Graduate Education

YIELD, SELECTIVITY, AND ALL THAT

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For chemically reacting systems, several measures are used for reaction "efficiency" as it relates to amount of reaction and/or distribution of reactants and products. These include terms such as "yield" and "selectivity" for products and "fractional conversion" for reactants. Such concepts are important in the economics of chemical processes, and it is equally important (from a pedagogical point of view) to have a clear interpretation of their meaning. In the literature, however, a great variety of both terminology and definitions is used. The situation was well illustrated years ago by comments by Yu,[1] Riesser,[2] Frye,[3] and Vogue.[4] The possibility of confusion was apparently not resolved then, and evidently still persists, as perusal of the literature shows.

The purpose of this note is to provide operational definitions that have the following characteristics for a reacting system, whether simple or complex:

- *Each measure is normalized to have values ranging between 0 and 1*
- *For products relative to a reactant with a common element (or radical) contained in no other reactant**
  - *yields are defined and normalized to sum to the fractional conversion of the reference reactant, and*
  - *selectivities are defined and normalized to sum to unity*

To define the various measures, we describe two equivalent approaches:

Stoichiometric Approach which uses stoichiometric coefficients obtained from an appropriate set of chemical equations representing the reacting system (the treatment given here is an extension of that given by Missen, *et al.*[5])

Nonstoichiometric Approach which uses element-conservation equations directly without chemical equations

The terms "stoichiometric" and "nonstoichiometric" are used in the same sense as in equilibrium algorithms (see, *e.g.*, Smith and Missen[6]).

We focus on overall measures rather than corresponding point or instantaneous measures. Definitions of the former stem only from considerations of conservation of mass and have no a priori connections with kinetics (rates) or thermodynamics (equilibrium), although they can be used in any application. The definitions are given for both closed and steady-state open/flow systems. For the former, "overall" refers to two states, initial and final, differing in time, and for the latter, it refers to inlet and exit streams of the control volume, wherever it is located.

We begin with the nonstoichiometric approach, since it is a precursor to the other. For this, we first give the element-conservation equations, followed by the definitions, and then an illustrative example. For the stoichiometric approach, we

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* *This situation formally covers what is usually envisaged; situations involving an element (or radical) common to more than one reactant are outside our scope.*

first outline the generation of chemical equations in a convenient canonical form, followed by the definitions and a repetition of the previous example.

ELEMENT-CONSERVATION EQUATIONS

For a closed reacting system, the element-conservation equations are

$$b_k = \sum_{i=1}^{N} a_{ki} n_i^{(0)} = \sum_{i=1}^{N} a_{ki} n_i; \qquad k = 1, 2, \ldots, M \qquad (1)$$

where b_k is the (constant) number of moles of element k, N is the number of system species, a_{ki} is the subscript to element k in the molecular formula of species i, $n_i^{(0)}$ is the initial number of moles of species i, n_i is the (final) number of moles of i at any subsequent time, and M is the number of elements in the N species.

For an open/flow reacting system *at steady state*, the corresponding equations are

$$\dot{b}_k = \sum_{i=1}^{N} a_{ki} \dot{n}_i^{in} = \sum_{i=1}^{N} a_{ki} \dot{n}_i^{ex} \qquad (2)$$

where $\dot{n}_i^{in}$ is the molar flow rate of species i at the inlet of the control volume (system), and $\dot{n}_i^{ex}$ is similarly the exit flow rate (we assume only one inlet and one exit stream for simplicity).

The subscripts a_{ki} form the (M x N) formula matrix **A** of the system

$$\mathbf{A} = \left(a_{ki}\right) \qquad (3)$$

with

$$\text{rank}(\mathbf{A}) = C \le M \qquad (4)$$

where C is the number of linearly independent element-conservation equations, Eq. (1) or (2).

