

# SIMPLIFYING CHEMICAL REACTOR DESIGN BY USING MOLAR QUANTITIES INSTEAD OF FRACTIONAL CONVERSION\*

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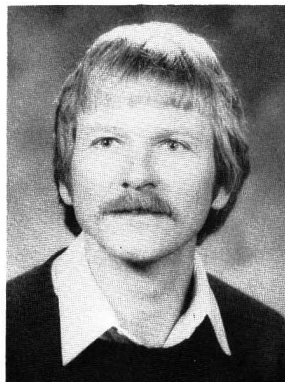
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**M**OST CHEMICAL REACTORS are nonisothermal, involve multiple reactions, have mole changes due to reaction, or have reactions with complicated rate expressions. In teaching reactor analysis, it is important that the techniques we present can be applied to these realistic situations; current approaches violate this principle.

In the textbooks on chemical reaction engineering,



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TABLE 1

## Chemical Reaction Engineering Texts Using Fractional Conversion as the Dependent Variable

Butt, 1980	Chen, 1983
Cooper, Jeffreys, 1971	Denbigh, Turner, 1981
Fogler, 1974; 1986	Froment, Bischoff, 1979
Hill, 1977	Holland, Anthony, 1979
Levenspiel, 1962, 1972	Levenspiel, 1979
Peters, Timmerhaus, 1980	Rase, 1977
Smith, 1956, 1972, 1980	Tarhan, 1983

authors use a variety of dependent variables in reactor mass balances (see Tables 1, 2). The tables show that fractional conversion is employed by a significant majority of authors. We argue here that using fractional conversion in these mass balances is extremely awkward and can lead to serious confusion. Molar quantities as dependent variables in reactor-analysis equations make instruction much easier and chemical reactor design more straightforward. We show this by comparing the use of molar quantities with using fractional conversion for different situations. We also discuss the advantages of using differential versions of reactor mass balances rather than the integrated forms.

## GAS-PHASE SYSTEMS

We begin with the steady-state, gas-phase, plug-flow reactor; extension of the principles to other situations is direct. Consider a gaseous reaction,  $A \rightarrow$  products. The reaction rate  $r_A$  is a function of the component concentrations; carrying out a molar balance on substance A over a differential control volume results in

$$\frac{dF_A}{dV} = r_A = f(C_A, C_B, \dots, C_1, \dots) \quad (1)$$

in which  $F_A$  is the molar flow rate of substance A at a point in the tube, and the  $C_i$ 's are concentrations at

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this point. To solve this equation, both  $F_A$  and  $r_A$  (and therefore the  $C_i$ 's) must be expressed in terms of a common dependent variable. Tables 1 and 2 show that the most common dependent variable is fractional conversion. This is the fraction of a substance's entering molar flow rate which has been converted. For a substance A,

$$F_A = F_{A0}(1 - x_A) \quad \text{or} \quad x_A = 1 - \left(\frac{F_A}{F_{A0}}\right) \quad (2)$$

Substituting Eq. (2) into Eq. (1) yields

$$F_{A0} \left(\frac{dx_A}{dV}\right) = -f(C_A, C_B, \dots, C_i, \dots) \quad (3)$$

To solve Eq. (3), the  $C_i$ 's must be expressed in terms of the fractional conversion. It will be shown that using fractional conversion in this way frequently leads to extremely awkward formulations of Eq. (1). In other situations, fractional conversion cannot be used at all as a dependent variable in reactor mass balances.

The molar flow rate of the principal component,  $F_A$  in Eq. (1), also can be used as the dependent vari-

able. In Eq. (1), the concentrations can be expressed in terms of the molar flow rates and the ideal gas law, *i.e.*,

$$C_i = y_i \left(\frac{P}{RT}\right) = \left(\frac{F_i}{F_T}\right) \left(\frac{P}{RT}\right) \quad (4)$$

and the various  $F_i$ 's can be related to the dependent variable,  $F_A$ , by reaction stoichiometry. This approach offers a simple means for solving Eq. (1).

