Chemical Reaction Engineering - Part 99 - Notation

Richard K. Herz, rherz@ucsd.edu, ReactorLab.net

Superscripts:

*	=	Indicates dimensionless variable.
' or "	=	Indicates terms have been grouped or ungrouped from previous line of derivation, e.g., $kS_a = k'$. Dimensional units may have changed. Some authors use ' to denote reactions catalyzed by solid "heterogeneous" catalysts with rate based on catalyst mass.
0	=	Thermodynamic standard state.
off	=	Indicates conditions that would exist at that time and location if all conditions are kept constant except that all chemical reactions have been turned off in the entire system.

Subscripts:

Subscripts on elements of matrices are given in the order: row, column, e.g., a_{rc} is the element in row r, column c of matrix **A**.

0	=	Initial or inlet conditions.
b	=	Back or reverse rate of reaction (see f = forward rate)
batch	=	Batch reactor.
bed	=	Bed of catalyst pellets or particles, adsorbent pellets or particles, or inert packing.
cat	=	Catalyst.
cstr	=	Continuous flow stirred tank reactor.
e	=	Element index, e = 1, 2, ..., E.
E	=	Number of elements in the non-inert components.
f	=	Forward rate of reaction (see b = back or reverse rate)
f	=	Final or outlet conditions
in	=	inlet or initial conditions
i	=	components index for non-inert components, i = 1, 2, ..., S. components present in two different isomeric (but not isotopic) forms or different phases (e.g., liquid water and water vapor) count as different components j.
j	=	Pathway index, for reaction pathways, j = 1, 2, ..., R. A rate equation is required for each pathway for reactor design problems. For a reversible reaction pathway, a rate equation is needed for both the forward and reverse directions of the pathway for reactor design problems.

NOTE: Schmidt uses j for components and i for reaction pathways.

m	=	Independent stoichiometric equation index, m = 1, 2, ..., M.
pfr	=	Plug Flow Reactor.
M	=	Number of independent stoichiometric equations. M = S - rank(**A**) >= S - E.
R	=	Number of reaction pathways
S	=	Number of non-inert components present in the system.
tot	=	total, e.g., total pressure or total number of moles including inerts.

English Symbols:

a_{ie}	=	a_{ie} = subscript of the element e in the molecular formula of component i. For example, the subscript of the element *H* in the component H_2O is 2.
$\mathcal{A}_i$	=	chemical name or formula of component *i* in general form of stoichiometric equation

A = pre-exponential factor in Arrhenius equation

A = Helmholtz free energy

b_e = Number of moles of element e in a simple system, (mol).

C_i = Concentration of non-inert component i, (mol/vol).

C_{pm} = Mass-average heat capacity (kJ/kg/K)

F_i = Molar flow rate of non-inert component i, (mol/time).

F_{total} = Total molar flow rate, including inert components, (mol/time).

G = Gibbs free energy.

H = Enthalpy.

k = Rate coefficient (dimensional units as required to balance units in component balance)

K_i = Adsorption equilibrium constant for component i in LHHW rate equation denominator.

K_j = Equilibrium constant for the reaction pathway j.

$K_{eq,k}$ = Equilibrium constant for independent stoichiometric equation k.

K_M = Constant in denominator of Michaelis-Mention rate equation for enzyme reaction.

M = Number of independent stoichiometric equations. M >= S - E.

M_i = Molecular weight of component i.

N_i = Number of moles of component i, (mol).

N_{tot} = Total number of moles, including inert components, (mol).

p_i = Partial pressure of component i, (atm).

P = Total pressure, including inert components, (atm).

r_{ij} = "Rate of generation by reaction" of component i in reaction pathway j. For "reactants," which are components which decrease in amount with extent of reaction, the "rate of generation by reaction," r_{ij} has a negative value. For "products," r_{ij} has a positive value. For a reversible reaction pathway, r_{ij} is the net rate of generation of i by both the forward and backward (reverse) directions of the reaction pathway. A rate equation is associated with all component i of each reaction pathway j. The corresponding rate equation for any other components in one pathway can be obtained from

$$\frac{r_{ij}}{\upsilon_{ij}} = \frac{r_{mj}}{\upsilon_{mj}} = \frac{r_{nj}}{\upsilon_{nj}} = \text{constant for all components in one reaction } j$$

r_i = "Rate of generation by reaction" of component i in all reaction pathways.

$$r_i = \sum_{j=1}^{R} r_{ij}$$

For "reactants," which are components which decrease in amount with extent of reaction, the "rate of generation by reaction" r_i has a negative value. For "products" r_i has a positive value. Use this relation for the term r_i in the mole balance for component i, substituting the rate equation for each pathway into the component balance using correct coefficent for component i in reaction pathway j.

NOTE: UNITS FOR RATES usually are (mol/"amt"/time), where "amt" is an amount of the phase in which the reaction is occurring. For homogeneous reactions, units are typically (mol/vol/time). For solid-catalyzed reactions of reactants in fluids (no homogeneous reactions in the fluid phase itself, only on the surface of the catalyst), units typically are (mol/vol/time) or (mol/wt/time), where vol & wt are the volume and weight of the solid catalyst, not the fluid.

R = Number of reaction pathways

R = R_g = Ideal gas constant.

R = Recycle ratio.

S_{DU} = Selectivity for desired component D vs. undesired component U. Warning: always check definition of selectivity.