MEASURES OF REACTION EFFICIENCY: NONSTOICHIOMETRIC APPROACH

Fractional Conversion

Fractional conversion (f) of a reactant is a measure of the amount of the reactant consumed. For any reactant r, f_r is defined as the ratio of the moles reacted to the initial moles:

$$f_r = \frac{n_r^{(0)} - n_r}{n_r^{(0)}}; \qquad f_r, n_r^{(0)} > 0 \quad \text{(closed system)} \qquad (5)$$

$$f_r = \frac{\dot{n}_r^{in} - \dot{n}_r^{ex}}{\dot{n}_r^{in}}; \qquad f_r, \dot{n}_r^{in} > 0 \quad \text{(flow system)} \qquad (6)$$

For either definition,

$$0 \le f_r \le 1 \qquad (7)$$

Yield of a Product with Respect to a Particular Reactant

The yield of a product species p with respect to a reactant species r is the ratio of the amount of p formed to the theoretical amount that would be formed if all of r were reacted to form p; that is, the moles of r reacted to form p per mole of r *initially.* More specifically, we define the yield $Y_{p/r,k}$ to be the ratio of the amount of element k reacted to form product p to the amount of element k in reactant r initially, where k is an element (or a radical) common to p and r. We assume there is only one reactant with the common element k. Thus

$$Y_{p/r,k} = \frac{a_{kp}}{a_{kr}} \left(\frac{n_p - n_p^{(0)}}{n_r^{(0)}} \right); \qquad n_r^{(0)} > 0 \quad \text{(closed system)} \qquad (8)$$

$$Y_{p/r,k} = \frac{a_{kp}}{a_{kr}} \left(\frac{\dot{n}_p^{ex} - \dot{n}_p^{in}}{\dot{n}_r^{in}} \right); \qquad \dot{n}_r^{in} > 0 \quad \text{(flow system)} \qquad (9)$$

From the definition,

$$0 \le Y_{p/r,k} \le 1 \qquad (10)$$

Furthermore

$$\sum_p Y_{p/r,k} = f_r \qquad \text{(all k)} \qquad (11)$$

Selectivity of a Product with Respect to a Particular Reactant

The selectivity (or fractional yield) of a product species p with respect to a particular reactant species r is a measure of the amount of r reacted to form p relative to the total amount of r *reacted*; that is, the moles of r reacted to form p per mole of r reacted. More specifically, we define the selectivity $\hat{S}_{p/r,k}$ to be the ratio of the amount of element k reacted to form product p to the total amount of element k reacted from r, where k is an element (or a radical) common to p and r. Again, we assume there is only one reactant with the common element k. Thus

$$\hat{S}_{p/r,k} = \frac{a_{kp}}{a_{kr}} \left(\frac{n_p - n_p^{(0)}}{n_r^{(0)} - n_r} \right); \qquad n_r^{(0)} > n_r \quad \text{(closed system)} \qquad (12)$$

$$\hat{S}_{p/r,k} = \frac{a_{kp}}{a_{kr}} \left(\frac{\dot{n}_p^{ex} - \dot{n}_p^{in}}{\dot{n}_r^{in} - \dot{n}_r^{ex}} \right); \qquad \dot{n}_r^{in} > \dot{n}_r^{ex} \quad \text{(flow system)} \qquad (13)$$

From the definition*

$$0 \le \hat{S}_{p/r,k} \le 1 \qquad (14)$$

Furthermore

$$\sum_p \hat{S}_{p/r,k} = 1 \qquad \text{(all k)} \qquad (15)$$

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* *Alternative definitions of selectivity involve the ratio of the amount formed of a product of interest to the amount formed of one, or more than one, other product. Such a quantity has a range of values of 0 to ∞, and there is a possibility of ambiguity (Schmidt[7]).*

From Eqs. (5), (8), and (12), or from (6), (9), and (13),

$$Y_{p/r,k} = f_r \hat{S}_{p/r,k} \qquad (16)$$

Example 1

Consider the partial oxidation of methane to obtain "synthesis gas" ($CO + H_2$) in a steady-state flow reactor; CO_2 and H_2O are also formed. For a feed gas containing 0.522 mol O_2/mol CH_4, suppose O_2 is completely reacted, 0.0524 mol CH_4 remain per mole of CH_4 in the feed, and 1.820 mol H_2 are produced per mole of CH_4 in the feed. Calculate at the exit

