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INVESTIGATING MASS TRANFER IN REACTIVE TURBULENT FLOW USING PASSIVE PARTICLE TRACKING

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ABSTRACT

In this work, particle tracking is used in conjunction with turbulent flow simulation to investigate the effects of the flow on turbulent mass transfer with a chemical reaction. The flow is simulated with a spectral methods-based direct numerical simulation (DNS) [1]. After the fluid flow reaches fully developed, stationary state, the mass transfer is simulated by releasing a large number of reactant particles into the flow field [2]. Two different cases are examined: (a) a homogeneous reaction case, where particles are released from the wall and then react in the flow field with a first order reaction, and (b) a surface reaction, where particles are released randomly on a cross section of the channel and then react with the wall.

The reaction equation can be written as: A → B, where A is the reactant and B is the product. In the case of the homogeneous reaction, each of the reactant particles can either react and transform into a product in every time step, or continue moving in the flow field without reacting. The probability of reaction follows a Poisson probability density function that depends on the reaction rate. In the case of the surface reaction, the reactant particle can transform into a product when it comes in contact with the wall (i.e., a diffusion-controlled reaction between the fluid and the channel wall is simulated). The rate of reaction between the fluid and the wall is related to the probability that a particle colliding with the wall will react with the wall. In both cases, in each simulation time step, the reactant particles move due to convection, which is determined by the DNS of the flow, and due to diffusion, which is simulated by a random Brownian motion that depends on the Schmidt number of the fluid [3,4].

The presentation will discuss the methodology for determining the bulk concentration, the wall concentration, and the mass transfer coefficient from and to the wall. All these can be calculated as a function of the channel length. The effects of the chemical reaction on the mass transfer coefficient in the case of a homogeneous reaction will be discussed. The main result is an enhancement of the mass transfer coefficient by a factor that can be as high as ten, depending on the fluid diffusivity. In the case of the

heterogeneous reaction, the effects of the flow and of the Schmidt number on the apparent reaction rate and on the mass transfer coefficient, as well as the entry effects on the rate of mass transfer will be explored. Although there is no effect of Schmidt number on the bulk concentration, the mass transfer coefficient is found to be higher for smaller Schmidt number fluids, but the nominal reaction rate does not appear to affect the mass transfer. The mass transfer coefficient is found to be independent of the reaction rate, but has a strong dependence on the fluid diffusivity.

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