



Direct Numerical Simulation of interfacial mass transfer into falling films



Christoph Albert^b, Holger Marschall^a, Dieter Bothe^{a,*}

^a Mathematical Modeling and Analysis, Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-Str. 10, 64287 Darmstadt, Germany

^b DFG International Research Training Group 1529, Mathematical Fluid Dynamics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany

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ABSTRACT

This contribution is concerned with interfacial mass transfer into falling films, for which detailed insight is achieved by means of Direct Numerical Simulation employing the Volume-of-Fluid method. As for the numerical model for mass transfer across the fluid interface of falling films, we employ the two-scalar approach.

We examine the influence of wave regimes and flow patterns on local Sherwood numbers and identify distinct mass transfer enhancement mechanisms taking effect in specific wave regimes.

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1. Introduction

Both in Process and Chemical Engineering, heat and mass transfer apparatus are in widespread use in which a continuous liquid phase is processed as a continuous thin film falling down flat or structured walls due to gravity. Henceforth we shall refer to such configurations as falling films. Falling films are used in a variety of industrial applications where large rates of heat or mass transfer are desired. Examples are cooling devices [23], gas absorbers [9,43], desalination units [29,45] and falling film microreactors [21,41].

In these falling film apparatus, interfacial waves are known to play a central role for heat and mass transfer enhancement and, hence, process intensification. It has been shown experimentally that the presence of surface waves has an intensifying effect on the observed heat transfer rates from the wall into the film [15], and that the wave effect is even larger for the transport of a chemical species from the gas into the liquid [3]. The observed transfer rates of a chemical species into the liquid depend to a large extent on the flow structure inside the nonlinear waves. The flow structure, in turn, depends on the wavelength of the perturbation from which it develops. As a consequence of these non-trivial interdependencies, detailed experimental studies providing insights into the local sub-processes are not available. Moreover, most numerical simulations are based on simplified model assumptions, the effect of which for a correct prediction of the complex interplay

between hydrodynamics and interfacial mass transfer into falling films would require research in itself.

The first numerical simulations of mass transfer into falling films were performed by Wasden and Dukler [39]. They used experimentally measured film thicknesses to compute the local flow fields, and solved a stationary species transport equation for a single wave. Boundary conditions in streamwise direction for the species concentration were computed by a solution of the concentration profile for a flat film. They found that the presence of surface waves results in velocity components normal to the interface, which in turn bring forth mass transfer enhancement. More recent simulations have been performed in [36,30], where the hydrodynamics was not modeled by the full Navier–Stokes equations, but by a simpler model derived by Shkadov [35], where the velocity profile is considered semi-parabolic at each streamwise direction. Both contributions look for an excitation frequency of the film that leads to a wave regime which is optimal in terms of achievable mass transfer rates. In [36], it is found that for low Reynolds numbers (Re), the variation of mass transfer rates exhibits two local maxima, whereas three peaks are found for higher Re. In [30], on the other hand, three peaks are found for low Reynolds numbers, and only two peaks are found for higher Re. In contrast to that, the experimental results in [44] show a single peak for low Reynolds numbers, and two for high Re.

In [4], the hydrodynamics of the falling film was captured by Direct Numerical Simulation (DNS), while the species concentration was solved for stationary conditions, employing the method of Wasden and Dukler [39]. They find that recirculation in the large waves causes a decrease in absorption rates, whereas the

* Corresponding author. Address: Petersenstr. 17, 64287 Darmstadt, Germany. Tel.: +49 6151 16 5363; fax: +49 6151 16 72022.

E-mail address: bothe@csi.tu-darmstadt.de (D. Bothe).

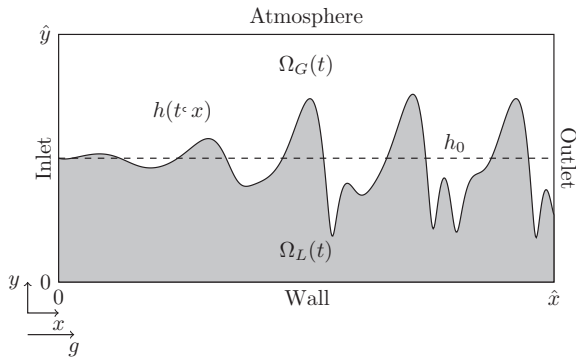


Fig. 1. Computational domain with wavy falling film.

absorption rates increase in the capillary wave region. Here, the effect of the choice of artificial boundary conditions is unclear.

Mass transfer simulations into falling films were also performed in [40]. The transient species transport equation was solved over the whole length of the film. They introduced a hydrodynamic parameter (the gradient of the vertical fluctuating velocity at the interface), and find that this parameter can be used to characterize species transfer across the gas–liquid interface. Unfortunately, the range of investigated hydrodynamic parameters was quite small, and local mass transfer rates were only provided for a single simulation.

In [20], a coupled heat/mass transfer problem is solved by a finite difference method. Results in the capillary wave regime are compared to results with a smooth film, and it is found that recirculation in the large waves results in enhanced transfer rates compared to the flat film.

