

A Critical Review of Chemical Reactors Design for Reversible Reactions (II)

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Abstract

The aim of this paper is to continue the presentation of correct relations of some chemical reactors design written for reversible reaction. Our discussion is based on a paper of R. Levine where this subject is analysed, but a lot of errors made by this author led to wrong solutions. This paper follows the presentation proposed by Levine, but in each situation where an error is occurred we try to correct it and finally to propose the wright solution for each type of analysed reaction. This part of review put in discussion the reversible production of a dimmer from twin or two different reactants

Key words: reactor, reversible reaction, dimmer

Introduction

This paper continues the discussion about a design approach for CSTR made by Ralf Levine in his article “CSTR Design for Reversible Reactions” published in Chemical Engineering, September 2009 [2].

We will analyse the article exactly in the manner of the presentation, using the same chemical reactions and the same number for the equation proposed by author, but we added a small star (*) for each equation corrected by us. Finally, all the equations with the sign (*) are those that are proposed to replace the equations with the same number from the original article.

This part of the review will put in discussion the reversible reaction for a dimmer production using two different or twin reactants. The reaction is carried out in a CSTR or in a plug-flow reactor. Finally, the volumetric efficiency is calculated in order to compare the performance of these two types of reactors.

Reversible Production of a Dimmer from Two Reactants

In this case, the author [2] considers that the reaction of dimmer production contains 2 reactants C and D, but all the equations were written for B and D, thus we will discuss the kinetics of the following reversible reaction: $B + D \Leftrightarrow P$

The reaction rate is presented in equation (15):

$$-r = k_F C_B C_D - k_R C_P \quad (15)$$

Where the equations for C_B and C_D are similar because $X_B = X_D = X_f$:

$$C_B = C_{B0} - C_{B0}X_f = C_{B0}(1 - X_f) \quad (16a^*)$$

$$C_D = C_{D0} - C_{B0}X_f = C_{B0}(M - X_f) \quad (16b^*)$$

where: $M = C_{D0}/C_{B0}$

$$C_{Pf} = C_{B0}X_f \quad (16b)$$

Results the expression of the reaction rate (17), as follows:

$$-r = k_F C_{B0}^2 \left[(1 - X_f)(M - X_f) - \frac{X_f}{KC_{B0}} \right] \quad (17)$$

where: $K = k_F/k_R$.

At equilibrium, the reaction rate is zero, and we present the correct expression (18a*) which replaces the wrong equation (18a):

$$0 = (1 - X_e)(M - X_e) - \frac{X_e}{KC_{B0}} = X_e^2 - \frac{MKC_{B0} + KC_{B0} + 1}{KC_{B0}} X_e + M \quad (18a^*)$$

The quadratic equation (18b*) is also different of equation (18b) proposed by author:

$$X_e = \frac{\frac{MKC_{B0} + KC_{B0} + 1}{KC_{B0}} \pm \sqrt{\frac{(MKC_{B0} + KC_{B0} + 1)^2}{K^2 C_{B0}^2} - 4M}}{2} \quad (18b^*)$$

To write a correct expression of reaction rate, we replaced the equilibrium constant from equation (17) with its expression as a function of X_e (ha*) and we obtain the equation (19*) which shows that the reaction rate becomes zero when $X_f = X_e$.

$$K = \frac{(C_P)_e}{(C_B)_e \cdot (C_D)_e} = \frac{C_{B0}X_e}{C_{B0}(1 - X_e) \cdot C_{B0}(M - X_e)} = \frac{X_e}{C_{B0}(1 - X_e)(M - X_e)} \quad (ha^*)$$

$$-r = k_F C_{B0}^2 \left[(1 - X_f)(M - X_f) - \frac{X_f}{\frac{X_e}{C_{B0}(1 - X_e)(M - X_e)} C_{B0}} \right] =$$

$$= k_F C_{B0}^2 \left[(1 - X_f)(M - X_f) - (1 - X_e)(M - X_e) \frac{X_f}{X_e} \right] \quad (19^*)$$

The volume of the first stage from CSTR series is calculated with equation (20*):

$$\frac{V_1}{vC_{B0}} = \frac{1}{k_F C_{B0}^2} \cdot \frac{X_1}{(1 - X_1)(M - X_1) - (1 - X_e)(M - X_e) \cdot \frac{X_1}{X_e}} \quad (20^*)$$

$$\frac{V_1(k_F C_{B0})}{v} = \frac{X_1}{(1-X_1)(M-X_1) - (1-X_e)(M-X_e)} \cdot \frac{X_1}{X_e} \quad (20a^*)$$

Also, for plug-flow reactor, the volume is calculated with equation (20b*):

$$\frac{V}{v}(k_F C_{B0}) = \int_0^{X_f} \frac{dX}{(1-X)(M-X) - (1-X_e)(M-X_e)} \cdot \frac{X}{X_e} \quad (20b^*)$$

Considering that in a series of CSTR all the stages are equal and are working in the same conditions, we can accept equation (13a) here marked with (21*), but we cannot accept equations (21) and (22) because $X_f \neq n \cdot X_1$ as we already shown [1].

$$V_T = nV_1 \quad (21^*)$$

$$\frac{V_T(k_F C_{B0})}{v} = \frac{n \cdot X_1}{(1-X_1)(M-X_1) - (1-X_e)(M-X_e)} \cdot \frac{X_1}{X_e} \quad (22^*)$$

The volumetric efficiency is obtained by equation (20b*) divided by equation (22*) as following:

$$\frac{V}{V_T} = \frac{\int_0^{X_f} \frac{dX}{(1-X)(M-X) - (1-X_e)(M-X_e)} \cdot \frac{X}{X_e}}{nX_1 \frac{(1-X_1)(M-X_1) - (1-X_e)(M-X_e)}{X_e}} \quad (23^*)$$

The equation (23*) is different of the efficiency calculated by the author, because his procedure is based on a wrong application of some chemical rules described at that moment.

