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## ARE CONVERSION, SELECTIVITY AND YIELD TERMS UNAMBIGUOUSLY DEFINED IN CHEMICAL AND CHEMICAL ENGINEERING TERMINOLOGY?

*This review shows and discusses the different definitions and use of conversion, selectivity and yield, with reference both to different reactor types and reaction schemes. Books or manuscripts focusing on kinetics prefer to express selectivity as the amount of the product desired weighted with respect to all the possible by-products. This definition, which is quite inapplicable if some by-products are non quantitatively well defined, may come directly from the comparison of the reaction rates bringing to the different species. By contrast, authors devoted to process or reactor design prefer a more practical definition of selectivity as amount of the desired product formed with respect to the key-reagent that reacted. A confusing situation may arise if such expression is used to define the yield. In such case the well known equation  $\text{yield} = \text{conversion} \times \text{selectivity}$  is inapplicable.*

### Introduction

In the chemical literature (in particular the one devoted to engineering topics) it is necessary to use the terms of conversion (X), selectivity (S) and yield (Y) due to their relevance in kinetic studies, in order to adequately dimension reactors, to choose the best conditions to maximize the production of a given compound, limiting the amount of by-products. Moreover, only if these terms are univocally defined it is possible to correctly compare different experimental results.

An inspection of a review [1] and some books [2-26] brought us to conclude that such terms have different meanings in many cases,

especially if selectivity and yield are of concern. This quite confusing situation was well commented in the past in ref. [10], p. 46, and [25], p. 70: "No universally agreed upon definitions exist for such terms-in fact quite the contrary. Rather than cite all the possible usage of these terms, many of which conflict, we shall define them as follows...".

Such statement has been repeated in the subsequent editions of this book.

Such confusing situation is still actual; in fact in a recent (2006) and excellent book [24] it is written in chap. 6, dedicated to multiple reactions: "As a consequence of the different definitions for selectivity

and yield, when reading literature dealing with multiple reactions, check carefully to ascertain the definition intended by the authors. From an economic standpoint it is the overall selectivities,  $S$ -, and yields,  $Y$ -, that are important in determining profits. However, the rate-based selectivities give insights in choosing reactor and reaction schemes that will help maximize the profit. However, many times there is a conflict between selectivity and conversion (yield) because you want to make a lot of your desired product (D) and at the same time minimized the undesired product (U). However, in many instances the greater conversion you achieve, not only you make more D, you also form more U". Among the cited textbooks the one by Fogler [24], contains, but not exhaustively, some interesting discussions about the topics of the present paper.

The most recent (2012) publication which is devoted to Chemical Terminology (IUPAC-Gold Book [26]) contains only short definitions of the title terms: selectivity definition is devoted to ion exchange chromatography, organic chemistry or analytical chemistry; the yield has been defined in the area of nuclear analytical chemistry and the conversion in the one of chemical kinetics.

Therefore it seems useful to perform a comparison among the variety of definitions of  $X$ ,  $S$ ,  $Y$  in order to rationalize the panorama of such terms. A previous review titled: "Yield in Chemical Reactor Engineering" has been published in 1966 by Carberry [1], dealing mainly with the different regimes (isothermal, non-isothermal, diffusional) in chemical reactors. *Note:* The symbols  $X$ ,  $S$ ,  $Y$  (with different sub or/and superscripts) are used in order to standardize the different symbols used in the cited literature with reference to the same meaning. In few cases different symbols are used and explained in the text. Similarly  $n$ ,  $F$ ,  $C$  are used as mole number, molar flux and molar concentration, respectively.

## 1. Discussion

### 1.1 The definition of conversion

With respect to the three topics of this paper there is no doubt that the conversion (and fractional conversion) definition is the one for which there is an explicit, and quite agreed, definition in the majority of the cited references [2-24]. In fact, the definition below reported is cited in the following references: [7], p. 17; [8], p. 24; [10], p. 46; [12], p. 300; [13], p. 33; [14], pp. 3, 317; [15], p. 5; [16], p. 91; [18], p. 13; [20], p. 47; [21], p. 351; [23], p. 152; [24], p. 38.

If in a reaction scheme, occurring in a closed or in a flow system in stationary conditions, a reactant A is involved in only one irreversible reaction of known stoichiometry, then the *conversion* (or *fractional conversion*, indicated usually as  $X_A$  or in some books as  $f$  [14, p. 3; 16, p. 91;] or  $\xi$  [8], p. 24) is the unique parameter to follow the course of the reaction at any time (closed system) or position (flow system). Considering a batch reactor (BR) or a flow reactor (FR) the most accepted definitions of  $X_A$ , as *fractional conversion*, are:

$$\text{for BR } X_A = \frac{\text{amount (moles) of A reacted/amount of A introduced in the system}}{n_{A0}} = \frac{(n_{A0}-n_A)}{n_{A0}} \quad (1)$$

$$\text{for FR } X_A = \frac{\text{flow (moles or weight) of A reacted/flow of A introduced in the system}}{F_{A0}} = \frac{(F_{A0}-F_A)}{F_{A0}} \quad (2)$$

Being  $n$  the moles or weight and  $F$  the flux, in moles or weight per unit time; the suffix 0 indicates the initial quantity or flow of the reagent A. The numerators of the equations (1) and (2) are defined as conversion. If the system is at constant density (on molar or mass basis) the symbol  $n$  can be changed in concentration ( $C_A$  and  $C_{A0}$ ) in moles or mass per unit volume [21, p. 351]. If there is a change,  $\epsilon_A$ , in the density (on molar or mass basis) the following definition of conversion is reported ([9], p. 59):

$$X_A = \frac{1 - \frac{C_A}{C_{A0}}}{1 + \frac{\epsilon_A C_A}{C_{A0}}} \quad (1')$$

where, supposing a linear variation of the volume  $V$  with the conversion:

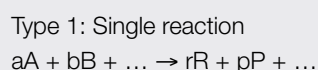
$$\epsilon_A = \frac{(V_{X_A \rightarrow 1} - V_{X_A \rightarrow 0})}{V_{X_A \rightarrow 0}} \quad (1'')$$

The equations (1) and (2) hold even if the reaction scheme is complex, i.e. if the reactant A takes part to parallel or series reactions. However, in this case, the fractional conversion parameter  $X_A$  is not sufficient to describe the course of the reaction and it is necessary to take into account the concepts of *selectivity* and *yield* (*vide infra*).

