Numerical evidence for a novel non-axisymmetric bubble shape regime in square channel Taylor flow

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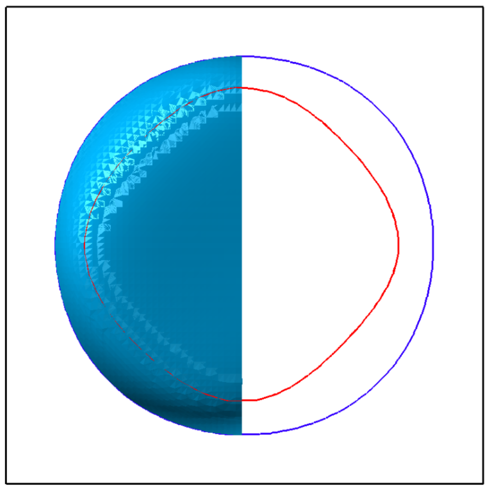
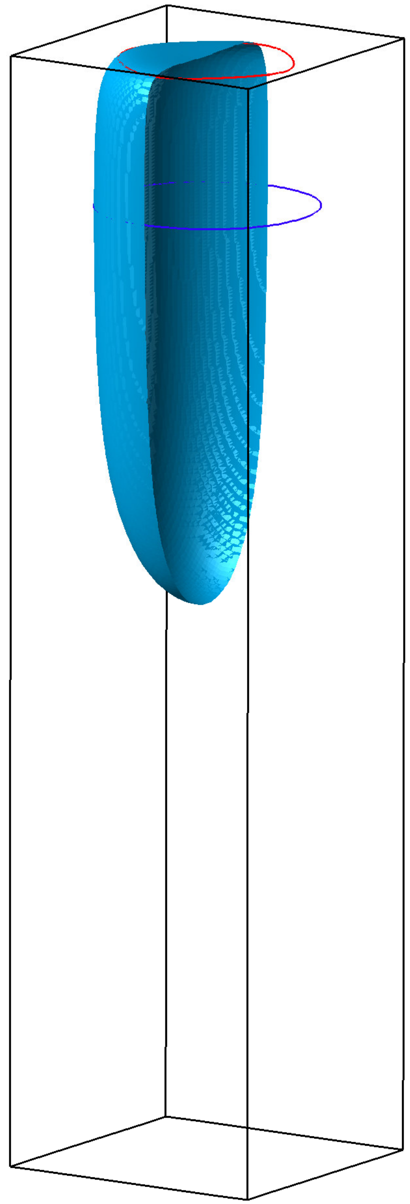




Outline

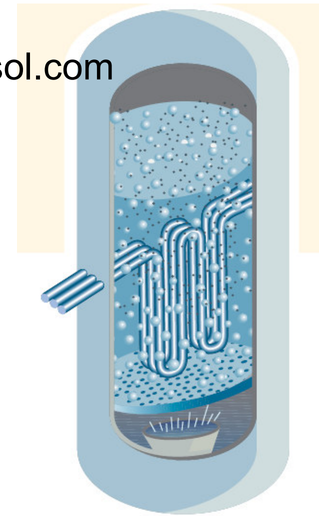
- Background
- Simulation model
  - Numerical method
  - Computational set-up
- Results
  - Bubble shape for different capillary numbers
  - Local interface curvature and pressure field
  - Transition from slug flow to annular flow
- Conclusions

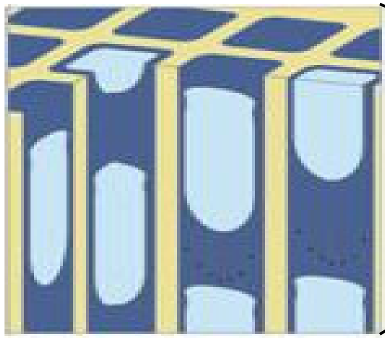
Background

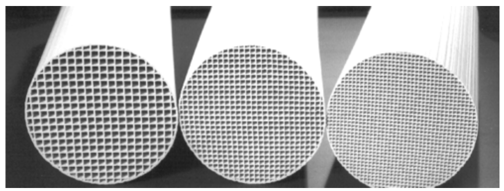
Fischer-Tropsch-Synthesis (conversion of CO & H_2 into liquid fuels)

