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**KINETICS OF COMPOSITE REACTIONS IN CLOSED
AND OPEN FLOW SYSTEMS**

(IUPAC Recommendations 1993)

Prepared for publication by

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Kinetics of composite reactions in closed and open flow systems (IUPAC Recommendations 1993)

Abstract

This paper is aimed at providing an accurate and non-ambiguous description of reaction systems occurring in closed or open systems and involving possible density changes during the reaction. Owing to its systematic character, the proposed method is well suited to implementation on the computer for quantitative calculations, as those which are required for chemical engineering applications.

The treatment proposed below is based on standard methods used in Chemical Reaction Engineering (CRE). Unfortunately, the notations universally accepted in the CRE community, which created the corresponding concepts, are different from those recommended in the "Green Book" [1] from IUPAC. This especially applies to the rate of reaction which is universally denoted r in the CRE literature instead of v , used by chemists. Related quantities such as the rate of production of species are denoted R_j (CRE) instead of r_j (IUPAC).

In order to avoid confusion among the chemist's community, the treatment below follows the Green Book's recommendations. However, as this report may also be used by chemical reaction engineers, a summary of the main relationships is given with CRE notations in the Appendix.

FOREWORD

The proposal below is the final version of a report prepared for the Commission on Chemical Kinetics of IUPAC. Comments on the first draft from Professors J.A. Kerr, K.J. Laidler, Yu.N. Molin and P.J. Van Tiggelen are gratefully acknowledged. The second draft was discussed at the 34th General Assembly, Boston, August 22nd-25th 1987 and the third draft at the 35th General Assembly, Lund, August 9th-15th 1989 by the commission. The fourth draft was further modified according to suggestions from Professor R.A. Alberty, which were particularly helpful. The present version takes into account remarks and criticisms from 15 experts (mainly chemists) among whom it was circulated. Their contribution is greatly acknowledged.

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1. STOICHIOMETRY OF A COMPOSITE REACTION NETWORK

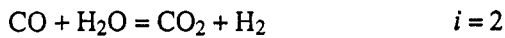
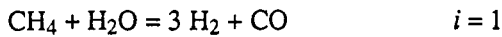
It is assumed that N species A_j , $j = 1, 2, 3, \dots, N$ are involved in a system of R independent reactions $i = 1, 2, 3, \dots, R$. In many situations, the reactions are assumed independent, which means that none of them can be obtained by a linear combination of the others. But they may involve common species. The independence assumption is not necessary and many relationships derived below also apply to any reaction network.

The stoichiometric equations are written

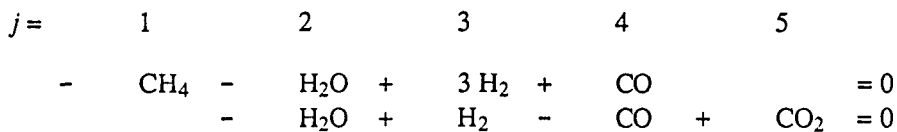
$$\sum_{j=1}^N v_{ij} A_j = 0 \quad i = 1, 2, \dots, R \quad (1)$$

The v_{ij} are the stoichiometric numbers. They may be considered as elements of a matrix \underline{v}^T of rank R (see section 9 below).

Example : steam reforming of methane. In traditional form, the chemical transformation may be described by two equations



In canonical form



the stoichiometric matrix is

$$\underline{v}^T = \begin{bmatrix} -1 & -1 & 3 & 1 & 0 \\ 0 & -1 & 1 & -1 & 1 \end{bmatrix}$$

In the case of one single reaction $R = 1$ and one has simply

$$\sum_{j=1}^N v_j A_j = 0$$

2. CLOSED SYSTEMS. RATES OF TRANSFORMATION OF SPECIES. RATES OF REACTION

Let n_j be the instantaneous amount of A_j in a closed system of volume V . For a single reaction, the rate of transformation of species A_j is defined as

$$r_j = \frac{1}{V} \frac{dn_j}{dt} = v_j v \quad (2)$$

This also constitutes a definition of the rate of reaction v which is thus independent of the considered species A_j

$$v = \frac{1}{v_j V} \cdot \frac{dn_j}{dt} \quad \text{The SI unit for } v \text{ is mol m}^{-3} \text{ s}^{-1} \quad (3)$$

It must be strongly emphasized that this relationship is only valid for a single reaction in a closed system.

