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Analysis of the wall mass transfer on spinning disks using an integral boundary layer method

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AUTHOR-HIGHLIGHTS

- Modeling liquid-to-wall species mass transfer on rotating substrates using IBL method.
- Development of velocity and concentration boundary layers from center.
- Validation against CFD and experimental data for $Sc=1200$.
- IBL model captures local Sherwood number very well in radial inner region.
- Deviations due to the significant effect of waviness on mass transfer in outer region.

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ABSTRACT

Spinning disk devices are widely used for wet surface processing to produce thin liquid films offering very intense heat and mass transfer rates. The present work computationally investigates in particular the liquid-to-wall reactive species mass transfer to describe wet surface etching in the limit of diffusion-controlled fast chemistry at very high Schmidt number ($Sc=1200$). The computations are carried out using a specially adapted Integral Boundary Layer (IBL) method, which accounts explicitly for the development of the velocity and species concentration boundary layers inside the liquid film. The presently used IBL method is proven to capture the radial variation of the wall mass flux and the directly related etching abrasion very well. It particularly provides a reliable description of the momentum and mass transfer in the central region of impingement, which had to be excluded in the most previous IBL based approaches. An Ekman number based criterion is deduced from the validation against CFD results and experiments, which allows to demarcate the outer radial region, where the typically emerging waviness of the liquid surface becomes significant for the wall mass flux. It is shown that the steady-state smooth film predictions of the IBL method generally start to deviate notably from the CFD and experimental data, as the local Ekman number exceeds a certain critical limit.

1. Introduction

The liquid-to-wall mass transfer of thin liquid films, which is radially spreading along rotating substrates driven by the centrifugal forces, is of high relevance in numerous chemical engineering applications. In the semiconductor industry, for example, spinning disk devices are used for the surface preparation of silicon wafers. One important process step in this particular application is the wet-chemical dissolution of the substrate coating using a liquid etchant. Two asymptotic regimes for wet chemical etching can be distinguished based on the Damköhler number

$$Da=\frac{\tau_{diff}}{\tau_{chem}}, \quad (1)$$

which basically relates the time scale of the diffusive mass transport of the etchant into the reactive layer, τ_{diff}, to the time scale of the chemical reaction, τ_{chem}. In the limit of very small Damköhler numbers the etching rate will be mainly controlled by the timescale of the chemical reaction. In the limit of large Damköhler numbers the chemistry is very fast in comparison to the transport of the etchant towards the solid surface, and the etching rate is essentially controlled by the diffusive mass flux of the primary etchant species.

The present work computationally investigates the hydrodynamics and species mass transfer of the thin film flow on spinning disks, with the focus in particular on the modeling of the process

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of wet chemical surface etching in the large Damköhler number regime.

The strong disparity of the two governing length scales, which is related to the disk size and the much smaller film height, greatly challenges any fully resolved numerical simulation of this thin film flow. In addition, when including species mass transfer in a binary mixture, involving a small molecular diffusivity of the primary component, the associated steep concentration gradients further increase the spatial resolution requirements, which lead to excessively high computational costs. The integral boundary layer (IBL) method offers a computationally efficient alternative approach to describe thin film flow including species mass transfer. The present work attempts to explore the potential and limits of the IBL method in providing valuable insight into the salient features of the process of wet chemical surface etching, as well as the underlying flow conditions covering the region of liquid impingement at the center to the outer edge of the disk.

Despite the high relevance for various engineering applications the species mass transfer in thin film flow on spinning disks was considered only in a few theoretical and numerical studies. Kaneko et al. (2007) carried out a direct numerical simulation of the governing Navier–Stokes equations assuming an axisymmetric flow field on an Eulerian mesh using the Volume-of-Fluid (VoF) method to track the evolution of the two-phase flow. They also included species transport in a binary mixture to model the diffusion controlled process of wet chemical etching of silicon wafers. Their CFD study was complemented by experiments, and the numerical predictions were found to be in good agreement with the experimentally observed etching rates.

