THE RATE OF REACTION: A DEFINITION OR THE RESULT OF A CONSERVATION EQUATION?*

ALBERTO E. CASSANO
Instituto de Desarrollo Tecnológico para la Ind. Química
3000—*Santa Fe, Argentina*

A quick survey of the classical literature on chemical kinetics and reactor analysis reveals different criteria concerning the definition of the rate of reaction. Relying on historical rather than rational bases, the following "definition" has been used:

$$r_i = \frac{dC_i}{dt} \qquad (1)$$

Eq. (1) was probably derived from the first physicochemical studies on rates of reaction developed in constant volume batch systems.

This "definition" has been used by Glasstone [1], Benson [2], Daniels [3], Laidler [4], Frost and Pearson [5], and Johnston [6], among others.

On the other hand, chemical engineers mainly engaged in design problems, distrusted the validity of the "definition," taking into account its inapplicability to reacting systems of variable volume. The alternative "definition" was based on the number of moles instead of concentration. The difference lies in defining beforehand an extensive rate of reaction which can then be turned into an intensive property dividing by the reaction volume.

$$r'_i = \frac{dN_i}{dt} \qquad (2)$$

$$r_i = \frac{1}{V_r}\frac{dN_i}{dt} \qquad (3)$$

The greater generality of expression (3) as compared to equation (1) is easily demonstratable, in either conceptual or mathematical terms.

The "definitions" belonging to the kind provided by equation (3) can be found in books such as those written by Hougen and Watson [7], Smith [8], Levenspiel [9], Walas [10], Boudart [11], Pannetier and Souchay [12]; and with explicitly stated limitations by Kramers and Westerterp [13], by Aris [14] and Denbigh [15] as well. Many other cases could be quoted.

A good example for analysis is the "Continuous Flow Stirred Tank Reactor" (CFSTR). In this particular case the product is continuously removed at the system outlet and it becomes evident that at the steady state dN_i/dt is zero (the product being species i) but the rate of reaction is utterly different from zero. Here, as Denbigh remarks, expression (3) is not valid, either. This author tries to narrow the applicability of the "definition" (3) to processes where the only change in reactant i is due to a chemical reaction. This would exclude any other form of physical phenomena causing changes in reactant concentration. The restriction seems valid for the CFSTR and for all forms of diffusive flows. Nevertheless, it does not seem so clear for the "Piston or Plug Flow Reactor" (PFR), in which if, on the limit, dt is taken as the reacting mass average residence-time in the elementary reaction volume of length dz, equation (3) may be properly applied with some substitutions.*

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This work shows the futility of arguing about the "definition" of the reaction rate and the convenience of dealing with the subject from a different viewpoint.

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*This paper is the result of mutually beneficial discussions on the subject with my former classmates Charles Allen and Sieghard Wanke. Any merit to this paper is theirs. Any errors in it are mine.

*It should be noticed that now v_z may be a function of z if changes in the number of moles take place.

the convenience of dealing with the subject from a different viewpoint, that is, drawing the necessary equations from a more fundamental principle, as the general mass conservation equation for multicomponent systems would be.

REDEFINITION OF THE PROBLEM FOR HOMOGENEOUS REACTORS

So far, it is obvious that the existing "definitions" seem to depend either on the author's personal likings or on the reactor to which the equations will be applied.

It seems logical to assume that any reaction rate should be a function not of the system in which it has been determined but only of temperature, pressure and concentration of the species participating in the reaction, just to mention the most commonly encountered variables affecting the rate. The reaction rate could be naturally influenced by the type of reactor-continuous or batchwise—but only up to the extent that it may affect concentrations, temperatures or pressures.

It is necessary to reconcile an expression derived from the ontological concept of the rate of reaction with a mathematical equation expressing exactly the same, involving the variables susceptible of experimental measurement.

Ontologically (and considered as an intensive property), "The rate of reaction is the change in the number of moles which takes place in unit time and unit reaction volume, due to a transformation of reactants into products."