On the contrary, in [1] the following expressions are reported: "Conversion or activity" (as synonymous definitions), or: "Conversion in terms of moles of reactant converted per unit time per unit volume of reactor", or: "Conversion per se indicates the speed of reaction". In some cases [14, 17, 19] the conversion or fractional conversion are defined without explicit mathematical expressions, like the equations (1) and (2), but only through a word expression. In particular, in ref. [19], p. 15, conversion is defined as "1 minus the fraction unreacted". In a unique case [17], p. 128, conversion is defined using an ambiguous expression, i.e.: "Conversion has several definitions and conventions. It is best to state the definition in the context of the problem being solved". In ref. [22], p. 26, the following expression is reported for an irreversible reaction A to products: "The quantity ( $C_X/C_{A0}$ ) is a fraction varying between zero (no conversion) and unity (complete conversion) for this irreversible reaction and is ordinarily called *fractional conversion* of the reactant X". The above reported definition is correct only by defining  $C_X = C_{A0} - C_A$ . Conversion is also related to the "degree of completion of a reaction" [10], p. 47.

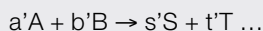
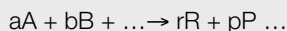
### 1.2 The definitions of selectivity

In order to discuss conveniently this topic, it is compulsory to refer to a scheme of irreversible reactions which include single, series or parallel reactions, i.e. a multiple reaction scheme, involving a desired product R and a reference (or limiting, or key) reagent A:

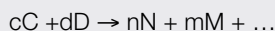
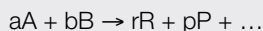


Type 2: Parallel reactions

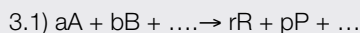
2.1) With the same reagents



2.2) With separate reagents and products (simultaneous reactions) ([7], p. 23; [22], p. 26)



Type 3: Series (or consecutive) reactions



It is useful to point out that the concept of selectivity is usefully applicable especially to a multiple reaction scheme, but in the considered literature some definitions are cited only with reference to Type 1 scheme (*vide infra*), where it would instead be sufficient to define the conversion and the stoichiometric ratio among the different products to calculate the amount of desired product at the end of the reaction or at the outlet of the reactor.

## 1.2.1 General definitions

A convenient definition of selectivity to the desired product R is the one that considers all (or some) the undesired product formed. Such definitions are prevalently given on a molar basis:

- in ref. [1], p. 41:

“Selectivity, at a point, is the rate of generation of a desired product relative to the generation of some undesired product”;

- in ref.s. [2], p. 158; [3], p. 232; [4], p. 127:

$$S_R = \frac{\text{moles of desired product formed}}{\text{moles of the undesired material formed}} \quad (3)$$

- in ref. [23], p. 153:

$$S_R = \frac{\text{moles of desired product formed}}{\text{moles of all the products formed}} \quad (3')$$

In ref. [24], p. 308, for flow reactors the overall selectivity is defined as:

$$S_{DU} = \frac{F_D}{F_U} = \frac{\text{Exit molar flow rate of the desired (D) product}}{\text{Exit molar flow rate of the undesired (U) product}} \quad (3'')$$

Or, for batch reactors:

$$S_{DU} = \frac{n_D}{n_U} \quad (3''')$$

being  $n$  the mole number at the end of the reaction time.

Here the undesired materials *formed* include also, in a multiple reaction scheme, the ones coming from other reagents than the key reagent A, such as M or N as defined in Type 2.2 (simultaneous reactions). Additional comments about Eq.s (3) and (3') are reported in paragraph 1.2.2.

Another definition considers the moles of R produced with respect to

the moles of the reference reagent A reacted:

$$S_{R/A} = \frac{\text{moles of R formed}}{\text{moles of A reacted}} \quad (4)$$

This definition is reported in most books: [5], p. 267; [7], p. 24; [8], p. 29; [10], p. 47; [12], p. 300; [13], p. 33; [16], p. 93; [18], p. 13; [21], p. 352; [22], p. 26; [23], p. 153. In some of the references above cited ([5, 8, 12, 13, 16, 23]) an explicit mathematical expression of (4) is given, with [5, 8, 13, 16] or without [12, 23] the stoichiometric coefficients; in the former case it results for the different types of reactors [16]:

for BR (batch reactor) at constant or variable density:

$$S_{R/A} = [(n_R - n_{R0}) / (n_{A0} - n_A)](a/r) \quad (5)$$

for FR (flow reactor) at constant or variable density:

$$S_{R/A} = [(F_R - F_{R0}) / (F_{A0} - F_A)](a/r) \quad (5')$$

for BR or FR at constant density:

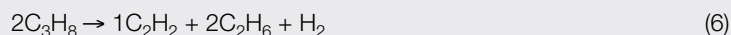
$$S_{R/A} = [(C_R - C_{R0}) / (C_{A0} - C_A)](a/r) \quad (5'')$$

Being:  $n$  the moles number,  $F$  the flux,  $C$  the concentration and the suffix 0 the initial value. Eq. (5) is equivalent to the following one:

$$S_{R/A} = \frac{\text{moles of A required to produce R}}{\text{moles of A reacted}} \quad (5''')$$

It is noteworthy to observe that in the majority of the cited references the definitions (4) and (5-5''') are referred to a multiple reaction scheme, but in some cases [12, 18] to Type 1 (single reaction) scheme, only. In the latter case it could be observed that the selectivity has a fixed value determined by the stoichiometric coefficients, as already observed. Indeed, for example, if we apply Eq. (5) to a Type 1 scheme, quantity  $(n_R - n_{R0})$  for Eq. (5), or the moles of the desired product (R) formed, for Eq. (3), can be evaluated from  $(n_{A0} - n_A)$  by considering the stoichiometry of the reaction, provided that it does not change with time or position.

An example is the following one, concerning a cracking reaction:



Considering:  $A=C_3H_8$ ;  $R=C_2H_2$ ,  $a=2$ ;  $r=1$ , it results:

$$\text{Eq. (3): } S_{R/A} = \frac{n_{\text{desired}}}{n_{\text{undesired}}} = \frac{(n_{A0} - n_A)1/2}{(n_{A0} - n_A)(1+1/2)} = \frac{(1/2)}{(1+1/2)} = \frac{1}{3}$$

$$\text{Eq. (5): } S_{R/A} = \frac{n_{\text{desired}}}{n_{\text{reacted}}} = \frac{(n_{A0} - n_A)1/2}{(n_{A0} - n_A)} = \left(\frac{2}{1}\right) = 1$$

The experimental evaluation of the selectivity for Type 1 reactions may not be exactly equal to the one calculated by applying the stoichiometry as above reported. This could happen if there are some analytical errors or due to a change of the reaction scheme; this is more evident when the conversion of the reactant increases. It is

reported ([18], p. 14) that the ratio (4) “often changes as the reaction progresses and the selectivity based on the final mixture composition should be called *average selectivity*”. A similar terminology, *overall or integral selectivity*, is reported for Eq. (5) too ([5], p. 268; [7], p. 24; [8], p. 85; [13], p. 33; [22], p. 26). This discussion justifies the application of Eq.s (5, 5', 5'') to Type 1 scheme.