#### DIFFERENTIAL OR INTEGRAL FORMS OF EQUATIONS?

For most realistic cases, reactor-analysis equations cannot be solved to give analytic closed-form solutions, and numerical techniques must be used. A method such as a Runge-Kutta technique can be used to solve the differential equation or equations directly. In many cases, an alternative attack is possible; the variables can be separated and the integrals evaluated using Simpson's rule or some other scheme.

We prefer the first approach, because separation of variables merely adds an unnecessary step which gives no advantage in solution technique. Moreover, direct solution of the differential equations yields the flow rates, concentrations, temperature, and pressure as functions of location or time in the reactor. This enables the analyst to establish the location or point in time of hot spots, critical concentrations, or dangerous pressures. This is not possible when the separated variables are integrated numerically; to obtain an equivalent result, separate integrations would have to be carried out for each location or time desired.

Most important, though, the approach involving direct solution of the differential equations is better because it can be extended to situations where the variables are not separable, such as nonisothermal reactors with heat exchange, many multiple-reaction systems, and most unsteady-state flow systems. For these reasons, we consider only the differential equations in our comparisons.

#### CONSTANT-DENSITY SYSTEMS

Constant mass-density reactor systems make a significant class that merits consideration. For example, most liquid-phase systems do not change density much during a chemical reaction. Thus the volumetric

**TABLE 2**

**Chemical Reaction Engineering Texts Using Dependent Variables Other Than Fractional Conversion**

Text	Variable Used
Aris, 1969	extent of reaction, $\epsilon = (F_i - F_{i0})/\alpha_i$
Carberry, 1976	*
Denbigh, 1966; Denbigh, Turner, 1971, 1981	moles product/unit mass
Hougen, Watson, 1947	moles converted/unit mass feed
Hill, 1977**	extent of reaction
Kramer, Westerterp, 1963	mass fraction formed or converted
Petersen, 1965	moles/amt. mass numerically equal to MW of feed
Walas, 1959	moles converted/unit mass feed

\*A single dependent variable is not used. A variable is chosen appropriate to the situation being considered.

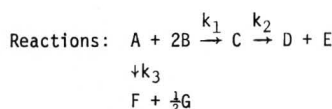
\*\*Fractional conversion is used in reactor equations (cf. Table 1), but extent of reaction is used in other contexts.

flow rate  $q$  in liquid-flow reactors is usually not altered significantly, and the molar concentration  $C_A$  can be set equal to  $F_A/q$ . For this reason, either concentrations or molar flow rates are useful variables in a flow reactor with a constant-density process. However, for an unsteady-state flow system, the numbers of moles of substances in the reactor are the only acceptable dependent variables. This is shown below in the second example.

## EXAMPLES

### Case 1: Isothermal multiple-reaction system

Reactor system: A gas-phase, steady-state, plug-flow reactor.



$$\begin{aligned} \text{Rate laws: } & r_A = -k_1 C_A^\alpha C_B^\beta - k_3 C_A^Y \\ & r_B = -2k_1 C_A^\alpha C_B^\beta \\ & r_C = k_1 C_A^\alpha C_B^\beta - k_2 C_C^\delta \\ & r_D = r_E = k_2 C_C^\delta; \quad r_F = 2r_G = k_3 C_A^Y \end{aligned}$$

