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An analysis for compressible flows in a packed bed with metathesis gas–solid reaction ☆

Yuanyong Jiang [a], Zeng-he Xu [a,*], Xiaofeng Peng [b]

[a] Engineering Mechanics Institute, Campus Box 265, Northeastern University, Shenyang 110004, China
[b] Department of Thermal Engineering, Tsinghua University, Beijing 100084, China

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ABSTRACT

Taking into consideration the mass exchange between gas and solid, and the density change of gas mixture due to reaction, a model is proposed for compressible flows in a packed bed with isothermal metathesis gas–solid reaction $a\mathrm{A}(g)+b\mathrm{B}(s)=c\mathrm{C}(g)+d\mathrm{D}(s)$, When $a\neq c$, the ratio c/a greatly affects the flows of gas mixture, but for $a=c$, this coupled model reduces to the non-coupled model. One-dimensional numerical solutions show that the velocity profiles obtained from coupled model greatly differ from that from the non-coupled model. The radius of pellets can change the velocity variation trend. The concentration profiles obtained from this coupled model also differ from that from the non-coupled model. A coupled model accounting for only mass exchange between gas and solid, but neglecting the density change of gas mixture due to reaction will produce an extra term, which results in a great deviation of the velocity and concentration from those from the more comprehensive coupled model.

1. Introduction

The metathesis gas–solid reaction $a\mathrm{A}(g)+b\mathrm{B}(s)=c\mathrm{C}(g)+d\mathrm{D}(s)$ in a packed bed is common practice in chemical and metallurgical industries. This kind of gas–solid reactions often takes place very rapidly due to high temperature. The transport phenomena, associated with the overall rate of a single pellet, have been received much attention [1–4]. The pores in a pellet are so small that a very great resistance to the gas flow is produced, so, the migration of gas species is induced mainly by concentration gradient rather than pressure gradient. This means that there is no necessary to consider the effect of convection on the gas–solid reaction taking place in a pellet, and nor, overall gas–solid reaction rate of a single pellet [1–4]. For reactors, however, the scales of pores have the same order as the pellets, and the force to drive gas component motion in reactors is mainly the pressure gradient, so it is necessary to investigate the interaction between the flows and rapid gas–solid reaction.

Although the general mass conservation equations in the presence of chemical reaction were presented in continuum theory for mixture [5] and in porous media flows [6], very few further analyses were reported on the compressible flows in a packed bed with gas–solid reaction. In addition, these equations often neglect the density change of fluid mixture during reaction process. If chemical reactions take place at very slow rate, or all fluid species are in liquid form, the density change of fluid mixture would be negligible. However for a rapid gas–solid reaction, the density change of gas mixture should be considered in an analysis.

Song et al. [7] discussed the effect of gas compressibility on gas–solid reaction, but neglected the interaction between flows and reaction. Xu et al. [8] analyzed the compressible flows in a packed bed with synthesis gas–solid reaction $a\mathrm{A}(g)+b\mathrm{B}(s)=d\mathrm{D}(s)$ and proposed a model coupling compressible flows with synthesis gas–solid reaction. Based on the previous works [7,8], an analysis is conducted for understanding the compressible flows in a packed bed with metathesis gas–solid reaction $a\mathrm{A}(g)+b\mathrm{B}(s)=c\mathrm{C}(g)+d\mathrm{D}(s)$. First, a model to couple compressible flows with metathesis gas–solid reaction is proposed, which is slightly different from the model presented in paper [8], then, the model, subject to specified initial and boundary conditions, is solved numerically by finite volume method [9,10]. The new model is compared with the available non-coupled models, and a discussion is conducted on the characteristics of the velocity and concentration profiles. Particularly, an emphasis is addressed on exploring the effect of the chemical properties of a metathesis reaction system, the radius of pellets and the length of a packed bed on the compressible flows and rapid metathesis gas–solid reaction.

2. Physical and mathematical model

Consider compressible flows in a packed bed with the isothermal metathesis gas–solid reaction $a\mathrm{A}(g)+b\mathrm{B}(s)=c\mathrm{C}(g)+d\mathrm{D}(s)$, as shown in Fig. 1. The gas–solid reaction and conversion of a pellet are sketched in Fig. 2. There are always some protecting gases in gas mixture not involved in gas–solid reactions, they are taken as inert gas, though they may be not inert chemically. Other important assumptions adopted here are: (i) each gas component in gas mixture

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* Corresponding author.
E-mail addresses: zenghexu@mail.neu.edu.cn, xuzenghe@yahoo.com.cn (Z. Xu).

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