In conclusion, in the absence of competing reactions (typically Type 1 scheme), if the overall selectivity is defined and calculated according to Eq.s. (5-5'') its value is 100% and, moreover, the Yield (see paragraph 1.3) is the same, as observed in ref. [13], p. 33.

For some types of reaction schemes (namely catalytic reactions where some products can have a doping effect on the catalyst) this overall selectivity is a degree of conversion. In such cases it is possible and useful to define a *local selectivity* (for FR) or *instantaneous selectivity* (for BR) ([13], p. 34), being calculated from a differential ratio.

For example  $dn_R/dn_A$  for Eq. (5), may be called *instantaneous (differential) selectivity* too, both for BR and FR ([5], p.268; [22], p. 26):

$$S'_{R/A} = \left[ \frac{dn_R}{-dn_A} \right] \left( \frac{a}{r} \right) \quad (7)$$

The correlation between  $S'_{R/A}$  and the overall selectivity  $S_{R/A}$ , as expressed by Eq.s. (5-5''), is calculated from the following equation [5], p. 268, for BR and FR by using Eq. (5), for instance:

$$S_{R/A} = - \left[ \frac{1}{(n_{A0} - n_A)} \right] \int_{n_{A0}}^{n_A} S'_{R/A} dn_A \quad (8)$$

In this equation the  $n_A$  value is determined as a function of the reaction time  $t$  (BR) or residence time  $\tau$  (FR) ([13], p. 35), being this last parameter determined from the ratio between the considered reaction volume,  $V$ , and the total volumetric flow rate  $v_T$ .

By contrast, for a CSTR (Continuously Stirred Tank Reactor) or MFR, (Mixed Flow Reactor, according to the nomenclature of ref. [2], p. 90), using moles number, it results, being  $n_R$  and  $n_A$  constant throughout the reactor ([15], p. 268):

$$S_{R/A} = S'_{R/A} = \frac{(n_R - n_{R0})}{(n_{A0} - n_A)} \left( \frac{a}{r} \right) \quad (9)$$

Equations like (7), written without stoichiometric coefficients, and (4), both using concentrations (C) instead of moles number (n), have been used in ref. [2], p. 156, to indicate the *instantaneous fractional yield* ( $\varphi$ ) and the *overall fractional yield* ( $\Phi$ ), respectively, both referred to R. It is useful to notice that equations like (8) and (9) written using concentrations (C) or fluxes (F) are all equivalent if the system has constant molar density.

Historically, the first distinction between overall selectivity, or simply selectivity, and an expression like Eq. (7) appeared in the Denbigh's book [6], p. 112, where the Eq. there numbered (4.16), indicated with  $\phi$  at first member, is identical to the present Eq. (7) at the second member, being  $\phi$  called *the infinitesimal yield* of the product R obtained from a reagent A in a Type 1 reaction.

### 1.2.2 Some ambiguous definitions

In ref. [1], p. 41, a word definition equivalent to Eq. (7) is referred to “yield at a point within the reactor”, instead of instantaneous or differential selectivity.

In ref. [2], p. 159, the definition reported in Eq. (3) is considered a source of problems if the undesired products are “a goulash of undesired material”. Therefore it is concluded to “stay away from selectivity and use the most clearly defined and useful fractional yield  $\varphi_{R/A}$ ” (see paragraph 1.3). This observation can be extended to Eq. (3'). It is not clear in this definition if the expression: “all products formed” may include or not the desired product too.

The scarce consideration of this selectivity definition may be the reason why this parameter is totally ignored in the second edition of a well-known book [11]. In strong disagreement with the previous statement, in ref. [18], p. 14, it is reported that “The selectivity is a very important parameter for many reaction systems”, being the selectivity definition the one reported in Eq.s (5-5'').

With reference to Type 1 scheme, in ref. [6], p. 98, two expressions are reported for the yield parameter (indicated as  $\Phi'$  and  $\Phi$ ):

$$\Phi' = \frac{(a \cdot \text{moles of R formed})}{(r \cdot \text{moles of A reacted})} \quad (10)$$

or as:

$$\Phi = \frac{(a \cdot \text{moles of R formed})}{(r \cdot \text{moles of A which were originally introduced in the system})} \quad (11)$$

Obviously these two definitions are not equivalent and, in particular, Eq. (10) is equivalent to *selectivity* as defined in Eq.s (5-5'') in the previously reported literature.

In ref. [10], p. 47, it is reported that selectivity, as defined by Eq. (4), is also called as “efficiency, conversion efficiency, specificity, yield, ultimate yield, or recycle yield”. This variety of definitions further justifies the unified discussion of the present paper.

In ref. [14], p. 317, in defining the selectivity it is reported that “Different conventions have been used in assigning numerical values to selectivity, but one that is often useful is the ratio of the limiting reagent that reacts to give the desired product to the amount that reacts to give an undesired product”. Such definition is too vague because the undesired product may be P, S, T, etc. in the previously reported schemes (paragraph 1.2).

In the same book, the Eq. therein defined as (9.0.2), the same as Eq. (4) of the present paper, connected with Type 1 scheme, is defined as yield, but previously it is reported that “It is also necessary to state whether the yield is computed relative to the amount of reactant introduced into the system or relative to the amount of reactant consumed.” Clearly Eq. (4) is relative to reactant (key-reagent) consumed, as Eq. 9.0.2, but this last equation is reported in most references as *selectivity* not as yield (see paragraph 1.2.1).

In ref. [16], p. 92, it is written: “The fractional yield of a product is a measure of how selective a particular reactant is in forming a particular

product, and hence is sometime referred to as *selectivity*. Two ways of representing selectivity are (1) the overall fractional yield (from the inlet to a particular point such as the outlet); and (2) the instantaneous fractional yield (at a point)". Then the equations identical to those (5-5") are reported as "overall fractional yield" of D (desired product) from a key reagent A, and indicated as  $\hat{S}_{D/A}$ .

