Absorption of gas by a falling liquid film

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Mathematical Modeling and Analysis

Center of Smart Interfaces/

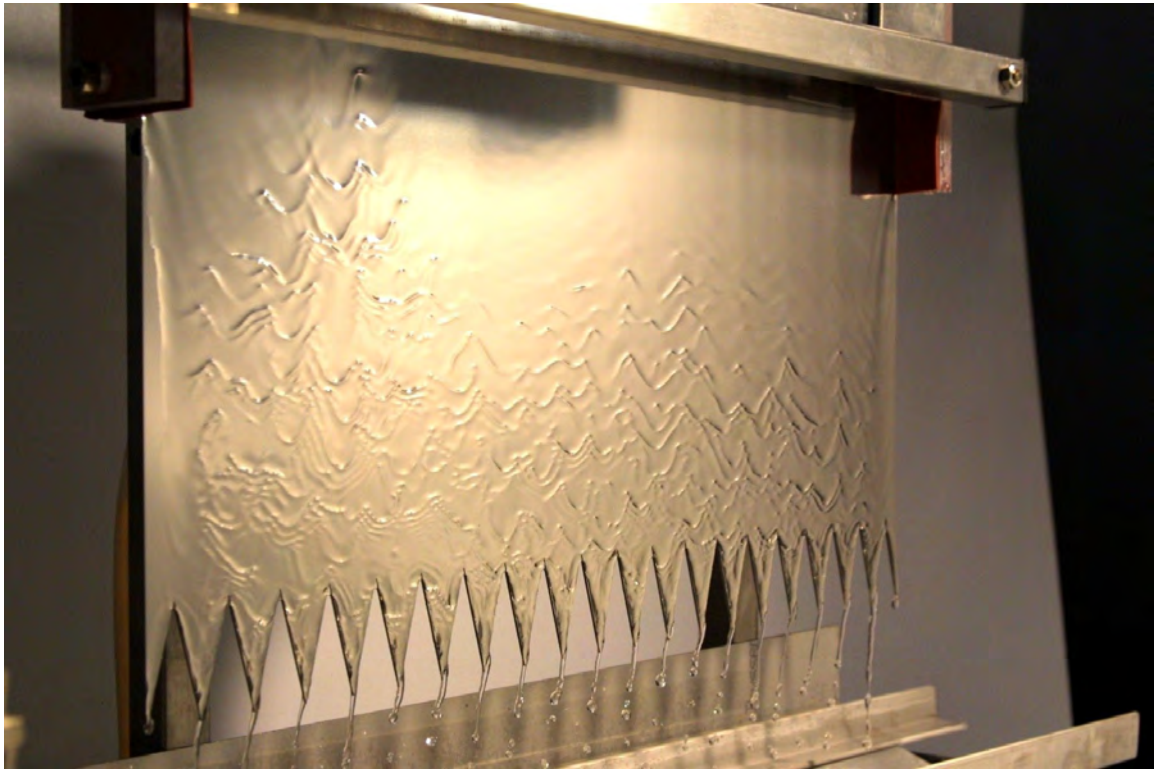
IRTG 1529

Darmstadt University of Technology

4th Japanese-German International Workshop

on Mathematical Fluid Dynamics , 30.11.2011

Wavy Falling Films



- Advantages
  - Good heat transfer due to small thickness
  - Large Interface
- Applications
  - Evaporation
  - Cooling
  - Absorption

Hydrodynamic Model

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Assumptions

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

$$\partial_t(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla p = \nabla \cdot \boldsymbol{S} + \rho \boldsymbol{g}, \qquad \Omega \setminus \Sigma$$

$$\nabla \cdot \boldsymbol{u} = 0, \qquad \Omega \setminus \Sigma$$

$$[\![p \boldsymbol{I} - \boldsymbol{S}]\!] \cdot \boldsymbol{n}_\Sigma = \sigma \kappa \boldsymbol{n}_\Sigma, \qquad \Sigma$$

$$[\![u]\!] = 0, \qquad \Sigma$$

$$\boldsymbol{S} = \eta(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)$$

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The Volume of Fluid Method

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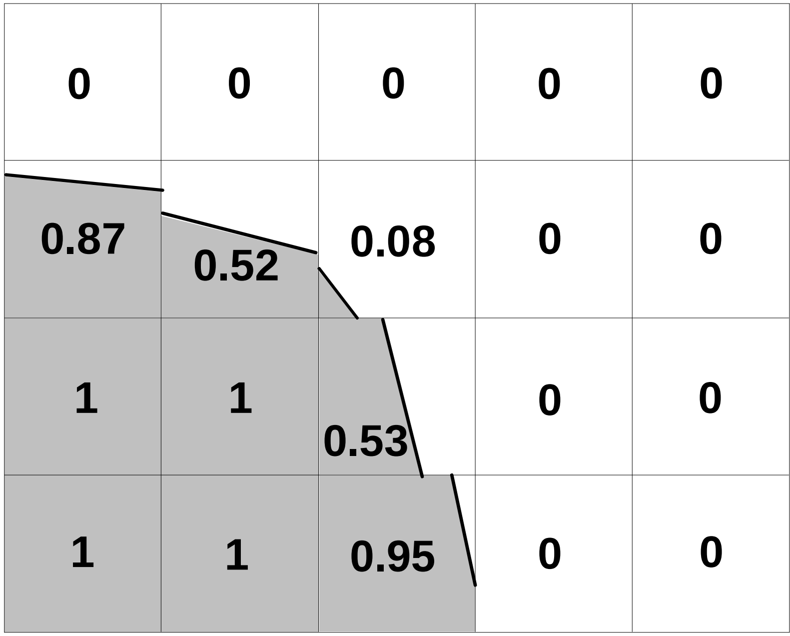
One Fluid Formulation:

$$\partial_t(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla p = \nabla \cdot \boldsymbol{S} + \rho \boldsymbol{g} + \delta \boldsymbol{f}_\Sigma$$

$$\nabla \cdot u = 0$$

$$\partial_t f + \boldsymbol{u} \cdot \nabla f = 0$$

- Density and viscosity depend on volume fraction
- Volume fraction has to be transported
- Additional surface tension force term f_Σ



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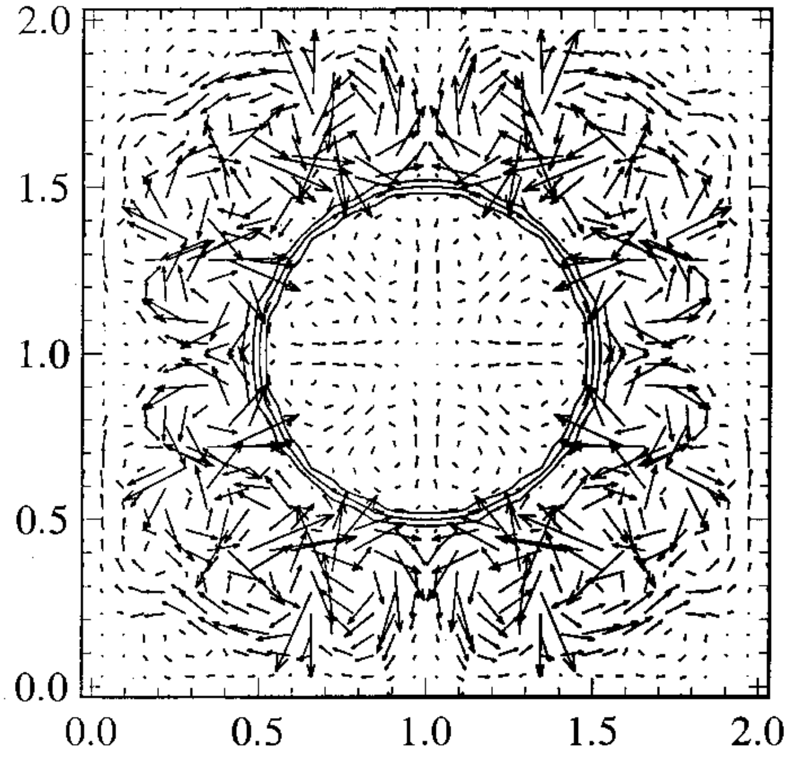
Parasitic Currents



Parasitic Currents in a VOF simulation of a static droplet

- VOF simulations suffer from unphysical oscillation of velocity, so-called parasitic currents
- Stem from numerical treatment of interfacial jump condition for stress:

$$[\![p\boldsymbol{I} - \boldsymbol{S}]\!] \cdot \boldsymbol{n}_\Sigma = \sigma \kappa \boldsymbol{n}_\Sigma$$

- Especially serious in stagnant flow situations
- Also problematic in simulations of falling films, which are convection dominated

