Lecture 23: Process modeling & balance laws

- Process modeling, structure and methodolgy
- Balance laws
  - Closure relations

Book: 10.4, 11.1-11.4

Process equations

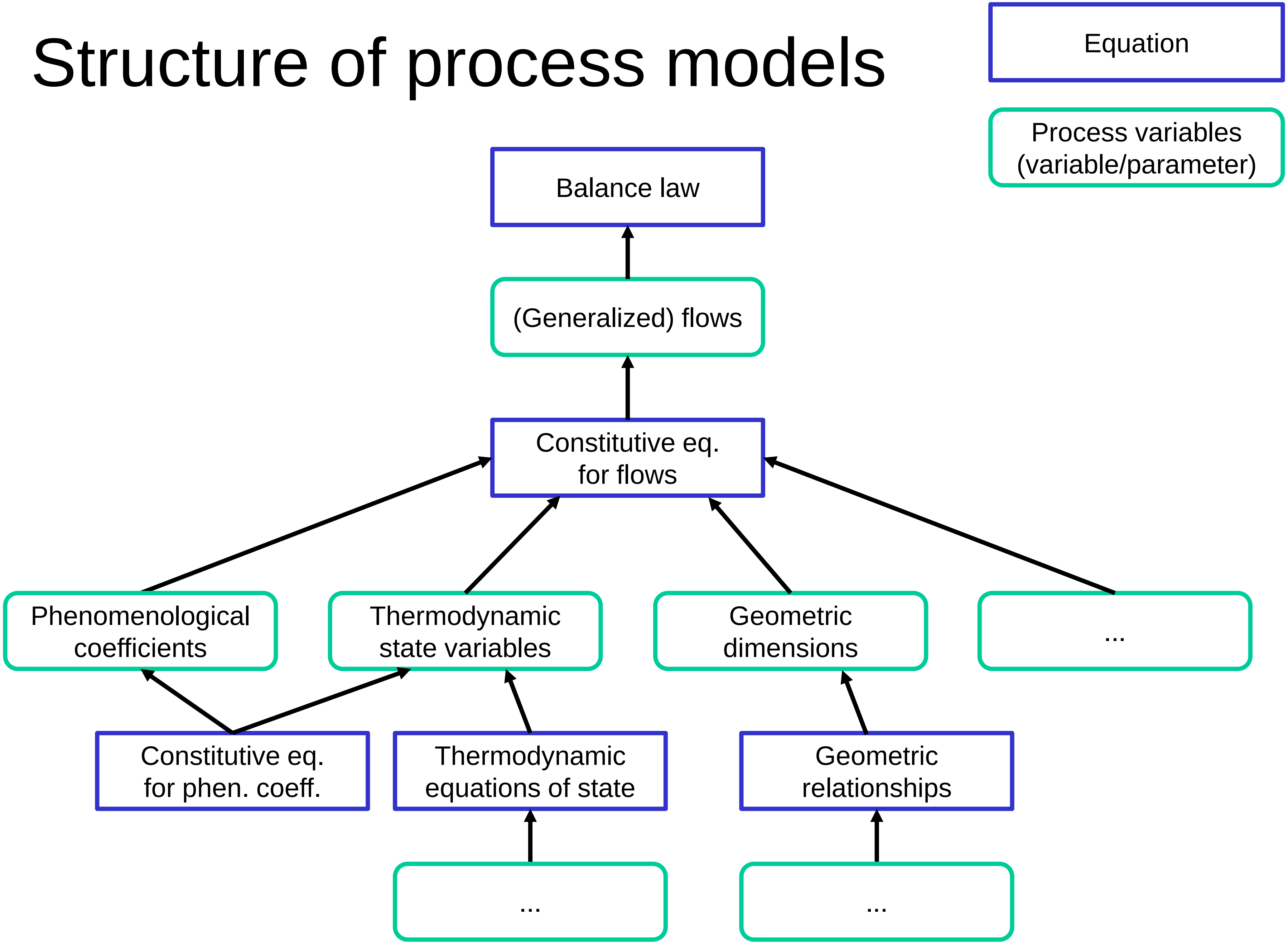
- Balance laws
  - Mass
  - Momentum
  - Energy
  - ...