Reversible Production of a Dimmer from Twin Reactants

The last case discussed by Levine [2] in his article is described by the reaction: $2A \Leftrightarrow P$

The reaction rate is:

$$-r = k_F C_{A0}^2 - k_R C_P \quad (24)$$

$$C_{Pf} = C_{A0} X_f \quad (25)$$

$$-r = k_F C_{A0}^2 (1-X_f)^2 - \frac{k_F}{K} C_{A0} X_f \quad (26)$$

$$-r = k_F C_{A0}^2 \left(1 - 2X_f + X_f^2 - \frac{1}{KC_{A0}} X_f\right) \quad (26a)$$

Here the author makes a new mistake and obtain a wrong equation (26b), but the correct expression of reaction rate is (26b*):

$$-r = k_F C_{A0}^2 \left(X_f^2 - \frac{2}{KC_{A0}} X_f + 1 \right) \quad (26b)$$

$$-r = k_F C_{A0}^2 \left(X_f^2 - \frac{2KC_{A0} + 1}{KC_{A0}} X_f + 1 \right) \quad (26b^*)$$

At the equilibrium, the reaction rate is zero, and it is obtained:

$$0 = X_e^2 - \frac{2KC_{A0} + 1}{KC_{A0}} X_e + 1 \quad (27a^*)$$

Solving the quadratic equation, we will obtain:

$$X_e = \frac{2KC_{A0} + 1 \pm \sqrt{4KC_{A0} + 1}}{2KC_{A0}} \quad (27b^*)$$

Replacing K in equation (26b*) with its expression calculated with equation (ja*), we obtain the correct expression of reaction rate (28*), which shows that reaction rate becomes zero when $X_f = X_e$:

$$K = \frac{(C_p)_e}{(C_A)_e^2} = \frac{C_{A0} X_e}{C_{A0}^2 (1 - X_e)^2} = \frac{X_e}{C_{A0} (1 - X_e)^2} \quad (ja^*)$$

$$-r = k_F C_{A0}^2 \left(X_f^2 - \frac{X_e^2 + 1}{X_e} X_f + 1 \right) \quad (28^*)$$

For plug-flow reactor the true equation is:

$$\frac{V}{v} (k_F C_{A0}) = \int_0^{X_f} \frac{dX}{X^2 - \frac{X_e^2 + 1}{X_e} X + 1} \quad (29^*)$$

Regarding multi stage CSTR, the expression for the first stage is given as equation (30*):

$$\frac{V_1 (k_F C_{A0})}{v} = \frac{X_1}{X_1^2 - \frac{X_e^2 + 1}{X_e} X_1 + 1} \quad (30^*)$$

Because $X_f \neq n \cdot X_1$, we cannot accept equation (31), but for $V_T = nV_1$, it is possible to calculate total volume V_T :

$$\frac{V_T}{v} (k_F C_{A0}) = \frac{nX_1}{X_1^2 - \frac{X_e^2 + 1}{X_e} X_1 + 1} \quad (31^*)$$

The volumetric efficiency is calculated with equation (32*):

$$\frac{V}{V_T} = \frac{\int_0^{X_f} \frac{dX}{X^2 - \frac{X_e^2 + 1}{X_e} X + 1}}{\frac{nX_1}{X_1^2 - \frac{X_e^2 + 1}{X_e} X_1 + 1}} \quad (32^*)$$

Regarding the volumetric efficiency, the equation (32*) is very different of equation proposed by author because he takes in consideration a wrong application of chemical rules.

Conclusion

This study presents a critical analysis of dimer production from twin or different reactants. The author [2] intension was to “create” short equations for different chemical reactions in order to use them in different programs for CSTR or plug-flow reactors design.

Unfortunately, the author made some errors and these “short” equations didn’t respect the fundamental laws of chemistry, so that we need to correct them in order to respect the chemical laws and to use after for different applications.

References

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2. Levine, R. – CSTR Design for Reversible Reactions, *Chemical Engineering*, Vol. 116, No.9, Sept. 2009, p.46.

O analiză critică a proiectării reactoarelor chimice pentru reacții reversibile (II)

Rezumat

Scopul acestei lucrări este să continuăm prezentarea relațiilor corecte pentru proiectarea unor reactoare chimice scrise pentru reacții reversibile. Analiza noastră are la bază un articol scris de R. Levine care se ocupă de acest subiect, dar face o serie de erori care conduc la soluții greșite. Lucrarea noastră urmărește prezentarea făcută de Levine, dar acolo unde apar greșeli, noi încercăm să le corectăm și în final propunem o soluție corectă pentru fiecare tip de reacție analizată. Această parte a analizei se ocupă de reacțiile reversibile pentru producerea unui dimer din doi reactanți identici sau diferiți.