For composite reactions, each reaction may contribute to the transformation (i.e. the formation or the consumption) of A_j whose rate of transformation is

$$r_j = \sum_{i=1}^R \nu_{ij} v_i \quad (4)$$

v_i is the rate of the i^{th} reaction. In the example of the steam reforming of methane above

$$r_{\text{CO}} = v_1 - v_2$$

$$r_{\text{H}_2} = 3v_1 + v_2$$

r_j was defined here as the rate of transformation per unit volume. This convention is well adapted to homogeneous reactions. The rate of transformation may be referred to other quantities, e.g. the mass of catalyst in the case of heterogeneous reactions. This point is thoroughly discussed in textbooks on Chemical Reaction Engineering. The case of homogeneous reactions is not restrictive and was chosen here only for illustration purpose.

3. CLOSED SYSTEMS. EXTENT OF REACTION

For one single reaction, De Donder [2] introduced the extent of reaction ξ such that

$$n_j = n_{j0} + \nu_j \xi \quad (5)$$

n_{j0} is the amount of A_j in a reference state (e.g. at the beginning of the reaction). For several simultaneous reactions (composite reactions), (5) may be easily generalized.

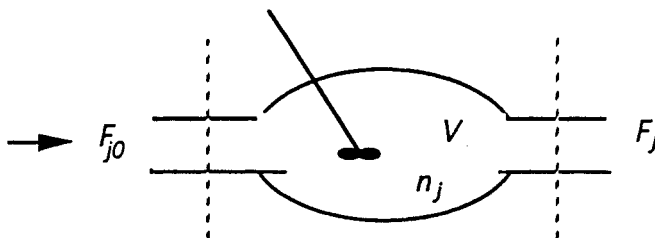
There are R independent chemical variables such that

$$n_j = n_{j0} + \sum_{i=1}^R \nu_{ij} \xi_i \quad (6)$$

We must note that with this notation, ξ_i has the dimension of n_j . This is a disadvantage if one wishes to measure the extent of reaction with a dimensionless quantity. This problem will be solved by introducing normalized extents of reaction in Section 6 below.

4. OPEN OR FLOW SYSTEMS (PURELY CONVECTIVE FLOW ONLY). EXPRESSION OF r_j

Let F_j be the molar flow rate of species A_j in a given cross-section (SI unit mol s^{-1}).



Assuming that the vessel is well-mixed and of uniform composition, the material balance of A_j in the reactor is written

$$F_{j0} + V r_j = F_j + \frac{dn_j}{dt} \quad (7)$$

(input)
(Chemical transformation)
(output)
(accumulation)

It is clear here that $r_j \neq \frac{1}{V} \frac{dn_j}{dt}$. The equality is true only if $F_j = F_{j0} = 0$ (closed system).

Thus, the rate of reaction must not be defined from $\frac{dn_j}{dt}$ in an open system.

At steady state

$$\frac{F_j - F_{j0}}{V} = r_j = \sum_i \nu_{ij} v_i \quad (8)$$

For a single reaction

$$\frac{F_j - F_{j0}}{V} = r_j = \nu_j v \quad (9)$$

This relationship is the basis of the measurement of reaction rates by use of a continuous stirred (well mixed) reactor.

5. EXTENT OF REACTION IN A FLOW SYSTEM AT STEADY STATE

From the stoichiometry, one may write $\left(\frac{dn_j}{dt} = 0\right)$

$$F_j = F_{j0} + \nu_j \dot{\xi} \quad (10)$$

and for simultaneous reactions

$$F_j = F_{j0} + \sum_i \nu_{ij} \dot{\xi}_i \quad (11)$$

However, $\dot{\xi}_i$ has the dimension of F_j (for which the SI unit is mol s⁻¹).