- Constitutive equations
  - For (generalized) flows
  - Thermodynamic equations of state (e.g. ideal gas law)
  - Phenomenological relationships (e.g. between friction force and flow in a pipe)
  - ...

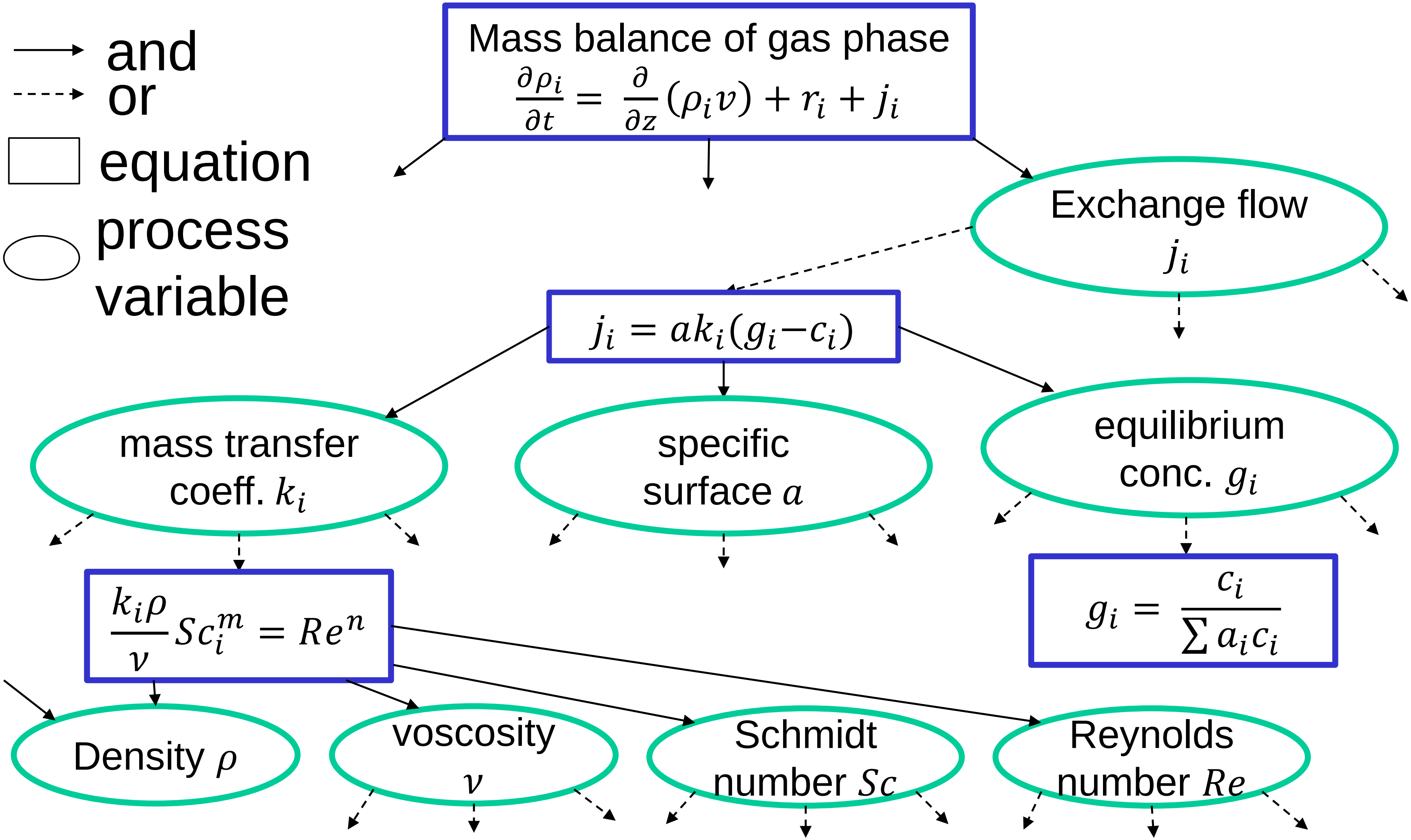
- Constraints
  - Geometric relationships
  - Equilibrium conditions
  - ...