Reactor design equations using molar flow rates:

$$\begin{aligned} \frac{dF_A}{dV} = & -k_1 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^{\alpha+\beta} (F_A)^\alpha (F_B)^\beta \\ & - k_3 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^Y (F_A)^Y \end{aligned} \quad (5)$$

$$\frac{dF_B}{dV} = -2k_1 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^{\alpha+\beta} (F_A)^\alpha (F_B)^\beta \quad (6)$$

$$\begin{aligned} \frac{dF_C}{dV} = & k_1 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^{\alpha+\beta} (F_A)^\alpha (F_B)^\beta \\ & - k_2 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^\delta (F_C)^\delta \end{aligned} \quad (7)$$

$$\frac{dF_D}{dV} = \frac{dF_E}{dV} = k_2 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^\delta (F_C)^\delta \quad (8)$$

$$\frac{dF_F}{dV} = 2 \left( \frac{dF_G}{dV} \right) = k_3 \left( \frac{1}{F_{A0} + F_B + F_E + F_G + F_I} \right) \left( \frac{P}{RT} \right)^Y (F_A)^Y \quad (9)$$

Reactor design equations using fractional conversions:

$$\begin{aligned} \frac{dX_A}{dV} = & k_1 F_{A0}^{\alpha+\beta-1} \left( \frac{1}{F_{A0}[1-X_A + (F_{B0}/F_{A0}) - X_{AC} + 1.5X_{AF}] + F_I} \right) \left( \frac{P}{RT} \right)^{\alpha+\beta} \\ & \cdot \left( (1 - X_A)^\alpha \left( \frac{F_{B0}}{F_{A0}} - 2X_{AC} \right)^\beta \right) \\ & + k_3 F_{A0}^{Y-1} \left( \frac{1}{F_{A0}[1-X_A + (F_{B0}/F_{A0}) - X_{AC} + 1.5X_{AF}] + F_I} \right) \left( \frac{P}{RT} \right)^Y (1-X_A)^Y \end{aligned} \quad (10)$$

$$\begin{aligned} \frac{dX_{AC}}{dV} = & k_1 F_{A0}^{\alpha+\beta-1} \left( \frac{1}{F_{A0}[1-X_A + (F_{B0}/F_{A0}) - X_{AC} + 1.5X_{AF}] + F_I} \right) \left( \frac{P}{RT} \right)^{\alpha+\beta} \\ & \cdot \left( (1 - X_A)^\alpha \left( \frac{F_{B0}}{F_{A0}} - 2X_{AC} \right)^\beta \right) \\ & - k_2 F_{A0}^{Y-1} \left( \frac{1}{F_{A0}[1-X_A + (F_{B0}/F_{A0}) - X_{AC} + 1.5X_{AF}] + F_I} \right) \left( \frac{P}{RT} \right)^Y (X_{AC})^Y \end{aligned} \quad (11)$$

$$\frac{dX_{AD}}{dV} = k_2 F_{A0}^{\delta-1} \left( \frac{1}{F_{A0}[1-X_A + (F_{B0}/F_{A0}) - X_{AC} + 1.5X_{AF}] + F_I} \right) \left( \frac{P}{RT} \right)^\delta (X_{AC})^\delta \quad (12)$$

$$\frac{dX_{AF}}{dV} = k_3 F_{A0}^{Y-1} \left( \frac{1}{F_{A0}[1-X_A + (F_{B0}/F_{A0}) - X_{AC} + 1.5X_{AF}] + F_I} \right) \left( \frac{P}{RT} \right)^Y (1-X_A)^Y \quad (13)$$

**Comments:** Using the fractional conversion in multiple-reaction systems requires the definition and use of several subsidiary fractional conversions. In this example,  $X_{AC}$  is the fraction of A converted only to C, not to D, E, F, or G;  $X_{AD}$  is the fraction of A converted only to D;  $X_{AF}$  is the fraction of A converted only to F, and  $X_A = X_{AC} + X_{AD} + X_{AF}$ . Not only are the mass balances much simpler when molar flow rates are used, but they do not require the tortured mental convolutions necessary for implementation of the subsidiary fractional conversions. The denominators in the mass balances are especially difficult for students to create correctly. As shown above, the molar flow rates are straightforward to define and use, even in complicated, multiple-reaction systems.