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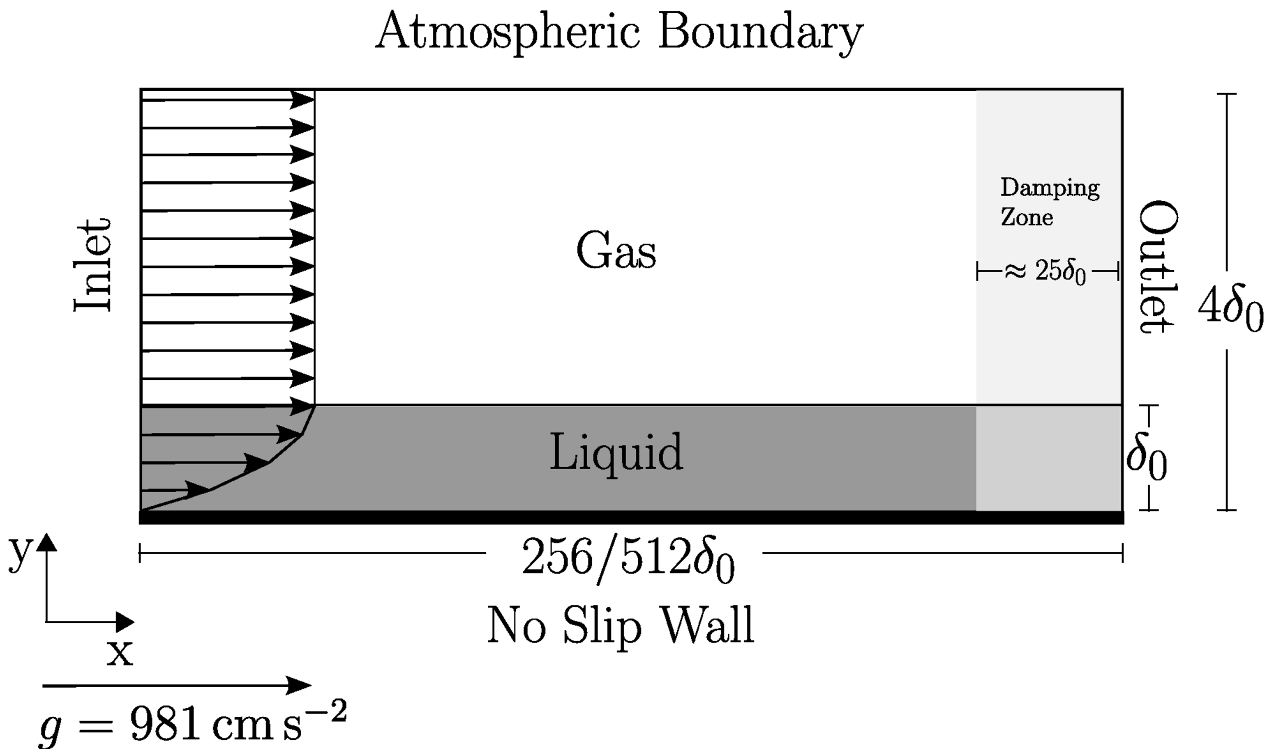
Numerical Setup



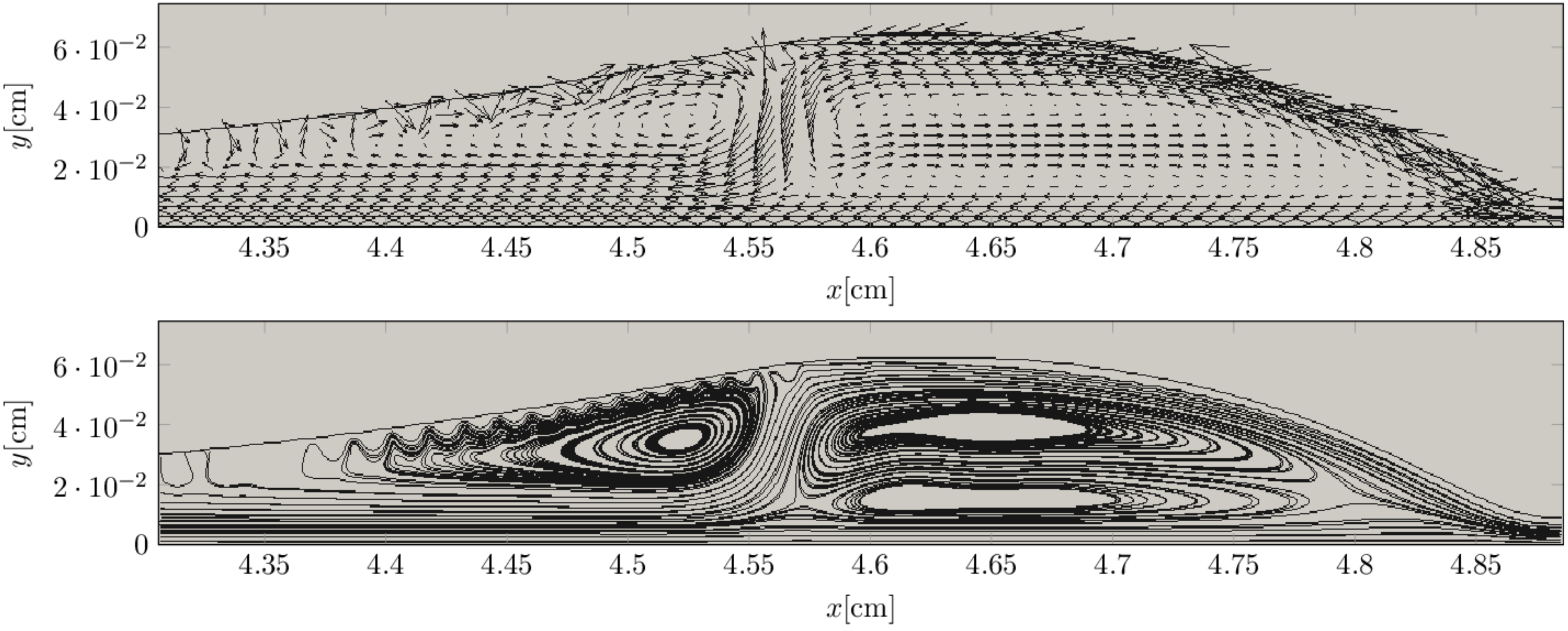
$$\boldsymbol{u}(t,y)\big|_{x=0}=\left(1+\epsilon\sin(2\pi\omega t)\right)\left(\frac{\rho_l}{\mu_L}g\,\delta_0^2\left[\frac{y}{\delta_0}-\frac{1}{2}\left(\frac{y}{\delta_0}\right)^2\right],0\right)$$

Continuum Surface Stress (CSS)

Body Force $\nabla \cdot \left(\|\nabla f\| \sigma \left(I - \vec{\boldsymbol{n}}_\Sigma \otimes \vec{\boldsymbol{n}}_\Sigma \right) \right),$

- Approximate $\vec{\boldsymbol{n}}_\Sigma$ 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 Hz

Continuum Surface Force (CSF)

Body Force $\sigma \kappa \nabla f$

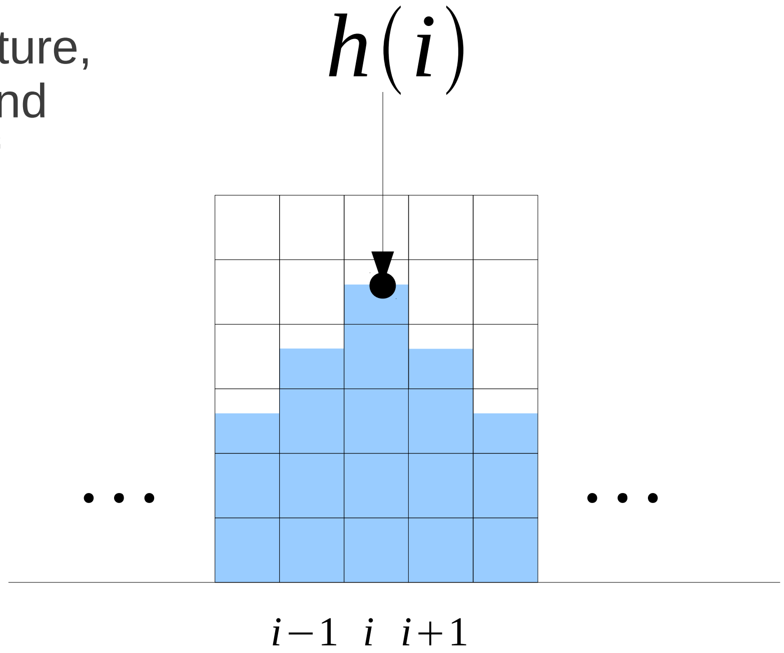
- In the case of a sphere and constant curvature, an exact balance between surface tension and pressure can be achieved: „Balanced Force“

  Renardy, J. Comput. Phys. 183 (2002)

