Process Model Formulation and Solution, 3E4

Section A: Process modelling concepts

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A few announcements

TA office hours:

- Vote for best times

Tutorial groups:

- **Group A:** Anyone
- **Group B:** A $\rightarrow$ K
- **Group C:** L $\rightarrow$ Z

First tutorial: 14 and 15 September

- MATLAB/Python refresher
- Tutorial posted on the website
- Software tutorial on the website: demo

Please print a copy of the tutorial, or work from the website at the tutorial.

Mathematical modelling

WIKIPEDIA:

"A mathematical model uses mathematical language to describe a system" (as opposed to a physical system)

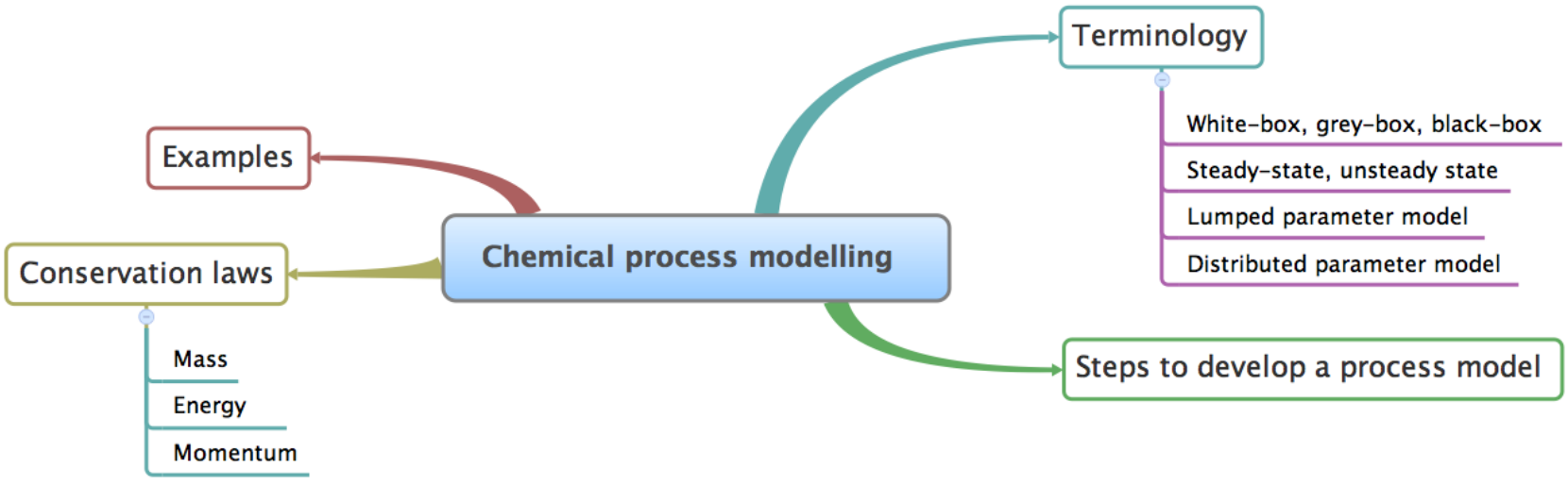
EYKHOFF (1974):

"A mathematical model is a representation of the essential aspects *of an existing system (or a system to be constructed) which presents knowledge of that system in* usable form*"*

GEORGE E. P. BOX:

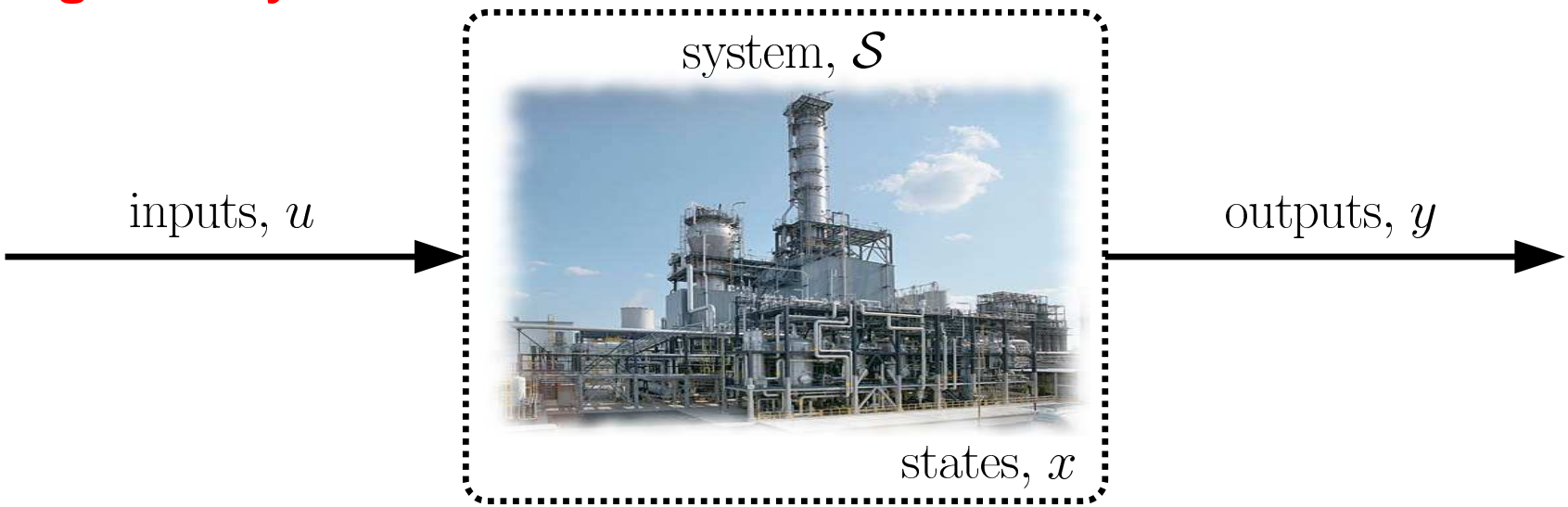
"[...] all models are approximations. Essentially, all models are wrong, but some are useful. However, the approximate nature of the model must always be borne in mind [...] "

Outline for this section



Notion of a process system

A general system



- **Process system:** A system in which physical and chemical processes are taking place; need to specify:
  1. boundaries
  2. inputs and outputs
  3. physico-chemical processes taking place

- **States:** Internal to the system; memory compressing all past input-output history

Mathematical model and modelling goals

A general mathematical model:

$$\begin{matrix}\text{dependent}\\ \text{variables } x, y\end{matrix} = \mathcal{M}\left(\begin{matrix}\text{independent}\\ \text{variables } t, z\end{matrix}, \text{ parameters } p, \begin{matrix}\text{input}\\ \text{variables } u\end{matrix}\right)$$

Typical modelling goals:

- **Steady-state/dynamic process simulation:** **3E04 + 3G04**
  - Given: (known) inputs u, model structure $\mathcal{M}$, model parameters p
  - Find: (predicted) outputs y
- **Process control:** **3P04 + 4E03**
  - Given: (desired) outputs y, model structure $\mathcal{M}$, model parameters p
  - Find: inputs u
- **Process design:** **3G04 + 4G03**
  - Given: (known) inputs u, (desired) outputs y, model structure $\mathcal{M}$
  - Find: model parameters p
- **System identification:** **4C03 + 4G03**
  - Given: (known) inputs u, (measured) outputs y
  - Find: model structure $\mathcal{M}$, model parameters p

Mathematical model structure, $\mathcal{M}$

Equation form of process models:

	steady-state problem	dynamic problem
lumped parameter	AEs	ODEs
distributed parameter	ODEs/PDEs	PDEs

AEs: Algebraic Eqs.
ODEs: Ordinary Differential Eqs.
PDEs: Partial Differential Eqs.

- These 4 types may use either linear or nonlinear equations

Modelling trade-offs:

- Reflect properties of the real system relevant to the modelling goals
- Be much cheaper and easier to handle than real system

Model classification (one viewpoint)

White-box models: (or **first-principles** models, or **mechanistic** models)

- Describe physico-chemical processes using *engineering knowledge*; e.g., conservation principles
- No direct use of measurement data
- Requires knowledge of physical constants (e.g. heat capacities, densities, *etc*)

Black-box models: (or **empirical** models)

- Describe physico-chemical processes using collected sets of *measurement data*; e.g., statistical methods
- No prior engineering knowledge of the system

Grey-box models: $\longleftarrow$ **most** practical process engineering models!