Of the differential equations presented for each approach, only three are necessary, since only three independent reactions occur. Stoichiometric equivalences can determine the other flow rates, *e.g.*,  $F_F = F_{A0} - (F_A + F_C + F_D)$ .

### Case 2: Isothermal stirred tank with outflow

Reactor system: A tank reactor with a steady out-

flow starting at  $t = 0$ . Initial charge contains reactant A and inerts; the outflow volumetric flow rate is  $q_f$ . This might describe a leaking nuclear waste site.



Rate law:  $r_A = -kC_A$

Reactor design equations using molar quantities:

$$\frac{dN_A}{dt} = -kN_A - q_f \left( \frac{N_A}{V} \right) \quad (14)$$

$$V = V_0 - q_f t \quad (15)$$

Reactor design equation using fractional conversion: *None possible.*

**Comments:** Using molar quantities, the mass balance can be integrated analytically; the solution is

$$N_A = N_{A0} e^{-kt} [1 - (q_f t / V_0)] \quad (16)$$

This is one of the simplest unsteady-state reactor systems, yet it appears impossible to express the mass balance in terms of fractional conversion without also including at least one molar quantity as a variable. Because A reacts, leaves, or remains in the reactor,

$$N_A(t) = N_{A0} [1 - X_A(t)] - q_f \int_0^t [N_A(\beta) / V(\beta)] d\beta \quad (17)$$

and  $N_A$  must also be included as a variable. Hill [11, p. 301] has noted this difficulty. In contrast, the substance A in a batch reactor is restricted to either reacting or remaining in the reactor, and  $N_A$  can be expressed as  $N_{A0}(1-X_A)$ . Similarly, in a steady-state, stirred-tank flow reactor, A either reacts or leaves, and  $F_A$  can be expressed as  $F_{A0}(1-X_A)$ . For unsteady-state systems with an outflow stream, too many possibilities are present, and fractional conversions cannot be used.

### Case 3: Reactor with an entering side stream

Reactor system: Steady-state, isothermal, plug-flow reactor with entering side stream  $F_{A10}$ . Feed contains A and inerts; the side stream entering the reactor at point  $V_1$  is pure A. This configuration avoids a high initial concentration of A in order to reduce production of undesired product C.



Rate laws:  $r_A = -k_1 C_A - 2k_2 C_A^2$

$r_B = k_1 C_A$ ;  $r_C = k_2 C_A^2$

Reactor design equations using molar flow rates:

$$F_A = F_{A0} - F_B - 2F_C \quad (18)$$

$$\frac{dF_B}{dV} = k_1 \left( \frac{1}{F_{A0} - F_C + F_I} \right) \left( \frac{P}{RT} \right) F_A \quad (19)$$

$$\frac{dF_C}{dV} = k_2 \left( \frac{1}{F_{A0} - F_C + F_I} \right)^2 F_A^2 \quad (20)$$

B.C.: At  $V = 0$ :  $F_A = F_{A0}$ ;  $F_{A0} = F_{A0}$   
 At  $V = V_1$ :  $F_{A1+} = F_{A1-} + F_{A10}$ ;  $F_{A0} = F_{A0} + F_{A10}$  (21)

Reactor design equations using fractional conversions:

$$X_A = X_{AB} + X_{AC} \quad (22)$$

$$\frac{dX_{AB}}{dV} = k_1 \left( \frac{1}{F_{A0}(1 - \frac{1}{2}X_{AC}) + F_I} \right) \left( \frac{P}{RT} \right) (1 - X_A) \quad (23)$$

$$\frac{dX_{AC}}{dV} = k_2 \left( \frac{1}{F_{A0}(1 - \frac{1}{2}X_{AC}) + F_I} \right)^2 \left( \frac{P}{RT} \right)^2 F_{A0} (1 - X_A)^2 \quad (24)$$

B.C.:

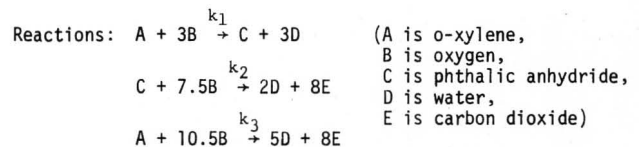
At  $V = 0$ :  $F_{A0} = F_{A0}$ ;  $X_{AB} = 0$ ;  $X_{AC} = 0$

At  $V = V$ :  $F_{A0} = F_{A0} + F_{A10}$ ;  $X_{AB1+} = (F_{A0} X_{AB1-}) / (F_{A0} + F_{A10})$ ;  
 $X_{AC1+} = (F_{A0} X_{AC1-}) / (F_{A0} + F_{A10})$  (25)

**Comments:** Here, use of fractional conversions not only makes the mass balances more involved, but severely complicates the boundary conditions.

### Case 4: Energy balance for reactor with heat transfer.

Reactor system: Nonisothermal, gas-phase, plug-flow reactor with heat transfer (catalytic oxidation of o-xylene to produce phthalic anhydride).



Rate laws [11]:

$$r_A = -k_1 C_A - k_3 C_A \quad [k_i = A_i \exp(-E_i/RT)]$$

$$r_B = -3k_1 C_A - 7.5k_2 C_C - 10.5k_3 C_A$$

$$r_C = k_1 C_A - k_2 C_C$$

$$r_D = 3k_1 C_A + 2k_2 C_C - 5k_3 C_A$$

$$r_E = 8k_2 C_C + 8k_3 C_A$$

Energy balance equation using molar flow rates:

**Another benefit to using the differential equations occurs because students tend to memorize the integrated forms for particular cases. They then use the integrated forms even when the variables are not separable. This happens much less frequently when the differential-equation approach is taught.**

$$\frac{dT}{dV} = \left( \frac{1}{F_A C_{PA} + F_B C_{PB} + F_C C_{PC} + F_D C_{PD} + F_E C_{PE} + F_I C_{PI}} \right) \cdot \left( \frac{1}{F_A + F_B + F_C + F_D + F_E + F_I} \right) \left( \frac{P}{RT} \right) \cdot \left[ A e^{-E_1/RT} (F_A)(-\Delta H_{r1}) + A_2 e^{-E_2/RT} (F_C)(-\Delta H_{r2}) + A_3 e^{-E_3/RT} (F_A)(-\Delta H_{r3}) - (4U/D)(T-T_{ex}) \right] \quad (26)$$

Energy balance equation using fractional conversions:

$$\frac{dT}{dV} = \left( \frac{1}{F_{A0} \{ (1-X_A) C_{PA} + [(F_{B0}/F_{A0}) - (3X_{AC} + 10.5X_{AE})] C_{PB} + X_{AC} C_{PC} + (3X_{AC} + 5X_{AE}) C_{PD} + 8X_{AE} C_{PE} \} + F_I C_{PI}} \right) \cdot \left( \frac{1}{F_{A0} (1-X_A + X_{AC} + 2.5X_{AE}) + F_{B0} + F_I} \right) \left( \frac{P}{RT} \right) \cdot \left[ F_{A0} [A_1 e^{-E_1/RT} (1-X_A)(-\Delta H_{r1}) + A_2 e^{-E_2/RT} (X_{AC})(-\Delta H_{r2}) + A_3 e^{-E_3/RT} (1-X_A)(-\Delta H_{r3})] - (4U/D)(T-T_{ex}) \right] \quad (27)$$

**Comments:** Only the energy balance is presented here; the superiority of the molar quantity approach in multiple-reaction mass balances was illustrated in Case 1. In energy balances as in mass balances, the molar-quantity approach is invariably more straightforward for all but the simplest systems. If fractional conversions are used, the denominators, especially in energy balances, become extremely complex and are difficult to derive and explain.