6. NORMALIZED EXTENTS OF REACTION

In order to define a dimensionless (or normalized) extent of reaction, applicable in closed as well as in open systems at steady state, it suffices to normalize $\dot{\xi}_i$ or $\dot{\xi}_j$ by an appropriate quantity.

Closed system : Let $n_0 = \sum_j n_{j0}$. For a single reaction, the normalized extent X is defined by

$$n_j = n_{j0} + n_0 \nu_j X \quad (12)$$

In the case of a non-equilibrated reaction, X increases from 0 (if the reference state is chosen at the beginning) up to a value X_L determined by the total consumption of the limiting reactant A_L ($n_L=0$)

$$X_L = \frac{n_{L0}}{(-\nu_L)n_0}$$

for simultaneous reactions

$$n_j = n_{j0} + n_0 \sum_{i=1}^R \nu_{ij} X_i \quad (13)$$

Comparing (6) and (13), one obtains

$$X_i = \dot{\xi}_i/n_0 \quad (14)$$

It is advantageous to consider that the sum $n_0 = \sum_j n_{j0}$ is concerned only with reacting species (e.g. those which are actually involved in the chemical reactions). Non-reacting or inert species (denoted by index I below) are not included in the sum, in order to give a broader range of variation to X_i , but this is only a matter of convention.

Open system at steady state : Let $F_0 = \sum_j F_{j0}$, then

$$F_j = F_{j0} + F_0 v_j X \quad (15)$$

or for composite reactions

$$F_j = F_{j0} + F_0 \sum_{i=1}^R v_{ij} X_i \quad (16)$$

$$\text{and } X_i = \dot{\xi}_i / F_0 \quad (17)$$

Obviously, X_i is the same for a closed or an open system.

The dimensionless extent of reaction is thus a vector \underline{X}^T whose components are the R values of X_i (see section 9 below).

The advantages of this definition are :

X_i is unique, both for closed or steady state open systems,

X_i is dimensionless,

X_i is exactly equal to the fractional conversion of the reactant in the case of a single reaction consuming this reactant, e.g.

$A \rightarrow \text{products}$

$$n_A = n_{A0} (1 - X_A) \quad X_A = X, \text{ extent of reaction}$$

In all other cases, the fractional conversion of a reactant A_j may be expressed as a function of the X_i but is a quantity of different nature.

Concluding remark

Other normalization factors for ξ_i are possible, depending on the problem. For instance, ξ_i may be normalized by the total mass m of the reacting phase $X'_i = \xi_i / m$ (closed system) or by the mass flowrate $X'_i = \dot{\xi}_i / Q_m$ (open system). But X'_i is no longer dimensionless.

7. DENSITY VARIATION DURING THE REACTION

Closed system : The variations of volume can be easily accounted for by using the concept of normalized extent of reaction. For a single reaction in the gas phase, in the presence of inerts (I) :

$$n_j = n_{j0} + v_j n_0 X$$

The total amount of substance is

$$n = \sum_{j=1}^N n_j + n_I = n_0 + n_I + n_0 \sum v_j X$$

Let

$$\Delta v = \sum_j v_j \quad (18)$$

$$I = n_I / n_0 \quad (19)$$

$$\alpha = \frac{\Delta v}{1+I} \quad (20)$$

The total amount of substance is

$$n = (n_0 + n_I) (1 + \alpha X) \quad (21)$$

In an ideal gas, $pV = nR_gT$, where R_g is the gas constant

Let the physical dilation factor (or volume strain) be

$$\beta = \frac{p_0 T}{p T_0} \quad (22)$$

then

$$V = \beta V_0 (1 + \alpha X) \quad (23)$$

The rate of reaction is such that

$$r_j = \frac{1}{V} \frac{dn_j}{dt} = v_j v = v_j \frac{n_0}{V} \frac{dX}{dt} \quad (24)$$

$$v = \frac{c_0}{\beta(1 + \alpha X)} \cdot \frac{dX}{dt} \quad (25)$$

where $c_0 = n_0/V_0$

More generally, defining the chemical dilation factor (or amount strain) as $\alpha = c_0 \Delta v_0$ with $\Delta c_0 = \sum_j v_j v_{j0}$, where v_{j0} is the molar volume of species A_j , (23) holds for any phase (especially for liquids). It is assumed here that partial molar volumes in mixture are the same as pure molar volumes.