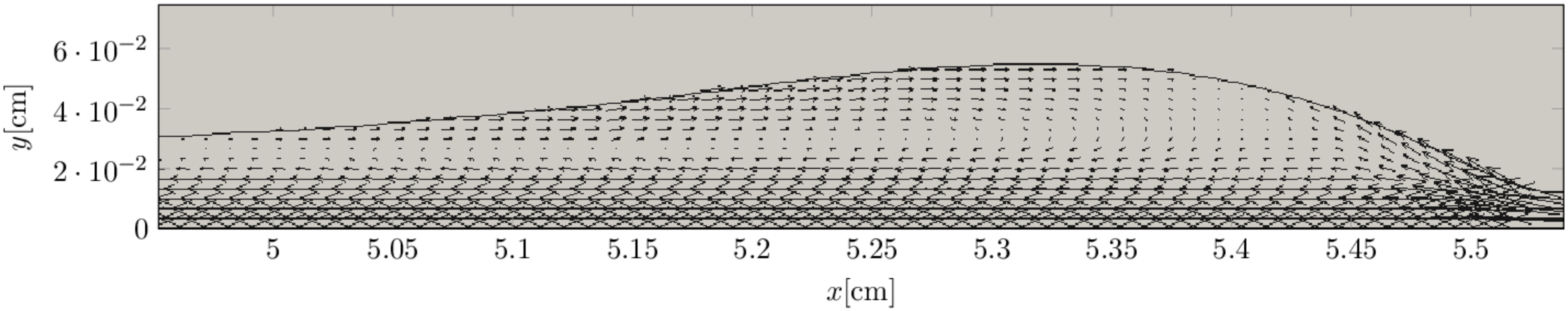
- Greatly reduces parasitic currents

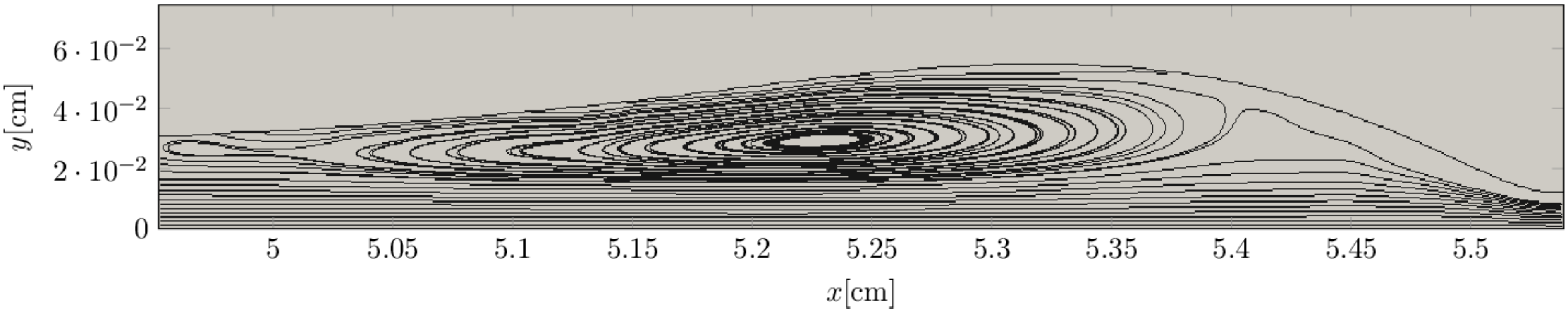
- Relies on „good“ curvature information

- Easy for a falling film: $\kappa = \frac{h_{xx}}{(1+h_x^2)^{\frac{3}{2}}}$



Falling Films with CSF





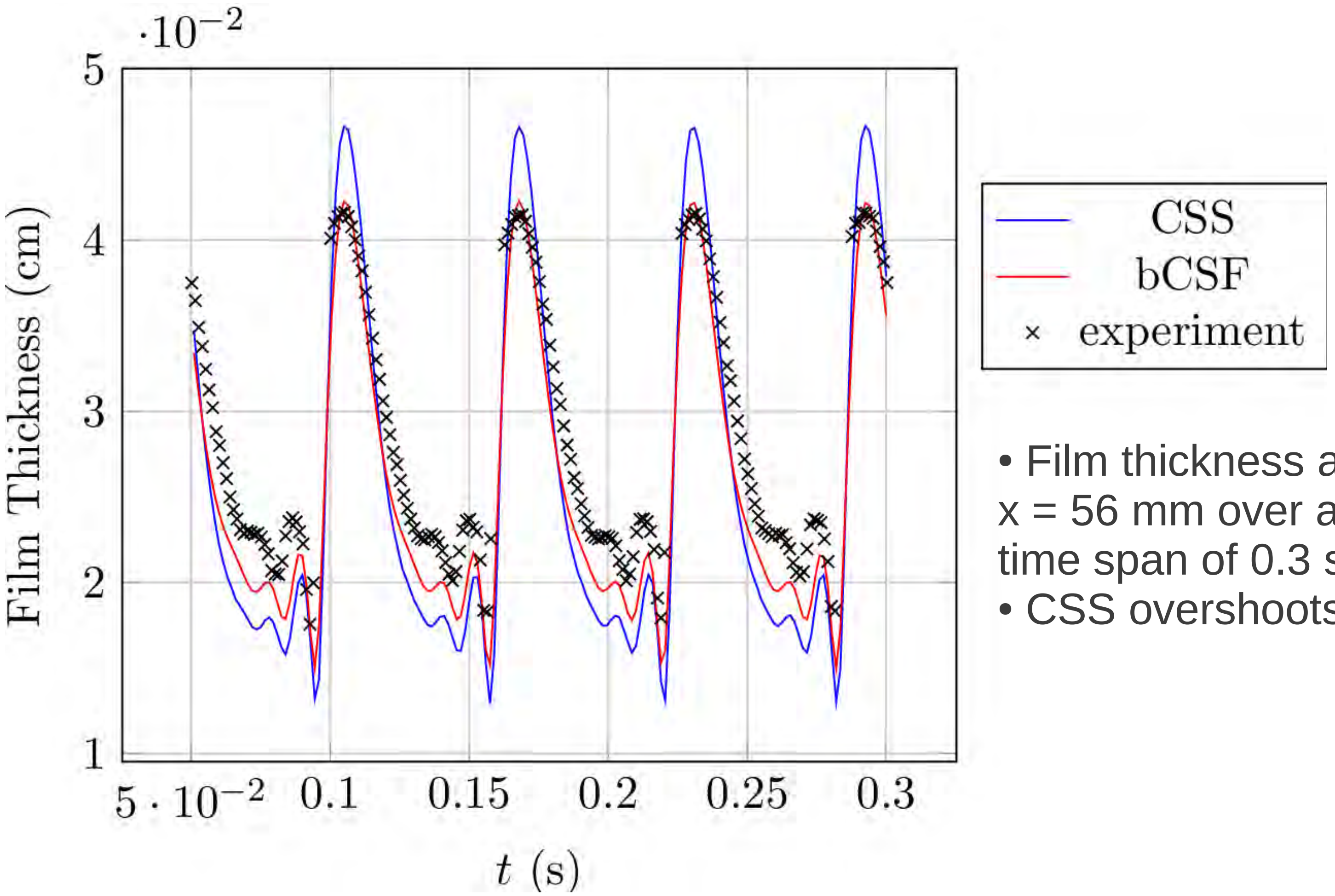
Water/Air, Re 60

- 16 cells per mean film thickness (0.265mm)
- A = 30%, f = 20 Hz

Comparison to experiment: Dietze

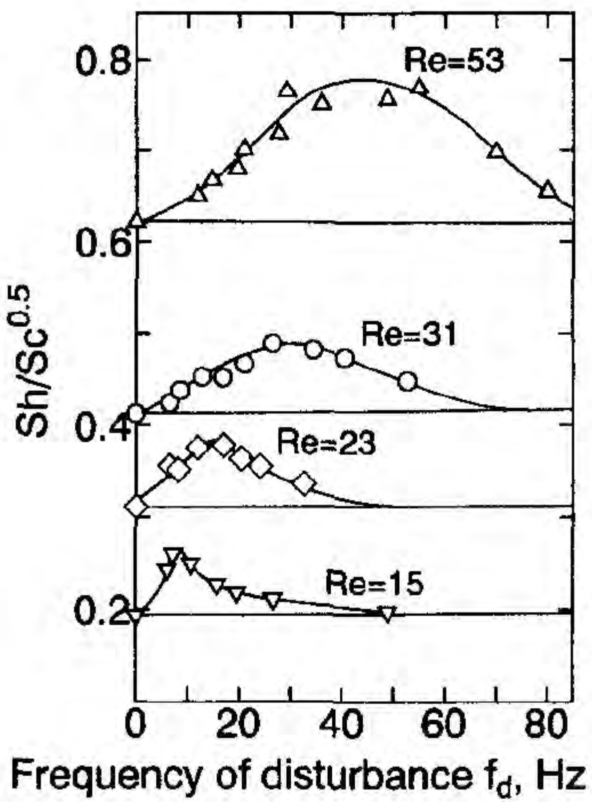
- Experimental data from G.F. Dietze, Flow Separation in Falling Liquid Films, 2010
  - DMSO/Air
  - $\nu = 2.85 \cdot 10^{-6} \frac{m^2}{s}, \rho = 1098.3 \frac{kg}{m^3}, \sigma = 0.0484 \frac{N}{m}$
  - Re = 8.6
  - f = 16 Hz
  - A = 40%
  - Resolution $\frac{\delta}{16}$

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

$$\mathrm{Sc} = \frac{\nu_L}{D} = 570$$

$$\mathrm{Sh} = \frac{k_L \delta_0}{D}$$

$$k_L = \frac{\Gamma}{L} \ln\left(\frac{C_S - C_{\mathrm{in}}}{C_S - C_{\mathrm{out}}}\right)$$