- Suitable *combination* of:
  - a priori engineering knowledge; e.g. model structure
  - measured data; e.g. kinetic and transport rates

Extra notes

See the Hangos and Cameron PDF download under *Suggested readings* on course website

Model development procedure

- **Step 1. Definition of the problem:**
  - inputs and outputs
  - desired accuracy, level of details, lumped vs. distributed, steady-state vs. dynamic

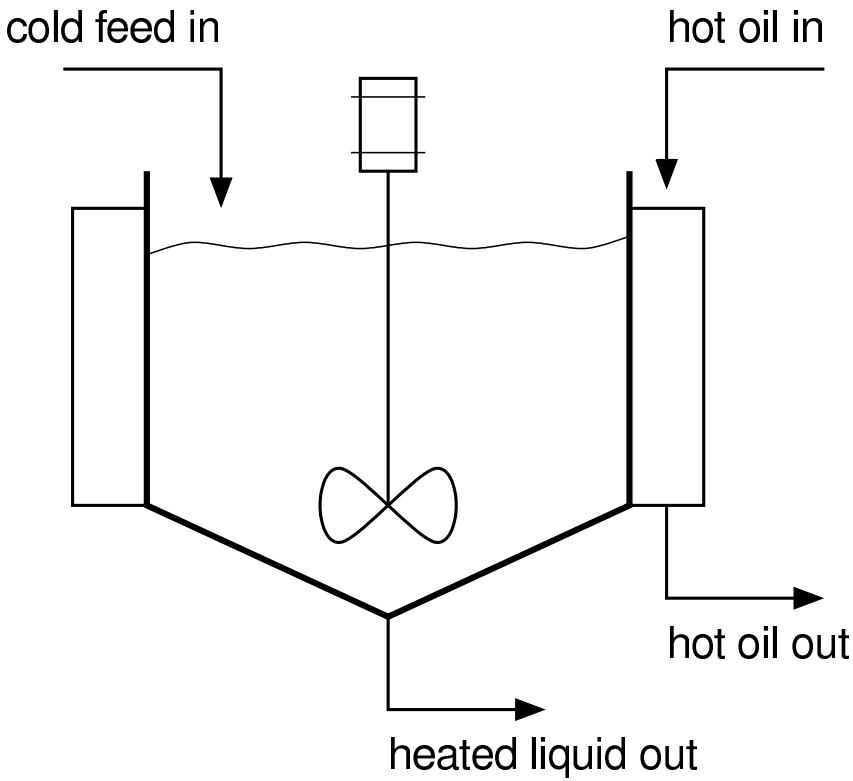
$$\begin{matrix}\text{dependent}\\ \text{variables } x, y\end{matrix} = \mathcal{M}\left(\begin{matrix}\text{independent}\\ \text{variables } t, z\end{matrix}, \text{ parameters } p, \begin{matrix}\text{input}\\ \text{variables } u\end{matrix}\right)$$

- **Step 2. Identification of the controlling mechanisms:**
  (those relevant to the modelling goal only!)
  - chemical reaction
  - diffusion of mass
  - conduction of heat
  - forced/free convection heat transfer
  - radiation heat transfer
  - turbulent mixing
  - fluid flow
  - evaporation

Example: Identifying key controlling mechanisms

Consider the modelling of a jacketed tank which is well-stirred and heated using a hot oil feed. The modelling goal is to predict the **dynamic** behaviour of the liquid **temperature** in the tank.

Question: Identify possible key controlling mechanisms?



Model development procedure (cont'd)

- **Step 3. Development of a set of model equations, $\mathcal{M}$:**
  Mixed set of differential equations (e.g., conservation balances) and algebraic equations (e.g., transfer rates, property relations)
- **3-a. System/subsystem boundary and balance volume**
  Identify where mass, energy, momentum is likely to accumulate

Example

What could be the relevant balance volumes to consider for the liquid heating system?

-
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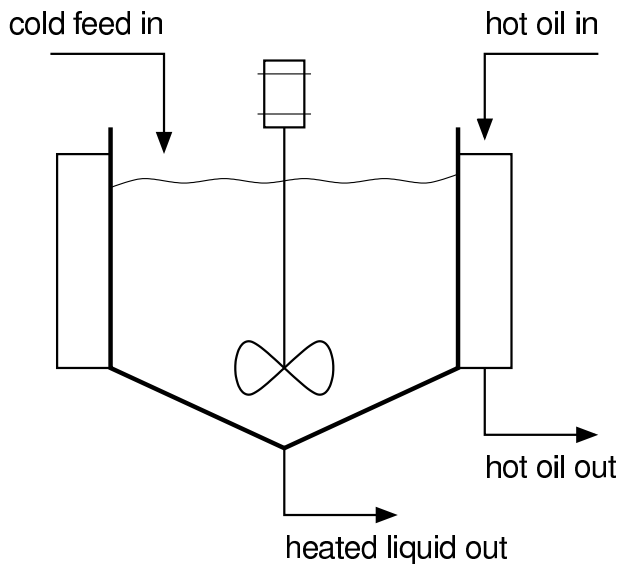