In our opinion, to avoid confusion, such *overall fractional yield*, but indicated with the letter S, should be called *overall selectivity* as discussed in the previous paragraph.

In ref. [17], p. 128, the overall selectivity is defined as "the ratio of the amount of one component produced to the amount of another component produced". This definition is completely new but it is again too vague. Moreover, in ref. [23], p. 153, the definition (3') is not equivalent to the one reported in (3). In fact, among all the formed products some may be desired, but they are not included in the numerator of (3) and (3') being different from R. Besides for some specific calculations the undesired products may be only some among all the products of a reaction, as reported in a numerical example in ref. [4], p. 128.

In connection with Eq.s (3") and (3'''), in ref. [24]), (reaction scheme at p. 307) only one undesired (U) product is cited. Therefore or U include all the undesired products formed or in presence of many products (see for example Eq. (6)) one must choose which of these is the undesired one. But if there is a "goulash" (see ref. [2], p. 159) of products, may be that some of these are not well identified, it is difficult to include in U all the undesired products, or to choose some of these as undesired. Such observations can be extended to the instantaneous selectivity (S') if this parameter is defined (ref. [24], p. 307) as:

$$S'_{DU} = \frac{r_D}{r_U} = \frac{\text{rate of formation of D}}{\text{rate of formation of U}} \quad (7')$$

In conclusion Eq.s (3"), (3''') and (7') may be too limiting in the case of multiple by-products. In this case, in our opinion, it is much better to use Eq.s (4) and the equivalent ones (5-5") or the equivalent equations for the instantaneous selectivity.

### 1.2.3 Parallel reactions

Such reaction scheme (Types 2.1 and 2.2) is considered in quite all the books cited in the references; it is connected with both the definitions (3) (see ref. [4], p. 128) and (4-5"). Basically, the terms overall selectivity and local (or differential) selectivity are applicable to scheme 2, but it is necessary to evaluate the moles of the key reagent reacted according to two or more reactions.

Detailed discussion of this case are reported in particular, sometime with numerical examples too, in ref.s [2], pp. 159-161; [5], pp. 267-272; [7], pp. 23-26 and 226-228; [13], pp. 34-45. In ref. [2], pp. 155-156, the selectivity, overall and instantaneous, is called respectively *overall fractional yield and instantaneous fractional yield*, but the definitions are the same as reported in Eq.s. (4) and (7).

Now we can consider the scheme 2.2 in order to calculate the overall

selectivity from the instantaneous one. It is convenient for all the types of reactors to rewrite Eq. (7) in terms of the two reaction rates  $r_{R/A}$  and  $r_{S/A}$ , which are relative to the formation of R and S from A, respectively:

$$S'_{R/A} = \frac{r_{R/A}}{(r_{R/A}+r_{S/A})} = \frac{dC_{R/A}}{(dC_{R/A}+dC_{S/A})} \quad (12)$$

$$S'_{S/A} = \frac{r_{S/A}}{(r_{R/A}+r_{S/A})} = \frac{dC_{S/A}}{(dC_{R/A}+dC_{S/A})} \quad (13)$$

To simplify, without a loss of a rigorous discussion, the different mathematical expressions reported in the literature, it may be useful to distinguish between the case in which  $r_{R/A}$  and  $r_{S/A}$  equations are different only due to the two kinetic constants  $k_{R/A}$  and  $k_{S/A}$ , i.e.:

$$r_{R/A} = k_{R/A} C_A^\alpha C_B^\beta \text{ and } r_{S/A} = k_{S/A} C_A^{\alpha'} C_B^{\beta'} \quad (14)$$

where it has been supposed that the reactions orders are  $\alpha=\alpha'$  and  $\beta=\beta'$ .

In this case, as outlined in ref. [13], p. 36, by substituting Eq.s (14) in (12) and (13) it results:

$$S'_{R/A} = \frac{k_{R/A}}{k_{R/A}+k_{S/A}} = \text{const} \quad (15)$$

$$S'_{S/A} = \frac{k_{S/A}}{k_{R/A}+k_{S/A}} = \text{const} \quad (16)$$

It is evident that assuming  $S'_{R/A}$  and  $S'_{S/A}$  a constant value then the overall selectivities, also  $S_{R/A}$  and  $S_{S/A}$ , will have the same values as (15) and (16), respectively. For a CSTR this derives by applying Eq. (9) and for a PFR or BR by the integration of Eq. (8'), where  $S'_{R/A}$ , under integral, has a constant value (15), and similarly for  $S_{S/A}$ .

In conclusion, if the reaction rates are different only for the kinetic constants then *for every types of reactor* the overall selectivities and the instantaneous selectivities have the same constant values for each desired product i:

$$S_{R/A} = S'_{R/A} = \frac{k_{R/A}}{\sum_i k_{i/A}} \text{ and } S_{S/A} = S'_{S/A} = \frac{k_{S/A}}{\sum_i k_{i/A}} \quad (17)$$

A more complex case is the one in which the rate equations have different expressions. In particular considering that a CSTR operates at the outlet concentration of the reactants, then instantaneous selectivity is always constant and equal to the overall one, but in general these values will depend on both the kinetic constants and on the values of  $C_A$  and  $C_B$  at the exit.

A different situation holds for a PFR or BR because in the Eq. (8') the upper limit of the integral ( $C_A$ ) should be evaluated at the maximum residence time for a PFR ( $\tau_{max}=V_R/V_T$ ) or to any other reactor volume  $V'_R < V_R$ ; for BR,  $C_A$  can assume all the values from 0 to the final reaction time.

For instance if  $\alpha=\beta=\beta'=1$  and  $\alpha'=2$ :

$$r_{R/A} = k_{R/A}C_A C_B \text{ and } r_{S/A} = k_{S/A}C_A^2 C_B \quad (18)$$

then, by applying Eq. (12) the instantaneous or local selectivity is:

$$S'_{R/A} = \frac{k_{R/A}C_A C_B}{k_{R/A}C_A C_B + k_{S/A}C_A^2 C_B} = \frac{k_{R/A}}{k_{R/A} + k_{S/A}C_A} \quad (19)$$

Similarly:

$$S'_{S/A} = \frac{k_{S/A}C_A^2 C_B}{k_{R/A}C_A C_B + k_{S/A}C_A^2 C_B} = \frac{k_{S/A}C_A}{k_{R/A} + k_{S/A}C_A} \quad (20)$$

For a CSTR the  $C_A$  value is the one at the exit of the reactor and the resulting overall selectivity is equal to the instantaneous one ( $S'_{R/A}$ ). The same holds for  $S'_{S/A}$ .

