Supplementary data

The present file collects fundamental mass balances, which are utilized for the purpose of reactors' sizing.

BALANCE EQUATION FOR BATCH REACTORS

Balance equations for batch reactors:

$$\mathrm{V}\frac{\mathrm{dc}}{\mathrm{dt}} = -\mathrm{Vr(c)} \tag{S.1}$$

By dividing through by the volume V, we obtain:

$$\frac{\mathrm{dc}}{\mathrm{dt}} = -\mathrm{r(c)} \tag{S.2}$$

Let c_0 be the initial concentration and c the concentration inside the reactor. The conversion X can be defined as:

$$\mathrm{X} = \frac{c_0 - \mathrm{c}}{c_0} \tag{S.3}$$

Solving for c:

$$\mathrm{c} = c_0(1 - \mathrm{X}) \tag{S.4}$$

Substituting this into the mass balance equation:

$$c_0\frac{\mathrm{dX}}{\mathrm{dt}} = \mathrm{r(X)} \tag{S.2}$$

Since r is a function of c, it must be expressed as a function of X. Performing the integration yields:

$$\int_0^{\mathrm{X(t)}} \frac{\mathrm{dX}}{\mathrm{r(X)}} = \int_0^{\mathrm{t}} \frac{\mathrm{dt}}{c_0} \tag{S.3}$$

This is the final equation describing reagent conversions as a function of time. As shown in Eq. S.6, it is not possible to achieve this without considering kinetics.

BALANCE EQUATIONS FOR FED-BATCH REACTORS

The same balance can be applied for the dimensioning of fed-batch reactors. As discussed in the present study, the second step of the reaction can be directly analyzed using Equations S.1–S.6. However, the initial phase requires accounting for the contribution from the added flow rate:

$$\mathrm{V}\frac{\mathrm{dc}}{\mathrm{dt}} = \mathrm{F_0} - \mathrm{Vr(c)}$$

(4)

where F^0 represents the inlet flow rate of the sodium hydroxide solution. The mass flow rate entering the reactor is given by:

$$F_0 = \mathrm{Q}c_0$$

(5)

Thus, the equation becomes:

$$\frac{\mathrm{dc}}{\mathrm{dt}} = \mathrm{D}c_0 - \mathrm{r(c)}$$

(6)

where D is the dilution rate defined as $\mathrm{D} = \frac{\mathrm{Q}}{\mathrm{V}}$.

BALANCE EQUATIONS FOR CSTR

The dimensioning of CSTRs is based on steady-state conditions. The balance equation is:

$$0 = \mathrm{Q_0 c_0} - \mathrm{Qc} - \mathrm{r(c)V}$$

(7)

Solving for V:

$$\mathrm{V} = \frac{\mathrm{Q_0 c_0} - \mathrm{Qc}}{\mathrm{r(c)}}$$

(8)

Alternatively, in terms of conversion X:

$$\mathrm{V} = \frac{\mathrm{c_0(Q_0} - \mathrm{Q} + \mathrm{X})}{\mathrm{r(X)}}$$

(9)

Similarly, it is not possible to dimension the reactor without knowledge of the reaction kinetics.

BALANCE EQUATIONS FOR PFR

PFR dimensioning is undertaken performing the balance along the x-axis. Imposing the balance along the length between what is consumed and what is transferred by the flow:

$$\frac{\mathrm{dF}}{\mathrm{dx}} = -\mathrm{Sr(c)}$$

(10)

Explicating F as the product of the volume flow rate and the concentration:

$$\mathrm{Q}\frac{\mathrm{dc}}{\mathrm{dx}} = -\mathrm{Sr(c)}$$

(11)

$$\frac{dc}{dx} = -\frac{S}{Q} r(c) \tag{12}$$

Substituting:

$$X = \frac{c_0 - c}{c_0} \tag{13}$$

The equation becomes:

$$\frac{dX}{dx} = \frac{S}{Qc_0} r(X) \tag{14}$$

This can be solved using integration:

$$\int_0^{X(t)} \frac{dX}{r(X)} = \int_0^t \frac{S}{Qc_0} dx \tag{15}$$

This equation allows for the dimensioning of the reactor and monitoring of the conversion along the equipment.