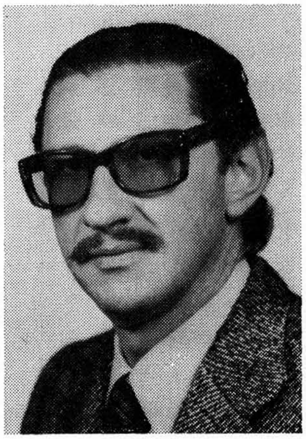
The mathematical expression of the above definition will be set equal to the kinetic equation of the chemical system under consideration; i.e. if such a definition is adequately represented by a mathematical proposition which will be called r, it is evident that:

$$r = \phi\ (C_1, C_2, \ldots .\ \text{etc. } T, P, \text{etc.}) \qquad (4)$$

where ϕ depends on the complexity of the reacting system (order, molecularity, activation energy, etc.). It is the concern of this work to determine the adequate formulation for the left-hand side of equation (4).

The problem at issue has been partially, even though quite accurately, discussed by Petersen [16] and also singularly viewed by Amdur and Hammes [17], particularly for batch reactors. The reader may resort to the quoted references.

In many cases, experimental measurements will register not only the change in concentration but also the resultant of the chemical process of reaction and the physical processes of diffusion, convection and volume changes. From this point of view, all the "definitions" previously analyzed are erroneous and inaccurate, and only applicable, at best, to systems universally used but no less particular (e.g. the constant volume stirred batch reactor, etc.).



Alberto E. Cassano is the founder and Chairman of INTEC; Professor at the Universidad Nacional del Litoral and Member of the Scientific Research Staff of the National Council for Scientific and Technological Research of Argentina. He received his Chemical Engineer's degree from the Facultad de Ingenieria Quimica of U.N.L. (Santa Fe, Argentina) and his Ph.D. degree from the University of California, Davis. His research interests are in Photochemical Reactors and Gas-Liquid Reactions Catalyzed by Solids. At present he is also responsible for a consulting contract (undertaken by INTEC) for the Argentinian Atomic Energy Commission engaged in the development of a Heavy Water Experimental Plant.

Petersen clearly points out that the left-hand side of equation (4) is a direct resultant of the experimental system employed in kinetic determinations, and that, therefore, there is no single definition which could be widely used, still less if the reacting system were non-isothermal. This statement can be effectively generalized and is the subject of the next paragraph.

SOLVING METHODS

If the rate of reaction is to be defined, the problem is usually reduced to finding the rate of change of the reacting species with respect to some independent variable (time in a batch reactor and position in many continuous reactors). The rate of change of the reacting species is generally measured considering the change in the number of moles of the said reactant or the rate of change in its concentration.

An apparent way of solving the problem would be to consider the reaction within a species material volume, instead of the generally used fixed control volume. But it is difficult to think of a species material volume since they are not preserved [18]. If the "particles" of the material volume are elements, the difficulty is overcome at the expense of a greater complexity. Therefore, this strategy is quite troublesome.

A more adequate way of looking into the problem for an isothermal system is to consider the various mechanisms which can bring about concentration changes of a reactant within a system and, then, determine which part of these total changes is due to the chemical reaction, subtracting all contributions other than the reaction.

This means to state in detail a mass conservation balance for a multicomponent system. Generally speaking, there are two categories of phenomena through which a species concentration may vary in a fixed volume in space: (1) The species may appear or disappear by chemical reaction and (2) There is a net flow of this species through the area of this volume element. This flow mechanism, be it diffusion, forced convection or any other means of mass transport, needs not be detailed here. The description of this flow will exclusively depend on the system at stake.

The general conservation equation may be thus written [19]:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{N}_i = r_i \tag{5}$$

or in a more general way: if a_i is the stoichiometric coefficient of species i:

$$r_i = r\, a_i \tag{6}$$

Then:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{N}_i = a_i\, r \tag{7}$$

This well known conservation equation is the only general formulation for homogeneous isothermal rates of reaction that is independent of the reaction system being employed. It clearly shows that the rate of reaction is the "source" or "sink" term in the mass inventory; therefore all the remaining non-zero terms resulting from taking r out of expression (7) must be substituted into the right-hand side of equation (4).

