



[The Engineering Of Chemical Reactions L D Schmidt Solution Manual 2](#)

or for species  $j$

$$C_j = [A_j]$$

In gases the most used quantity for the density of species  $j$  is the partial pressure  $P_j$ . This can be related to concentration and mole fraction  $y_j$  through the relations

$$y_j = \frac{N_j}{\sum N_j} = \frac{N_j}{N}$$

and

$$P_j = y_j P = C_j RT$$

where  $P$  is the total pressure and  $N$  is the total number of moles in the system. In this equation we assume ideal gases ( $PV = NRT$ ) to relate partial pressure to concentration, while for **nonideal** gases (not considered here) we would need an equation of state to describe the density of each chemical species.

For liquid solutions we could use

$$x_j = \frac{N_j}{\sum N_j}$$

where  $x_j$  is the mole fraction of species  $j$  in liquid solution. However, we will use only the concentration,  $C_j = N_j / V$ , throughout this text.

For an irreversible reaction we can frequently describe the rate to a good approximation as

$$r = k \prod_{j=1}^R C_j^{m_j}$$

where  $m_j$  is the order of the reaction with respect to the  $j$ th species and the product extends over all species in the reaction with  $m_j = 0$  for species that do not affect the rate of reaction. If the rate is proportional to the concentration of a species raised to a power ( $m_j$ ), we say that this form of the rate expression is described by "power-law kinetics." This empirical function is frequently used to describe reaction rates, but it frequently is not accurate, especially with surface or enzyme-catalyzed reactions, which we will consider later.

Several alternate definitions of the reaction rate are used in different texts. In our notation we will always write a chemical reaction as an equation and then define the rate of that reaction as the positive rate of change for that particular stoichiometry. Consider the reaction



In an alternate definition of reaction rates, one writes a rate as *the rate of formation of each species*. In that notation one would define  $r_A$ ,  $r_B$ , and  $r_C$ , with the definitions

$$r_A = -2k[A]^2 = -2r$$

$$r_B = +k[A]^2 = r$$

$$r_C = +3k[A]^2 = +3r$$



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