Instead, for a PFR (or BR) the overall selectivity is evaluated by applying Eq. (8') and Eq. (19):

$$S_{R/A} = - \frac{1}{(C_{A0} - C_A)} \int_{C_{A0}}^{C_A} \left( \frac{k_{R/A}}{(k_{R/A} + k_{S/A}C_A)} \right) dC_A = \left( \frac{1}{(C_{A0} - C_A)} \frac{k_{R/A}}{k_{S/A}} \right) \ln \left( \frac{(k_{R/A} + k_{S/A}C_{A0})}{(k_{R/A} + k_{S/A}C_A)} \right) \quad (21)$$

In the paragraph 1.3, dedicated to the yield, it is discussed how the different equations used to calculate the instantaneous or local selectivity strongly influence the estimation of the total production of R and S depending on the reactor type.

### 1.2.4 Series (or consecutive) reactions

The discussion for this type of reactions is limited to the case  $A \xrightarrow{k_1} R \xrightarrow{k_2} S$ .

Type 3 reaction scheme is referred to different expressions found in the literature, for example: consecutive reactions ([6], p. 25; [8], p. 108; [9], p. 70); reaction sequential ([7], p. 27); series reactions ([2], p. 192; [3], p. 452; [13], p. 45). This topic is discussed in quite all the referred books and in particular in: [2], pp. 194-197; [3], pp. 461-464; [6], pp. 99-104; [7], pp. 228-231; [8], pp. 109-123; [13], pp. 45-48.

Discussing the behaviour of the different types of reactors, in connection with series reactions, it is useful to observe that for PFR and CSTR the residence time distribution represents the extremes in mixing behaviour ([7], p. 223); besides PFR and BR can be discussed together being the reaction time ( $t$ ) in BR substituted in PFR by a residence time ( $\tau$ ), which is the ratio between the considered real volume,  $V$ , and the volumetric flux  $v_T$ , being  $0 < V \leq V_{max}$  ([13], pp. 20-22).  $V_{max}$  is the volume of a CSTR which (for a positive order reaction rate) is always greater than that of a PFR to achieve the same reagent conversion at the same total flux. For a reaction order less than zero the opposite is true. For a CSTR instead it is better to use the mean residence time  $\bar{\tau} = V_{max}/v_T$ . Therefore in the literature the comparison is made between PFR and CSTR.

Type 3 scheme is well studied in all kinetic books where the mathematical expressions show how the concentration of A continuously decreases as a function of time, R reaches a maximum and S monotonously increases. This behaviour influences strongly and differently PFR and

CSTR systems. Several types of calculations are presented in the literature concerning the two mentioned kinds of reactors; it is possible to summarize such calculations in four items:

- i) concentration ratios  $C_A/C_{A0}$ ,  $C_R/C_{A0}$ ,  $C_S/C_{A0}$ , expressed as a function of the ratio between the kinetic constants  $k_2/k_1$ , with comparison between the residence time of different reactor types;
- ii) ratio between the overall selectivity toward R ( $S_{R/A}$ ) or S at the same conversion of the key reagent A ( $x_{A,max}$ );
- iii) optimum values of the residence time ( $\tau_{opt}$ ) and mean residence time ( $\bar{\tau}_{opt}$ ) to obtain the maximum concentration of R, and the corresponding conversion of A ( $x_{A,max}$ );
- iv) instantaneous selectivity towards R and S ( $S'_{R/A}$ ,  $S'_{S/A}$ ) for a PFR. Indeed, as previously indicated (Eq. (9) for a CSTR it results  $S_{R/A} = S'_{R/A}$ . All the previous items can be solved by using the classical fundamental equations for a PFR and CSTR, as below reported, using the concentrations of A, R, S (respectively  $C_A$ ,  $C_R$ ,  $C_S$ ), being the suffix "0" the initial value.

For a PFR:

$$\frac{C_A}{C_{A0}} = e^{-k_1\tau} = 1 - X_A \quad (22)$$

$$\frac{C_R}{C_{A0}} = \left[ \frac{k_1}{(k_2 - k_1)} \right] (e^{-k_1\tau} - e^{-k_2\tau}) \quad (23)$$

or

$$\frac{C_R}{C_{A0}} = \left\{ \frac{1}{(k_2/k_1 - 1)} \right\} (e^{-k_1\tau} - e^{-k_2\tau}) \quad (23')$$

$$\frac{C_S}{C_{A0}} = (1 - e^{-k_1\tau}) - \left[ \frac{1}{(k_2/k_1 - 1)} \right] (e^{-k_1\tau} - e^{-k_2\tau}) \quad (24)$$

For a CSTR:

$$\frac{C_A}{C_{A0}} = \frac{1}{(1 + k_1\bar{\tau})} = 1 - X_A \quad (25)$$

$$\frac{C_R}{C_{A0}} = \frac{k_1\bar{\tau}}{(1 + k_1\bar{\tau})(1 + k_2\bar{\tau})} \quad (26)$$

$$\frac{C_S}{C_{A0}} = \frac{(k_1\bar{\tau})(k_2\bar{\tau})}{(1 + k_1\bar{\tau})(1 + k_2\bar{\tau})} \quad (27)$$

The results of the calculations lead to the following remarks.

Item i): a very useful equilateral diagram, having on the three sides  $C_A/C_{A0}$ ,  $C_R/C_{A0}$ ,  $C_S/C_{A0}$  (all three ratios varying from 0 to 1), is obtained ([8], p. 115). Such calculation is easily performed using the following sequence, where  $k_2/k_1 = k$  is fixed: choosing a ratio  $C_A/C_{A0}$  between 0 and 1 from Eq.s (22) and (25) the products  $k_1\bar{\tau}$  and  $k_2\bar{\tau}$  are calculated and therefore  $\tau/\bar{\tau} = a$  is determined. Then  $(k_2/k_1) \times (\tau/\bar{\tau}) = ka = k_2\tau/k_1\bar{\tau}$  and, therefore,  $k_2\tau = (ka)k_1\bar{\tau}$ . Similarly,  $k_1\bar{\tau} = k_2\bar{\tau}$ . The four values  $k_1\tau$ ,  $k_2\tau$ , and  $k_1\bar{\tau}$ ,  $k_2\bar{\tau}$  together with  $k_2/k_1 = k$  allow the calculation of  $C_A/C_{A0}$  and  $C_R/C_{A0}$  (Eq.s (23'), (26),

respectively). Then,  $C_S/C_{A0}=1 - C_A/C_{A0}-C_R/C_{A0}$ .