So far, it is obvious that the existing "definitions" seem to depend either on the author's personal likings or on the reactor to which the equations will be applied.

APPLICATION TO COMMON REACTING SYSTEMS

EQUATION (7) WILL now be used to obtain the adequate expressions for some classical reacting systems. The following homogeneous isothermal systems will be considered:

1) **Isothermal constant volume batch reactor**
2) **Isothermal variable volume batch reactor**
3) **Steady state, isothermal continuous plug flow reactor**
4) **Steady state, isothermal continuous flow stirred tank reactor**

In every case, the adequate assumptions will be made in order to allow an analytical description of the flux $\mathbf{N}_i$ so as to simplify the rate expression.

ISOTHERMAL CONSTANT VOLUME BATCH REACTOR

IF WE ASSUME THAT properties are constant in the whole volume of the reactor (especially concentration and temperature), then the divergence of the flux becomes zero since $\mathbf{N}_i$ will be independent of position. Therefore, if $\nabla \cdot \mathbf{N}_i = 0$, equation (7) is reduced to:

$$r = \frac{1}{a_i}\frac{dC_i}{dt} \tag{8}$$

where the derivative is now total insofar as concentration will be a function of time only.

ISOTHERMAL VARIABLE VOLUME BATCH REACTOR

IF WE ASSUME THAT the expansion of volume is slow so that, as in the previous case, such properties as concentration, pressure and temperature are independent of their position within the reactor, no diffusional effects whatsoever will result, and the flow will be caused only by expansion.

In this case, by definition:

$$\mathbf{N}_i = C_i\, \mathbf{v}_i^*$$

but, as all species expand at the same rate:

$$\mathbf{v}_i = \mathbf{v}_j = \mathbf{v} = \mathbf{v}^*$$

the velocity of all species coincides with the global velocity of the system.

With the previous relationships, equation (7) results:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (C_i\, \mathbf{v}) = a_i\, r$$

But, since it has been assumed that concentration is independent of position $\nabla C_i = 0$. Then:

$$\frac{\partial C_i}{\partial t} + C_i\, (\nabla \cdot \mathbf{v}) = a_i\, r \tag{9}$$

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RATE OF REACTION

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The evaluate $\nabla \cdot \mathbf{v}$ the continuity equation is used (see ref. 19):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad (10)$$

But for this system $\nabla \rho = 0$. Besides $\rho = m/V$ and $\partial m/\partial t = 0$ because the total mass of the system is constant in time. Substituting these relationships into equation (10) and operating:

$$\nabla \cdot \mathbf{v} = \frac{1}{V}\frac{\partial V}{\partial t} \qquad (11)$$

Substituting C_i by N_i ($C_i = N_i/V$) and performing the differentiation, the equation for r, in the case of an isothermal variable volume batch reactor, results:

$$r = \frac{dN_i}{a_i V(t)\, dt} \qquad (12)$$

The partial differential is now a total differential insofar as N_i is a function of time only. It must be noticed, however, that we should know the relationship existing between the change of volume and the reaction extent, i.e., if the extent of the reaction is expressed in terms of conversion, there should be at hand a relationship of the following type: V (t) = V (V_o,x). In most gaseous systems a linear variation of volume with conversion is often assumed (9).

STEADY STATE ISOTHERMAL CONTINUOUS PLUG FLOW REACTOR

UNDER STEADY CONDITIONS, general equation (7) is reduced to:

$$\nabla \cdot \mathbf{N}_i = a_i r$$

If, according to the model it is supposed that there are no diffusion or dispersion effects, the mass flux is only due to the global convective flow. Hence:

$$\mathbf{N}_i = C_i \mathbf{v}$$

from where we finally have:

$$r = \frac{d(C_i v_z)}{a_i\, dz} \qquad (13)$$

since in this reactor the flow is uni-directional. (Direction z has been chosen as representative of the model).

