Environment and tools

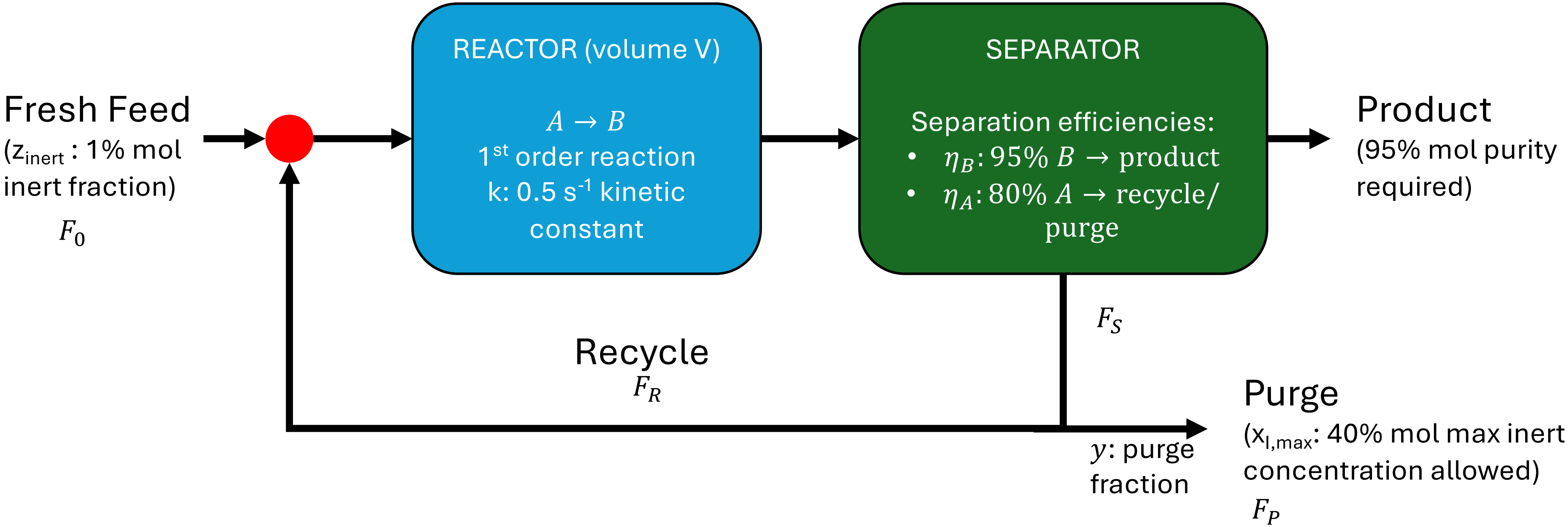
Amply validated, fast, easy-to-use, **open-source**, customizable

Open-source symbolic calculation through algorithmic differentiation, numeric optimization oriented

Standard in the class of **open-source** nonlinear programming (NLP) solvers

Example 1

Reactor, Separator and Recycle: optimal design and operation



Reactor, Separator and Recycle: optimal design and operation

Let's build the problem...

Decision Variable/s

$$\min_{w \in \mathbb{R}^{n_w}} F(w, p)$$

Objective function

Subject to

$$G(w, p) = 0$$
$$H(w, p) \leq 0$$

Constraints

Reactor, Separator and Recycle: optimal design and operation

Let's build the problem…

1) Objective function: Revenue - Costs

F = Product Revenues – CAPEX – OPEX [$/year]

2) Decisions variables, Parameters, Constraints (in our case)