S = Number of non-inert components present in the system.
S = Entropy.
S_a = Area of active surface in a heterogeneous catalyst (area / volume) or (area / mass)
T = Temperature, (K).
v = volumetric flow rate, (vol/time). This is lower-case v.
V = Volume of fluid phase in homogeneous reaction, (vol). This is upper-case V.
V_{bed} = Volume of catalyst bed or monolith in solid-catalyzed reaction, (vol).
V_{cat} = Volume of catalyst particles, pellets or solid fraction of monolith (vol)

$$V_{cat} = (1 - \varepsilon_{bed}) V_{bed}$$

W_{cat} = Weight of catalyst in solid-catalyzed reaction (wt)

$$W_{cat} = \rho_{bed} V_{bed} = \rho_{cat} V_{cat}$$

X_i = Fractional conversion of non-inert reactant component i (dimensionless)
= $(N_i^{off} - N_i)/N_i^{off}$ for batch systems, where $N_i^{off} = N_{i0}$ for simple batch reactors
= $(F_i^{off} - F_i)/F_i^{off}$ for flow systems, where $F_i^{off} = F_{i0}$ for simple flow reactors (e.g., ideal CSTR and PFR)
y_i = Mole fraction of component i.
Y_D = Yield of desired component D. Warning: always check definition of yield.

Greek:

α, β = Order (exponent, raise to power) of concentration in rate equation.
α_i = Activity of component i.
ξ_m = Stoichiometric extent for independent stoichiometric equation m.
Units: (mol) for batch reactors, (mol/time) for flow reactors (e.g., CSTR, PFR).
χ_m = Stoichiometric extent in Schmidt's book
ε_{bed} = Void fraction of catalyst bed or monolith, (dimensionless).
ϕ_i = Fugacity of component i, (pressure).
γ_i = Activity coefficient of component i.
φ_i = Fugacity coefficient of component i.
μ_i = Chemical potential of component i.
ρ_{bed} = Density of catalyst bed or monolith, (wt / vol).
ρ_{cat} = Density of catalyst pellets, or solid fraction of monolith (wt / vol),
= $\rho_{bed} / (1 - \varepsilon_{bed})$.
υ_{ij} = Stoichiometric coefficient of component i in stoichiometric equation j. For a stoichiometric equation written in the conventional manner, coefficients are negative for components on the left-hand side of the equation and coefficients are positive for components on the right-hand side. For example, in the stoichiometric equation [CO + 1/2 O_2 = CO_2] the stoichiometric coefficient of the component O_2 is -1/2 and the coefficient of CO_2 is +1. This sign convention can be remembered by re-writing a stoichiometric equation in the "general form" with all components moved to the right-hand side of the equation, for example: 0 = - CO - 1/2 O_2 + CO_2 (see "General Form" below)

Vectors:

$\vec{a}_i$ = Column vector representing the molecular formula of component i, (E rows). For example, for the elements [Si, H, Cl], the column vector $(1, 2, 2)^T$ represents dichlorosilane, SiH_2Cl_2.

$\vec{b}$ = Element abundance vector, a column vector listing the number of moles of each element present in a simple system, (E rows) $\vec{b} = \boldsymbol{A}\,\vec{n}$

$\vec{N}$ = Composition vector, a column vector listing the number of moles of each non-inert components present in a batch system, (S rows). Also, "component abundance vector."

$\vec{F}$ = Composition vector, a column vector listing the molar flow rate of each non-inert component present in a flow system, (S rows). Also, "component abundance vector."

$\vec{\upsilon}_m$ = Stoichiometric column vector representing independent stoichiometric equation m (S rows). For example, for the components [CO, O_2, CO_2, H_2, H_2O] the column vector $(-1, -1/2, 1, 0, 0)^T$ represents: $0 = -CO - 1/2\ O_2 + CO_2$; $\mathbf{0} = \boldsymbol{A}\,\vec{\upsilon}_m$

Matrices (for multiple reaction systems, M > 1, R > 1):

Matrices are in bold text. Subscripts on elements of matrices are given in the order: row, column, e.g., a_{rc} is the element in row r, column c of matrix **A**.

A = Formula matrix (E rows, S columns) = $\left(\vec{a}_1, \vec{a}_2, .., \vec{a}_S\right)$;
$\vec{b} = \boldsymbol{A}\,\vec{n}$; $\mathbf{0} = \boldsymbol{A}\,\vec{\upsilon}_m$; $\mathbf{0} = \boldsymbol{A}\,\boldsymbol{Y}$

I = Identity Matrix.

Y = Complete stoichiometric matrix of independent stoichiometric equations, (S rows, M columns) = $\left(\vec{\upsilon}_1, \vec{\upsilon}_2, .., \vec{\upsilon}_M\right)$; $\mathbf{0} = \boldsymbol{A}\,\boldsymbol{Y}$

General Form of Stoichiometric Equations:

Stoichiometric equations describe how the relative amounts of the reactive components change in order to conserve the mass of each element, since, in chemical reactions, elements are not transformed into other elements.

General form of stoichiometric equation describing for equation j

$$\mathbf{0} = \boldsymbol{A}\,\vec{\upsilon}_j$$

$$\mathbf{0} = \sum_{i=1}^{S} \upsilon_{ij}\,\vec{a}_i$$

The above equations are usually written with each $\vec{a}_i$ replaced by the chemical formula of the components it represents: e.g., $= (1, 2, 2)^T$ in the [Si, H, Cl] system would be replaced by SiH_2Cl_2. In the conventional form of a stoichiometric equation, the general form is re-written with the "reactants" or components with negative υ_i moved to the left-hand side of the equation.