If the total number of moles is not preserved and, furthermore, if the reaction takes place in a gaseous phase, equation (13) is not so useful for v_z will become a function of z and it will not be possible to take it out of the differential. If the number of moles stays constant, equation (13) is reduced to:

$$r = \frac{v_z\, dC_i}{a_i\, dz} \qquad (14)$$

which, obviously, also includes the assumption that pressure changes along the reactor are small (due to losses by friction, for example) because otherwise v_z would not be independent of z, either.

Equation (13) can be adequately modified to become useful even in those cases in which the number of moles is not constant.

To do so, we simply transform the equation and work in terms of mass fractions (w). Recalling that:

$$C_i = \frac{\rho\, w_i}{M_i}$$

In this equation w_i is the mass fraction of component i and M_i its molecular weight. Substituting in equation (13):

$$\frac{d}{dz}\left[\frac{\rho\, w_i}{M_i} v_z\right] = a_i r \qquad (15)$$

and since the mass flow rate G_o is constant: $\rho\, v_z = G_o$ = constant; hence, the rate of reaction can be written as:

$$r = \frac{G_o\, dw_i}{a_i M_i\, dz} \qquad (16)$$

STEADY STATE, ISOTHERMAL CONTINUOUS FLOW STIRRED TANK REACTOR

The SSICFSTR is an ideal type of system, in which concentration of reactants does not depend upon time or position within the reactor. The mathematical description of the flow within the reactor is exceedingly difficult, as we are dealing with a highly idealized case which, consequently, cannot be fully achieved in practice. Nevertheless, in many cases the deviations are almost negligible and the system has been successfully modelled. The exact mathematical description cannot be accomplished because the model implies a transport of mass, instantaneously, over finite distances.

But the difficulty may be overcome if we do away with the necessity of describing the internal pattern of the flow inside the reactor. To do so, the general equation (7) is integrated over the

This statement sums up the whole problem: The rate of reaction expression is the "sink" or "source" term in the continuity equation for multicomponent systems which will take into account the creation or destruction of the said species by chemical reaction.

volume of the reactor so as to obtain a macroscopic balance.

$$\int_V \frac{\partial C_i}{\partial t}\, dV = - \int_V (\nabla \cdot \mathbf{N}_i)\, dV + \int_V a_i\, r\, dV \quad (17)$$

Under steady state conditions the left-hand side is zero and, as the assumptions of the model grant that all properties within the reactor are constant, r is not a function of the space coordinates and it may be taken out of the integral. With this, the previous equation is reduced to:

$$a_i\, r\, V_R = \int_V (\nabla \cdot \mathbf{N}_i)\, dV \quad (18)$$

Applying the divergence theorem to the right-hand side of equation (18), we obtain:

$$a_i\, r\, V_R = \int (\mathbf{N}_i \cdot \mathbf{n})\, dA \quad (19)$$

The integration performed over the whole surface of the reactor may be evaluated because the flux is non-zero only at the inlets and outlets.

$$\int_A (\mathbf{N}_i \cdot \mathbf{n})\, dA = \int_{In.} (\mathbf{N}_i \cdot \mathbf{n})\, dA + \int_{Out.} (\mathbf{N}_i \cdot \mathbf{n})\, dA \quad (20)$$

On the right-hand side, the first term represents the inlet flow of component i and the second one, the outlet flow. Taking into account the directions of unit normal vectors **n**, the final equation is:

$$r = \frac{1}{a_i V_R} (F_{i,\ outlet} - F_{i,\ inlet}) \quad (21)$$

which is the expression usually written for the reaction rate in a continuous stirred tank reactor. **The integration of the differential equation (7), so accomplished, brings about a macroscopic balance for species i, which is usually the starting point of the derivations in the books on applied kinetics. In this work we have followed this approach in order to demonstrate the absolute generality of equation (7).**

In the following section, this analysis will be extended to two more complex experimental systems, the recycle reactors. These are often useful for obtaining kinetic data.