These relationships can be easily extended to the case of composite reactions.

(23) is generalized to

$$V = \beta V_0 \left(1 + \sum_i \alpha_i X_i \right) \quad (26)$$

where

$$\alpha_i = \frac{\Delta v_i}{1+I} = \frac{\sum_j v_{ij}}{1+I} \quad \text{for gases} \quad (27)$$

and

$$\alpha_i = c_0 \Delta v_{i0} = c_0 \sum_j v_{ij} v_{j0} \quad \text{for any phase}$$

But, now the relationship between v_i and X_i may involve the normalized extents of all reactions

$$v_i = \frac{c_0}{\beta \left(1 + \sum_i \alpha_i X_i \right)} \cdot \frac{dX_i}{dt} \quad (28)$$

Open flow system at steady state

Analogous relationships are obtained for the volumetric flow rate Q simply by replacing V by Q

$$Q = \beta Q_0 \left(1 + \sum_i \alpha_i X_i \right) \quad (29)$$

8. EXPRESSION OF VARIOUS QUANTITIES INVOLVED IN KINETIC LAWS

From relationships (13), (16), (23), (29) it is easy to express other quantities of interest as a function of the X_i , namely

$$\text{concentrations} \quad c_j = n_j / V = F_j / Q$$

$$\text{partial pressures (ideal gas)} \quad p_j = c_j R_g T$$

$$\text{mole (or amount) fractions} \quad x_j = p_j / p = n_j / n$$

This formalism may thus be efficiently utilized to write down material balances in chemical reactors (1).

It must be again emphasized that the often quoted expression for the rate of reaction

$$v = \frac{1}{\nu_j V} \frac{dn_j}{dt}$$

is only valid in a closed system (batch reactor) and for a single reaction. In a constant volume reactor, and only in this case, it becomes

$$v = \frac{1}{\nu_j} \frac{dc_j}{dt} \quad (30)$$

In an open-flow reactor at steady state

$$v = \frac{1}{\nu_j V} (F_{j,\text{out}} - F_{j,\text{in}}) \quad (31)$$

and at non-steady state

$$v = \frac{1}{\nu_j V} \left(\frac{dn_j}{dt} + F_{j,\text{out}} - F_{j,\text{in}} \right) \quad (32)$$

In the case of a composite reaction network ($i = 1, 2, \dots, R$), the rate of a particular reaction cannot be directly defined from the change of amount (or flow rate) of a given species because these quantities may depend on the rate of all reactions occurring simultaneously. If however the rates of all reactions are known except one (say $i = 1$), it is possible to deduce ν_1 from

$$\nu_1 = \frac{1}{\nu_{1j}} \left(r_j - \sum_{i=2}^R \nu_{ij} \nu_i \right) \quad (33)$$

with

$$r_j = \frac{F_{j,\text{out}} - F_{j,\text{in}}}{V} + \frac{1}{V} \frac{dn_j}{dt} \quad (34)$$

But this method is not frequently used.

It must be also noted that all the treatments in this report are concerned with purely convective flow. The case of simultaneous convection and diffusion of species would require special consideration.

9. MATRIX NOTATION

The relationship above can be given a more condensed form by use of matrix notation. There are two possible conventions.

