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Mass Transport/Diffusion and Surface Reaction Process with Lattice Boltzmann

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Abstract. Multi-component flow with chemical reactions is a common problem in different industrial applications: the mixing chamber of a reaction injection molding (RIM) machine; the dynamics of diesel soot particles interacting with a porous-ceramic particulate filter; reactive transport in porous media; bio-chemical processes involving enzyme-catalyzed kinetics. In all these cases, mass diffusion/convection and wall or volume chemical interactions among components play an important role. In the present paper we underline the importance of diffusion/convection/reaction mechanisms in bio-chemical processes using the Lattice Boltzmann (LB) technique. The bio-application where we studied diffusion/convection/reaction mechanisms is the quorum-sensing pathway for the bio-synthesis of the AI-2, a molecule that allows the bacteria to launch a coordinated attack on a host immune system (see [9,10] for more details of the bio-application). The overall goal is to create a micro-device to screen potential drugs that inhibit AI-2 bio-synthesis. The Michaelis-Menten saturation kinetic model is implemented at the reactive surface and the results are shown in terms of two dimensionless numbers: Damkohler (*Da*) and Peclet (*Pe*) number. For high *Pe* number a small conversion of reactants into products is obtained at the reactive surface, but the overall flux of products is high; moreover, a fast saturation of the conversion of reactants to products is obtained for high *Da* numbers. The trade-off for setting the *Pe* and *Da* numbers depends on the specific application and the technologies used in the micro-device (e.g., sensitivity of the detector, cost of reactants).

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1 Introduction

Bio-sensors and bio-chips are one of the most useful and challenging application based on microfluidic devices for different kinds of problems like DNA analysis, protein separation, antibiotics screening [9, 10]. Using of microdevices is ideal for parallel and automatic drugs screening, and it allows using small volume of expensive reagents. The bio-application that we are focusing on in this paper, in order to study diffusion/convection/reaction mechanisms using Lattice Boltzmann technique, is the quorum-sensing pathway for the bio-synthesis of the AI-2, a molecule that allows the bacteria launching a coordinate attack on a host immune system. The overall goal is to create and to optimize a microdevice to screen potential drugs that inhibit the AI-2 bio-synthesis (see [9, 10] for more details).

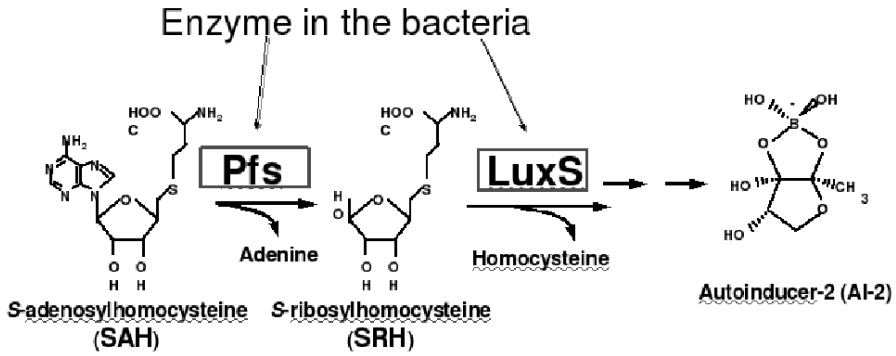

Figure 1: Schematic representation of the quorum sensing pathway (figure from [9,10]): the complex molecular SAH reacts with the enzyme Pfs giving adenine and SRH as product. The SRH reacts with the enzyme LuxS giving the by-product homocysteine and the autoinducer-2 (AI-2) (see [9, 10] for more details).

The quorum sensing pathway involve two kinds of enzymes: either the Pfs or LuxS (see Fig. 1). It is clear from the scheme in Fig. 1 that one mole of SAH that reacts with the enzyme Pfs gives one mole of adenine and one mole of SRH. The by-product adenine is not involved in the successive steps of the reaction, so a common simplification is to consider a reaction where one mole of SAH produces one mole of SRH. A microdevice that can mimic the quorum sensing pathway is a microchannel with two patches on the bottom surface. The enzymes Pfs and Luxs are attached on the surface of the patches with a fixed superficial concentration so that the two patches can be considered as reactive surfaces: when a molecule of a reactant reaches the surface of the patch it can react with the attached enzyme to generate a molecule of product. At the inlet of the microchannel is introduced a potential inhibitors of the AI-2 whose efficiency is analyzed through the microdevice [9,10]. A scheme of the microdevice is shown in Fig. 2; Fig. 3 shows the microchannel used in the experiment [9,10]. In order to optimize the microdevice in terms of maximum sensitivity, minimal sample requirement and fastest screening times, the quorum-sensing pathway was simulated with a LB code, and the results were compared with available experimental analysis [9, 10]. The experimental analysis [9, 10] was con-