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Gas–liquid mass transfer enhancement by catalyst particles, a modelling study



P.W.A.M. Wenmakers^a, J.A.A. Hoorn^a, J.A.M. Kuipers^b, N.G. Deen^{c,*}

^a DSM Ahead – Research and Development, Advanced Chemical Engineering Solutions (ACES), P.O. Box 18, 6160 MD Geleen, The Netherlands

^b Multiphase Reactors Group, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

^c Multiphase and Reactive Flows Group, Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, the Netherlands

HIGHLIGHTS

- The presence of catalyst particles on the enhancement of gas absorption is studied.
- The enhancement factor is numerically calculated as function of all key parameters.
- These parameters are catalyst concentration, particle size and diffusion coefficients.
- A homogeneous model is derived that can adequately describe the results.

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ABSTRACT

In this paper we studied the effect of catalyst particles on the enhancement of the gas–liquid mass transfer due to a first order heterogeneously catalyzed reaction. The enhancement factor was obtained by solving the liquid side unsteady reaction–diffusion equation accounting for the presence of the particles. The results are compared with an analytical model that was derived assuming a homogeneous distribution of the particles in the liquid film. It was found that the enhancement factor increases with increasing catalyst concentration and increasing rate of reaction, as expected. As the particle diameter is increased, the enhancement factor decreases due to an increasing degree of diffusion limitation.

The results of the homogeneous model match well with the results of the numerical simulations within a 10% error. Therefore it is concluded that the homogeneous model can be used to predict the enhancement of the mass transfer due to the presence of catalytic particles.

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1. Introduction

In chemical industry the importance of multiphase reactors is eminent already for decades. Still today there are enough challenges left to further improve performance of these reactors to maintain profitability and also to meet more strict (future) environmental targets. Especially for reactor systems in large bulk chemical plants every small fraction in reactor performance increase can be a substantial overall improvement. Not only in increased reactor yield as such but also separation downstream can be positively affected. Studies to support the fundamental understanding of the mechanisms taking place in the reactors and at the same time extending

engineering skills are still very worthwhile to do. One of the more complicated multiphase systems is the so-called gas–liquid–solid reactor where gaseous and liquid components are allowed to react by means of a solid (supported) catalyst. A proper understanding of the hydrodynamics, mass transfer, heat transfer, and kinetics is required for the proper design of such a reactor. For slurry reactors, where the small catalyst particles are dispersed throughout the liquid phase, the gas to liquid mass transfer is one of the critical aspects.

It is known that the rate of gas–liquid mass transfer can be significantly influenced by the presence of small particles in the liquid, either being gas-absorbing or reactive particles (Ramachandran, 2007; Ruthiya et al., 2004; Wimmers et al., 1984, 1988; Wimmers and Fortuin, 1988b; Holstvoogd et al., 1988; Holstvoogd and Van Swaaij, 1990). The presence of the small particles near the gas–liquid interface can increase the liquid side concentration gradient of the transferred

* Corresponding author.

E-mail address: N.G.Deen@tue.nl (N.G. Deen).

component, thereby increasing the mass transfer rate. Depending on the lyophobicity the particles can actually adhere to the gas–liquid surface (Wimmers and Fortuin, 1988a; Omota et al. 2006a,b; Verrelli et al., 2011), thus reducing the diffusion distance between the gas–liquid interface and the (catalyst) particles. The enhancement of mass transfer due to the presence of catalyst particles near the gas–liquid surface has been investigated in a couple of earlier papers, see e.g. Ruthiya et al. (2004, 2005), Ramachandran (2007). Especially Ramachandran (2007) presents a thorough review on the modelling approaches followed. Typically a continuum approach is adopted where the steady state diffusion-reaction equation is solved. In some cases also the effect of internal diffusion is taken into account via the effectiveness factor. However, the presence of the particles themselves and the reaction occurring within the particles will result in the presence of spatial concentration gradients in all directions, not only perpendicular to the gas–liquid interface. The particles themselves can also be seen as an obstruction within the fluid, thus hindering mass transfer towards the bulk of the liquid. These aspects are typically not taken into account within the available models. Also, as stated earlier, the internal diffusion is approximated by the effectiveness factor approach which per definition does not account for local concentration variations around the catalyst particle.

Nowadays, the computing power and the availability of commercial software allows for a much more detailed consideration of transport phenomena and related problems. The integration between software packages facilitates the accurate representation of more complex geometrical structures and to arrange for a sequence of simulations. Therefore, a large number of simulations can be conducted and run even on a standard workstation. Therefore, the effect of particles near the gas–liquid interface can now be studied numerically in more detail.