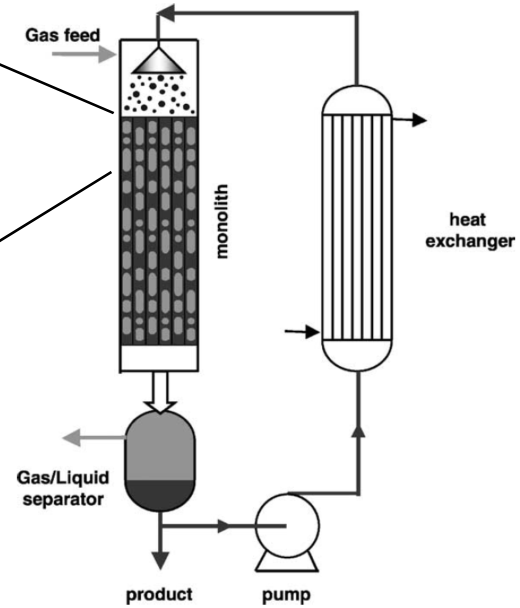
- Sasol Inc: 6 Mio. t fuel per year by bubble column reactors (diam. 12 m)
- Monolith reactors with Taylor flow offer higher yield by similar selectivity
  Güttel et al. Ind. Eng. Chem. Res. 47 (2008) 6589