Also called «closure relations» as they «close» the balance laws (such that #equations = #variables)

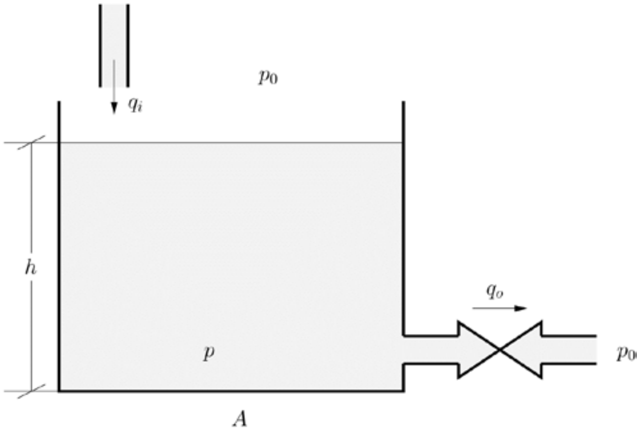
Structure of process models



Example – structure of process models



Example: Tank



- Mass balance: $\overset{1}{\frac{dm}{dt}} = (\overset{2}{q_i} - \overset{3}{q_0})\overset{4}{\rho}$
- Constitutive equation: $q_0 = \overset{5}{C}\sqrt{\overset{6}{p} - \overset{7}{p_0}}$ (2)

  $p = p_0 + \rho \overset{8}{g} \overset{9}{h}$ (3)
- Constraints: $m = \overset{10}{V}\rho$ (4)

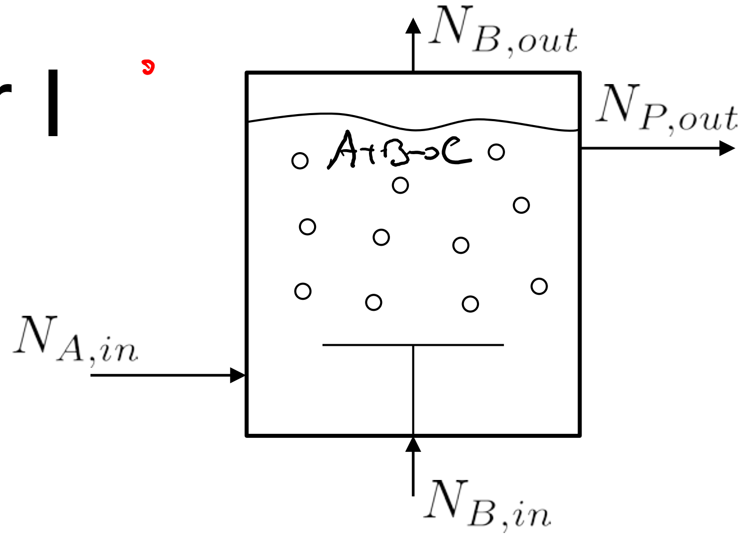
  $V = \overset{11}{A}h$ (5)
- How many variables?
- Need to define parameter and inputs
  - Parameters: C, g, A, ρ
  - Inputs: q_i, p_0