In the present study the enhancement of gas–liquid mass transfer was studied using 3D unsteady simulations using the COMSOL Multiphysics software environment. The diffusion of the gaseous component through a suspension of catalyst particles was studied for various cases, viz. effect of:

1. particle configuration, i.e. randomly distributed particles versus closely packed particles,
2. particle diameter,
3. particle volume fraction,
4. rate of reaction, i.e. different reaction rate coefficients (this also directly relates to the degree of internal diffusion limitation), and
5. liquid diffusivity.

In addition to the 3D simulations a homogenous model was derived that incorporates the combined effects of the catalyst particles and internal diffusion limitation on the overall rate of mass transfer through the gas–liquid interface. The results of the homogeneous model have been compared with the rigorous simulations in COMSOL Multiphysics.

The outline of our paper is as follows: first the adapted modelling approach for gas–liquid mass transfer through a suspension of catalyst particles is described. Subsequently the derivation of the homogeneous model for the enhancement factor for gas–liquid mass transfer is presented, followed by a comparison of the results obtained from the homogeneous and detailed models. Finally it is shown that the homogeneous model is capable of providing adequate estimates of the enhancement factor using either graphs or (relatively) simple algebraic expressions.

The presented graphs and expressions can be used to estimate the degree of enhancement on gas–liquid mass transfer for a plethora of reactor systems, since no assumptions are made on this part. Using knowledge (or assumptions) on the local catalyst concentration and the kinetics thus allows the engineer to account for gas–liquid mass transfer enhancement, resulting in a more accurate

design. Heterogeneously catalyzed reactions are abundant in industry for e.g. oxidation, hydrogenation, and Fischer–Tropsch, see e.g. Youssef et al. (2013).

2. Theory

The enhancement of gas absorption into the liquid phase by means of heterogeneous catalyst particles has already been studied for many decades, see e.g. Ruthiya et al. (2005), Ramachandran (2007), Wimmers et al. (1984), both experimentally and theoretically. In these publications a number of modeling approaches have been followed to describe the enhancement of gas absorption. Ramachandran (2007) gives an overview of the various methodologies applied. All of these models, in one way or another, describe the enhancement of the absorption by concentration depletion within the film layer. The different models vary in level of complexity from pseudo-homogeneous models to more complex cell models which take into account various distances of the catalyst particle from the gas–liquid interface. Some of these models employ the classical resistances in series approach (see Fig. 1) to describe the observed rate of absorption:

$$R_{Av} = \left(\frac{1}{k_{gl}a_{gl}} + \frac{1}{k_{ls}a_{ls}} + \frac{1}{\eta k_r} \right)^{-1} \frac{p_A}{H_A} \quad (1)$$

while others start from the stationary reaction-diffusion equation. In some studies even the effect of internal diffusion limitation by means of the so-called effectiveness factor (η) is accounted for. These studies typically have derived their relations on (pseudo) steady state assumptions. In this work two approaches have been followed to study the enhancement of the gas absorption by catalyst particles residing inside the liquid-side mass transfer boundary layer:

1. Detailed unsteady simulation of diffusion into a liquid film filled with reactive catalyst particles using COMSOL Multiphysics.
2. Derivation of an unsteady homogeneous model for diffusion into a liquid containing catalyst particles.

2.1. Numerical model

COMSOL Multiphysics 4.3a has been used to model the diffusion of the gas into a liquid film filled with catalyst particles. For practical reasons only a small part of a gas–liquid interface has been modelled, therefore curvature of the gas–liquid interface is neglected, i.e. the gas–liquid interface has been modelled as a flat interface. The catalyst particles are assumed spherical and homogeneous, i.e. no pores have been modelled explicitly where the (effective) diffusion coefficient throughout the solid is assumed to be constant. The presence of the solid catalyst particles within the liquid film has been represented in two ways:

1. The particles are randomly distributed.

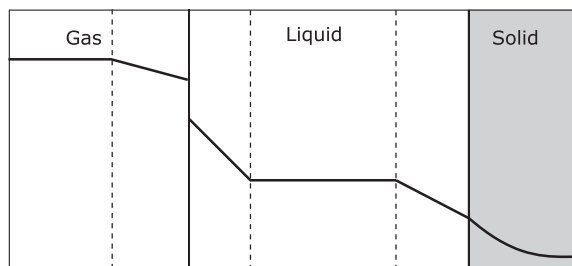


Fig. 1. Schematic representation of the concentration profile for a heterogeneously catalyzed gas–liquid reaction, showing the resistances in series.

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