www.sasol.com









Monolith-Loop-Reaktor
de Deugd et al. Cat. Today 79 (2003) 495

Goal

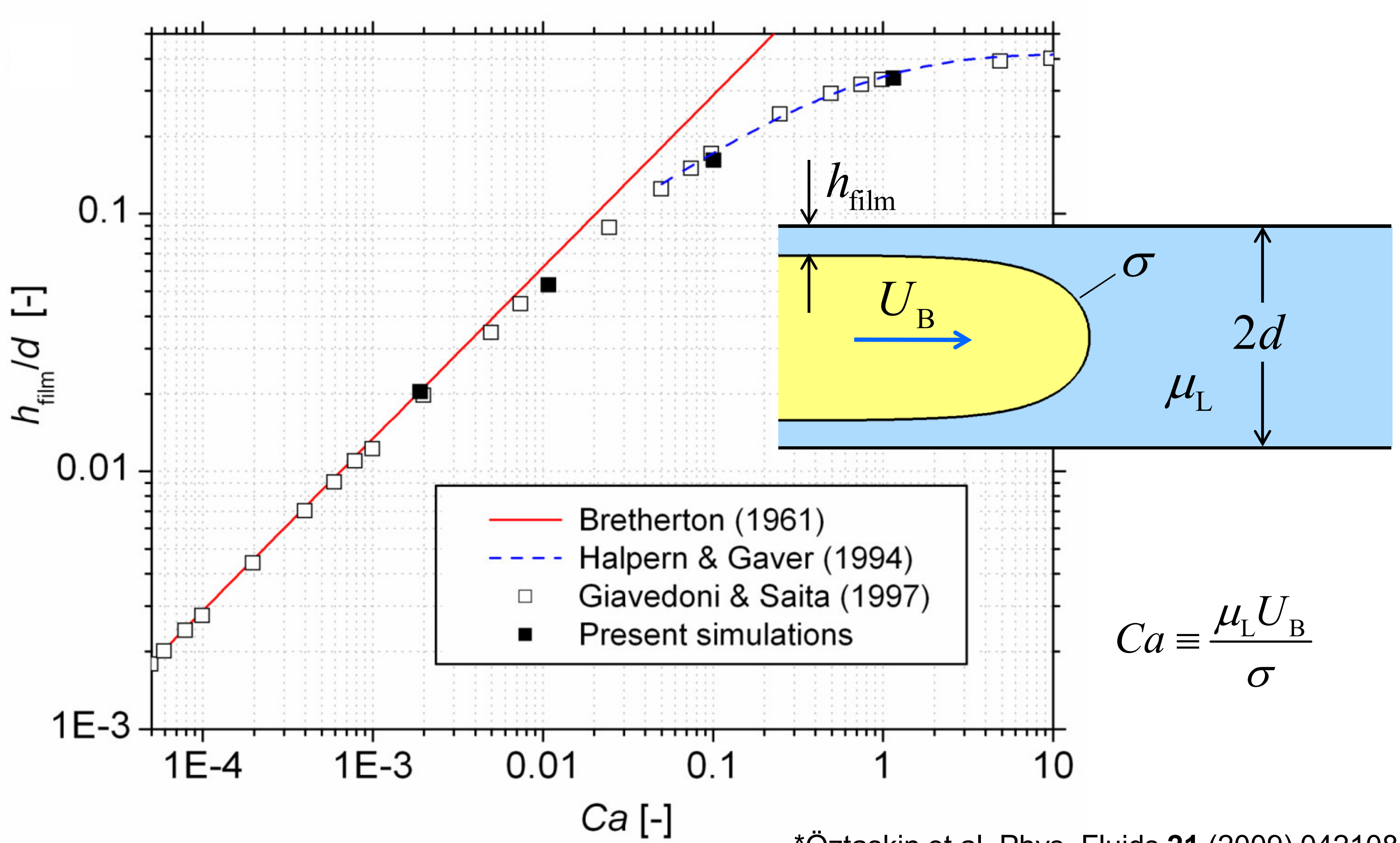
- Investigate hydrodynamics of Taylor flow in a single square mini-channel by detailed numerical simulations