Species Transport in Falling Films: Model

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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

$$\partial_t c + \boldsymbol{u} \cdot \nabla c = D \Delta c, \qquad \Omega^G(t) \cup \Omega^L(t)$$

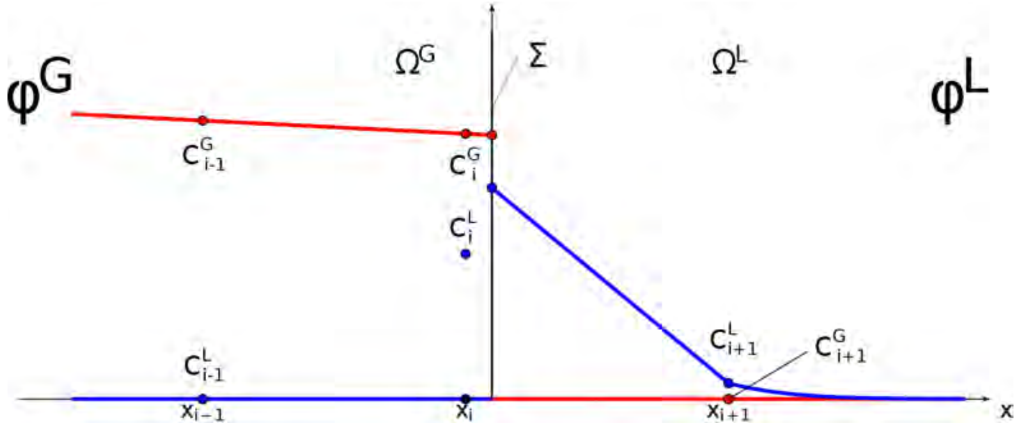
$$[\![-D \nabla c]\!] \cdot \boldsymbol{n}_\Sigma = 0, \qquad \Sigma$$

$$c_L = H c_G, \qquad \Sigma$$

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



$$\phi^G = c\,\chi_{\Omega_G}$$

$$\phi^L = c\,\chi_{\Omega_L}$$

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Calculations

Water film at 18°C in „Oxygen“ atmosphere

Resolution $\frac{\delta_0}{16}$

$\mathrm{Re}=31$

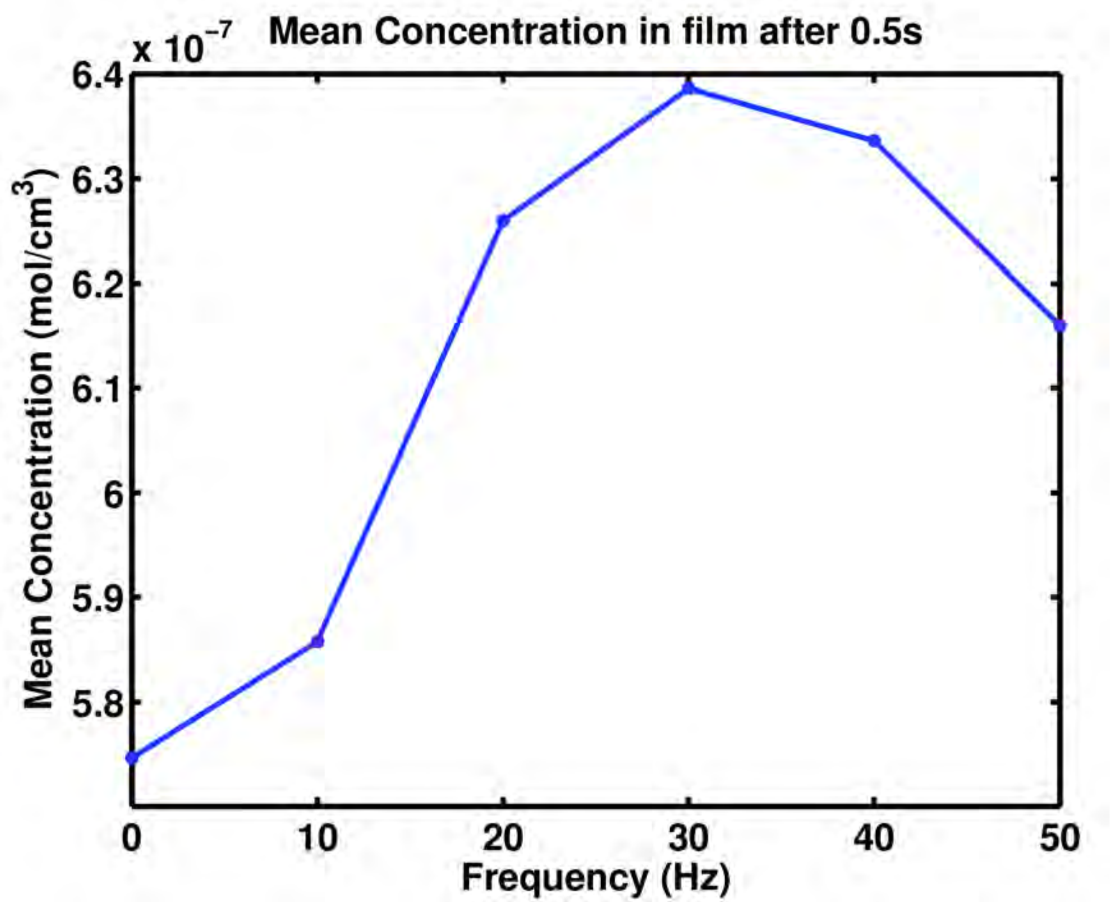
$Sc=50$

$k_{H,cc}=0.0270$

$c_G=4.19\text{e-}5$

$c_{L,0}=2.37\text{e-}7$

$D=2.14\text{e-}4$



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Validation: Method

Solve stationary advection diffusion problem

$$u(y)\partial_x c = D\partial_y^2 c$$

on domain

$$[0, x_{max}]\times[0, \delta_0]$$

with boundary conditions.