Model development procedure (cont'd)

- **Step 3. Development of a set of model equations, $\mathcal{M}$:**
  Mixed set of differential equations (e.g., conservation balances) and algebraic equations (e.g., transfer rates, property relations)

- **3-b. Define the characterizing variables**
  Inputs and outputs: flows, mass/molar conc., temperatures, pressures, etc.
  Internal states: related to the main mass, energy and momentum holdups
- **3-c. Establish the balance equations**
  Mass, energy and momentum balances for *each* subsystem
- **3.d. Specify the constitutive equations**
  Rate expressions: heat, mass and momentum transfer between subsystems
  Property relations: e.g., equations of states, physico-chemical properties
  Balance volume relations: if multiple phases are present
- **3.e. Modelling assumptions**
  Usually built up incrementally, in parallel to steps 3-a to 3-d.

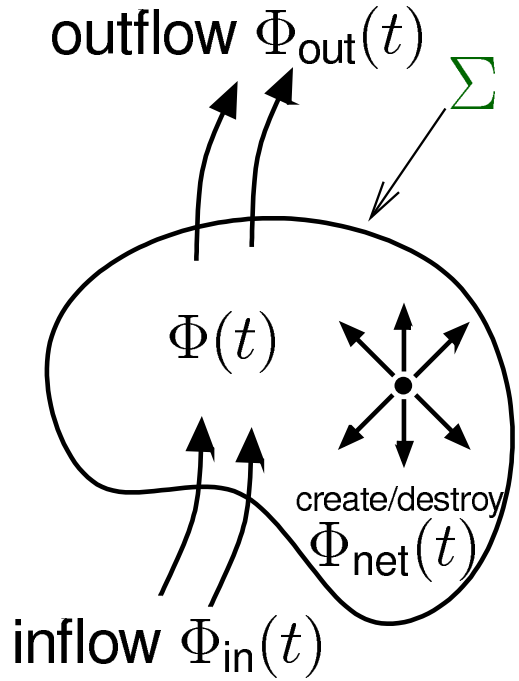
Conservation balances for lumped systems

General form:

- No spatial variation in states
- Leads to models represented by ODEs in time

$$\frac{\mathrm{d}\Phi(t)}{\mathrm{d}t} = \Phi_{\text{in}}(t) - \Phi_{\text{out}}(t) + \Phi_{\text{net}}(t)$$

$\Phi(t)$	conserved extensive quantity
$\frac{d\Phi(t)}{dt}$	rate of change of Φ
$\Phi_{\text{in}}(t)$	inflow of Φ into boundary Σ
$\Phi_{\text{out}}(t)$	outflow of Φ out of boundary Σ
Φ_{net}	net generation = created $\Phi(t)$ - destroyed $\Phi(t)$ within boundary Σ



Incremental model building:

1. Do an overall mass balance (a.k.a. total bass balance)
2. Do a mass balance for each component
3. Do an energy balance for each boundary

Conservation balances for mass

Total mass balance, $\Phi \triangleq$ mass $= M$

$$\left\{ \begin{array}{c} \text{rate of accum.} \\ \text{of mass} \end{array} \right\} = \left\{ \begin{array}{c} \text{mass flow} \\ \text{in} \end{array} \right\} - \left\{ \begin{array}{c} \text{mass flow} \\ \text{out} \end{array} \right\}$$

$$\frac{\mathrm{d}M(t)}{\mathrm{d}t} = \sum_{k=1}^{n^{\mathrm{in}}} F_k^{\mathrm{in}}(t) - \sum_{k=1}^{n^{\mathrm{out}}} F_k^{\mathrm{out}}(t) \quad \text{in [kg/s]}$$

Given initial condition: $M(t_0) = M^{(0)}$

Workshop

- Why **not** perform a *"conservation balance for volume"*?

