Absorption of gas by a falling liquid film

Christoph Albert    Dieter Bothe
Mathematical Modeling and Analysis
Center of Smart Interfaces/
IRTG 1529
Darmstadt University of Technology

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Wavy Falling Films

- Advantages
  - Good heat transfer due to small thickness
  - Large Interface

- Applications
  - Evaporation
  - Cooling
  - Absorption
Hydrodynamic Model

Assumptions

- Incompressible, Newtonian two-phase flow
- No phase transition
- Constant surface tension

\[
\begin{align*}
\partial_t (\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p &= \nabla \cdot S + \rho g, & \Omega \setminus \Sigma \\
\nabla \cdot u &= 0, & \Omega \setminus \Sigma \\
[p I - S] \cdot n_\Sigma &= \sigma \kappa n_\Sigma, & \Sigma \\
[u] &= 0, & \Sigma \\
S &= \eta (\nabla u + (\nabla u)^T)
\end{align*}
\]
The Volume of Fluid Method

One Fluid Formulation:
\[
\partial_t (\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p = \nabla \cdot S + \rho g + \delta f_{\Sigma} \\
\nabla \cdot u = 0 \\
\partial_t f + u \cdot \nabla f = 0
\]

- Density and viscosity depend on volume fraction
- Volume fraction has to be transported
- Additional surface tension force term \( f_{\Sigma} \)
Parasitic Currents

- VOF simulations suffer from unphysical oscillation of velocity, so-called parasitic currents

- Stem from numerical treatment of interfacial jump condition for stress:

\[ \left[ pI - S \right] \cdot n_\Sigma = \sigma \kappa n_\Sigma \]

- Especially serious in stagnant flow situations

- Also problematic in simulations of falling films, which are convection dominated
Numerical Setup

\[ u(t, y)|_{x=0} = (1 + \varepsilon \sin(2\pi \omega t)) \left( \frac{\rho_l}{\mu_L} g \delta_0^2 \left[ \frac{y}{\delta_0} - \frac{1}{2} \left( \frac{y}{\delta_0} \right)^2 \right], 0 \right) \]
Continuum Surface Stress (CSS)

Body Force \[ \nabla \cdot (||\nabla f|| \sigma (I - \hat{n}_\Sigma \otimes \hat{n}_\Sigma)) \],

- Approximate \( \hat{n}_\Sigma \) by differentiating a smoothed \( f \)-field
- Momentum conservative
- Standard Surface Tension model in FS3D; delivers good results in many two-phase flow situations.
Falling Films with CSS

Water/Air, Re 60

- 16 cells per mean film thickness (0.265mm)
- $A = 30\%, f = 20\,\text{Hz}$
Continuum Surface Force (CSF)

Body Force \( \sigma \kappa \nabla f \)

- In the case of a sphere and constant curvature, an exact balance between surface tension and pressure can be achieved: „Balanced Force“
  

- Greatly reduces parasitic currents

- Relies on „good“ curvature information

- Easy for a falling film:
  
  \[
  \kappa = \frac{h_{xx}}{(1 + h_x^2)^{3/2}}
  \]
Falling Films with CSF

Water/Air, Re 60
- 16 cells per mean film thickness (0.265mm)
- A = 30%, f = 20 Hz
Comparison to experiment: Dietze

- Experimental data from G.F. Dietze,
  Flow Separation in Falling Liquid Films, 2010

  - DMSO/Air
  - $\nu = 2.85 \cdot 10^{-6} \frac{m^2}{s}$, $\rho = 1098.3 \frac{kg}{m^3}$, $\sigma = 0.0484 \frac{N}{m}$
  - Re = 8.6
  - f = 16 Hz
  - A = 40%
  - Resolution $\frac{\delta}{16}$
Comparison to experiment: Film thickness

- Film thickness at $x = 56$ mm over a time span of 0.3 s
- CSS overshoots
Species Transport in Falling Films

Data from Yoshimura et.al., 1996

Transport of Oxygen into a water film at 18°C

\[
Sc = \frac{\nu_L}{D} = 570
\]

\[
Sh = \frac{k_L \delta_0}{D}
\]

\[
k_L = \frac{\Gamma}{L} \ln \left( \frac{C_S - C_{in}}{C_S - C_{out}} \right)
\]
Species Transport in Falling Films: Model

Assumptions:

• Dilute system => species bears no mass or momentum, and does not affect viscosity
• No adsorption at the interface => surface tension stays constant
• No chemical reaction
• Local thermodynamic equilibrium at the interface => Henry's law holds
• Constant Henry coefficient

\[ \partial_t c + u \cdot \nabla c = D \Delta c, \quad \Omega^G(t) \cup \Omega^L(t) \]
\[ \left[-D \nabla c \right] \cdot n_\Sigma = 0, \quad \Sigma \]
\[ c_L = H c_G, \quad \Sigma \]
Numerical Approach

Two scalar approach with one-sided concentration gradient transfer flux

- Concentration is advected in the same way as volume fraction
- Two concentrations stored in each interfacial cell
- Both concentrations and Henry's law yield interfacial concentration
- Concentration gradient in liquid phase computed between interface and some value in bulk by subgrid model
- Diffuse flux from gas to liquid according to Fick's Law

\[
\phi^G = c \chi_{\Omega_G} \\
\phi^L = c \chi_{\Omega_L}
\]
Calculations

Water film at 18°C in „Oxygen“ atmosphere

Resolution \( \frac{\delta_0}{16} \)

\( \text{Re} = 31 \)
\( \text{Sc} = 50 \)
\( k_{H,cc} = 0.0270 \)
\( c_G = 4.19 \times 10^{-5} \)
\( c_{L,0} = 2.37 \times 10^{-7} \)
\( D = 2.14 \times 10^{-4} \)
Validation: Method

Solve stationary advection diffusion problem on domain with boundary conditions.

\[ u(y) \partial_x c = D \partial_y^2 c \]
\[ [0, x_{max}] \times [0, \delta_0] \]

\[ c \bigg|_{x=0} = c_{L,0} \]
\[ \partial_y c \bigg|_{y=0} = 0 \]
\[ \partial_x c \bigg|_{x=10cm} = 0 \]
\[ \partial_y c \bigg|_{y=\delta_0} = k_{H,cc} c_G \]

Solved with Matlab ODE Solver, by defining x as pseudotime.
Validation: Result
0 Hz

Planar Interface
Pure Diffusion
• Time-periodic wave structures appear
• Large Wave humps, preceded by several smaller capillary waves
20 Hz

- Filaments of high concentration in the large wave humps
- Develop along the streamlines of the large vortex
- Touch the interface at a hyperbolic point
20Hz

- Highly non-monotonous concentration profiles
20 Hz

- Strong contribution from the capillary wave region
20 Hz

- Flow up the wall in the reference frame of the wall
20 Hz

Pressure in film according to Young-Laplace: $\Delta p \sim \sigma \kappa$

Increase in pressure large enough to drive water up the wall

Compare Dietze et al., J. Fluid Mech., 637, 2009
30 Hz

- Less capillary waves
- Wave length, peak height, and wave velocity decrease
40 Hz

- No capillary waves; waves become sinusoidal
- Wave length, peak height, and wave velocity decrease further
At this Reynolds Number, there exists backflow even when Capillary Waves are absent.
At this Reynolds Number, concentration profiles are monotonous.
Re 15 / 15Hz

Concentration Profiles at different positions

Concentration (mol cm$^{-3}$) vs. y (cm)
Re 15 / 15Hz

- No Vortex relative to wave velocity
Thank you for your attention!