$$c|_{x=0} = c_{L,0}$$

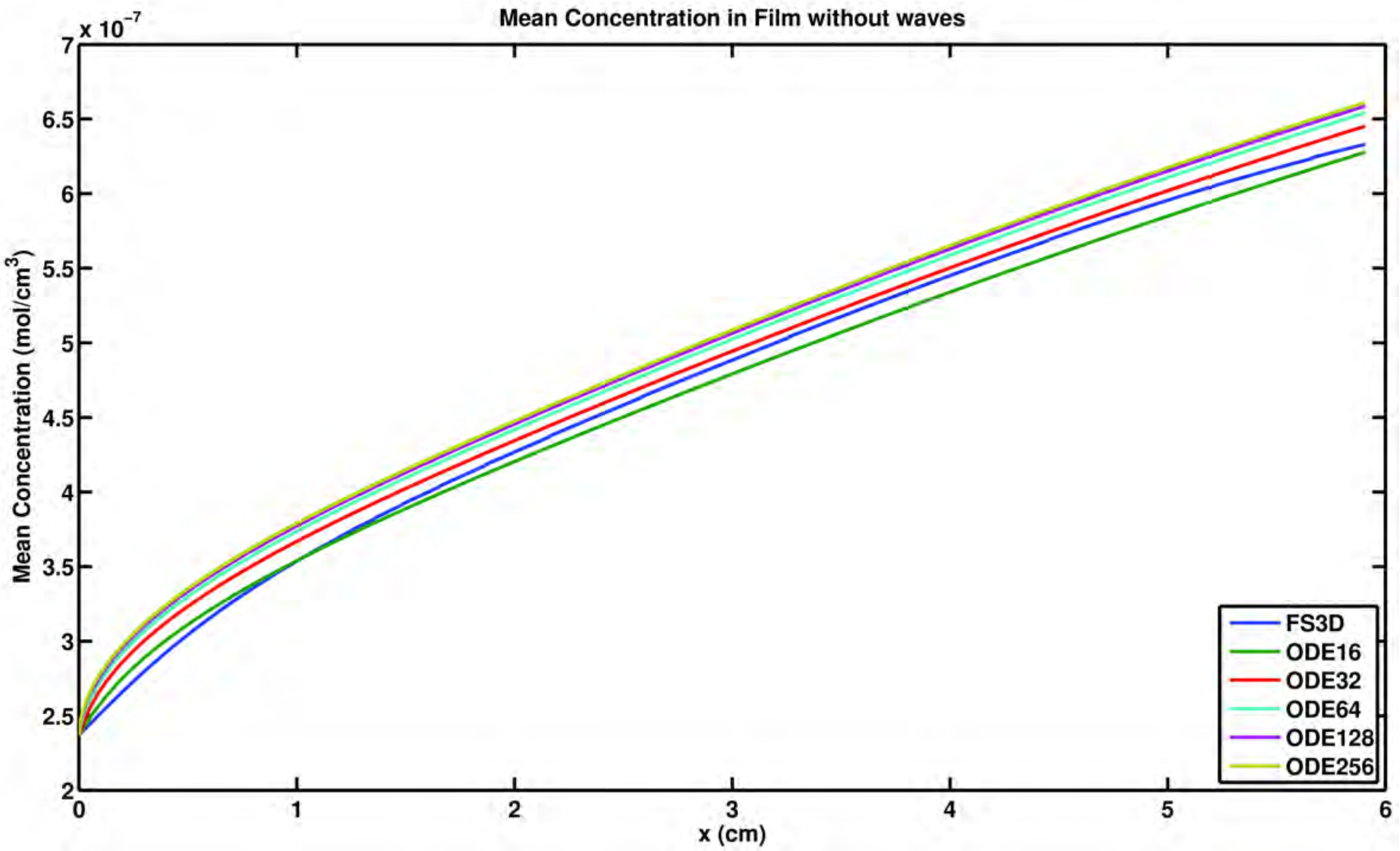
$$\partial_y c|_{y=0} = 0$$

$$\partial_x c|_{x=10\mathrm{cm}} = 0$$

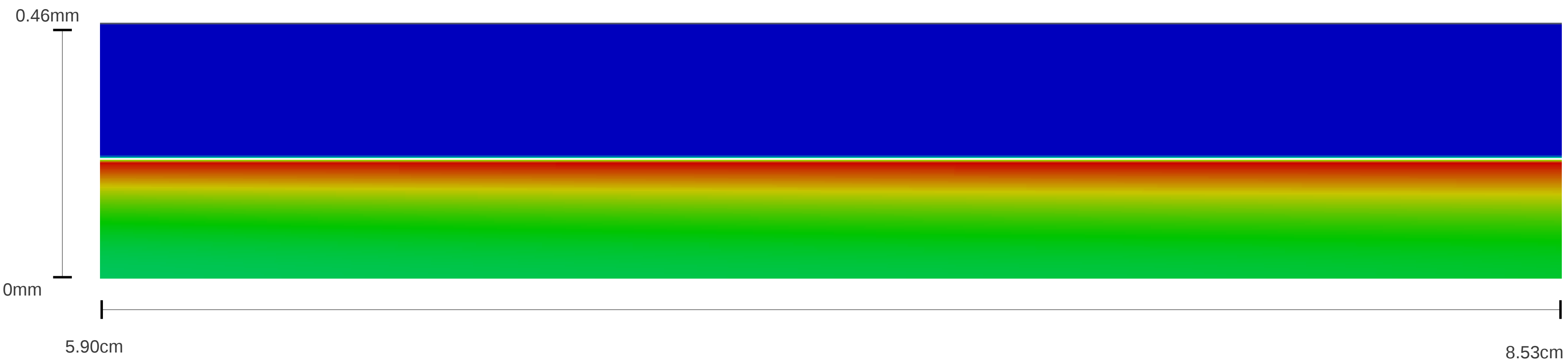
$$\partial_y c|_{y=\delta_0} = k_{H,cc}\, c_G$$

Solved with Matlab ODE Solver, by defining x as pseudotime.

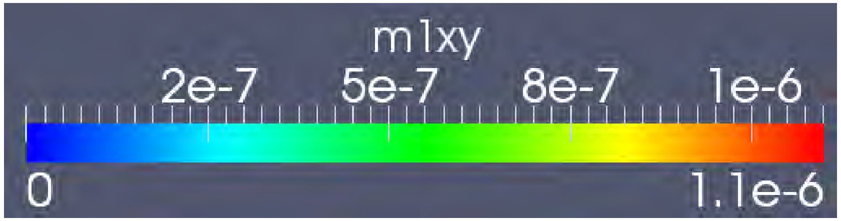
Validation: Result



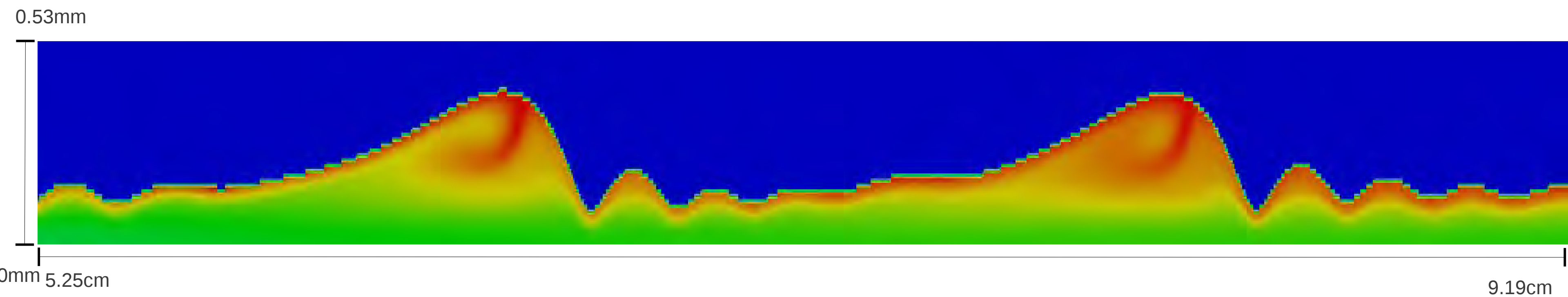
0 Hz



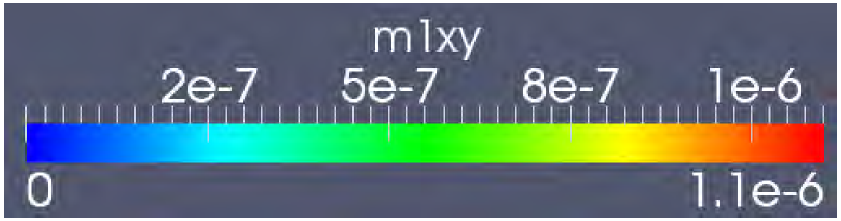
Planar Interface
Pure Diffusion



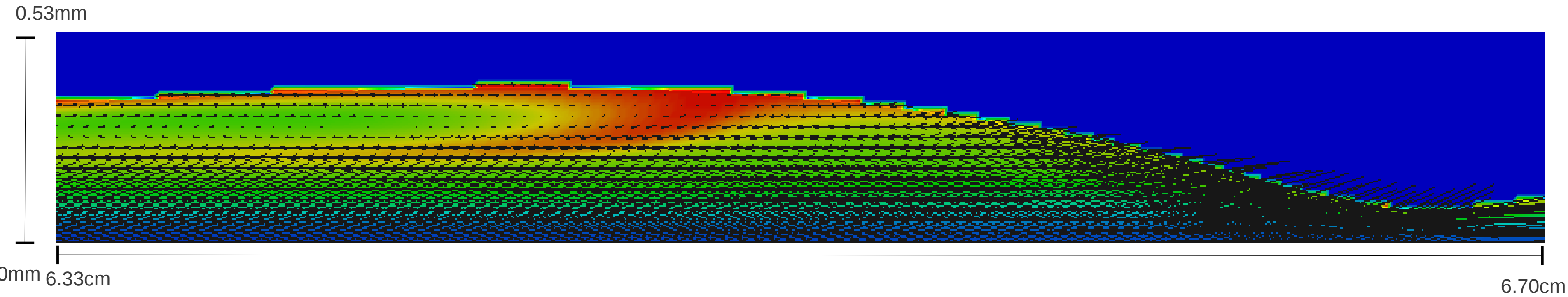
20 Hz



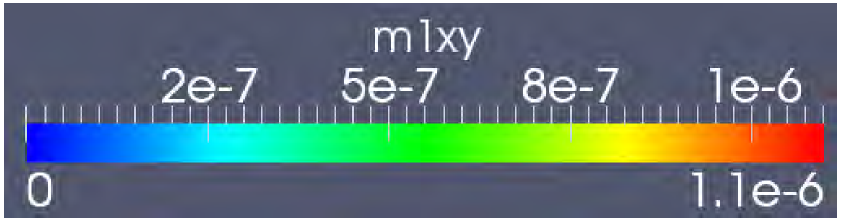
- Time-periodic wave structures appear
- Large Wave humps, preceeded by several smaller capillary waves