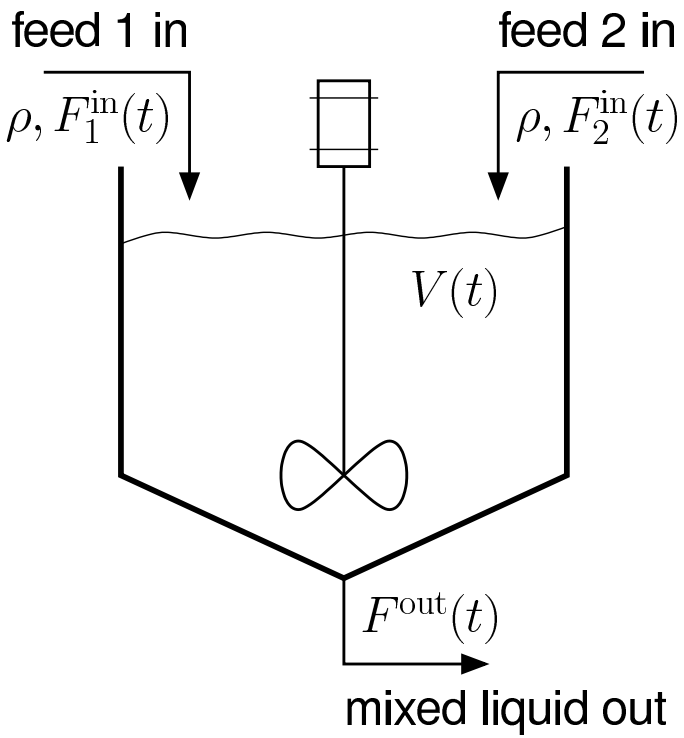
At steady-state ...

- Leads to an algebraic equation:

$$0 = \sum_{k=1}^{n^{\mathrm{in}}} F_k^{\mathrm{in}}(t) - \sum_{k=1}^{n^{\mathrm{out}}} F_k^{\mathrm{out}}(t) \qquad \text{units are in } \left[\frac{\text{mass}}{\text{time}}\right]$$

Example: Total mass balance in a stirred tank

Consider the modelling of a stirred tank, fed with two inlet streams.



Assumptions:

- Perfect mixing
- Equal and constant liquid densities

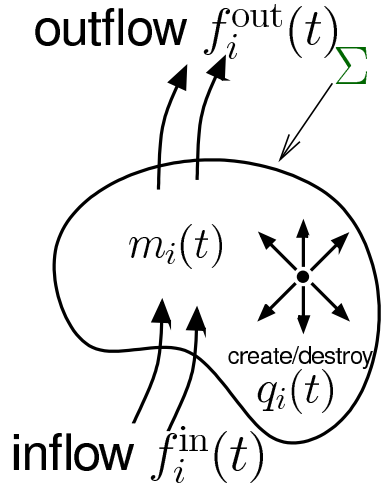
Modelling goals:

- Predict the dynamic behaviour of the liquid volume in the tank
- Which condition must hold at steady-state?

Conservation balances for mass (cont'd)

Component mass balances, $\Phi \triangleq m_i$, with $\sum_i m_i(t) = M(t)$

$$\left\{ \begin{array}{c} \text{rate of accum.} \\ \text{of species } i \end{array} \right\} = \left\{ \begin{array}{c} \text{mass flow} \\ \text{in of sp. } i \end{array} \right\} - \left\{ \begin{array}{c} \text{mass flow} \\ \text{out of sp. } i \end{array} \right\} + \left\{ \begin{array}{c} \text{rate of formation} \\ \text{of sp. } i \end{array} \right\}$$



$$\frac{\mathrm{d}m_i(t)}{\mathrm{d}t} = \sum_{k=1}^{n^{\text{in}}} f_{i,k}^{\text{in}}(t) - \sum_{k=1}^{n^{\text{out}}} f_{i,k}^{\text{out}}(t) + q_i(t)$$

Given initial condition: $m_i(t_0) = m_i^{(0)}$, with $f_{i,k}$ in $\left[\frac{\text{mass}}{\text{time}}\right]$

Component mole balances, $n_i \triangleq \frac{m_i}{W_i} = \frac{m_i}{\text{molar mass of } i}$

$$\frac{\mathrm{d}n_i(t)}{\mathrm{d}t} = \sum_{k=1}^{n^{\text{in}}} \tilde{f}_{i,k}^{\text{in}}(t) - \sum_{k=1}^{n^{\text{out}}} \tilde{f}_{i,k}^{\text{out}}(t) + \tilde{q}_i(t) \quad \text{with } \tilde{f}_{i,k} \text{ in } \left[\frac{\text{mol}}{\text{time}}\right]$$