Simulation model

- Governing equations*
  - Navier-Stokes equation in single field formulation with surface tension term for two incompressible immiscible Newtonian fluids with constant physical properties
- Numerical method*
  - Volume-of-fluid method with PLIC reconstruction
  - Finite volume discretization an a staggered 3D Cartesian grid
  - Projection method for pressure-velocity coupling
  - Explicit 3rd order Runge-Kutta time integration scheme
  - In-house computer code TURBIT-VOF

* for details see Öztaskin, Wörner, Soyhan, Phys. Fluids **21** (2009) 042108

Code validation by 2D Bretherton problem*

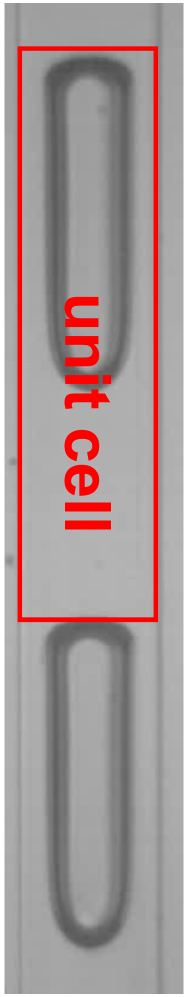


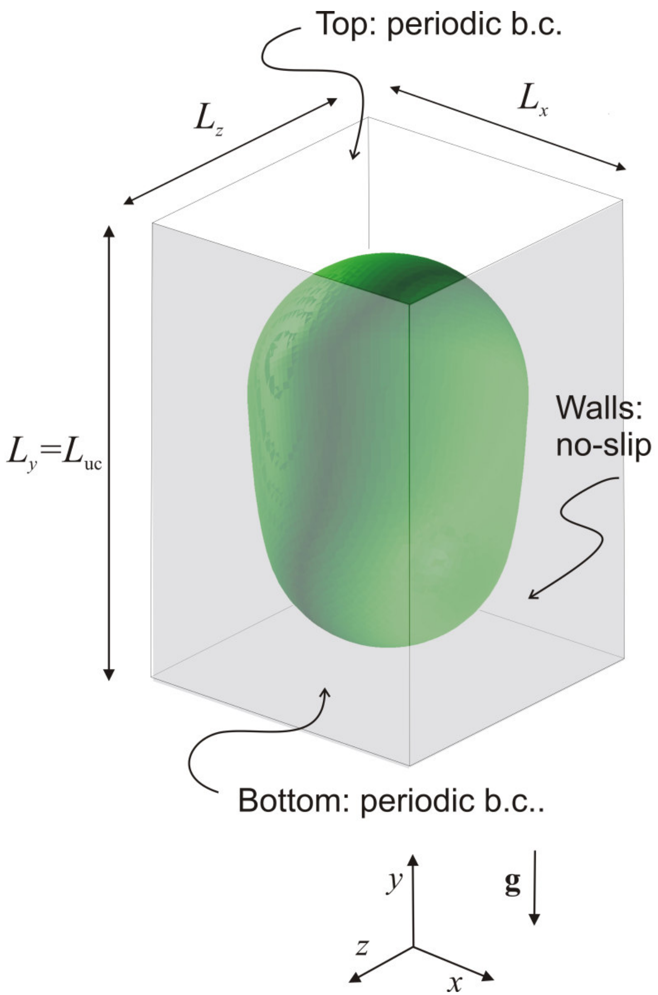
$$Ca \equiv \frac{\mu_L U_B}{\sigma}$$

*Öztaskin et al. Phys. Fluids **21** (2009) 042108

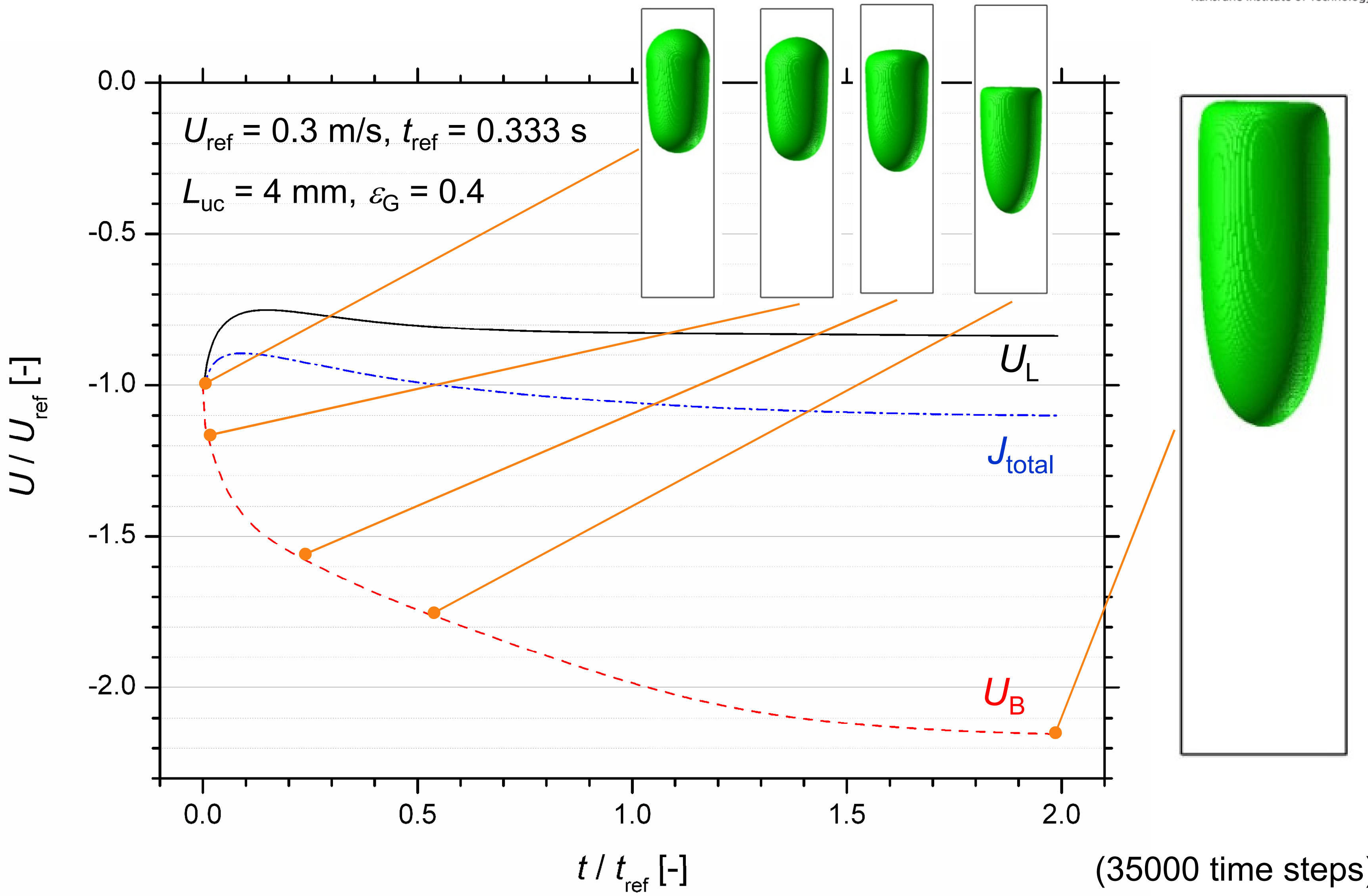
Computational set-up for Taylor flow

- Set-up
  - co-current downward flow of squalane ($C_{30}H_{62}$) and nitrogen
  - consideration of **one unit cell**
  - square channel with internal cross section 1 mm × 1 mm
  - periodic boundary conditions in vertical (axial) direction
- Parameter
  - gas content: ε_G = 0.2 or 0.4
  - unit cell length: L_y = 4 or 6 mm (grid up to 80×480×80 cells)
  - pressure drop across the unit cell is prescribed (but varied for different cases)





