

THE EFFECTS OF INTERACTIONS BETWEEN LIQUID FILM AND BULK LIQUID ON GAS-LIQUID REACTIONS IN WELL-MIXED REACTORS

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INTRODUCTION

Gas treating and liquid phase production processes are the two most common applications of gas-liquid reactions in the chemical and biochemical industries. The theories on gas-liquid reactions can be retrieved from a vast variety of monographs and texts available in the literature [1-6]. Examples of gas treating processes include gas scrubbing and product purification while oxidation, hydrogenation, and polymerization represent liquid phase processes. The mathematical description and representation of the steady state operation of gas-liquid reactors has been largely based on the two-film theory, with molecular diffusion being considered to be the dominant transport mechanism in the gas and liquid films on either side of the gas-liquid interface. Classification of gas-liquid reactions in the past has been based on comparison of characteristic times for diffusional mass transfer and chemical reaction in liquid film near the gas-liquid interface. The fast chemical reactions occur almost entirely in liquid film and the very slow reactions are confined to bulk liquid. Gas-liquid reactions that do not belong to either class are frequently encountered in liquid phase production processes and have received less attention and have been assumed to be confined to either liquid film or bulk liquid for simplification of modeling and design of reactors. Reactions in the liquid phase help enhance the mass transfer by reducing the mass transfer resistance and increasing the driving force. The extensive literature on gas-liquid reactions has, with a few exceptions [7-10] been devoted to reactions that are considered to be completed entirely in liquid film (fast reactions) and reactions that are relegated to bulk liquid (reactions that are not fast). A unified approach for modeling of gas-liquid reactors is provided here considering the reaction occurring over the entire liquid phase, with at least one species participating in the reaction scheme being volatile. The two-way linkages between liquid film and bulk liquid, largely ignored previously, are properly accounted for in the present approach. The dispositions of concentration profiles for various reactant and product species in the liquid film are presented and discussed for a perfectly mixed reactor. The implications of these dispositions on parameters such as enhancement factors, liquid phase utilization factors, and distribution of the extent of reactions between liquid film and bulk liquid are discussed. A first-order reaction is considered as a specific example. Variation in relative importance of reactions in liquid film with respect to reactions in bulk liquid with variations in process parameters is also examined. Details of this effort are available in Parulekar and Saidina Amin[11].

PROBLEM FORMULATION

The process with molecular diffusion and chemical reaction with at least one of the species being volatile is described as follows.



The mass balance equations in the liquid film can be solved to produce analytical expressions for the concentration dispositions in the film. The boundary conditions at the gas-liquid interface for a species vary depending on whether or not the species is volatile. Interactions between the bulk liquid and the liquid film are accounted for by linking the mass balances in the bulk liquid and the liquid film. The same applies for the gas phase. For a first-order reversible reaction, the relevant material balances for the bulk gas and bulk liquid phases and flux balances at the gas-liquid interface represent

a set of linear algebraic relations among interfacial and bulk phase concentrations of reactant and product species. The appropriate species concentrations can be obtained analytically via simultaneous solution of the appropriate linear algebraic equations. Hence, no prior assumption is made on whether the distribution of reaction is largely in the liquid film or in the bulk liquid.

RESULTS AND DISCUSSION

The performance and the design of the reactors can be assessed from variables such as the ratios between the concentration of species J in phase P and the concentration of species J in phase P when the extent of reaction in liquid film is assumed to be negligible, Z_{JP} , the enhancement factors of species J, E_J , the extents of reactions in liquid film, ζ , and the liquid utilization factors, η_L . The dispositions of concentrations in the liquid film for volatile A and volatile B are shown in Figures 1a and b respectively for irreversible reaction. The profile of B in Figure 1c shows a maximum giving rise to supersaturation, wherein B is produced more near the gas-liquid interface because of higher conversion in this portion of the liquid phase.