Item ii): The relation between  $\tau$  and  $\bar{\tau}$  to achieve the same conversion,  $x_A$ , at the same volumetric flux, in PFR and CSTR, respectively, is easily obtained by using Eq.s (22) and (25). It results ([7], p. 228):

$$\tau = [\ln(1+k_1\bar{\tau})]/k_1 \quad (28)$$

$$\text{or: } \tau = [\ln(A)]/k_1 \quad (28')$$

being  $A=1+k_1\bar{\tau}$ .

The expression for  $S_{R/A}$ (PFR) is obtained by using Eq. (5'') in which Eq.s (22) and (23) are included. It results ([7], pp. 29, 228):

$$S_{R/A}(\text{PFR}) = [k_1/(k_2-k_1)](e^{-k_1\tau} - e^{-k_2\tau})/(1 - e^{-k_1\tau}) \quad (29)$$

Similarly, using Eq.s (25) and (26) in Eq. (5''),  $S_{R/A}$ (CSTR) is calculated

([7], p. 228):

$$S_{R/A}(\text{CSTR}) = [1/(1-k)][(A/B-1)/(A-1)] \quad (30)$$

where  $B=1+k_2\bar{\tau}$ .

At last, it should be remarked that Eq.s (29) and (30) hold for  $C_{B0}=0$ , not explicitly indicated in the selected reference.

To calculate the ratio  $S_{R/A}(\text{PFR})/S_{R/A}(\text{CSTR})$  at the same conversion  $x_A$ , it is necessary to substitute  $\tau$  in Eq. (29) a expressed by the Eq. (28). Therefore:

$$S_{R/A} = [1/(k-1)][(1/A-1/A^k)/(1-1/A)] \quad (31)$$

Finally the main result for item ii) is obtained by the ratio between Eq.s (31) and (30) ([7], p. 229):

$$R = S_{R/A}(\text{PFR})/S_{R/A}(\text{CSTR}) = [1-A^{(1-k)}]/(1-A/B) \quad (32)$$

A convenient diagram of the ratio  $R$  as a function of conversion  $x_A$  and  $k$  is reported in the cited reference.

Two observations, never reported in literature, can be made concerning Eq.s (28) and (29). The ratio

$$\tau/\bar{\tau} = \ln(1+k_1\bar{\tau})/k_1\bar{\tau} \quad (33)$$

depends only on the kinetic constant  $k_1$ ; the second member of this equation is a function only of  $k_1\bar{\tau}$ , and it has a decreasing value lower than 1. This analysis brings directly to the important conclusion that a PFR requires a lower residence time than a CSTR to reach the same conversion of the key reagent. The second observation is that an easy algebra applied to Eq. (30), by substituting  $A=1+k_1\bar{\tau}$ ;  $B=1+k_2\bar{\tau}$ ;  $k=k_2/k_1$  shows that:

$$S_{R/A}(\text{CSTR}) = 1/B = 1/(1+k_2\bar{\tau}) \quad (34)$$

Therefore for a CSTR the selectivity  $R/A$  does not depend from the kinetic constant  $k_1$ . This conclusion is rather surprising, but it is confirmed by a simple numerical comparison between Eq.s (30) and (34), which indeed return the same value when fixing  $\bar{\tau}$ ,  $k_1$ ,  $k_2$ , indeed independent on  $k_1$ . Furthermore, Eq. (34) proved much more reliable than Eq. (30), since it leads continuous and monotonously variable values from 0 to 1 for  $S_{R/A}$ (CSTR), whereas Eq. (34) is not applicable for  $k_1 \rightarrow 0$  and  $k_1=k_2$ , for which indeterminate forms are obtained. The same situation occurs also for Eq. (29). The independence of the selectivity of an intermediate from the kinetic constant for its formation, but only for that describing its consumption rate is not very intuitive and deserves a deeper investigation which goes beyond the scope of this work. However, a first attempt to interpret such intriguing observation is that explicit expressions to calculate selectivity for the intermediate in consecutive reaction paths have been derived for the simplest case only, i.e. first order reactions.

In this way an increase of  $k_1$  brings about an increase of concentration of the intermediate  $R$ , with consequent increase of its consumption rate. Therefore, for instance any increase of  $k_1$  does not bring to any net accumulation for  $R$  since its depletion is accelerated too due to an increased availability of this reactant.

Should the reactions exhibit different reaction orders, likely the dependence on  $k_1$  would be evident.

Item iii): The optimum residence time  $\tau_{opt}$  or  $\bar{\tau}_{opt}$  to obtain the maximum concentration of  $R$  is discussed in many books; we will consider some of them [ref.s. 2, pp. 195-196; 3, pp. 463-467; 6, pp. 101-102; 8, pp. 111-114; 13, pp. 46-47]. The starting point is to solve the equation  $dC_R/d\tau=0$  (for PFR) and  $dC_R/d\bar{\tau}=0$  (for CSTR).

The results are:

$$\tau_{opt}(\text{PFR}) = [\ln(k_2/k_1)]/(k_2-k_1) \quad (35)$$

$$\bar{\tau}_{opt}(\text{CSTR}) = 1/(k_1k_2)^{1/2} \quad (36)$$

Eq. (36) is also reported in ref. [13], p. 47.

In [7], p. 230 a sophisticated analysis is performed, which brings to the equation:

$$\bar{\tau}_{opt}(\text{CSTR}) = [(k_1k_2)^{1/2} - 1]/[k_1-k_2(k_1k_2)^{1/2}] \quad (37)$$

After some algebraic manipulations it can be demonstrated that such equation is perfectly reducible to the simpler one (36). In [3] it seems that  $\bar{\tau}_{opt}(\text{CSTR})$  is not discussed in order to obtain an equation like (36), while in [2], p. 196 the following equation is reported:

$$\bar{\tau}_{opt}(\text{CSTR}) = 1/(k_1k_2)^{1/2} \quad (38)$$

or:

$$\bar{\tau}_{opt}(\text{CSTR}) = k_2/(k_1k_2)^{1/2} \quad (38')$$

Obviously such equations do not coincide with Eq. (36). In the cited

ref. [2] the considered reaction scheme is more complicated than:  $A \rightarrow R \rightarrow S$ , because both A and R can react to give other 2 products different from R and S. Eq. (36) has been written by supposing that the reaction scheme is only as above reported.