Given initial condition: $n_i(t_0) = n_i^{(0)}$

Constitutive equations: reaction rates – Refresher

Reaction rate:

- Moles of sp. i formed/consumed per unit time and per unit volume,

$$r_i \triangleq \frac{1}{V}\frac{\mathrm{d}n_i}{\mathrm{d}t}, \qquad n_i\text{: moles of species } i$$

- Moles of sp. i formed/consumed per unit time, $\tilde{q}_i \triangleq r_i V$
- Mass of sp. i formed/consumed per unit time, $q_i \triangleq W_i r_i V$

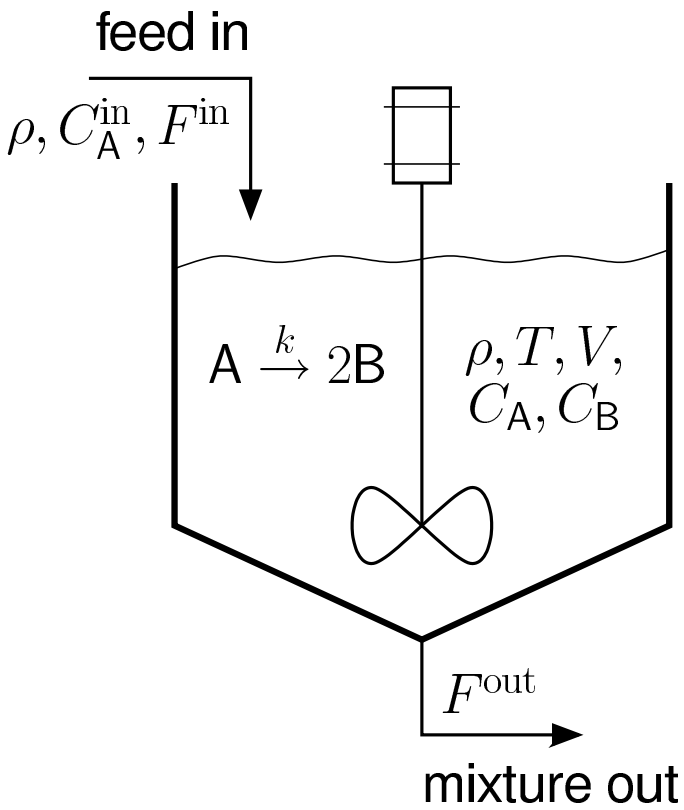
Overall reaction rate: $\nu_\mathrm{A}\mathrm{A} + \nu_\mathrm{B}\mathrm{B} \xrightarrow{r} \nu_\mathrm{C}\mathrm{C} + \nu_\mathrm{D}\mathrm{D}$

$$r \triangleq \frac{r_\mathrm{A}}{\nu_\mathrm{A}} = \frac{r_\mathrm{B}}{\nu_\mathrm{B}} = \frac{r_\mathrm{C}}{\nu_\mathrm{C}} = \frac{r_\mathrm{D}}{\nu_\mathrm{D}}, \quad \text{with:} \begin{cases} \text{reactants:} & \nu_\mathrm{A}, \nu_\mathrm{B} < 0 \\ \text{products:} & \nu_\mathrm{C}, \nu_\mathrm{D} > 0 \end{cases}$$

- Typical form: $r = k\, f(C_\mathrm{A}^\alpha, C_\mathrm{B}^\beta, \ldots)$; order $= \alpha + \beta + \cdots$
- First-order reaction, $\mathrm{A} \xrightarrow{r} \mathrm{P}$: $r = kC_\mathrm{A}$
- Temperature dependence (Arrhenius): $k = k_0 \exp\left(-\frac{E}{RT}\right)$

Application: Mass/mole balances in a CSTR

Consider the modelling of a CSTR, fed with a single inlet stream.



Assumptions:

- **A1:** Perfect mixing
- **A2:** Equal inflow and outflow
- **A3:** Constant liquid density
- **A4:** Single first-order reaction

Modelling goals:

- Predict the dynamic behaviour of the species concentrations $C_{\mathrm{A}}, C_{\mathrm{B}}$ in the reactor for a change in inlet conc. $C_{\mathrm{A}}^{\mathrm{in}}$
- Calculate the steady-state concentration of species A in the reactor