Let $\Delta n_j = n_j - n_{j0}$. Expression (6) can be written

$$\Delta n_j = \sum_{i=1}^R v_{ij} \xi_i \quad j = 1, 2, \dots, N \quad (35)$$

In matrix notation

$$\begin{bmatrix} \Delta n_1 \\ \Delta n_2 \\ \cdot \\ \cdot \\ \Delta n_j \\ \cdot \\ \cdot \\ \Delta n_N \end{bmatrix} = \begin{bmatrix} v_{11} \dots \dots v_{1R} \\ v_{21} \dots \dots v_{2R} \\ \dots \dots \dots \\ v_{j1} \dots v_{ji} \dots v_{jR} \\ \dots \dots \dots \\ v_{N1} \dots \dots v_{NR} \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \\ \cdot \\ \xi_i \\ \cdot \\ \xi_R \end{bmatrix} \quad (36)$$

or in more condensed form

$$\underline{\Delta n} = \underline{\nu} \underline{\xi} \quad (37)$$

where $\underline{\Delta n}$ is the amount of change vector, $\underline{\nu}$ is a form of the stoichiometric matrix with N rows (species) and R columns (reactions) and $\underline{\xi}$ is the extent of reaction vector.

Introducing dimensionless quantities

$$Y_j = \Delta n_j / n_0 \quad \text{and} \quad X_i = \xi_i / n_0$$

(37) is written

$$\underline{Y} = \underline{\nu} \underline{X} \quad (38)$$

where

$$\underline{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \cdot \\ \cdot \\ Y_i \\ \cdot \\ \cdot \\ Y_N \end{bmatrix} \quad \text{and} \quad \underline{X} = \begin{bmatrix} X_1 \\ X_2 \\ \cdot \\ \cdot \\ X_i \\ \cdot \\ \cdot \\ X_R \end{bmatrix}$$

The rate of transformation vector is then given from (4) i.e. $r_j = \sum_i v_{ij} v_i$, by

$$\underline{r} = \underline{v} \underline{v} \quad (39)$$

where

$$\underline{r} = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_i \\ \vdots \\ r_N \end{bmatrix} \quad \text{and} \quad \underline{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_i \\ \vdots \\ v_R \end{bmatrix}$$

\underline{v} is the rate-of-reaction vector.

However, there is a second possibility which is closer to the usual way to write composite reaction systems. In the standard chemical notation, the reactions are written one below the other and appear in successive rows whereas the species are written along horizontal lines. This leads to the transposed stoichiometric matrix already defined above.

$$\underline{v}^T = \begin{bmatrix} v_{11} \dots \dots v_{1N} \\ v_{21} \dots \dots v_{2N} \\ \dots \dots \dots \\ v_{i1} \dots v_{ij} \dots v_{iN} \\ \dots \dots \dots \\ v_{R1} \dots \dots v_{RN} \end{bmatrix}$$

\underline{v}^T denoting the transposed of the matrix \underline{v} , the relationship above is then written in this second convention

$$\underline{\Delta n}^T = \underline{\xi}^T \underline{v}^T \quad (40)$$

where $\underline{\Delta n}^T$ and $\underline{\xi}^T$ are row vectors. Similarly, (38) and (39) become, respectively

$$\underline{Y}^T = \underline{X}^T \underline{v}^T \quad (41)$$

and

$$\underline{r}^T = \underline{v}^T \underline{v}^T \quad (42)$$

Actually, the whole treatment proposed in the preceding sections is based on this convention, which is of course equivalent to the first one, the latter being more classical, from the standpoint of matrix algebra.

To be entirely correct, equations (4) and (6) should thus be written

$$r_j = \sum_i v_i v_{ij} \quad \text{and} \quad n_j = n_{j0} + \sum_i \xi_i v_{ij}$$

Example :

Coming back to the steam reforming of methane

	$j =$	1	2	3	4	5					
$i = 1$	-	CH ₄	-	H ₂ O	+	3H ₂	+	CO	= 0		
$i = 2$			-	H ₂ O	+	H ₂	-	CO	+	CO ₂	= 0

$$y = \begin{bmatrix} -1 & 0 \\ -1 & -1 \\ 3 & 1 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}$$

$$y^T = \begin{bmatrix} -1 & -1 & 3 & 1 & 0 \\ 0 & -1 & 1 & -1 & 1 \end{bmatrix}$$