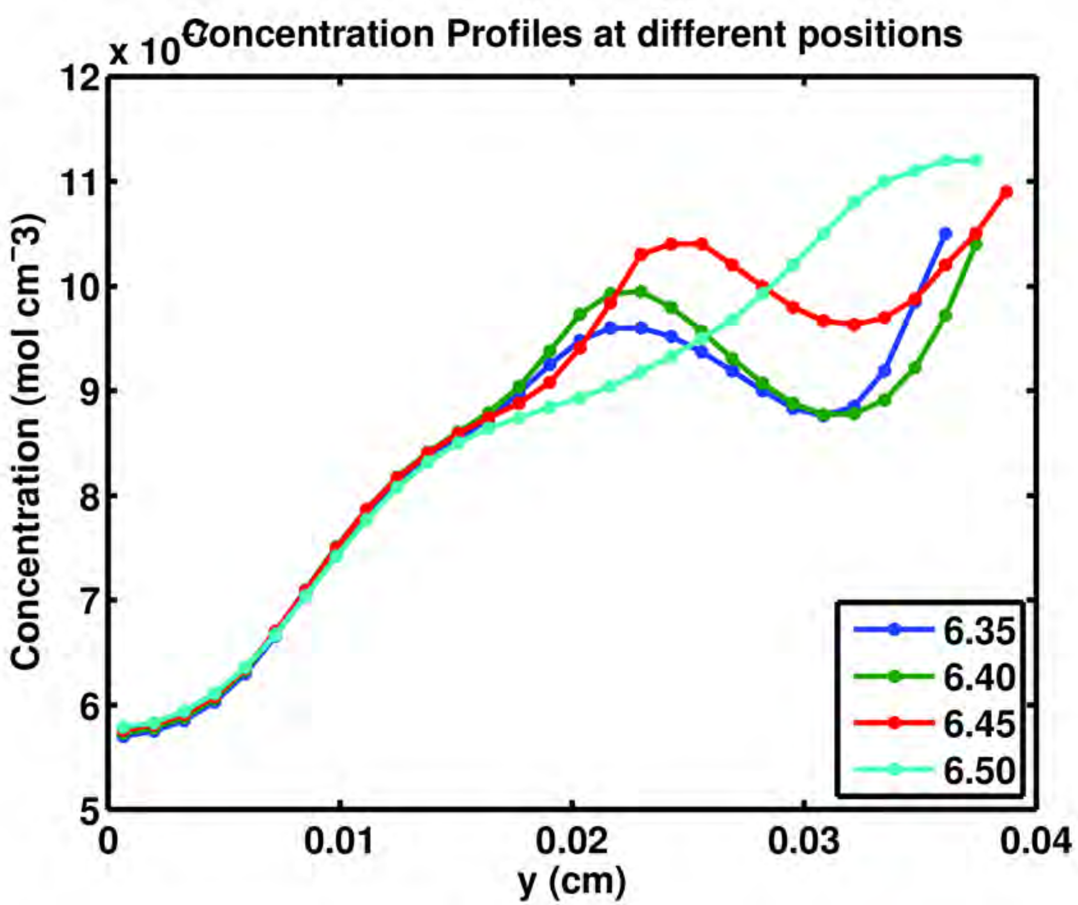
20 Hz



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

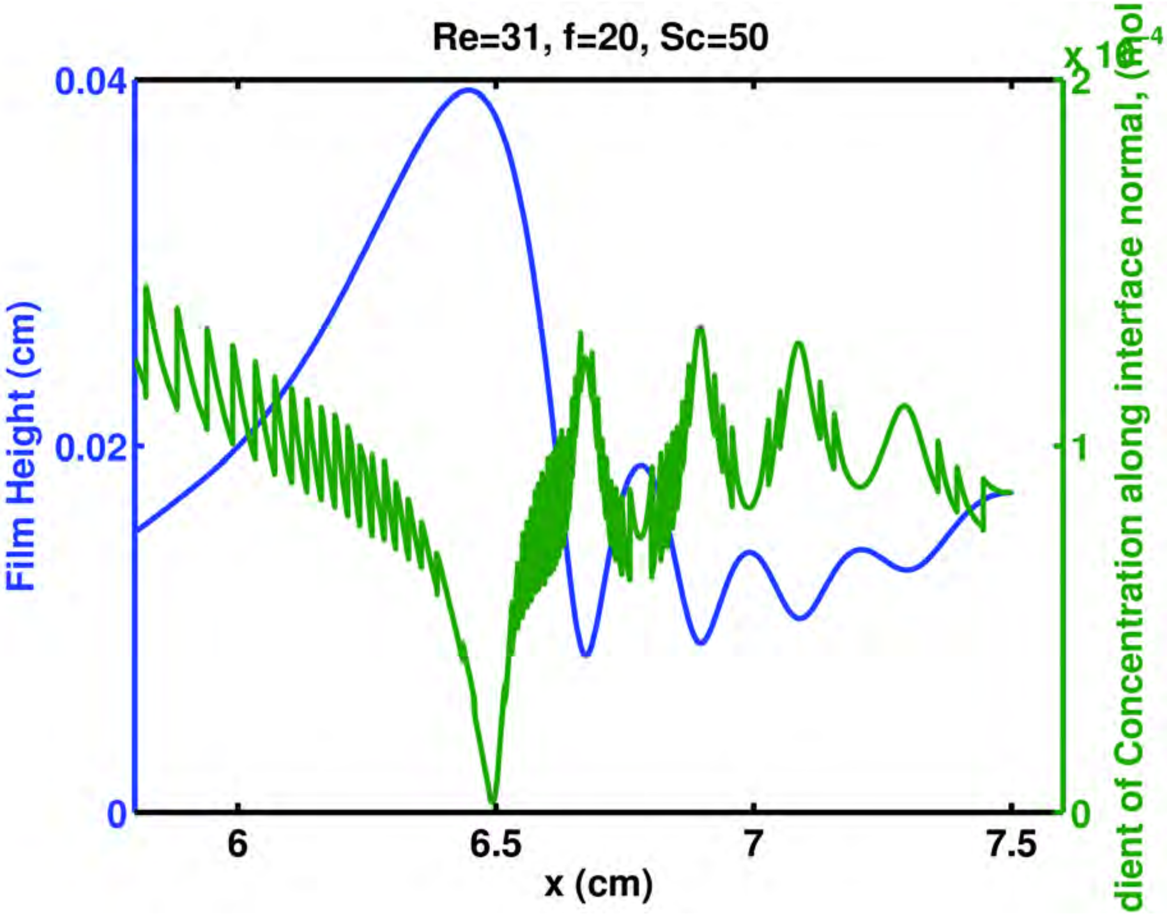


20Hz



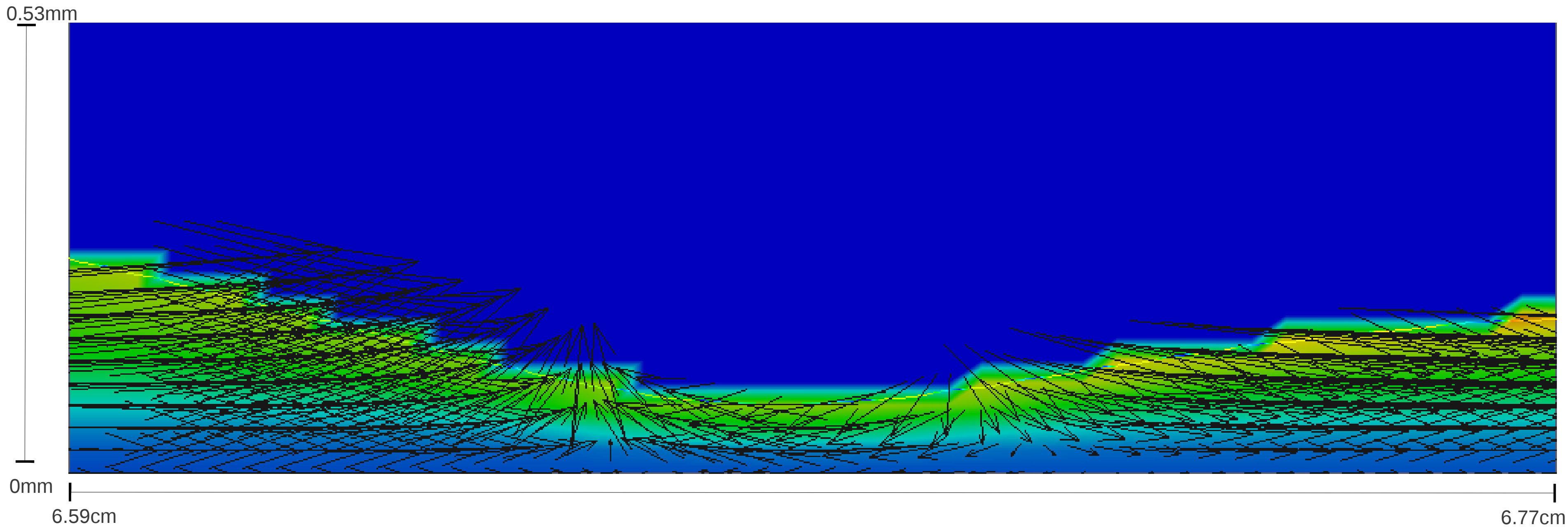
- Highly non-monotonous concentration profiles

20 Hz



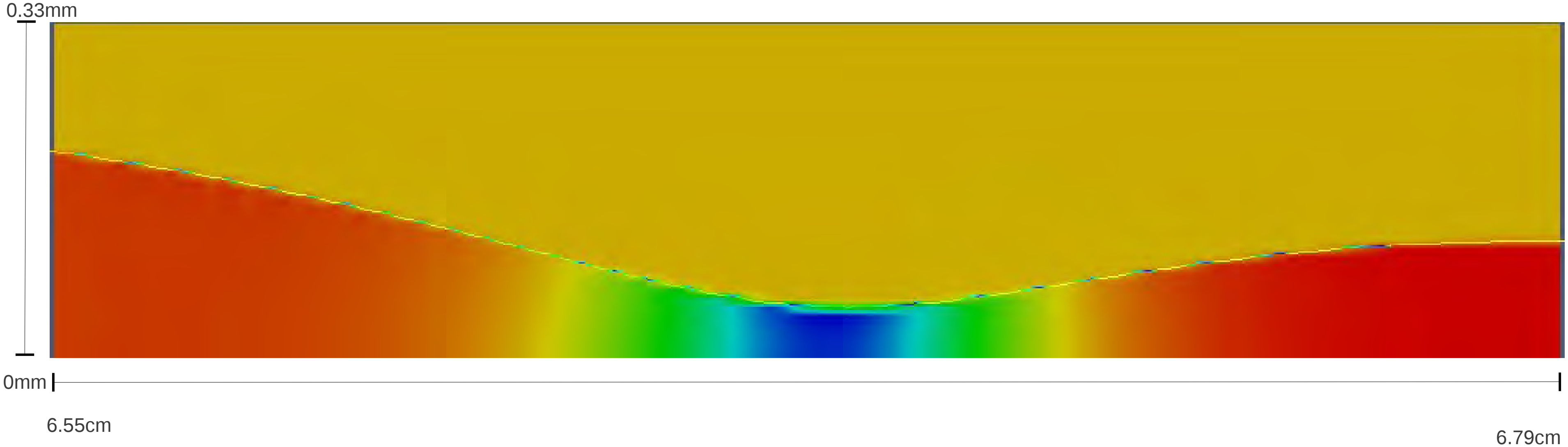
- Strong contribution from the capillary wave region