(a) f_{CH_4}

(b) $Y_{CO_2/CH_4,C}$ and $Y_{CO/CH_4,C}$

(c) $\hat{S}_{CO_2/CH_4,C}$ and $\hat{S}_{CO/CH_4,C}$

(d) $Y_{H_2/CH_4,H}$ and $Y_{H_2O/CH_4,H}$

(e) $Y_{H_2/CH_4,H}$ and $Y_{H_2O/CH_4,H}$

Solution: Represent the system by

$$\{(CH_4, O_2, CO, H_2, CO_2, H_2O), (C, H, O)\}$$

Choose a basis amount of 1 mol CH_4 in the feed. Numbering the species and elements in the order listed, we write the element-conservation equations, (2), for C, H, and O, respectively, as

$$\dot{n}_1^{ex} + \dot{n}_3^{ex} + \dot{n}_5^{ex} = \dot{n}_1^{in} + \dot{n}_3^{in} + \dot{n}_5^{in} = 1 \qquad (17)$$

$$4\dot{n}_1^{ex} + 2\dot{n}_4^{ex} + 2\dot{n}_6^{ex} = 4\dot{n}_1^{in} + 2\dot{n}_4^{in} + 2\dot{n}_6^{in} = 4 \qquad (18)$$

$$2\dot{n}_2^{ex} + \dot{n}_3^{ex} + 2\dot{n}_5^{ex} + \dot{n}_6^{ex} = 2\dot{n}_2^{in} + \dot{n}_3^{in} + 2\dot{n}_5^{in} + \dot{n}_6^{in} = 2(0.522) \qquad (19)$$

From the data given

$$\dot{n}_1^{ex} = 0.0524, \quad \dot{n}_2^{ex} = 0, \quad \dot{n}_4^{ex} = 1.820$$

Solving Eqs. (17) to (19) in the remaining three unknown exit flow rates, we obtain

$$\dot{n}_3^{ex} = 0.9264, \quad \dot{n}_5^{ex} = 0.0212, \quad \dot{n}_6^{ex} = 0.0752$$

(a) From Eq. (6),

$$f_{CH_4} = \frac{\dot{n}_1^{in} - \dot{n}_1^{ex}}{\dot{n}_1^{in}} = 1 - 0.0524 = 0.9476$$

(b) From Eq. (9),

$$Y_{CO_2/CH_4,C} = \frac{a_{15}}{a_{11}} \frac{\dot{n}_5^{ex} - \dot{n}_5^{in}}{\dot{n}_1^{in}} = \frac{1}{1} \frac{0.0212 - 0}{1} = 0.0212$$

$$Y_{CO/CH_4,C} = \frac{a_{13}}{a_{11}} \frac{\dot{n}_3^{ex} - \dot{n}_3^{in}}{\dot{n}_1^{in}} = \frac{1}{1} \frac{0.9264 - 0}{1} = 0.9264$$

$$\sum_p Y_{p/CH_4,C} = f_{CH_4}$$

(c) From Eq. (13),

$$\hat{S}_{CO_2/CH_4,C} = \frac{a_{15}}{a_{11}} \frac{\dot{n}_5^{ex} - \dot{n}_5^{in}}{\dot{n}_1^{in} - \dot{n}_1^{ex}} = \frac{1}{1} \frac{0.0212 - 0}{1 - 0.0524} = 0.0224$$

$$\hat{S}_{CO/CH_4,C} = \frac{a_{13}}{a_{11}} \frac{\dot{n}_3^{ex} - \dot{n}_3^{in}}{\dot{n}_1^{in} - \dot{n}_1^{ex}} = \frac{1}{1} \frac{0.9264 - 0}{1 - 0.0524} = 0.9776$$

$$\sum_p \hat{S}_{p/CH_4,C} = 1$$

Alternatively, the selectivities can be calculated from Eq. (16) and the results of (a) and (b).