Convention 1

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ -1 & -1 \\ 3 & 1 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$$

$$\begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ -1 & -1 \\ 3 & 1 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

Convention 2

$$[Y_1 Y_2 Y_3 Y_4 Y_5] = [X_1 X_2] \begin{bmatrix} -1 & -1 & 3 & 1 & 0 \\ 0 & -1 & 1 & -1 & 1 \end{bmatrix}$$

$$[r_1 r_2 r_3 r_4 r_5] = [v_1 v_2] \begin{bmatrix} -1 & -1 & 3 & 1 & 0 \\ 0 & -1 & 1 & -1 & 1 \end{bmatrix}$$

REFERENCES

- [1] "IUPAC Green Book" "Quantities, Unit and Symbols in Physical Chemistry", Blackwell Sci. Publisher, Oxford (1988)
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APPENDIX: MAIN RELATIONSHIPS

NOTATION USED IN CHEMICAL REACTION ENGINEERING

r_i stands for the rate of reaction i

\mathcal{R}_j stands for the rate of transformation of species A_j

Closed system, single reaction ($i=1$)

Rate of transformation of species A_j

$$\mathcal{R}_j = \frac{1}{V} \frac{dn_j}{dt}$$

Rate of reaction

$$r = \frac{1}{\nu_j V} \frac{dn_j}{dt}$$

Composite reactions :

$$\mathcal{R}_j = \sum_{i=1}^R \nu_{ij} r_i$$

Material balance in a well mixed open system

$$F_{j0} + V\mathcal{R}_j = F_j + \frac{dn_j}{dt}$$

Matrix notation

$$\underline{\mathcal{R}} = \begin{bmatrix} \mathcal{R}_1 \\ \mathcal{R}_2 \\ \vdots \\ \mathcal{R}_j \\ \vdots \\ \mathcal{R}_N \end{bmatrix} \quad \underline{r} = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_i \\ \vdots \\ r_R \end{bmatrix}$$

$$\underline{\mathcal{R}} = \underline{\nu} \underline{r} \quad (\text{convention 1})$$

$$\underline{\mathcal{R}}^T = \underline{r}^T \underline{\nu}^T \quad (\text{convention 2})$$

SUMMARY OF NOTATIONS AND DEFINITIONS

Name	Symbol	Definition	SI unit	Notes
Example of a matrix	\underline{A}	-	-	
Transposed matrix	\underline{A}^T	-	-	
Species	A_j	-		-
Total concentration of reacting species	c_0	$c_0 = n_0/V$	mol m ⁻³	
Concentration of species A_j	c_j	$c_j = n_j/V = F_j/Q$	mol m ⁻³	
Molar flow rate of species A_j	F_j	-	mol s ⁻¹	
Total molar flow rate of reacting species in reference state	F_0	$F_0 = \sum_j F_{j0}$	mol s ⁻¹	
Molar flow rate of inert or non-reacting species	F_I	-	mol s ⁻¹	
Total molar flow rate of species	F	$F = \sum_j F_j + F_I$	mol s ⁻¹	
Index of reaction	i	-	-	
Inert ratio	I	$I = n_I/n_0 = F_I/F_0$	-	
Index of species	j	-	-	
Total mass of the reacting system	m	-	kg	
Amount of species A_j	n_j	-	mol	
Total amount of reacting species in reference state	n_0	$n_0 = \sum_j n_{j0}$	mol	
Amount of inert or non-reacting species	n_I	-	mol	
Amount of limiting reactant	n_L	-	mol	

Summary of notations and definitions (contd.)