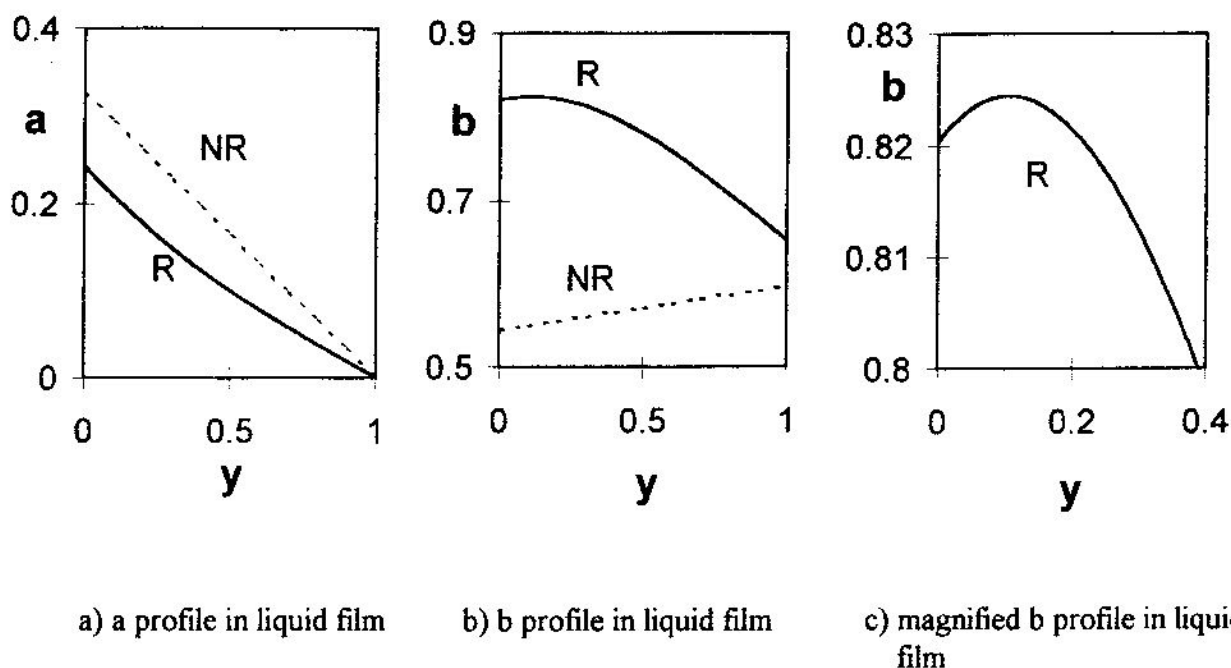


FIGURE 1: Profiles of dimensionless A and B in liquid film for $\gamma' = 1.3$

Figure 2a depicts the dependence of Z_{JP} on the dimensionless reaction parameter, γ . For example, at $\gamma=1$, Z_{JP} deviate from unity on both sides revealing that it is risky to neglect the reaction in the film. The negative enhancement factor has no physical meaning except to show there is a maximum in B somewhere in the film. E_B^* , the augmentation factor, provided an alternative definition to the enhancement factor and Figure 2b exhibits the variation with γ with no discontinuity.