Structural index:

	q_0	p	V	h
(2)	x	x		
(3)		x		x
(4)			x	
(5)				x

→ regular str. index

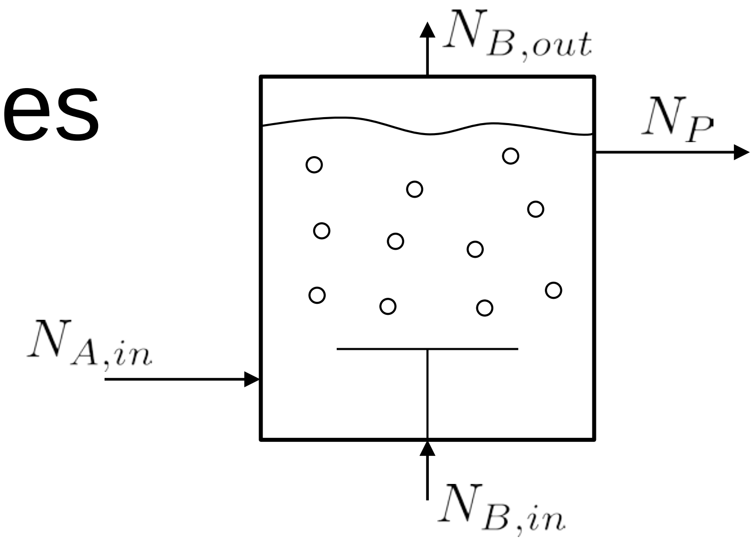
Example: Bubble reactor I



Model reactor as quasi-homogenous

- Assumptions:
  - Ideally mixed
  - Inflows are pure substances
  - Substance A and C are in liquid phase, substance B is gaseous
  - The total surface area of the bubbles depends on the inflow B
    - $S_R = S_R(N_{B,in})$
  - The reaction rate can be calculated based on the concentration of A and the pressure in the reactor
    - $R_0 = R_0(c_{A,liq}, p)$
  - Densities ρ_A and ρ_C and mole masses M_A and M_C are constant and known
  - The gas phase can be described by the ideal gas law
    - $p\, V_{gas} = n_B R_m T$
  - The volume of the reactor is constant and known

Bubble reactor – Balances

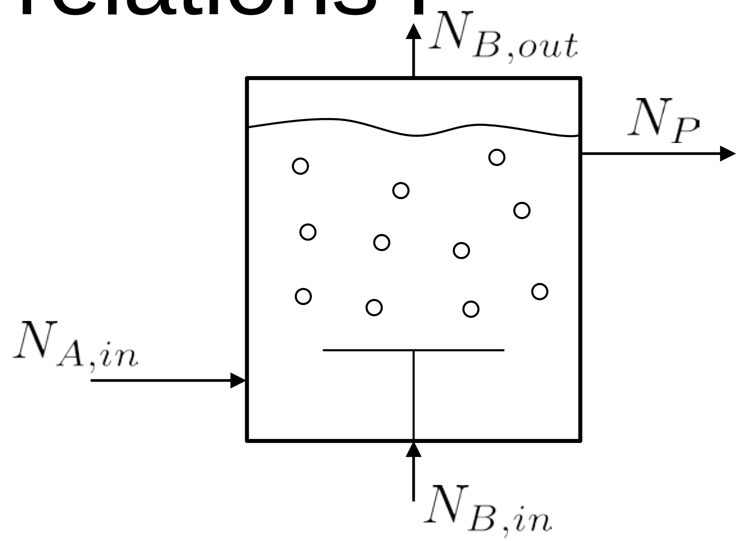


(1) $$\frac{d\overset{(1)}{n}}{dt} = \overset{2}{N_{A,in}} + \overset{3}{N_{B,in}} - \overset{4}{N_{B,out}} - \overset{5}{N_P} + \overset{6}{S_R}\,(\overset{7}{R_A} + \overset{8}{R_B} + \overset{9}{R_C})$$

(2) $$\frac{d\overset{10}{n_A}}{dt} = N_{A,in} - \overset{11}{x_A} N_P + S_R R_A$$

(3) $$\frac{d\overset{12}{n_B}}{dt} = N_{B,in} - N_{B,out} + S_R R_B$$

Bubble reactor – closure relations I



(4) $S_R = S_R(N_{B,in})$

(5) $R_A = -R_0$ [13]