#### ADDITIONAL ADVANTAGES TO MOLAR QUANTITIES

When fractional conversion is used as a dependent variable in mass and energy balances, additional parameters are sometimes introduced to simplify the forms of the equations. For example, parameters have been defined for molar ratios of feeds and for volume change upon reaction [15, 11, 8]. Introduction of these parameters is not necessary when molar quantities are used; rather, retention of the molar quantities in the numerical algorithm makes these parameters unnecessary.

Earlier, we presented several advantages of using differential equations instead of using the integrated forms. Another benefit to using the differential equa-

tions occurs because students tend to memorize the integrated forms for particular cases. They then use the integrated forms even when the variables are not separable. This happens much less frequently when the differential-equation approach is taught.

#### CONCLUDING REMARKS

Teaching of undergraduate reactor design can be improved by using molar quantities as variables in the differential equations for the mass and energy balances. This approach has several advantages over the more common approach of using fractional conversion in the integrated versions of the balances:

1) Most industrial reactor systems contain multiple reactions, nonisothermal reactors, pressure drop, complicated rate expressions, and reactions with mole changes. The equations must be solved numerically, and this approach can be directly applied to these systems. If students are taught other methods, they must still learn this approach to do practical calculations since fractional conversions are unsuitable as a design variable for complicated systems.

2) For semibatch reactors, unsteady-state CSTR's, and systems with side streams, fractional conversion cannot be defined easily. The use of molar quantities in these systems is straightforward.

3) Separate parameters are not needed to handle mole changes in gas-phase reactions.

4) By solving the differential equations instead of separating the variables and integrating the balances, the flow rates and temperatures are obtained at points along the reactor length (or molar amounts are obtained as functions of time in a batch reactor) instead of only at the end point.

5) Molar quantities are physically more interpretable variables in many cases. For example, the molar flow rate does not change when the temperature or pressure changes, or when inerts are added. On the other hand, the concentration changes when temperature, pressure, or amount of inerts is changed, and the parameter accounting for volume variation changes when inerts are added. *The molar flow rate will change only due to chemical reaction when no material is removed or added before the reactor exit.*

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## NOMENCLATURE

### Roman

- A pre-exponential factor in Arrhenius expression for reaction-rate "constant," various units  
 C concentration, mol/m<sup>3</sup>  
 C<sub>p</sub> molar heat capacity, J/(mol)(K)  
 D diameter of tubular reactor, m  
 E activation energy of reaction, J/mol  
 F molar flow rate, mol/s  
 ΔH<sub>r</sub> change in enthalpy upon reaction, J/mol  
 k reaction-rate "constant," various units  
 N number of moles in reactor, mol  
 P total pressure in reactor, Pa  
 q volumetric flow rate, m<sup>3</sup>/s  
 R universal gas constant, (Pa)(m<sup>3</sup>)/(mol)(K) or J/(mol)(K)  
 r reaction rate, mol created/(m<sup>3</sup>)(s)  
 T temperature, K; without subscript, the temperature of the reacting fluid, K  
 t time, s  
 U overall heat transfer coefficient between reacting fluid and external heating or cooling medium, J/(s)(m<sup>2</sup>)(K)  
 V reactor volume or volume of reacting mixture, m<sup>3</sup>  
 X fractional conversion, dimensionless  
 y mole fraction, dimensionless

### Greek

- α stoichiometric coefficient, dimensionless  
 β dummy variable in Eq. (17), s  
 ε extent of reaction, mol/s

### Subscripts

- A, B, C, D, E, F, G of substances A, B, C, D, E, F, or G  
 ex of external heating or cooling medium  
 f final value or relating to the effluent stream  
 I of inert components  
 i of the i'th component or of the input stream  
 O at the entrance to the reactor or at time zero  
 T total amount  
 1 referring to point 1 in reactor  
 1,2,3 referring to Reaction 1, 2, or 3

### Superscripts

Superscripts indicate order of reaction with respect to the superscripted term. □