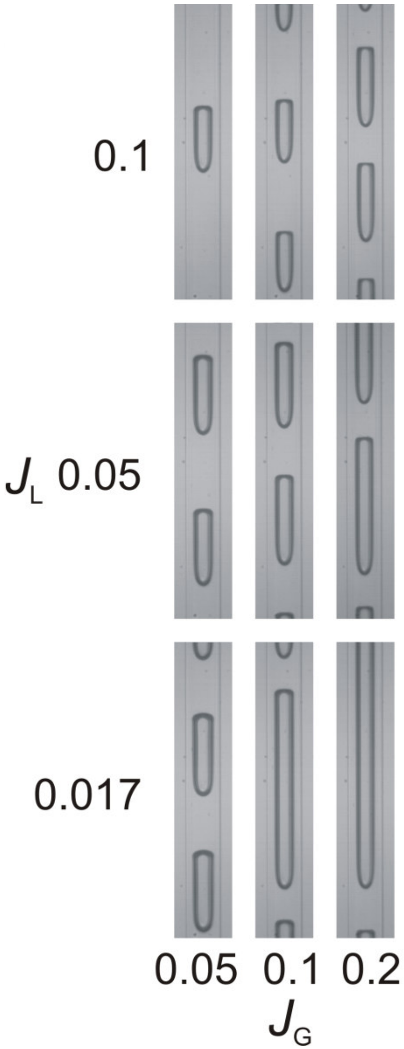
Evolution in time

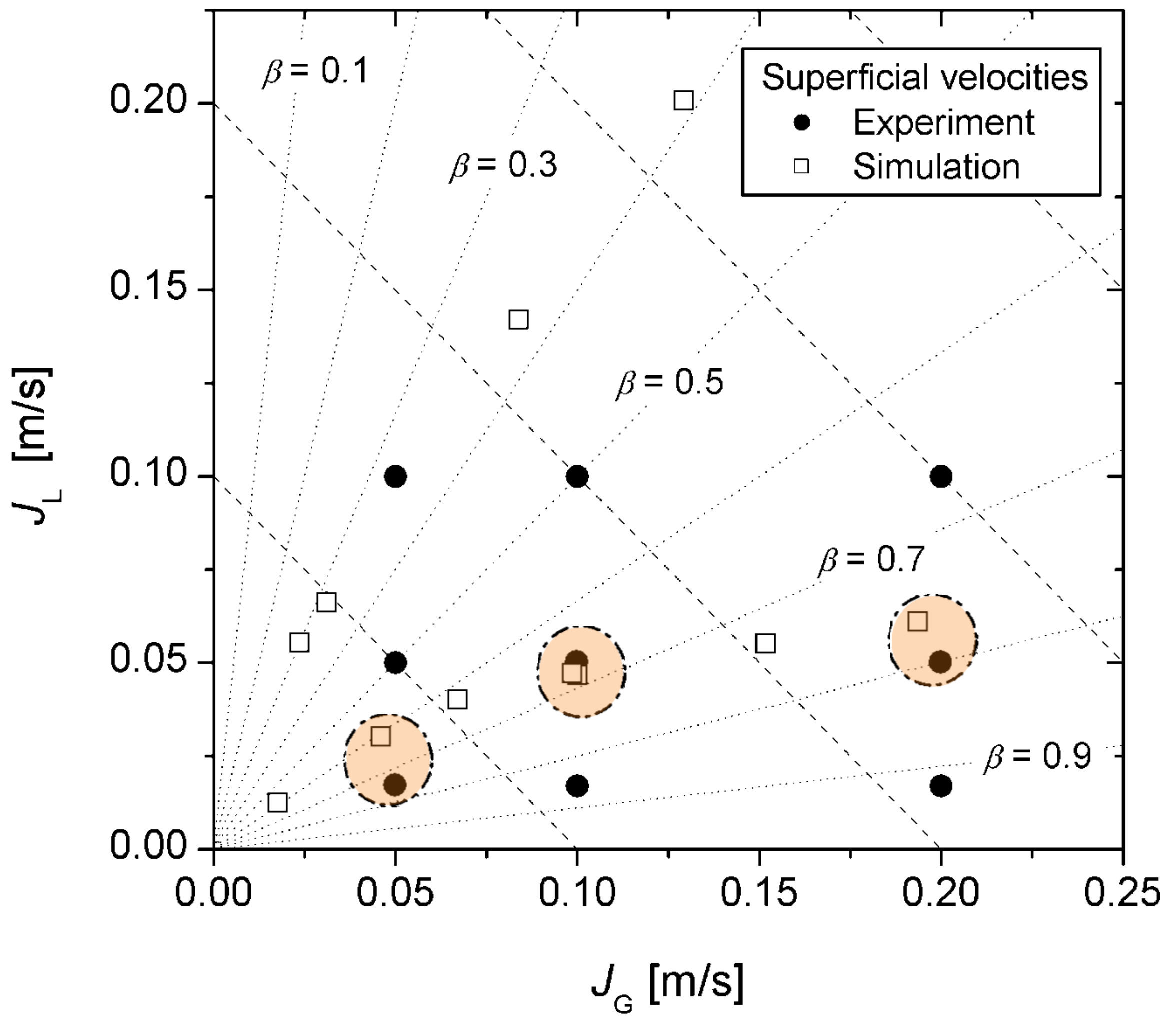


(35000 time steps)