(d)

$$Y_{H_2/CH_4,H} = \frac{a_{24}}{a_{21}} \frac{\dot{n}_4^{ex} - \dot{n}_4^{in}}{\dot{n}_1^{in}} = \frac{2}{4} \frac{1.820 - 0}{1} = 0.910$$

$$Y_{H_2O/CH_4,H} = \frac{a_{26}}{a_{21}} \frac{\dot{n}_6^{ex} - \dot{n}_6^{in}}{\dot{n}_1^{in}} = \frac{2}{4} \frac{0.0752 - 0}{1} = 0.0376$$

$$\sum_p Y_{p/CH_4,H} = f_{CH_4}$$

(e)

$$\hat{S}_{H_2/CH_4,H} = \frac{a_{24}}{a_{21}} \frac{\dot{n}_4^{ex}}{\dot{n}_1^{in} - \dot{n}_1^{ex}} = \frac{2}{4} \frac{1.820}{1 - 0.0524} = 0.9603$$

$$\hat{S}_{H_2O/CH_4,H} = \frac{a_{26}}{a_{21}} \frac{\dot{n}_6^{ex}}{\dot{n}_1^{in} - \dot{n}_1^{ex}} = \frac{2}{4} \frac{0.0752}{1 - 0.0524} = 0.0397$$

$$\sum_p \hat{S}_{p/CH_4,H} = 1$$

CHEMICAL EQUATIONS

The genesis of chemical equations from element-conservation equations is described by Smith and Missen,[8,9] and we only outline the essential features here. The equations are of the form

$$\sum_{i=1}^{N} \nu_{ij} A_i = 0\,; \qquad j = 1, 2, \ldots, R \qquad (20)$$

where A_i is the molecular formula of species i, ν_{ij} is the stoichiometric coefficient of species i in chemical equation j (+ for "products" written on the right side, and – for "reactants" written on the left side), and R is the maximum number of linearly independent chemical equations given by

$$R = N - \text{rank}(\mathbf{A}) = N - C \qquad (21)$$

Here, C, as defined by Eq. (4), is also the number of component species, and R is also the number of noncomponent species (these terms are discussed further below).

Equations (20) are obtainable by reduction of matrix **A** to unit matrix form, **A***. In **A***, C is the number of unit (column) vectors, and the remaining columns represent stoichiometric vectors, one vector for each noncomponent species. This method of generating chemical equations is called the *matrix reduction method* (MRM). It may be implemented by "hand" manipulation for systems that are not too complex, but for general purposes, a Java applet has been provided by Smith, *et al.*,[10] for computer implementation.

The MRM generates a proper (but nonunique) set of chemical equations (20) in *canonical form.* In this form, each noncomponent species appears only once, and each equation can be regarded as representing the formation of one mole of a noncomponent species from the set of component species. A *conventional canonical set* results on elimination of fractions and minus signs.

The link between nonstoichiometric and stoichiometric approaches can be further realized from the general solution of Eqs. (1) or (2) as a set of linear equations:

$$n_i = n_i^{(0)} + \sum_{j=1}^{R} \nu_{ij}\xi_j \, ; \qquad i = 1, 2, \ldots, N \quad \text{(closed system)} \qquad (22)$$

$$\dot{n}_i^{ex} = \dot{n}_i^{in} + \sum_{j=1}^{R} \nu_{ij}\dot{\xi}_j \, ; \qquad i = 1, 2, \ldots, N \quad \text{(flow system)} \qquad (23)$$

where the parameter ξ_j or $\dot{\xi}_j$ is the extent-of-reaction variable introduced in 1920 by De Donder.[11]

MEASURES OF REACTION EFFICIENCY: STOICHIOMETRIC APPROACH

Fractional Conversion

From Eqs. (5) and (6), and Eqs. (22) and (23), in terms of ξ_j and $\dot{\xi}_j$,

$$f_r = -\frac{\sum_{j=1}^{R} \nu_{rj}\xi_j}{n_r^{(0)}} \qquad \text{(closed system)} \qquad (24)$$

$$f_r = -\frac{\sum_{j=1}^{R} \nu_{rj}\dot{\xi}_j}{\dot{n}_r^{(0)}} \qquad \text{(flow system)} \qquad (25)$$

Equations (24) and (25) also satisfy Eq. (7).