From the values of  $\bar{\tau}_{opt}$  and  $\bar{\tau}_{opt}$  the corresponding values of the optimum conversion,  $X_{A,opt}$ , is calculated by inserting such values in Eq.s (22), for PFR, and (25) for CSTR; this substitution is made by using Eq.s (32) and (33). The results is ([3], p. 463):

$$X_{A,opt}(PFR) = 1 - (k_2/k_1)^{1/(1-k_2/k_1)} \quad (39)$$

or using  $k=k_2/k_1$ :

$$X_{A,opt}(PFR) = 1 - (k)^{1/(1-k)} \quad (39')$$

Besides using the basic equation (25) and (35) it results:

$$X_{A,opt}(CSTR) = 1 - 1/[1+k_1/(k_1 k_2)^{1/2}] \quad 0$$

or ([8], p. 114):

$$X_{A,opt}(CSTR) = 1/(1+k^{1/2}) \quad (40')$$

The optimum selectivity for R is easily obtained by using Eq. (5") in which  $C_A$  and  $C_R$  are calculated by using Eq.s (22) and (23) at  $\tau=\tau_{opt}(PFR)$ , to give Eq. (35), or Eq.s (25) and (26) at  $\bar{\tau}=\tau_{opt}(CSTR)$ , to obtain Eq. (36).

Item iv): The last subject of this discussion concerns only PFR because, as previously discussed, the differential,  $S'_{R/A}$ , and overall selectivities,  $S_{R/A}$ , in CSTR are the same.

Few books discuss this subject for Type 3 reactions (consecutive reactions). The equation for  $S'_{R/A}(PFR)$  can be calculated both by applying Eq. (7), written using concentration and assuming  $a=r$ :

$$S'_{R/A} = dC_R/dC_A = (k_1 C_A - k_2 C_R)/(k_1 C_A) \quad (7')$$

or by using the derivative of the yield with respect to conversion (see next paragraph). In the first case,  $C_A$  and  $C_R$  as described by Eq.s (22) and (23) respectively, are substituted in Eq. (7). The result is:

$$S'_{R/A}(PFR) = 1 - \left( \frac{k_1}{k_1 - k_2} \right) \left[ \frac{k_2}{k_1} \left( 1 - \frac{e^{k_1 \tau}}{e^{k_2 \tau}} \right) \right] \quad (41)$$

or

$$S'_{R/A}(PFR) = \frac{1}{\frac{k_2}{k_1} - 1} \left[ \frac{k_2}{k_1} \left( \frac{e^{k_1 \tau}}{e^{k_2 \tau}} - 1 \right) \right] \quad (41')$$

### 1.3 The definition of yield

This topic is the title of a paper published in the past by Carberry [1]. Miscellaneous definitions are offered in the cited literature. Let us group such definitions in some items, starting from the letters used to identify the yield:

i) the majority of the definitions uses the letter Y; sometimes the suffix I and j or A and R (or similar letters) are used to indicate the key reagent I or A and the desired product j or R (see: [1], [5], p. 268; [7], p. 23; [9], p. 70; [13], p. 33; [14], p. 317; [16], p. 92; [18], p. 13; [21], p. 353; [22], p. 26; [23], p. 154; [24], p. 309);

ii) the Greek letter  $\Phi$  or  $\varphi$  ([2], p. 156; [6], p. 98) or  $\eta$  ([8], p. 29) are used too;

iii) in all the other cited references the initial definition is given by a suitable expression, avoiding a specific letter.

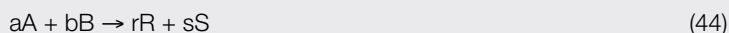
Considering the content of such definitions, the majority uses the following expression, with Y and a molar basis [3, p. 232; 8, p. 29; 10, p. 47; 12, p. 300; 21, p. 353; 23, p. 154]:

$$Y_{ij} = \frac{\text{moles of desired product j formed from moles of i reacted}}{\text{moles of i present initially}} \quad (42)$$

Or [7, p. 23; [13] p. 33; 16, p. 92; 22, p. 26]

$$Y_{ij} = \frac{\text{moles of i reacted to form j}}{\text{moles of i present initially}} \quad (43)$$

The two definitions, above reported, are equivalent, if we consider the reaction scheme:



Considering the definition (42) it results:

$$Y_{R/A} = \left( \frac{n_R - n_{R0}}{n_{A0}} \right) \frac{a}{r} \quad (45)$$

But:  $(n_R - n_{R0})/(a/r)$  are the moles of A reacted to give R, as the definition (43).

It has been observed ([13], p. 33) that if there is only one product, then Eq. (45) is the A conversion,  $x_A$ , because  $(n_R - n_{R0})/(a/r) = n_{A0} - n_A$  and  $x_A = (n_{A0} - n_A)/n_{A0}$ .

Some confusing situations, with respect to the definitions above given arise if we consider [2, 6, 14, 20] where the yield is defined as:

(overall fractional) yield ( $\Phi$  in [2], p. 156):

$$\text{Yield } (\Phi) = \frac{\text{all R formed}}{\text{all A reacted}} \quad (46)$$

or [6], p. 98; [14], p. 317; [20], p. 48:

$$Y_{R/A} = \left[ \frac{n_R - n_{R0}}{n_{A0} - n_A} \right] \frac{a}{r} \quad (47)$$

( $Y_{R/A}$  is indicated as  $\Phi'$  in ref. [6])

or (Instantaneous) Fractional Yield ( $\varphi$  in [2]):

$$\varphi = \frac{dC_R}{-dC_A} \quad (48)$$

Such equations are the same as overall selectivity (5-5") or differential



selectivity (7) discussed in the previous paragraph.

Other definitions are:

- Yield = (moles of desired product formed)/(moles that would have been formed if there were no side reactions and the limiting reactant had reacted completely [4], p. 127;

- Yield (Theoretical) = amount of product that would be formed if all the reactant were converted to the desired product [19], p. 15;

- Yield (Theoretical) = ratio of the rate generation of a desired product R ( $r_R$ ) to the rate of consumption of a key reactant A ( $r_A$ ) [9], p. 70;

- Yield = amount of desired product produced relative to the amount that would be formed if there were no by product and the main reaction went to completion [18], p. 13.

### 1.3.1 Application of Eq.s (42), (43).

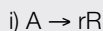
Taking into account definitions (42), (43) and the ones of conversion (1) and selectivity (5) it is obvious to obtain the well-known correlation among Y, X, S:

$$Y_{R/A} = X_A S_{R/A} \quad (49)$$

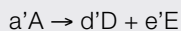
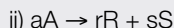
Such equation can be utilized both for parallel and series reactions in order to calculate the selectivity using the yield and viceversa.