F_0: Fresh Feed Flow

F_S: Outlet Separator Flow

F_R: Recycle Flow

F_P: Purge Flow

k: kinetic constant

V: reactor volume

$x_{I,max}$: max inert concentration allowed

Product purity required

z_{inert} : feed inert fraction

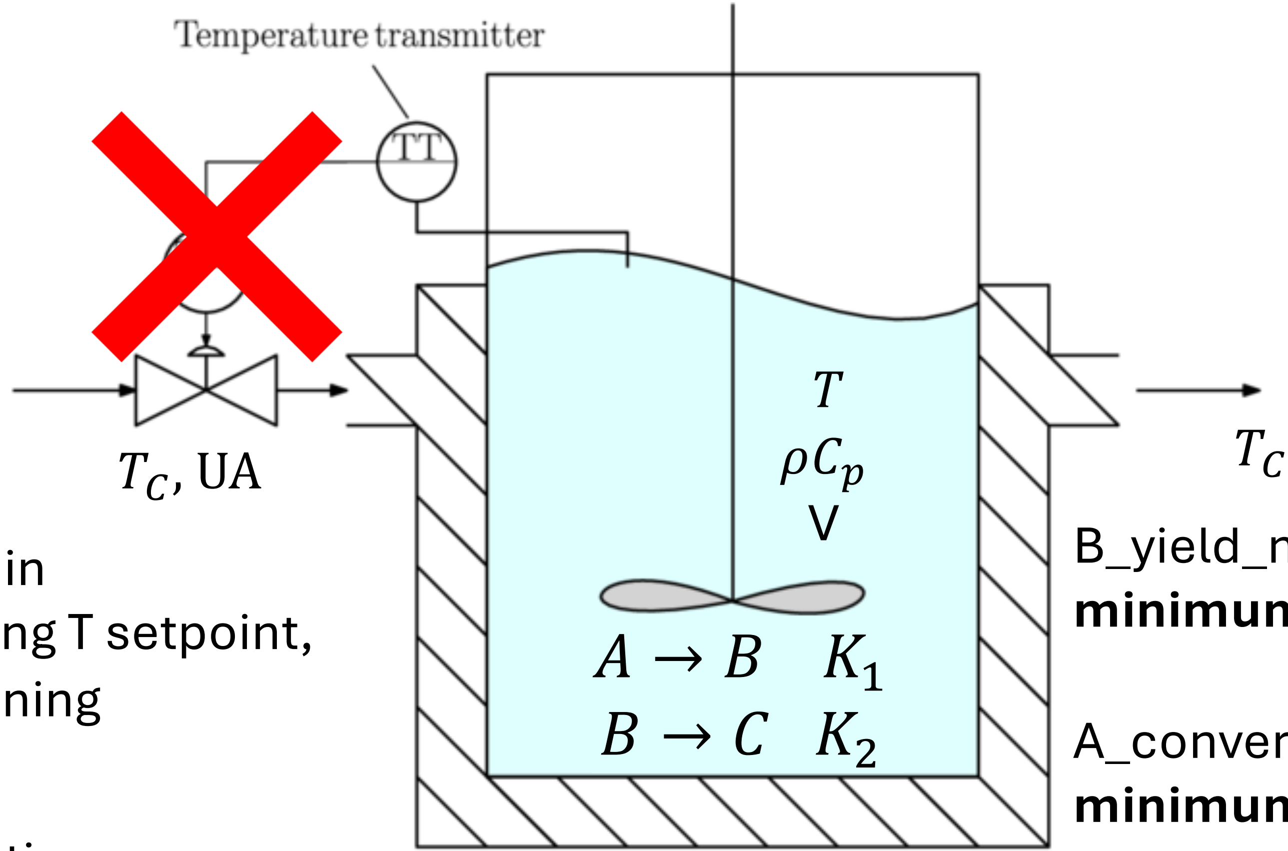
y: purge fraction

Separation efficiencies:

- η_B: $B \Rightarrow$ product
- η_A: $A \Rightarrow$ recycle/purge

Example 2

Optimal control of batch reactor



t_service = 15 min
Loading, Reaching T setpoint, Unloading, Cleaning

t_min = 5 min
Minimum batch time

B_yield_min = 0.3
minimum yield of B

A_conversion_min = 0.4
minimum conversion of A

Optimal control of batch reactor

Let's build the problem...

Decision Variable/s

$$\min_{w \in \mathbb{R}^{n_w \times N}} \int_0^{t_\mathrm{f}} F_c(w(t), p)\,dt$$

Objective function

Subject to

$$w(0) = w_0$$
$$\dot{w}(t) = f_c(w(t), p)$$
$$h(w(t), p) \leq 0$$
$$h_N\left(w\left(t_f\right), p\right) \leq 0$$

Constraints

Optimal control of batch reactor

Let's build the problem…

1) Objective function: Revenue - Costs

F = Product Revenues – ~~CAPEX~~ – OPEX [$/year]

2) Decisions variables, Parameters, Constraints (in our case)

C_0: Initial concentration

$k_0, E/R$: kinetic parameters

T_{amb}: Ambient temperature

ΔH_r: reaction heat

UA, ρC_p: thermal exchange capacity

V: reactor volume

B_yield_min: min yield of B

A_conversion_min: min conversion of A

N: time control intervals

t_f: final batch time

$T_{\min}, T_{\max}$: reactor temperature ranges

$Tc_{\min}, Tc_{\max}$: service fluid temperature ranges

T: reactor temperature/s

Tc: service fluid temperature/s

C_{A,B,C}: species concentrations

$Encost$: energy cost

Contacts

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