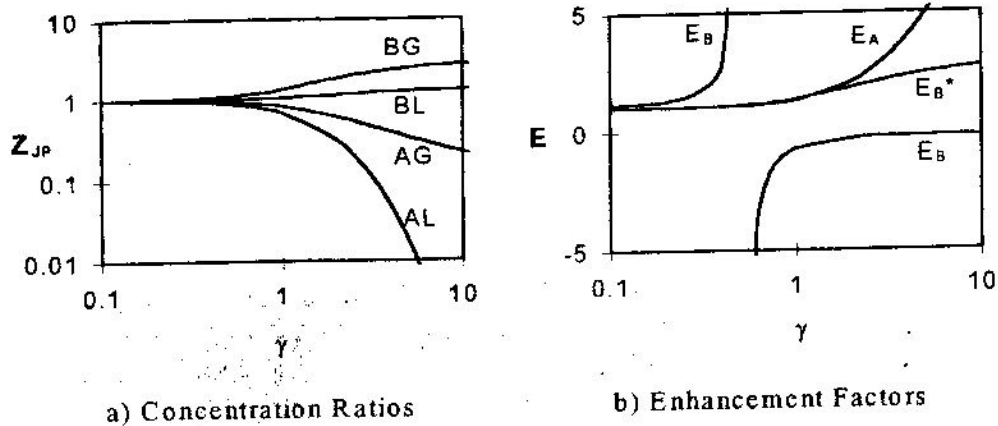


FIGURE 2 : Effect of interactions on concentration ratios and enhancement factors

For the reversible reaction, Figures 3a and b illustrate the liquid utilization factor and the extent of reaction, respectively, when the equilibrium constant, K , is varied for volatile A and B as γ' (or k) is increased. As k increases, the utilization factor of the liquid phase increases and the reaction is more concentrate and more in the liquid film. For all γ' investigated, the total reaction is always less than the reaction if the whole liquid phase is treated as a well-mixed reactor. The effect of irreversibility increases the driving forces, thus reduces the extent of reaction for $\gamma'=1.0$ and 1.3, but not for $\gamma'=2.0$ and 10.0. Similar effects are observed for the liquid utilization factor. At low K , when the reversible effect is more pronounced, the liquid utilization factor remains constant but then deviate with increasing K . At $\gamma'=1.0$ and 1.3, the extent of reaction is more in the bulk and η_L decreases with K . At $\gamma'=2.0$, η_L is not much affected by K ; at $\gamma'=10.0$, η_L increases with K , as expected.

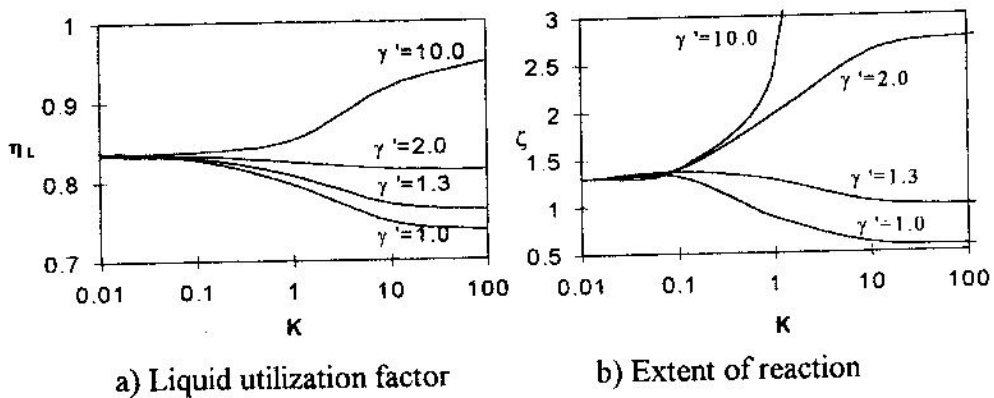


FIGURE 3: Performance of a reactor

CONCLUSIONS

The determination as to when to neglect or include reaction in the bulk liquid or liquid film cannot solely depend on the film parameters of the liquid film. There is no unique rule-of-thumb for reactions that are neither fast nor slow on relative importance of the extent of reaction in the liquid film and in the bulk liquid. Numerical illustrations demonstrate that an unwarranted confinement of liquid phase reactions to either liquid film or bulk liquid can lead to incorrect design of and erroneous prediction of performance of gas-liquid reactors. The interactions between the liquid film and bulk liquid are necessary to envisage a more realistic description of the diffusion-reaction phenomena in a well-mixed reactor.

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