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A supporting formulation for introducing gas–liquid reactions

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ABSTRACT

In spite of the widespread industrial application of non-catalytic or homogeneously catalyzed gas–liquid reactions (GLRs), many undergraduate chemical engineering curricula do not include this subject and heterogeneous catalysis provides the only example of a heterogeneous chemical reaction system.

Textbooks dealing with GLRs describe and formulate separately the different processes affecting the rate of chemical absorption, without providing a clear picture of the overall problem, which is highly desirable for the identification of effects and understanding of their interplay.

As an attempt to provide a different alternative for teaching GLRs, a general approximate formulation for the transport/reaction problem, in terms of a global enhancement factor (GEF) for a single chemically absorbed species, including all possible effects on the basis of the two-film model is presented here.

This contribution includes the development of the approximation for the GEF, an analysis of different regimes, which in part can be directly adopted for teaching, and an evaluation of the precision of the GEF estimation, mainly devoted to the lecturer.

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Keywords: Gas–liquid reactions; Global enhancement factor; Two-film model; Approximate solution; Chemical engineering curricula

1. Introduction

Gas–liquid reactions (GLRs), either non-catalytic or homogeneously catalyzed, are employed in many important industrial processes, as it has been summarized in specialized books (e.g. Astarita et al., 1983; Danckwerts, 1970; Doraiswamy and Sharma, 1984; Kaštánek et al., 1993) and chemical reaction engineering textbooks (e.g. Froment et al., 2011; Westerterp

et al., 1984). Frequent uses of GLRs concern the purification of a gas stream by absorption of undesirable species enhanced by chemical reaction, but many applications include the synthesis of more valuable products or the purification of liquid streams.

In spite of the practical significance of GLRs and of their specific features, many undergraduate chemical engineering curricula do not include this subject and heterogeneous

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catalysis provides the only example of a heterogeneous chemical reaction system. Actually, GLRs is not a short subject to deal with, as it involves a reference to different models for describing the transport/reaction process at a local level (i.e. film, penetration or surface-renewal models), the formulation and solution of the problem with one of these models and its application for design, analysis and selection of several possible types of gas–liquid contactors.

In comparison to heterogeneously catalyzed reactions, GLRs introduces two distinct features, as regards the local transport/reaction problem. On one hand, there are two reaction domains for a reactant A transferred from the gas. Fast reactions start, and frequently end, taking place close to the gas–liquid interface, where diffusion still governs mass transfer, and slower reactions proceed mainly in the liquid bulk. On the other hand, when reaction occurs close to the interface, the liquid reactant (say B) has to diffuse towards the interface, i.e. in direction opposite to that of A. As the reader acquainted with the subject should know, these features introduce distinct operation regimes, and formulation for the overall rate of chemical absorption becomes more complex than the counterpart in heterogeneous catalysis.

Available textbooks dealing with GLRs describe and formulate separately the different processes affecting the rate of chemical absorption. Perhaps the most important point to remark is the almost independent treatment of slow and fast reaction regimes. Different stages are also used for linear and non-linear kinetics and for cases limited or not by mass transfer resistance in the gas phase. Although this approach presents the merit of a gradual introduction of topics, it is our impression that a rather lengthy description arises without providing an overall picture of the problem, which is highly desirable for the identification of effects and understanding of their interplay.

An opposite alternative for the description of the transport/reaction process in GLRs is to present a unified treatment including simultaneously all significant effects. Then, the description of any conceptual or practical issue can be backed up by the available general formulation. It can be argued that developing a general formulation may not be appealing from a didactic point of view, particularly for a subject that, as discussed before, presents a significant degree of complexity. However, if heterogeneous catalysis is lectured before, the situation is different, as the basic notion of coupling between mass transport and chemical reaction would be already introduced, along with conservation equations and some approximations used for their solution. In our teaching experience, the background from heterogeneous catalyzed reactions greatly facilitates the presentation of a general solution for GLRs.

It is the objective of this contribution to develop a general approximate formulation for the transport/reaction problem in GLRs and show how it could be employed to present the different possible regimes and their significance. To be specific in outlining the scope of the formulation, we point out that the film model is employed for both sides of the gas–liquid interface (two-film model) under the assumptions of a single isothermal irreversible reaction of the type $A_{(G)} + bB_{(L)} \rightarrow \text{products}$, with irreversible kinetics $r = kC_A^m C_B^n$ ($m, n \geq 0$), reactant B being non-volatile and constant transport and phase equilibrium properties. A general picture of the situation to be evaluated on the basis of the two-film model is given in Fig. 1, where local values of partial pressure of A in the gas stream (p_{AG}) and liquid bulk concentrations (C_{BL} and

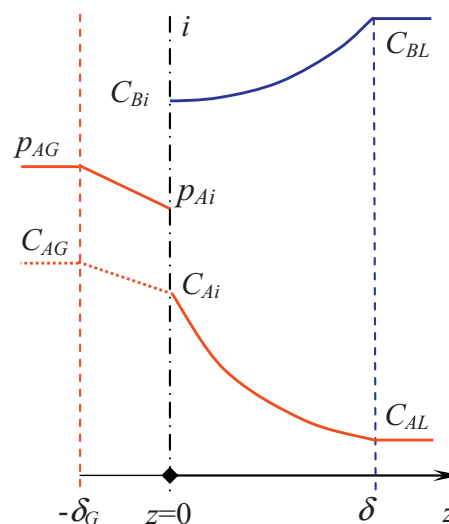


Fig. 1 – Generic profiles of the gas and liquid reactants, A and B respectively, through the gas and liquid films.

C_{AL}) are assumed to be known. Evaluating the flux of A at the interface, \mathcal{N}_{Ai} , is the main target. The processes defining the flux \mathcal{N}_{Ai} are: mass transfer of A in both films, mass transfer of B in the liquid film, chemical reaction in the liquid film under variable concentrations C_B and C_A , and chemical reaction in the liquid bulk under uniform concentrations C_{BL} and C_{AL} . The simultaneous effect of these processes will be analyzed along with the kinetic features represented by reaction orders m, n .

The manuscript is organized as follows. Section 2 summarizes some basic definitions, mainly concerned with physical absorption of A. An approximated solution for the problem of absorption with chemical reaction is presented in Section 3. A significant concept, neglecting the accumulation rate of A in the liquid stream, is introduced in Section 3.1. The different regimes of operation are described in Sections 4–7. While a large part of the material presented in Sections 2–7 can be directly employed for teaching, Sections 8–10 are more specialized and mainly directed to teachers: Section 8 accounts for the magnitude and relevance of errors from the approximated formulation, Section 9 presents a criterion for acceptance of the hypothesis of negligible rate of accumulation of A in the liquid stream for the analysis of gas–liquid contactors and Section 10 extends the analysis of Section 3 to a more generalized kind of irreversible kinetics. Finally, Section 11 mainly intends to summarize the relevant aspects of the present formulation in teaching GLRs.

2. Physical transport on both sides of the interface

It will be assumed for the analysis at a given position of a gas–liquid contactor that transport properties, including mass transfer coefficients, and the solubility in the liquid of reactant A are not composition dependent. This is in practice the case for a diluted system concerning species A and B. Also, local thermal equilibrium is assumed. At these conditions, the quoted transport and thermodynamic properties can be estimated beforehand.

Either for physical or chemical absorption, \mathcal{N}_{Ai} can be expressed as the flux through the gas film,

$$\mathcal{N}_{Ai} = k_{GA}^0 (p_{AG} - p_{Ai}), \quad (1)$$

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