(6) $R_B = -R_0$

(7) $R_C = R_0$

(8) $R_0 = R_0(c_{A,liq}$ [14], p [15]$)$

(9) $x_A = \dfrac{n_A}{n_A + n_C}$ [16]

(10) $n = n_A + n_B + n_C$

(11) $c_{A,liq} = \dfrac{n_A}{V_{liq}}$ [17]

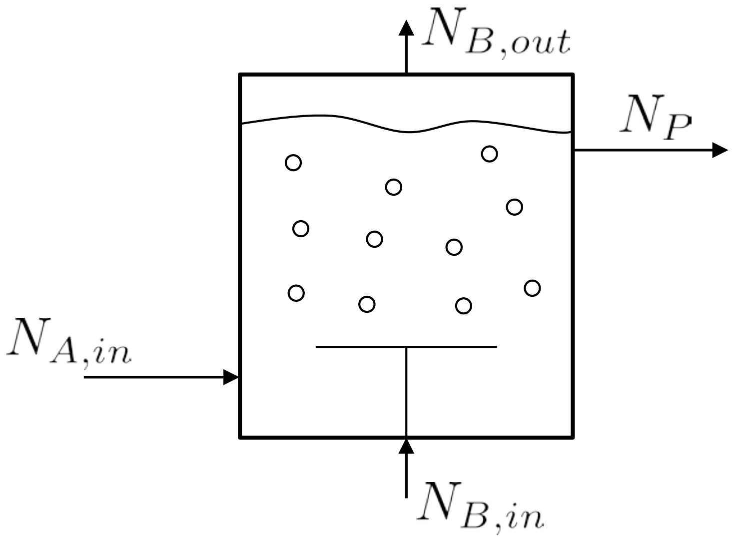
(12) $V_{liq} = \underbrace{n_A M_A \cdot \frac{1}{\rho_A}}_{V_A} + \underbrace{n_C M_C \frac{1}{\rho_C}}_{V_C}$ [18] [19] [20] [21]

(13) $p V_{gas} = n_B R_m T$ [22] [23] [24]

(14) $V = V_{gas} + V_{liq}$ [25]

Bubble reactor – DoF

$$\left.\begin{array}{ll}\text{Equation:} & \#14 \\ \text{Variables:} & \#25\end{array}\right\} \quad \text{DoF } \#11$$



- Variables: $[n; N_{A,in}; N_{B,in}; N_{B,out}; N_P; S_R; R_A; R_B; R_C; n_A; x_A; n_B; R_0; c_{A,liq}; p; n_C; V_{liq}; M_A; \rho_A; M_C; \rho_C; V_{gas}; R_m; T; V]$