APPLICATION TO ISOTHERMAL RECYCLE REACTORS

RECYCLE REACTORS HAVE been widely used since the publication of the original papers by Hougen [20], Perkins and Race [21], Biskis and Smith [22], Korbach and Stewart [23], and **Cassano, Matsuura and Smith [24] as a means of** retaining the differential operation of the reactor and, at the same time, eliminating the restrictions of inaccuracy in the analysis of the small composition changes.

Moreover, control of the flow rates in the recycle allows the reduction of diffusional resistances and the elimination of temperature gradients. Difficulties may be centered around the effects of reaction by-products, the considerably longer time usually needed to obtain the steady state condition in the recycling section of the apparatus and the difficulty in operating under pre-fixed concentration conditions. (The last two are especially important for the continuous type).

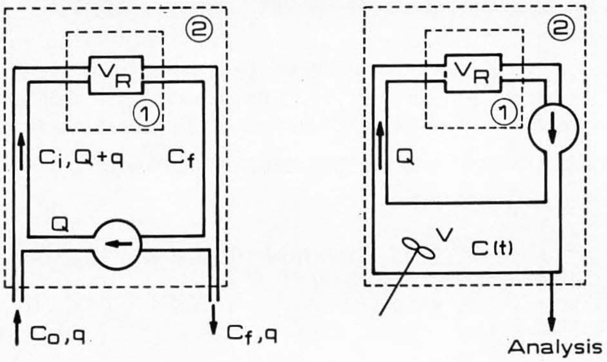
Once more, "general definitions" will be useless and we shall have to resort to the general mass inventory. In order to simplify the matter, let us consider the case when the total number of moles is constant.

ISOTHERMAL CONTINUOUS RECYCLE REACTOR

FIGURE 1 (A) SHOWS the system under consideration. Operating conditions must be adjusted in order to fulfill the following assumptions:

1) The operation in V_R is differential, i.e., the outlet concentration $C_{i,f}$ is very close to the inlet concentration of the reactor $C_{i,i}$.
2) Differences in concentration between $C_{i,o}$ and $C_{i,f}$ are accurately measured.
3) High recycling flow rate (Q).

When Q → ∞ the whole reactor, analyzed in the control volume (2), is an excellent approximation to a continuous flow stirred tank reactor, working at differential conversions as the reacting mixture goes through the control volume (1). The General equation (7) will be applied to each of these systems.



(A) (B)

FIGURE 1

Under steady state conditions, the concentration in the reactor is independent of time. The differential equation is reduced to:

$$\nabla \cdot \mathbf{N}_i = \mathbf{r}_1\, \mathbf{a}_i \qquad (22)$$

On the other hand, the operational characteristics allow us to neglect any form of dispersion or diffusion effects. Consequently:

$$\mathbf{N}_i = C_i\, \mathbf{v} \qquad (23)$$

If the differential equation (22) is integrated over the control volume, the result is:

$$\int_V (\nabla \cdot \mathbf{N}_i)\, dV = \int_V r_1\, a_i\, dV$$

On the left-hand side we shall apply the divergence theorem and on the other side we shall take into account the fact that the reactor is differential. Substituting expression (23) yields:

$$\int_A (\mathbf{n} \cdot C_i\, \mathbf{v})\, dA = r_1\, a_i \int_V dV$$

and finally:

$$(q + Q)\ (C_{i,f} - C_{i,i}) = a_i\, r_1\, V_R \qquad (24)$$

On the other hand, if the whole system (2) is treated as a CFSTR the application of equation (21) will yield:

$$q\ (C_{i,f} - C_{i,o}) = r_2\, a_i\, V_R \qquad (25)$$

In equation (25) we have V_R only on the right-hand side, because it is the only part of the total volume where r is different from zero. But the global velocity r_2 has to be equal to that produced in the reactor itself, that is to say r_1. If it is shown that r_1 accurately represents a differential rate of reaction, then the values which may be obtained through the application of equation (25) will portray the exact rate of reaction and not an average value. This will be true if $C_{i,i}$ is very close to $C_{i,f}$ as has been initially assumed. The only remaining doubt would be to know how these conditions could be accomplished. As $r_1 = r_2$, we have:

$$(q + Q)\ (C_{i,f} - C_{i,i,}) = q\ (C_{i,f} - C_{i,o})$$

$$C_{i,i} = \frac{Q\, C_{i,f} - q\, C_{i,o}}{q + Q}$$

If, as was first assumed, Q is sufficiently high, $Q >> q$ and therefore $C_{i,i} \cong C_{i,f}$.

For isothermal continuous recycle reactors, working under the conditions stated above, an adequate expression for the rate of reaction results:

$$r = \frac{q\ (C_{i,f} - C_{i,o})}{a_i\, V_R} \qquad (26)$$

Notice that the condition of a high recycling flow, necessary for the differential operation in V_R, coincides with the requirements for the operation of the global system as a continuous stirred tank reactor. The extension to a system with variable number of moles only complicates the algebra.

ISOTHERMAL BATCH RECYCLE REACTOR

FIGURE 1 (B) illustrates the system under consideration. For extremely slow reactions and for cases where one wishes to avoid serious limitations in the size of the samples for analysis, this is an adequate experimental device. Within this system there are no disadvantages such as those pointed out for a continuous recycle reactor, but an experimental problem may arise: the existence of a recycling device (with movable parts in most cases) could introduce contamination of the reacting mixture from the outside. For a batch system, the impurity level will grow with time. This is not so severe in continuous systems.

The operating conditions are as follows:

1) The operation in V_R is differential.
2) For reasonable intervals of time, concentration differences are accurately measured in V.
3) High recirculating flow, and adequate mixing in V.

We treat the whole system as a batch reactor: if the recirculating flow is high, the concentration will be uniform. Hence, $\nabla \cdot \mathbf{N}_i = 0$ and results:

$$\int_V \frac{dC_i}{dt}\, dV = \int_V a_i\, r\, dV$$

Since according to previous assumptions, concentration is not a function of position, the total derivative has been employed and it may be taken out of the volume integral. On the right-hand side, the integral will be different from zero only in those portions of the volume where r is different from zero. Due to the differential performance of V_R, one then obtains:

$$\frac{dC_i}{dt}(V + V_R) = a_i\, r\, V_R$$

and the rate of reaction, when there is no variation in the number of moles, is finally:

$$r = \frac{(V + V_R)\, dC_i}{V_R\, dt} \qquad (27)$$

This equation must be corrected for additional changes of concentration, in case the sample volumes for analysis were significant. A great relationship of V/V_R reduces this problem, but may largely prolong the necessary reaction time to attain accurately measured conversions.

Abalance in the reactor itself shows the conditions for the differential operation of V_R. At each cycle the reactor behaves as a steady state isothermal continuous plug flow reactor.

$$\nabla \cdot \mathbf{N}_i = a_i\, r$$

$$\int_V (\nabla \cdot \mathbf{N}_i)\, dV = \int_V a_i\, r\, dV$$

Assuming, for the time being, an average value of r, the result will be:

$$Q\,(C_{i,f} - C_{i,i}) = a_i\, r_{avg}\, V_R$$

where $C_{i,f}$ and $C_{i,i}$ are the outlet and inlet concentrations of reactor V_R at each cycle. If the rate of reaction has a finite value and, as previously assumed, Q is high, the difference between inlet and outlet concentrations will be small. By increasing Q the difference could be made small enough to turn r_{avg} into a differential rate of reaction. Notice that this condition was also assumed as necessary to propose a uniform composition model. It must also be noticed that an adequate experimental device should minimize the volumes of the connecting lines between the reactor V_R and the tank V.