Name	Symbol	Definition	SI unit	Notes
Total amount of species	n	$n = \sum_j n_j + n_I$	mol	
Total number of reacting species	N	-	-	
Index of reference state	0	-	-	
Total pressure	p	-	Pa	
Partial pressure of species A_j	p_j	-	Pa	
Volumetric flow rate	Q	-	$\text{m}^3 \text{s}^{-1}$	
Mass flow rate	Q_m	-	kg s^{-1}	
Rate of production of species A_j	r_j	$r_j = \sum_i \nu_{ij} \nu_i$	$\text{mol m}^{-3} \text{s}^{-1}$	1
Number of independent reactions	R	-	-	
Ideal gas constant	R_g	$R_g = \frac{pV}{nT}$	$\text{J.K}^{-1} \text{mol}^{-1}$	
Time	t	-	s	
Temperature	T	-	K	
Rate of reaction (single reaction)	ν	$\nu = \frac{1}{\nu_j V} \frac{dn_j}{dt}$ (single reaction in a closed system)	$\text{mol m}^{-3} \text{s}^{-1}$	
Rate of reaction (composite reactions)	ν_i	see r_j	$\text{mol m}^{-3} \text{s}^{-1}$	2

Notes

- (1) These are the only observable quantities, which can be deduced from a material balance over species A_j .
- (2) This quantity denotes the rate of reaction i in a system of simultaneous reactions. Its definition can be understood from the overall rate or production of a species A_j (see corresponding definitions).

Summary of notations and definitions (contd.)

Name	Symbol	Definition	SI unit	Notes
Molar volume of species A_j	v_j	$v_j = 1/c_j$	$\text{m}^3 \text{mol}^{-1}$	
Mole or amount fraction of species A_j	x_j	$x_j = n_j/n$	-	
Normalized extent of reaction (single reaction, molar reference)	X	$X = \xi/n_0$	-	
Normalized extent of reaction (composite reactions, molar reference)	X_i	$X_i = \xi_i/n_0$	-	
Fractional conversion of species A	X_A	$X_A = 1 - n_A/n_{A0}$ (closed system)	-	
Normalized extent of reaction (composite reactions, mass reference)	X'_i	$X'_i = \xi_i/m = \xi_i/Q_m$	mol kg^{-1}	
Limiting value of normalized extent of reaction	X_L	$X_L = \frac{n_{L0}}{(-v_L)n_0}$	-	
Dimensionless increase of amount of species A_j	Y_j	$Y_j = \Delta n_j/n_0$	-	
Chemical dilation factor (or amount strain) (single reaction)	α	$\alpha = \frac{n - n_0 - n_I}{X(n_0 + n_I)}$ (closed system)	-	
Chemical dilation factor (or amount strain) of reaction i	α_i	$\alpha_i = c_0 \Delta v_{i0}$	-	
Physical dilation factor (or volume strain) (ideal gas)	β	$\beta = \frac{p_0 T}{p T_0}$	-	
Increase of amount of species A_j	Δn_j	$\Delta n_j = n_j - n_{j0}$	mol	
Reaction variation of molar volume for reaction i	Δv_i	$\Delta v_i = \sum_j v_{ij} v_j$	$\text{m}^3 \text{mol}^{-1}$	
Reaction variation of stoichiometric number (single reaction)	Δv	$\Delta v = \sum_j v_j$	-	
Reaction variation of stoichiometric number for reaction i (composite reactions)	Δv_i	$\Delta v_i = \sum_j v_{ij}$		

Summary of notations and definitions (contd.)

Name	Symbol	Definition	SI unit	Notes
Stoichiometric number (single reaction)	ν_j	$\sum_j \nu_j A_j = 0$	-	
Stoichiometric number of species A_j in reaction i (composite reactions)	ν_{ij}	$\sum_j \nu_{ij} A_j = 0$	-	
Extent of reaction (single reaction)	ξ	$n_j = n_{j0} + \nu_j \xi$ (closed system)	mol	
Extent of reaction (composite reactions)	ξ_i	$n_j = n_{j0} + \sum_i \nu_{ij} \xi_i$	mol	
Rate of conversion (single reaction)	$\dot{\xi}$	$F_j = F_{j0} + \nu_j \dot{\xi}$ (open flow system) Steady state	mol s ⁻¹	
Rate of conversion (composite reactions)	$\dot{\xi}_i$	$F_j = F_{j0} + \sum_i \nu_{ij} \dot{\xi}_i$ (open flow system) Steady state	mol s ⁻¹	