Yield of a product with respect to a particular reactant

Corresponding to Eqs. (8) and (9), we have

Closed system

$$Y_{p/r,k} = \frac{\nu_{rp}}{\nu_p}\left(\frac{n_p^{(0)} - n_p}{n_r^{(0)}}\right) = -\frac{\nu_{rp}\xi_p}{n_r^{(0)}}; \qquad p = C+1, C+2, \ldots, N \qquad (26)$$

Flow system

$$Y_{p/r,k} = -\frac{\nu_{rp}\dot{\xi}_p}{\dot{n}_r^{(0)}}; \qquad p = C+1, C+2, \ldots, N \qquad (27)$$

where ν_{rp} is the stoichiometric coefficient for reactant r in the chemical equation involving noncomponent product species p in the canonical set, corresponding to that for p, ν_p. Equations (26) and (27) also satisfy Eqs. (10) and (11).

Selectivity of a product with respect to a particular reactant

Corresponding to Eqs. (12) and (13), we have

Closed system

$$\hat{S}_{p/r,k} = \frac{\nu_{rp}}{\nu_p}\left(\frac{n_p^{(0)} - n_p}{n_r^{(0)} - n_r}\right) = \frac{\nu_{rp}\xi_p}{\sum_{j=1}^{R} \nu_{rj}\xi_j}; \qquad p = C+1, C+2, \ldots, N \qquad (28)$$

Flow system

$$\hat{S}_{p/r,k} = \frac{\nu_{rp}\dot{\xi}_p}{\sum_{j=1}^{R} \nu_{rj}\dot{\xi}_j}; \qquad p = C+1, C+2, \ldots, N \qquad (29)$$

Equations (28) and (29) satisfy Eqs. (14) and (15). Equation (16) also applies.

Example 2

Repeat Example 1 using the stoichiometric approach.

Solution: We are required to calculate the yield and selectivity of two sets of products with respect to the reactant CH_4. One set involves CO and CO_2 with the common element C; the other involves H_2 and H_2O with the common element H. We cannot satisfy both these requirements with one canonical set of equations, since, as shown below, C=3 and there are only 6–3=3 noncomponent species, not 4. We therefore construct 2 canonical sets, in one of which CO and CO_2 are noncomponents, and in the other, H_2 and H_2O are noncomponents. In each case, we choose a basis amount of 1 mol CH_4 in the feed.

Canonical set A: Represent the system by

$$\{(CH_4, O_2, H_2, CO, CO_2, H_2O), (C, O, H)\}$$

The MRM produces the following set in conventional canonical form:

$$2CH_4 + O_2 = 4H_2 + 2CO$$
$$CH_4 + O_2 = 2H_2 + CO_2$$
$$O_2 + 2H_2 = 2H_2O$$

in which the noncomponents are CO and CO_2, as desired, together with H_2O, which does not enter into the calculations for parts (b) and (c); $\dot{\xi}_j$ are represented by $\{\dot{\xi}_{1A}, \dot{\xi}_{2A}, \dot{\xi}_{3A}\}$ for the equations in the order given. We can calculate the values of $\dot{\xi}_j$ from the information given for CH_4, O_2, and H_2, respectively, and the chosen basis amount:

$$1 - 2\dot{\xi}_{1A} - \dot{\xi}_{2A} = 0.0524 \qquad (30)$$

$$0.522 - \dot{\xi}_{1A} - \dot{\xi}_{2A} - \dot{\xi}_{3A} = 0 \qquad (31)$$

$$4\dot{\xi}_{1A} + 2\dot{\xi}_{2A} - 2\dot{\xi}_{3A} = 1.82 \qquad (32)$$

The solution of these three equations is

$$\left\{\dot{\xi}_{1A}=0.4632,\ \dot{\xi}_{2A}=0.0212,\ \dot{\xi}_{3A}=0.0376\right\}$$

Canonical set B: Represent the system by

$$\{(CH_4, O_2, CO, H_2, CO_2, H_2O), (C, O, H)\}$$

by interchanging H_2 and CO. The resulting conventional canonical set is

$$2CH_4+O_2=2CO+4H_2$$
$$2CO+O_2=2CO_2$$
$$2CH_4+3O_2=2CO+4H_2O$$

in which the noncomponent species are H_2 and H_2O, as desired, and CO_2, which does not enter into the calculations in parts (d) and (e); ξ_j are now represented by $\left\{\dot{\xi}_{1B}, \dot{\xi}_{2B}, \dot{\xi}_{3B}\right\}$.