#### 1.3.1.1 Parallel reactions

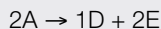
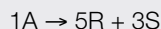
We will consider two reaction schemes:



Exemplified as:



Exemplified as:



For scheme i) according to Eq. (45):

$$Y_{R/A} = \left( \frac{n_R - n_{R0}}{n_{A0}} \right) \cdot \frac{1}{1} \quad (51)$$

$$Y_{S/A} = \left( \frac{n_S - n_{S0}}{n_{A0}} \right) \cdot \frac{1}{2} \quad (52)$$

Therefore:

$$Y_{R/A} + Y_{S/A} = \frac{(n_R - n_{R0}) + (n_S - n_{S0})/2}{n_{A0}} \quad (53)$$

The numerator of (50) is the number of moles of A reacted, i.e.  $n_{A0} - n_A$ , hence:

$$Y_{R/A} + Y_{S/A} = \frac{n_{A0} - n_A}{n_{A0}} = X_A$$

Therefore:

$$\sum_i Y_{i/A} = X_A \quad (54)$$

Taking into account Eq. (49) it derives:

$$S_{R/A} = \frac{Y_{R/A}}{\sum_i Y_{i/A}} \quad (55)$$

$$S_{S/A} = \frac{Y_{S/A}}{\sum_i Y_{i/A}} \quad (56)$$

Considering now the scheme ii), where a variety of products are formed, we may write four equations like (51) and (52) for the products R, S, D, E with stoichiometric coefficients 1/5, 1/3, 2/1, 2/2, respectively, but it is easy to demonstrate that the total conversion  $X_A$  can be calculated from Eq. (54), but using for each reaction only one product, i.e. for example:

$$X_A = Y_{R/A} + Y_{D/A} \quad (57)$$

#### 1.3.1.2 Consecutive reactions

The reaction scheme is the same as reported in paragraph 1.2.

A convenient discussion for such topic, in order to correlate selectivity and yield is presented in ref. [8], p. 108-114, both for PFR and CSTR reactors.

In the second case, the selectivity will include both the overall ( $S_{R/A}$ ) and the instantaneous one ( $S'_{R/A}$ ). A general procedure for both the types of reactors can be obtained from the derivative of Eq. (49) with respect to  $X_A$ :

$$S'_{R/A} = \frac{dY_{R/A}}{dX_A} \quad (58)$$

Besides,  $S'_{R/A}$  is obtained from an equation derived from (7') and using equation (45):

$$S'_{R/A} = 1 - k \frac{Y_{R/A}}{1 - X_A} \quad (59)$$

The dependence of the conversion  $X_A$  and  $Y_{R/A}$  from  $\tau$  and  $\tau^-$  for PFR/BR or CSTR respectively are obtained from equations (22), (25) and (26)

The final results are as below reported:

i) PFR/BR

$$S_{R/A} = \frac{1 - X_A}{(k-1)X_A} \left[ 1 - (1 - X_A)^{k-1} \right] \quad (60)$$

$$S'_{R/A} = \frac{1}{k-1} \left[ k(1-X)^{k-1} - 1 \right] \quad (61)$$

$$Y_{R/A} = \frac{1 - X_A}{k-1} \left[ 1 - (1 - X_A)^{k-1} \right] \quad (62)$$

ii) CSTR

$$S_{R/A} = S'_{R/A} = \frac{Y_{R/A}}{X_A} = \frac{1 - X_A}{(k-1)X_A + 1} \quad (63)$$

$$Y_{R/A} = \frac{X_A(1 - X_A)}{(k-1)X_A + 1} \quad (64)$$

## Conclusions

The aim of the present review, probably one of the very few published about the topics reported in the title, is to show and compare the different definitions and use of conversion, selectivity and yield, with reference both to the reactor types and the different reaction schemes shown in paragraph 1.2. Some definitions appear to have more consent than others in the analysed literature: for conversion, Eq.s (1, 2); for the (overall) selectivity, Eq.s (4, 5-5<sup>''</sup>); for the local and instantaneous (differential) selectivity, Eq.s (7-9); for the yield, Eq.s (42, 43, 45).

Obviously, as underlined in the sentence of [10] and [25], cited in the Introduction, there are some conflicting definitions, which are discussed in this review. In general, the most confusing concepts seem selectivity and yield. Apparently, the different definitions arise from the topic covered by the reference considered. Indeed, books or manuscripts focusing on kinetics prefer to express selectivity as the amount of the product desired weighted with respect to all the possible by-products. This definition may

come directly from the comparison of the reaction rates bringing to the different species.

In our opinion this definition is hardly applicable if all the by-products are not quantitatively defined.

By contrast, authors devoted to process or reactor design prefer a more practical definition of selectivity as the ratio between the amount of the desired product formed with respect to the key-reagent reacted.

If this definition is instead applied to define the yield, as for instance in [2, 4], then the product of this yield and the conversion as defined by Eq.s (1, 2) gives the most used definition of yields (Eq. 42), i.e. the ratio between the amount of the desired product formed and the key-reagent fed. In our opinion the useful equation  $\text{yield} = \text{conversion} \times \text{selectivity}$  must be maintained, but this imply to define the selectivity as in Eq. (4) or (7).

Anyway, the authors hope that the present review could give an help to standardize the definitions and the symbology of such important parameters in the chemical engineering publications.

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# RIASSUNTO

## **Conversione, selettività, resa sono termini definiti in modo non ambiguo nella letteratura chimica e di ingegneria chimica?**

Questa rassegna prende in considerazione e discute le differenti definizioni e usi dei termini conversione, selettività, resa, con riferimento sia ai diversi tipi di reattori che schemi di reazione. I libri e i lavori dedicati principalmente alla cinetica preferiscono esprimere la selettività come rapporto tra l'ammontare del prodotto desiderato e quello di tutti i possibili sottoprodotti. Questa definizione, che non è applicabile se tutti i sottoprodotti non sono quantitativamente determinati, deriva direttamente dal confronto delle velocità di formazione per le differenti specie chimiche. Gli autori che si dedicano a studi riguardanti processi o reattori chimici preferiscono invece una definizione più pratica di selettività, ovvero il rapporto tra l'ammontare del prodotto desiderato formato con quello del reagente chiave reagito. Una situazione che può creare confusione nasce se quest'ultima definizione di selettività è invece usata per definire la resa. In tal caso la ben nota equazione  $\text{resa} = \text{conversione} \times \text{selettività}$  risulta non applicabile.