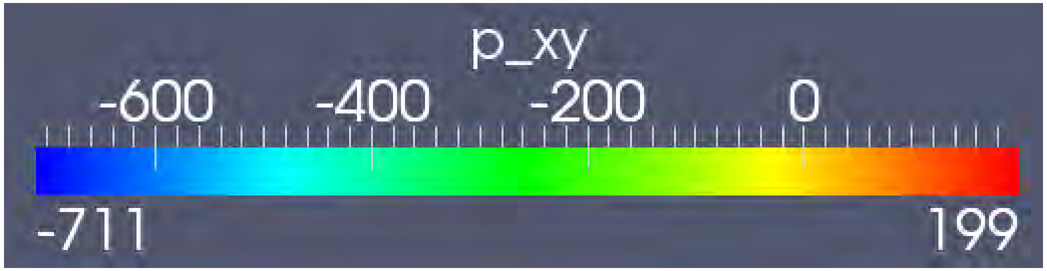
20 Hz



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

20 Hz



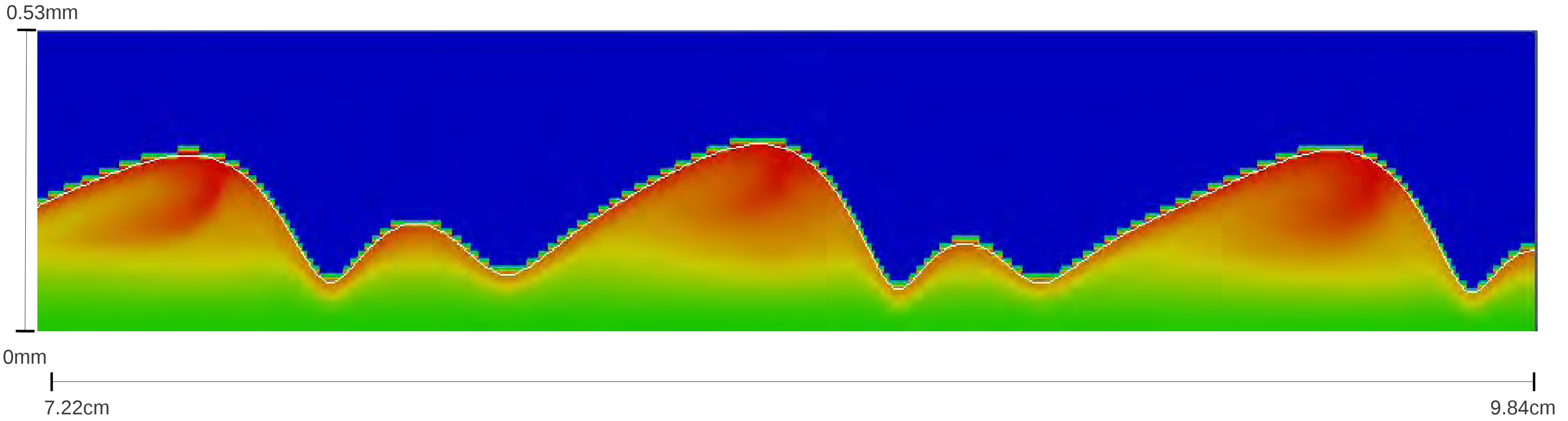


Pressure in film according to Young-Laplace: $\Delta p \sim \sigma \kappa$

Increase in pressure large enough to drive water up the wall

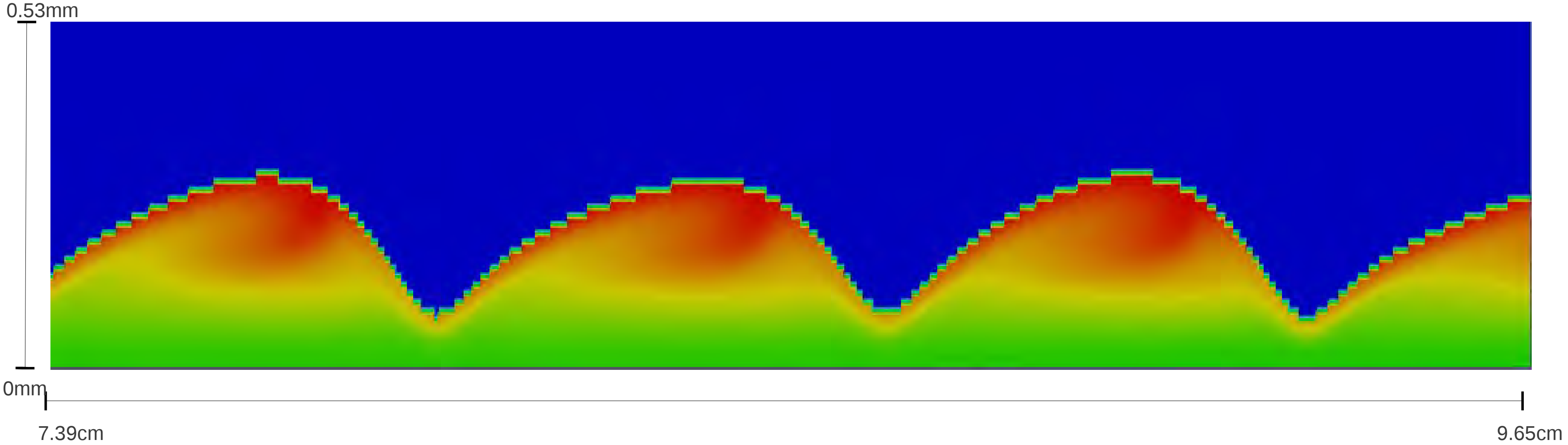
Compare Dietze et al., J. Fluid Mech., 637, 2009

30 Hz



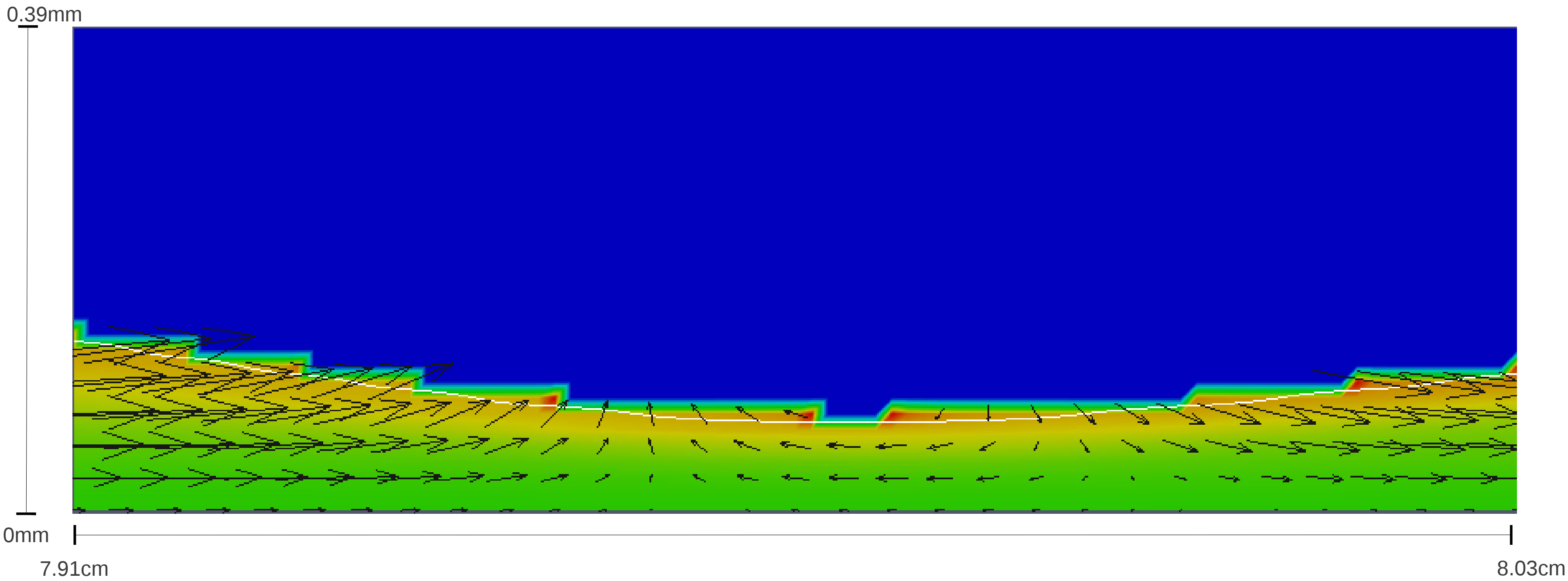
- Less capillary waves
- Wave length, peak height, and wave velocity decrease