The present contribution is concerned with the complex interplay of hydrodynamics and interfacial mass transfer into falling films. Since falling films exhibit a transient hydrodynamic nature and complex interfacial structures, their detailed experimental examination is difficult. Hence, we utilize DNS based on the Volume-of-Fluid (VOF) method along with the two-scalar approach of Bothe and Fleckenstein [5] in order to study the interdependency of hydrodynamics of wavy laminar films and mass transfer taking place across the deforming fluid interface. The simple scenario of a falling film on a flat vertical wall shall serve as a prototype case for mass transfer across the interface within (laminar) wavy film regimes. The arising non-trivial flow structures and species concentration patterns are studied, and the pertinent mass transfer enhancement mechanisms are identified. In particular, we examine the influence of wave regimes and flow patterns on local Sherwood numbers.

The remainder of this work is organized as follows: in Section 2 the governing equations for both hydrodynamics and interfacial mass transfer into falling films are presented. More precisely, we detail on the sharp interface model for hydrodynamics and interfacial mass transfer. Section 3 briefly describes the employed numerical methods. Section 4 sets forth the computational setup adopted both for validation (Section 5) and results (Section 6). Results are thoroughly discussed in Section 6. Finally, we provide conclusions regarding the obtained results in Section 7.

2. Sharp-Interface model

We consider a continuous thin film of a viscous fluid falling down a vertical flat wall due to gravity. Moreover, we account for the absorption of a weakly soluble gas into the liquid phase. This allows us to neglect any feedback of species concentration

on the hydrodynamics. For this case, the overall resistance to interfacial mass transfer is considered to be inside the liquid film.

The Squire Theorem [38], which states that the critical Reynolds number for two dimensional perturbations of parallel flow between fixed walls is lower than the critical Reynolds number for three dimensional perturbations, was extended to the case of falling liquid films in [42]. At the same time, it is known from experiments that the primary instability of the falling film is two-dimensional, see for example [26]. Therefore, we here consider the two-dimensional case only. This also allows for a sufficiently high spatial resolution, which is of significant importance for performing true DNS.

Let $\Omega = (0, \hat{x}) \times (0, \hat{y})$ be the domain occupied by both phases (cf. Fig. 1). The x -axis is aligned with the wall and points in streamwise direction, while the y -axis points in cross-streamwise direction, away from the wall. It is assumed that the position of the interface, separating gas and liquid, is given by a height function $h(t, x)$ over the x -axis. With this notation, the interface position is determined as

$$\Sigma(t) = \{(x, y) \in \Omega : y = h(t, x)\}. \quad (1)$$

The domain occupied by the liquid is given by

$$\Omega_L(t) = \{(x, y) \in \Omega : y < h(t, x)\}; \quad (2)$$

the domain occupied by the gas is given by

$$\Omega_G(t) = \{(x, y) \in \Omega : y > h(t, x)\}. \quad (3)$$

2.1. Hydrodynamics

As for the mathematical model, we employ a sharp interface continuum mechanical model, i.e. the two-phase Navier–Stokes equations, assuming a sharp jump of material properties at the interface. The fluid interface is a surface of discontinuity separating both fluid phase regions Ω_L and Ω_G ($\Omega = \Omega_L(t) \cup \Omega_G(t) \cup \Sigma(t)$), for which we consider two incompressible, Newtonian, immiscible fluids under isothermal conditions and without phase change.

The equations for conservation of mass and (linear) momentum in the bulk $\Omega_L \cup \Omega_G$ are

$$\rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{g} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (x, y) \in \Omega, \quad (4)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (x, y) \in \Omega, \quad (5)$$

where $\mathbf{u} = (u, v)$ is the velocity, p the pressure, and \mathbf{g} the gravitational acceleration. The phase dependent material parameters μ and ρ denote the dynamic viscosity and mass density of the fluids.

Table 1

Material parameters and dimensionless groups used for Direct Numerical Simulations.

Parameter	Symbol	Value	Unit
Density liquid	ρ_L	9.98744e–1	g cm ^{–3}
Viscosity liquid	μ_L	1.068e–2	g s ^{–1} cm ^{–1}
Density gas	ρ_G	1.3138e–3	g cm ^{–3}
Viscosity gas	μ_G	2.0274e–4	g s ^{–1} cm ^{–1}
Surface tension	σ	7.3638e1	g s ^{–2}
Gravitational acceleration	g	9.81e2	cm s ^{–2}
Inlet concentration of oxygen, liquid	$c_{ij, in, L}$	2.37e–7	mol cm ^{–3}
Inlet concentration of oxygen, gas	$c_{ij, in, G}$	4.186e–5	mol cm ^{–3}
Henry constant	H	2.70e–2	
Diffusivity of oxygen, gas	D_G	2.0173e–1	cm ² s ^{–1}
Diffusivity of oxygen, liquid, Sc = 15	$D_{L, 15}$	7.1290e–04	cm ² s ^{–1}
Diffusivity of oxygen, liquid, Sc = 30	$D_{L, 30}$	3.5645e–04	cm ² s ^{–1}
Diffusivity of oxygen, liquid, Sc = 50	$D_{L, 50}$	2.1387e–04	cm ² s ^{–1}
Diffusivity of oxygen, liquid, Sc = 100	$D_{L, 100}$	1.0693e–04	cm ² s ^{–1}
Diffusivity of oxygen, liquid, Sc = 200	$D_{L, 200}$	5.3467e–05	cm ² s ^{–1}
Diffusivity of oxygen, liquid, Sc = 400	$D_{L, 400}$	2.6734e–05	cm ² s ^{–1}
Kapitza Number	Ka	3.1497e + 003	

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