Many concepts proposed for the mathematical modeling of film flow on rotating disks are restricted to large radii, where an asymptotic solution for the flow field can be obtained, and the influence of the inertial and Coriolis forces is negligible (Rauscher et al., 1973). Peev et al. (2005) applied a method, known as method of Leveque (see, e.g., Bird et al., 1960), to compute the radial variation of the solid–liquid mass transfer coefficient. This method, which was also utilized by Burns and Jachuck (2005), is basically devised for the high Schmidt-number regime, where the profile of the radial velocity inside the very thin concentration boundary layer can be assumed as approximately linear. The resulting simplified convection–diffusion equation for the species mass fraction can then be solved analytically in terms of Gamma functions. A comparison of this analytical solution against the experimental results of Peev et al. (2005) and Burns and Jachuck (2005) showed satisfactory agreement for the first, but considerable deviations for the latter. Rahman and Faghri (1993) presented a steady-state analytical solution for the gas absorption at the gas–liquid interface and the solid dissolution at the disk surface. In their approach the radial convection velocity is prescribed using the semi-parabolic profile, which represents the exact analytical far-field solution for the steady-state smooth-film on rotating disks. Their analytically obtained solutions in terms of confluent hypergeometric functions provided a very plausible description of the concentration field, predicting a radial decrease of the Sherwood number as the thickness of the concentration boundary layer increases. The limits of this analytical approach, which are due to the assumption of a far-field solution for the radial profile, were unveiled in a comparison against a fully three-dimensional numerical simulation, obtained for a pie-shaped slice of the disk as computational domain. Accordingly, a good agreement between the numerical results and the analytical solution was found in the radially outer region, while notable deviations were seen in the radially inner region, as inertial effects, which are neglected in the far-field solution, dominate. As such this analytical approach is basically unable to predict the local minimum in the Sherwood number associated with the local maximum in the film thickness near the center, as it is observed in the numerical results.

The basic idea of the integral boundary layer (IBL) approximation consists in the reduction of the dimensionality of the problem applying a depth-averaging over the film thickness to the governing set of equations. This method has already been successfully used to analyze the fluid dynamics of thin film flow on spinning disks in various previous studies (see, e.g., Kim and Kim, 2009; Sisoev et al., 2003). Matar et al. (2005) included a convection–diffusion equation for the concentration of a gas phase, which is absorbed at the liquid surface. They obtained results for a wide range of flow conditions and their predictions for the averaged Sherwood number were compared against the experimental data of Aoune and Ramshaw (1999) showing good agreement.

The present work essentially attempts to extend the scope of these previous studies by including the wall mass transfer and diffusion-controlled surface etching chemistry into the IBL formulation considering in particular the regime of large Schmidt numbers. The operating liquid is assumed as a binary mixture of a primary etchant component diluted into a chemically inert carrier component. As such, the present study also intends to provide essential input for the modeling of surface etching processes on rotating disks in the limit of large Damköhler numbers.

2. Mathematical modeling

2.1. Governing equations

The problem is considered as axisymmetric and steady. It is mathematically described using a non-dimensionalized formulation with the characteristic scaling quantities introduced by Rauscher et al. (1973). Their scaling analysis starts from the definition of a radial velocity scale at a given radial distance $\tilde{r}$ associated with a film height $\tilde{\delta}$

$$u_0 = \frac{Q}{2\pi\tilde{r}\tilde{\delta}}. \tag{2}$$

In the asymptotic limit of large radii the radial momentum balance is essentially governed by the centrifugal and viscous forces, such that

$$\mathcal{O}(\Omega^2\tilde{r}) \sim \mathcal{O}\left(\nu\frac{Q/2\pi\tilde{r}\tilde{\delta}}{\tilde{\delta}^2}\right) \tag{3}$$

Describing the negligible small effect of the inertial forces in terms of a small Rossby number

$$Ro = \frac{u_0}{\tilde{r}\Omega} = \left(\frac{Q^2}{4\pi\nu\Omega\tilde{r}^4}\right)^{1/3} \ll 1 \tag{4}$$

leads to the definition of a radial length scale

$$l_0 = \left(\frac{9Q^2}{4\pi^2\nu\Omega}\right)^{1/4}, \tag{5}$$

such that Eq. (4) is satisfied at large radii $\tilde{r}/l_0 \gg 1$. Introducing l_0 into the momentum balance (3) gives

$$\delta_0 \sim \left(\frac{\nu}{\Omega}\right)^{1/2}\left(\frac{l_0}{\tilde{r}}\right)^{2/3}, \tag{6}$$

from which the definition of the vertical length scale

$$\delta_0 = \left(\frac{\nu}{\Omega}\right)^{1/2} \tag{7}$$

is obtained. Expression (3) can be also rewritten as product of the local Ekman and Rossby numbers, i.e.

$$\underbrace{\left(\frac{\nu}{\Omega\tilde{\delta}^2}\right)}_{Ek}\underbrace{\left(\frac{\tilde{u}}{\tilde{r}\Omega}\right)}_{Ro} \sim \mathcal{O}(1). \tag{8}$$