40 Hz



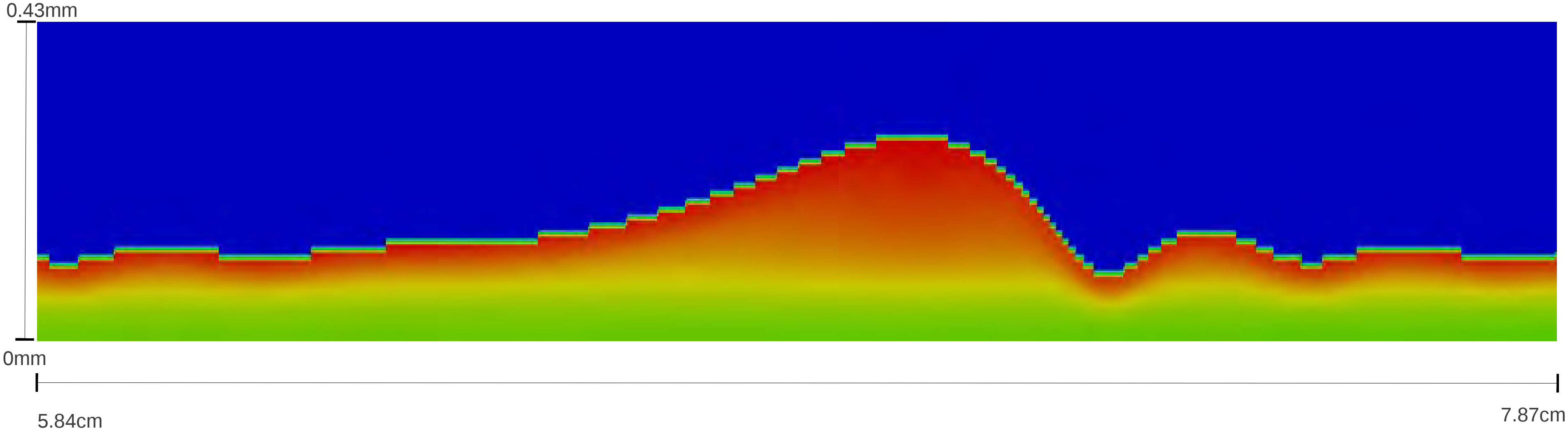
- No capillary waves; waves become sinusoidal
- Wave length, peak height, and wave velocity decrease further

40 Hz



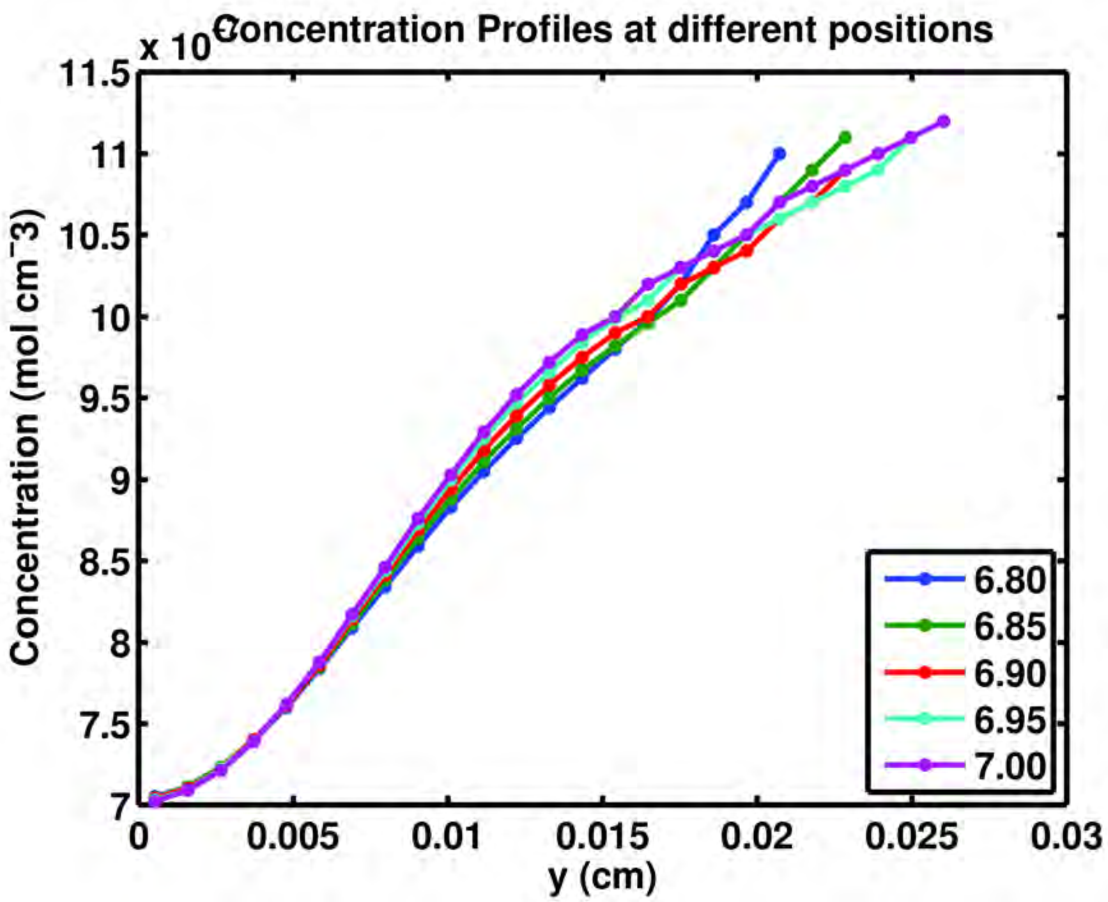
- At this Reynolds Number, there exists backflow even when Capillary Waves are absent

Re 15 / 15Hz



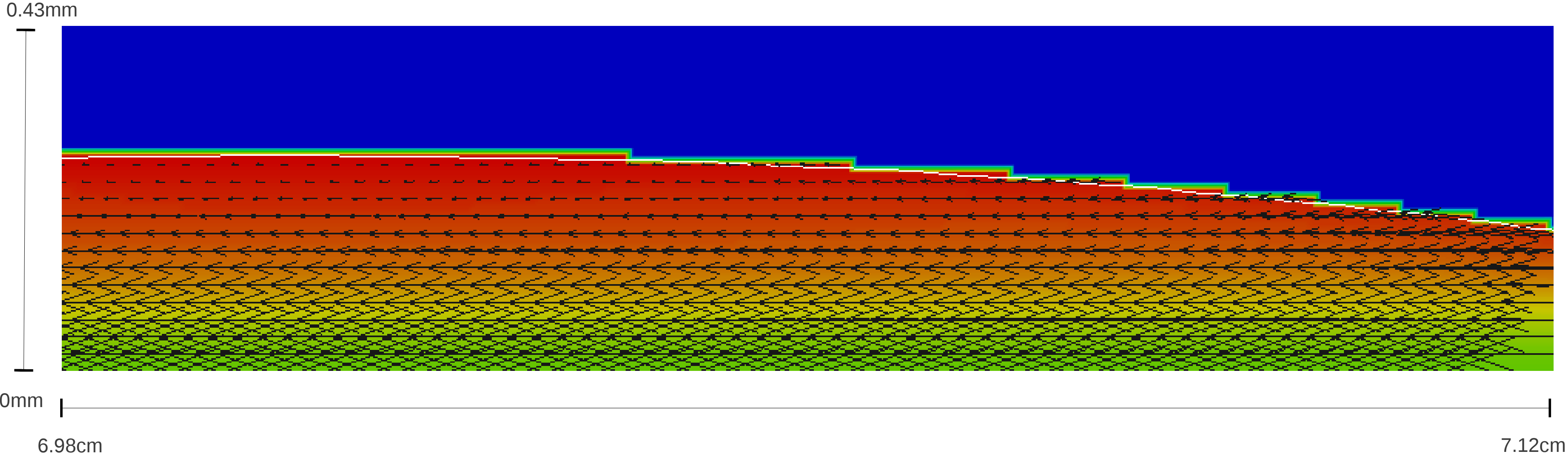
- At this Reynolds Number, concentration profiles are monotonous

Re 15 / 15Hz



Concentration Profiles at different positions
x 10
11.5
11
10.5
10
9.5
9
8.5
8
7.5
7
0
0.005
0.01
0.015
0.02
0.025
0.03
y (cm)
Concentration (mol cm^-3)
6.80
6.85
6.90
6.95
7.00

Re 15 / 15Hz



- No Vortex relative to wave velocity

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Thank you for your attention!

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