HETEROGENEOUS SYSTEMS OF REACTION

IN THIS WORK WE have emphasized the analysis of the different isothermal homogeneous reacting systems. The adequate treatment for heterogeneous reactions (catalyzed and non-catalyzed) is outside its scope.

It is not far-fetched, however, to notice that, in most cases, the flaws of the so-called definitions are even more evident within these systems. The problem may be summarized as follows:

1) **At the microscopic level all heterogeneous reactions take place at interphases.**
2) **Even at the macroscopic level, many heterogeneous reactions take place at interphases.**
3) **In many cases the rate of reaction takes place not only inside the control volume but on its boundaries as well.**
4) **Hence, accurately speaking, the rate of reaction will, in many cases, be a boundary condition of the general mass conservation equation.**
5) **When this happens at the microscopic level (in the case of a catalyst, for example), an "effective" rate has been used due to the difficulty in solving the conservation equations with complicated geometrics for the boundary conditions.**
6) **At the macroscopic level (for example, the case of free radical termination reactions on the walls of a reactor) when the rates of reaction are boundary conditions, the conservation equations are complicated, since diffusional terms cannot be neglected. See for example reference [25].**
7) **Even ontologically, the rates of reaction in heterogeneous systems undergo a change, insofar as their intensive character is attained by means of an expression referring to the area of this boundary (real or ideal).**

All this makes even more evident the futility of trying to establish a general "definition" of a reaction rate.

CONCLUSIONS

IN THE PREVIOUS sections, six different expressions have been attained for the rate of reaction: equations (8), (12), (21), (26) and (27). Many others could be found for other physical systems using equation (7) as a starting point. Quoting Petersen [16]: "to argue that any of these (rate of reaction expressions) is more correct than all of the others as its defining equation, is to confuse a conservation equation with a definition." This statement sums up the whole problem. *The rate of reaction expression is the "sink" or "source" term in the continuity equation for multicomponent systems which will take into account the creation or destruction of the said species by chemical reaction.*

The rates of reaction thus attained will be independent of the system used to measure them (provided it is a homogeneous reaction). This means that the kinetic expression of the rate of reaction $r = \phi\ (T, C_i, P, \text{etc.}\ .\ .\ .\ .\ .)$, if determined using equation (7) as a starting point, will be independent of the physical device employed to obtain the kinetic data.

There may exist a sound definition of an extensive rate of reaction based on the concept of the "extent of reaction," both introduced by De Donder [26], which may be useful for thermodynamic calculations but the idea becomes devoid of general validity when one needs an intensive property. For the purposes of reaction engineering this is legitimate but it is of little help.

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NOMENCLATURE

A : Area (cm^2)
a : Stoichiometric coefficient
C : Concentration (mole•cm^{-3})
F : Molar flow rate (mole•s^{-1})
G_o : Mass flow rate per unit area (gr•s^{-1}•cm^{-2})
M : Molecular weight (gr•mole^{-1})
m : Mass (gr)
N : Number of moles
$\mathbf{N}$: Molar flux (mole•cm^{-2}•s^{-1})
$\mathbf{n}$: Outwardly directed unit normal vector
P : Pressure (Kgf•cm^{-2})
Q : Volumetric recycle flow rate (cm^3•s^{-1})
q : Volumetric input flow rate (cm^3•s^{-1})
r : Rate of reaction (intensive) (mole•cm^{-3}•s^{-1})
T : Temperature (°K)
t : Time (s)
V : Volume (cm^3)
v : Linear velocity (cm•s^{-1})
V_R : Volume of reactor (cm^3)
w : Mass fraction
x : Conversion
ρ : Density (gr•cm^{-3})
ϕ : Kinetic expression for rate of reaction (mole•cm^{-3}•s^{-1})
∇ : Vector operator

Subindices and Supraindexes

avg : Average value
i : Indicates species or initial condition, according to context
f : Final condition
o : Inlet condition
R : Indicates reactor
z : Indicates direction
— : Indicates vector
* : Indicates molar average velocity

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