Direct Numerical Simulation of turbulence in rotor-stator spinning disc reactors: prediction of mass transfer and micromixing efficiency

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Highlights

- The mechanism behind G/L-mass transfer in an rs-SDR is indentified
- DNS of turbulent flow around a bubble shows turbulence focuses in the liquid film
- Vortex stretching in the liquid film increases vorticity in one direction in the film
- DNS of reaction, convection and diffusion in an rs-SDR is used to analyse micromixing

1. Introduction

The rotor-stator spinning disc reactor is a novel type of chemical reactor for multiphase processes in chemical industry. In this type of reactor, a disc (the rotor) is rotating at high angular velocities of up to 4,000 rpm in a narrow cylindrical encasing (the stator). The distance between the rotor and the stator is typically one to a few millimetres. In this configuration, there exists a large velocity gradient in the reactor contents over the span of the rotor-stator gap leading to high shear forces. In turn, this shear leads to the formation of increasingly smaller droplets and bubbles with an increasing disc speed, which have a large specific surface area a [1,2]. In addition, the high velocity of the disc leads to a flow field of high turbulence intensity with inherently low micromixing times down to 0.113 ms [3]. Due to this effect, there is a large surface renewal rate of liquid elements close to the interface. This lowers the resistance to mass transfer so that the mass transfer coefficient is increased. It is the combination of these two effects that lies at the heart of the spinning disc reactor's performance. In fact, it has been shown experimentally that gas-liquid mass transfer coefficients per volume of gas can be as high as $k_{GL}a_{GL}$ = 20.5 $m_L^3\,m_G^{-3}\,s^{-1}$ [4], about 40 times higher than typical values in bubble columns [5]. This allows reactions to be performed at intensified conditions and close to their intrinsic kinetic speeds. Moreover, the rapid rate of micromixing prevents the formation of hotspots and increases selectivity and product quality.

Traditional theories describing mass transfer rates, such as Higbie penetration theory [6], greatly underpredict the experimental values of the mass transfer coefficients [7,8]. Typical experimental values for the mass transfer coefficients are of the order $k_{GL} = O(10^{-3}) - O(10^{-2})$ $m_L^3\,m_i^{-2}\,s^{-1}$, while predictions using penetration theory range from $k_{GL} = O(10^{-5}) - O(10^{-4})$ $m_L^3\,m_i^{-2}\,s^{-1}$ which are more in line with non-intensified process equipment. The large mismatch between experiments and theory suggests that a fundamentally different mass transfer mechanism is responsible for the observed increase in gas-liquid mass transfer in a rotor-stator spinning disc reactor.

2. Methods

Direct Numerical Simulations for gas-liquid mass transfer studies were performed using the method of Verzicco and Orlandi (1996) [9]. Simulation of turbulent micromixing was performed using an in-house developed C++ code for reaction, convection and diffusion adopting a TVD scheme for convection.

3. Results and discussion

The vorticity of the flow field was found to be focussed in the thin liquid film between the moving boundaries and the bubble surface. More specifically, due to vortex stretching, the component of vorticity perpendicular to the flow and parallel to the interface were significantly increased as the liquid flow was forced in the narrow film between the bubble and the moving boundary. When the magnitude of the turbulent fluctuations were subsequently taken to be proportional to the turbulent dispersion coefficients in a mass balance over the liquid film, correlations for the gas-liquid mass transfer coefficients could be obtained as a function of the Reynolds number and film thickness. The order of magnitude of the so obtained mass transfer coefficients were in the range $k_{GL} = O(10^{-2})\ m_L^3\ m_i^{-2}\ s^{-1}$, which agrees well with the experimental values.

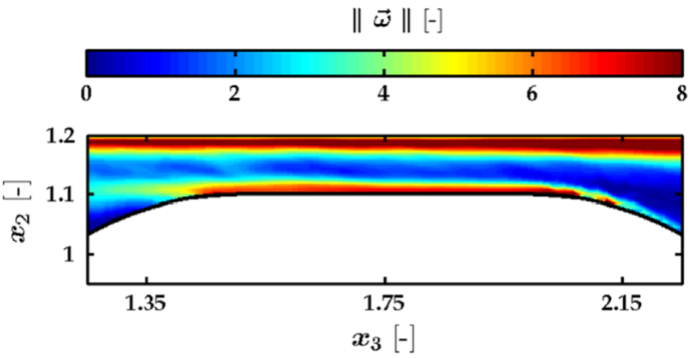

Figure 1. Typical vorticity field in the thin liquid film between a gas bubble and the moving wall [9].

4. Conclusions

Using Direct Numerical Simulation of the Navier-Stokes equation, and the equation of continuity, it was found that vortex stretching in the thin liquid film between a bubble and a moving wall increased vorticity in the film. The turbulence intensity in this film was subsequently taken as a measure to estimate the turbulent dispersion coefficients in a mass balance over the liquid film to come to estimates of the gas-liquid mass transfer coefficient in a rotor-stator spinning disc reactor. Using this approach, the order of magnitude of $k_{GL} = O(10^{-2})\ m_L^3\ m_i^{-2}\ s^{-1}$ was found to be more in line with experimental values than traditional mass transfer theory. The mechanism behind the intensification of gas-liquid mass transfer in a rotor-stator spinning disc reactor thus relies on vortex stretching in the thin liquid film, leading to locally more intense turbulence in this film and thus higher turbulent dispersion.

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Keywords
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