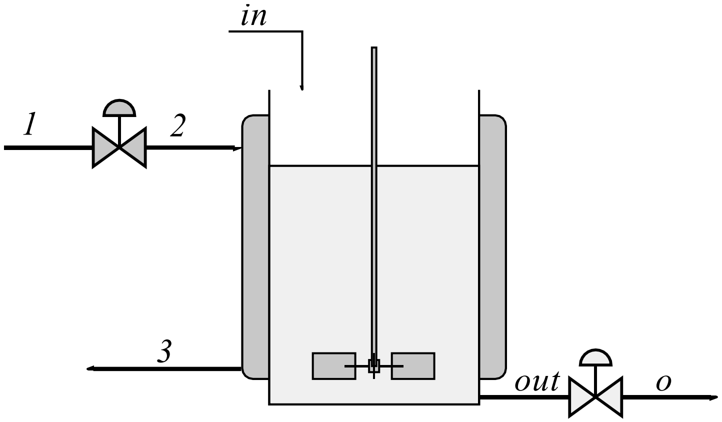
$$H_1 = H_2$$

$$f\left(T_1, P_1, H_1, x_1\right) = 0$$

$$f\left(T_2, P_2, H_2, x_2\right) = 0$$

$$m_1 = \rho_1 C_v \sqrt{\frac{P_1 - P_2}{\tilde{\rho}_1}}$$

$$f\left(T_1, P_1, x_1, \rho_1\right) = 0$$



$$m_{2,i} - m_{3,i} = 0 \quad \forall i$$

$$m_{3,i} = m_3 x_{3,i} \qquad \forall i$$

$$m_2 = \sum_{i=1}^{NC} m_{3,i}$$

El calor es opuesto al que cede o pierde el reactor.

$$m_2 H_2 \boxed{-Q} - m_3 H_3 = 0$$

$$f\left(T_3, P_3, H_3, x_3\right) = 0$$

Balances del lado de la camisa para el reactor (MS)

$$m_{1,i} - m_{2,i} = 0 \quad \forall i$$

$$m_{2,i} = m_2 x_{2,i} \quad \forall i$$

$$m_2 = \sum_{i=1}^{NC} m_{2,i}$$

$$H_1 = H_2$$

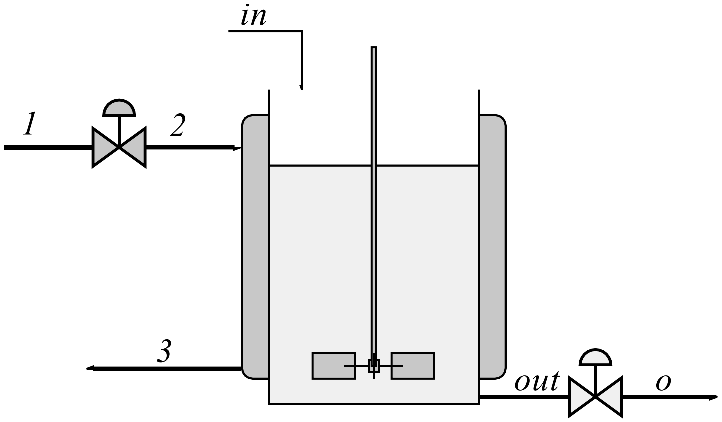
$$f\left(T_2, P_2, H_2, x_2\right) = 0$$

$$m_1 = \rho_1 C_v \sqrt{\frac{P_1 - P_2}{\tilde{\rho}_1}}$$

$$m_{2,i} - m_{3,i} = 0 \quad \forall i$$

$$m_{3,i} = m_3 x_{3,i} \quad \forall i \qquad m_2 H_2 - Q - m_3 H_3 = 0$$

$$m_2 = \sum_{i=1}^{NC} m_{3,i} \qquad f\left(T_3, P_3, H_3, x_3\right) = 0$$



$$m_2 \;\; m_{2,i} \;\; x_{2,i} \;\; T_2 \;\; H_2 \;\; P_2$$

$$m_3 \;\; m_{3,i} \;\; x_{3,i} \;\; T_3 \;\; H_3 \;\; P_3$$

Q ya esta contabilizada en el reactor

Ecuaciones: 7+4NC

Variables: 8+4NC

Reactor de una entrada y salida gravitatoria por válvula con camisa de enfriamiento