The equations corresponding to Eqs. (30), (31), and (32) are, respectively,

$$1-2\dot{\xi}_{1B}-2\dot{\xi}_{3B}=0.0524 \tag{33}$$

$$0.522-\dot{\xi}_{1B}-\dot{\xi}_{2B}-3\dot{\xi}_{3B}=0 \tag{34}$$

$$4\dot{\xi}_{1B}=1.82 \tag{35}$$

The solutions of these 3 equations is

$$\{\dot{\xi}_{1B}=0.455,\ \dot{\xi}_{2B}=0.0106,\ \dot{\xi}_{3B}=0.0188\}$$

(a) From Eq. (25) and either canonical set, A or B,

$$f_{CH_4}=0.9476$$

(b) From Eq. (27) and canonical set A,

$$Y_{CO/CH_4,C}=-\frac{-2\dot{\xi}_{1A}}{1}=2(0.4632)=0.9264$$

$$Y_{CO_2/CH_4,C}=-\frac{-1\dot{\xi}_{2A}}{1}=0.0212$$

as required by Eq. (11), the sum of the yields equals f_{CH_4}.

(c) From Eq. (29) and canonical set A,

$$\hat{S}_{CO/CH_4,C}=\frac{-2\dot{\xi}_{1A}}{-2\dot{\xi}_{1A}-1\dot{\xi}_{2A}-0\dot{\xi}_{3A}}=\frac{2(0.4632)}{2(0.4632)+0.0212}=0.9776$$

$$\hat{S}_{CO_2/CH_4,C}=\frac{-1\dot{\xi}_{2A}}{2(0.4632)+0.0212}=0.0224$$

As required by Eq. (15), the sum of the selectivities equals 1. Alternatively, the selectivities can be calculated from Eq. (16) and the results of (a) and (b).

(d) From Eq. (27) and canonical set B,

$$Y_{H_2/CH_4,H}=-\frac{-2\dot{\xi}_{1B}}{1}=2(0.455)=0.910$$

$$Y_{H_2O/CH_4,H}=-\frac{-2\dot{\xi}_{3B}}{1}=2(0.0188)=0.0376$$

The sum of the yields equals f_{CH_4}.

(e) From Eq. (16) and the results of (a) and (d),

$$\hat{S}_{H_2/CH_4,H}=Y_{H_2/CH_4,H}/f_{CH_4}=0.910/0.9476=0.9603$$

$$\hat{S}_{H_2O/CH_4,H}=Y_{H_2O/CH_4,H}/f_{CH_4}=0.0376/0.9476=0.0397$$

The sum of the selectivities equals 1.

The results of Example 2 are the same as those of Example 1.

COMPARISON OF STOICHIOMETRIC AND NONSTOICHIOMETRIC APPROACHES

The stoichiometric and nonstoichiometric approaches for defining yield, selectivity, etc., are equivalent, and which one is used is largely a matter of convenience or personal preference. The stoichiometric approach usually lends itself more naturally to situations in which chemical *reactions* are specified explicitly, as in chemical kinetics and chemical reaction engineering. But it requires additional effort to generate a proper set of chemical equations, most conveniently in canonical form; furthermore, more than one canonical set may be required for the complete treatment of a system, as shown in Example 2. Nevertheless, the generation of chemical equations reduces the number of problem variables, $\{\xi_j\}$, to be solved for, in comparison with the number of problem variables, $\{n_j\}$, in the nonstoichiometric approach. Offsetting this, we do not require the generation of chemical equations in the latter.

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