parameter: $p = [V, \rho_A, \rho_C, M_A, M_C, R_m]^T$

inputs: $u = [N_{A,in}; N_{B,in}; N_{B,out}; N_P; T]$

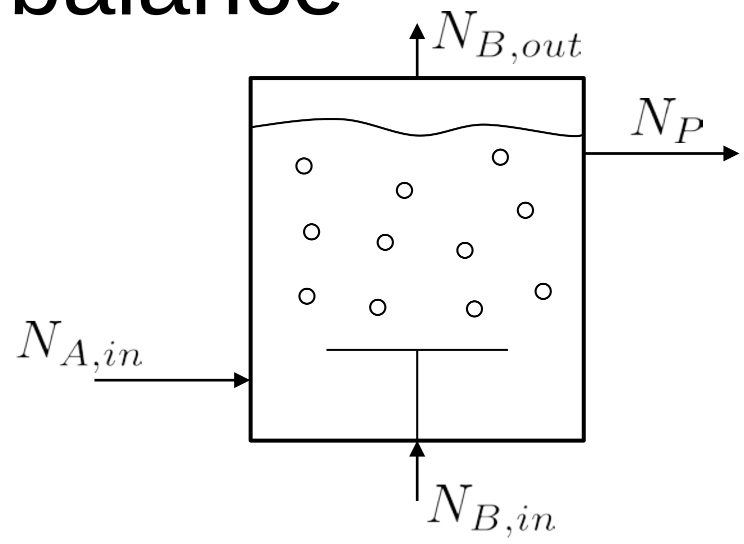
$\rightarrow$ 11 DoF fixed

Bubble reactor – structural index

	S_R	R_A	R_B	R_c	R_0	n_C	x_A	$c_{A,liq}$	p	V_{gas}	V_{liq}
(4)	X										
(5)		X			X						
(6)			X		X						
(7)				X	X						
(8)					X			X	X		
(9)						X	X				
(10)						X					
(11)								X			X
(12)						X					X
(13)									X	X	
(14)										X	X

→ structural index : regular

Bubble reactor – energy balance

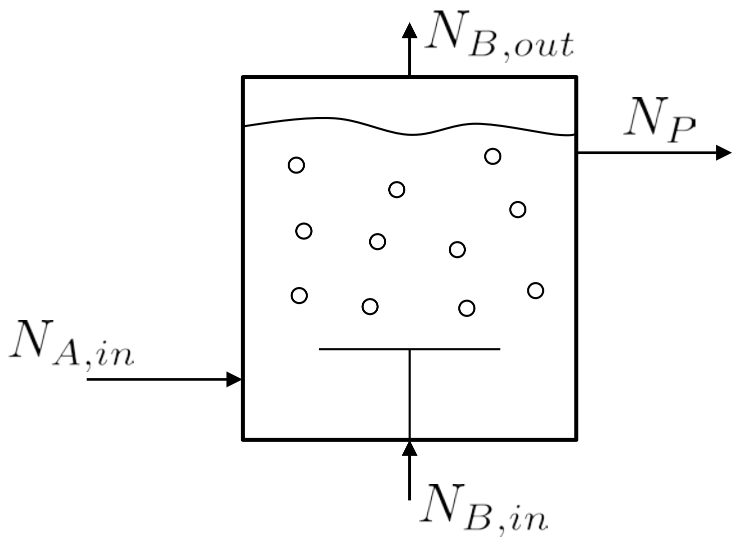


$$(15) \qquad \frac{dU}{dt}^{26} = N_{A,in}\, h_{A,in}^{27} + N_{B,in}\, h_{B,in}^{28}$$

$$- N \quad .. \; h_B^{29} - N_P\, h_P^{30}$$

Bubble reactor – closure relations II

- Assumptions: Adiabat reactor
  - Specific enthalpies of inputs are model inputs
  - Spedific enthalpies of pure substances A, B, C are given by $h_i = h_i(T, p)$



(16) $h_B = h_B(T,p)$

(17) $h_P = x_A \overset{33}{h_A} + \overset{31}{x_C} \overset{32}{h_C}$

(18) $h_A = h_A(T,p)$

(19) $h_C = h_C(T,p)$

(20) $x_C = \dfrac{n_C}{n_C + n_A}$

(21) $U = {}^{34}H - pV$

(22) $H = n_A h_A + n_B h_B + n_C h_C$

Bubble reactor – structural index II

- Variables: $[n; N_{A,in}; N_{B,in}; N_{B,out}; N_P; S_R; R_A; R_B; R_C; n_A; x_A; n_B; R_0; c_{A,liq}; p; n_C; V_{liq}; M_A; \rho_A; M_C; \rho_C; V_{gas}; R_m; T; V; U; h_{A,in}; h_{B,in}; h_B; h_P; h_A; x_C; h_C; H]$

#34 variables - #22 equations : #12 DoF

Inputs : $[N_{A,in}; N_{B,in}; N_{B,out}; N_P; h_{A,in}; h_{B,in}]$

Parameter $[V, \rho_A, \rho_C, M_A, M_C, R_m]$

	h_B	h_P	x_C	h_C	h_A	T	H	n_C	p	x_A
(16)	X					X			X	
(17)		X	X	X	X					X
(18)					X	X			X	
(19)				X		X			X	
(20)			X					X		
(21)							X		X	
(22)	X			X	X		X	X		

→ regular