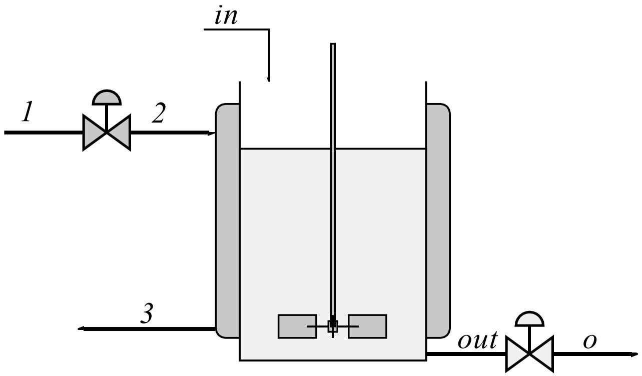
$r_i \quad V \quad m_{out} \quad x_{out,i}$

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

$Q \quad C_{out,i} \quad \rho_{out} \quad \boxed{P_s} \boxed{P_o}$

$m_2 \quad m_{2,i} \quad x_{2,i} \quad T_2 \quad H_2 \quad P_2$

$m_3 \quad m_{3,i} \quad x_{3,i} \quad \boxed{T_3} \quad H_3 \quad \boxed{P_3}$



Variables: 18+7NC

Ecuaciones: 14+7NC

GL: 4

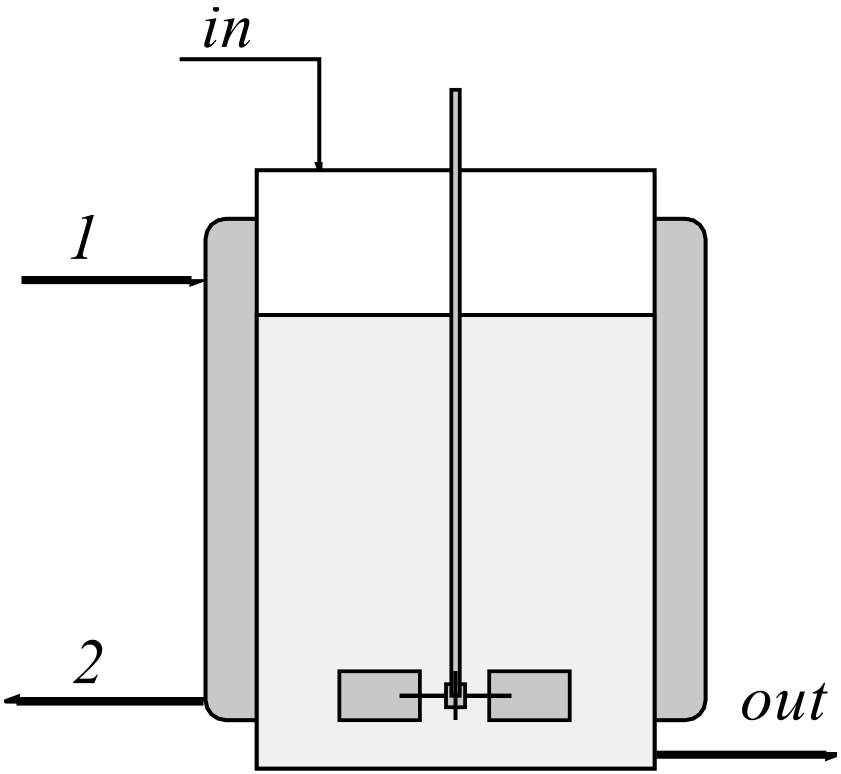
Ecuaciones: 7+3NC

Ecuaciones: 7+4NC

Variables: 10+3NC

Variables: 8+4NC

Ejemplo



$$A \leftrightarrow B + C$$

$$\left(-r_A\right) = k_D \times C_A - k_I \times C_B \times C_C$$

$$r_D = k_D \times C_A$$

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

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

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

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

Ejemplo

Hipótesis:

- Reacción reversible exotérmica
- Reactor Mezcla completa. La camisa de refrigeración también se considera mezcla completa.
- Los coeficientes cinéticos son conocidos ya que son función de la temperatura (funcional tipo Arrhenius).
- Hold up de vapor despreciable. Evaporación del líquido despreciable.
- Presión en el cuerpo de vapor del reactor es conocida.
- 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

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

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

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

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

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

La reacción es exotérmica, buscamos que el calor sea positivo

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

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

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

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

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

Utilizamos el calor de formación como entalpia de de referencia

Reactor CSTR (MS)

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

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

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

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

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

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

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

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

Variables: 20

Ecuaciones: 18

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

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

$$Q \;\; C_i \;\; \rho$$

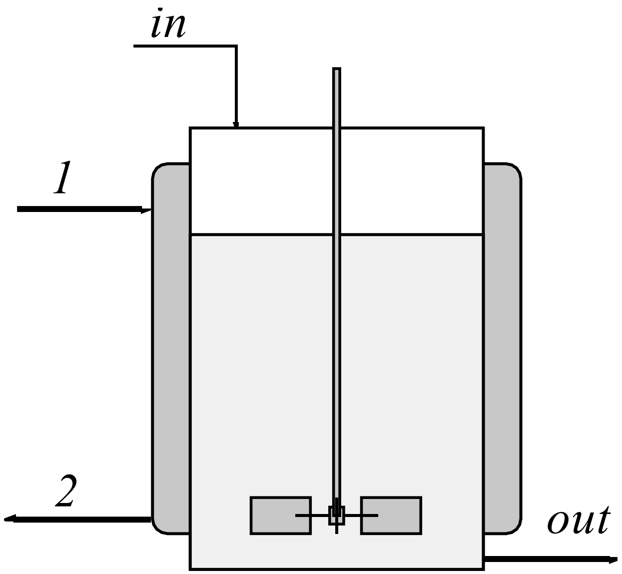
Balances del lado de la camisa para el reactor

$$m_1 - m_2 = 0$$

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

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

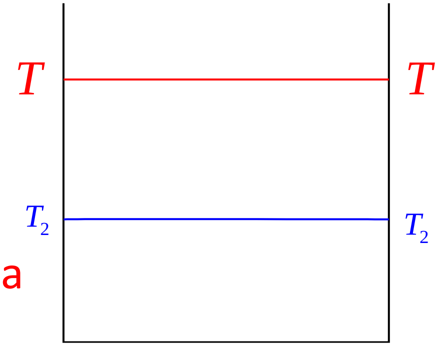
$$m_1 H_1 + Q - m_2 H_2 = 0$$



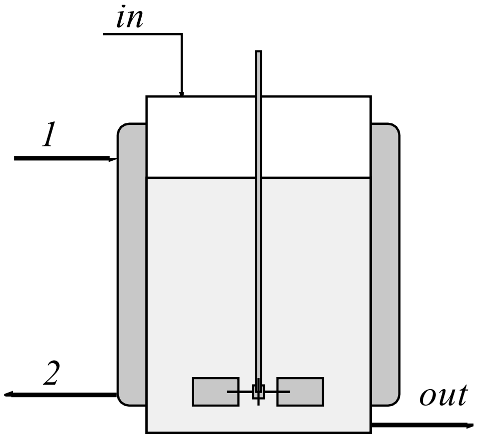
$$Q = UA\Delta t_c$$

$$\Delta t_c = T - T_2$$

Camisa mezcla completa



Balances del lado de la camisa para el reactor (MS)



$$m_1 - m_2 = 0$$

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

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

$$Q = UA\Delta t_c$$

$$\Delta t_c = T - T_2$$

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

Variables: 4

Ecuaciones: 5

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

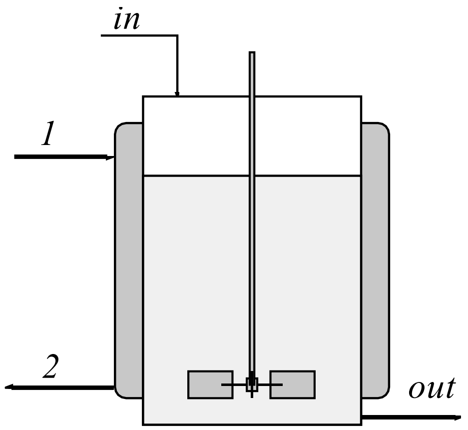
Balances del lado de la camisa para el reactor (MS)

$r_i \; \boxed{V} \; m \; m_i \; x_i$

$H \; T \; k_D \; k_I$

$Q \; C_i \; \rho$

$m_2 \; T_2 \; H_2 \; \Delta t_c$



Variables: 20

Ecuaciones: 18

Variables: 4

Ecuaciones: 5

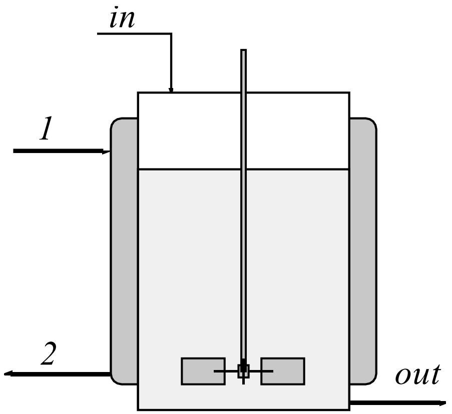
Variables: 24

Ecuaciones: 23

GL: 1

Estrategia de resolución

Propongo: T



Resuelvo el reactor CSTR isotérmico a la temperatura propuesta.

Calculamos la temperatura de salida de la camisa:

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

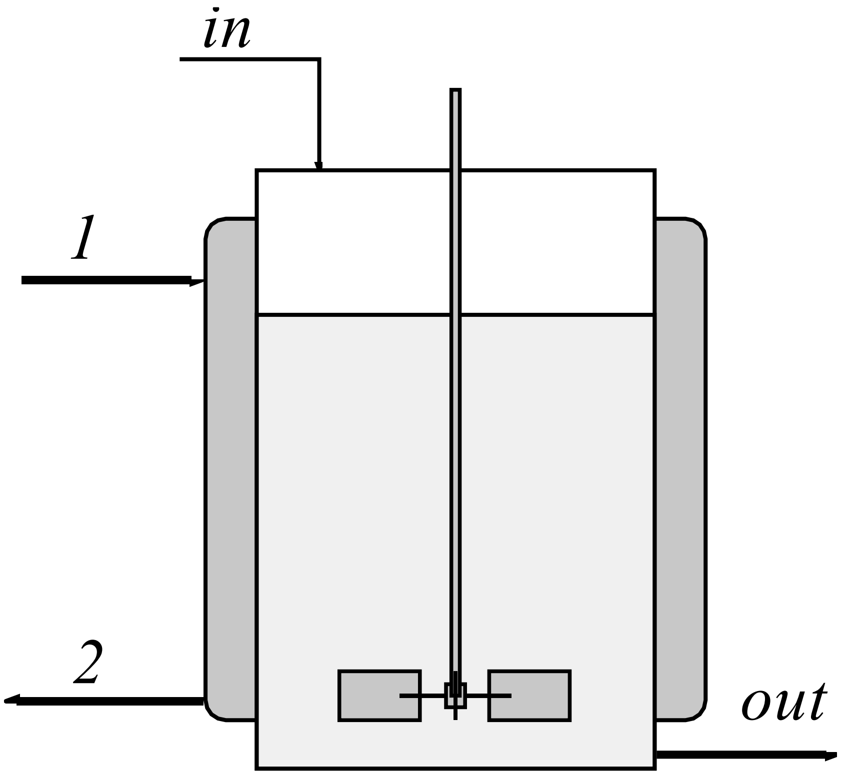
Chequemos la ecuación de transferencia de calor:

$$\Delta t_c = T - T_2$$

$$Q^* = UA\Delta t_c$$

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

Ejercicio



$$A \rightarrow 2B$$

$$r_D = k_D \times C_A$$

Ejemplo

Hipótesis:

- Reacción endotérmica.
- 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).
- Hold up de vapor despreciable. 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.