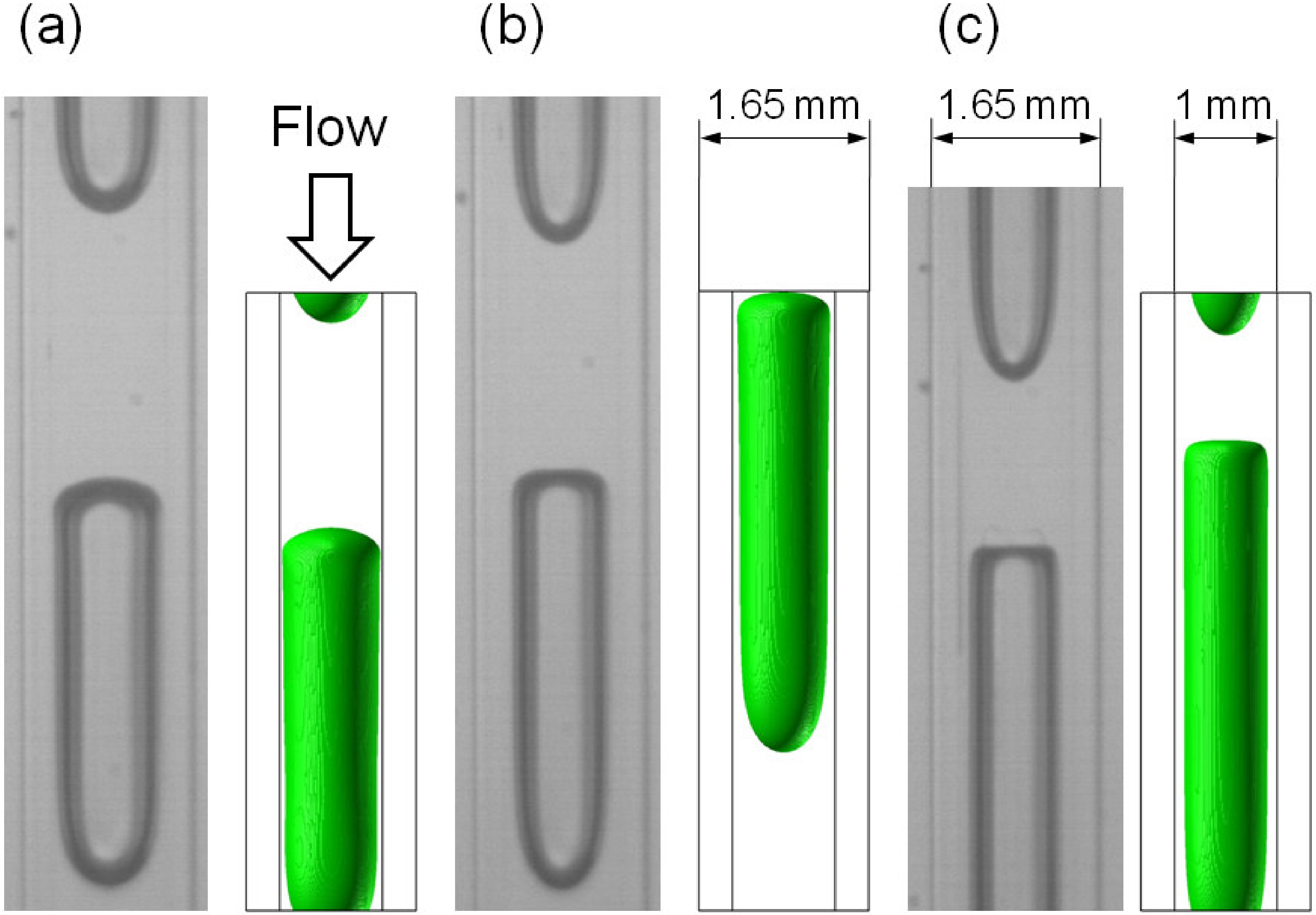
Experiments of TECHNISCHE UNIVERSITÄT DRESDEN (T. Bauer, R. Lange)

(Pressure = 20 bar)





Comparison of bubble shape*



*Keskin et al., AIChE Journal, in press

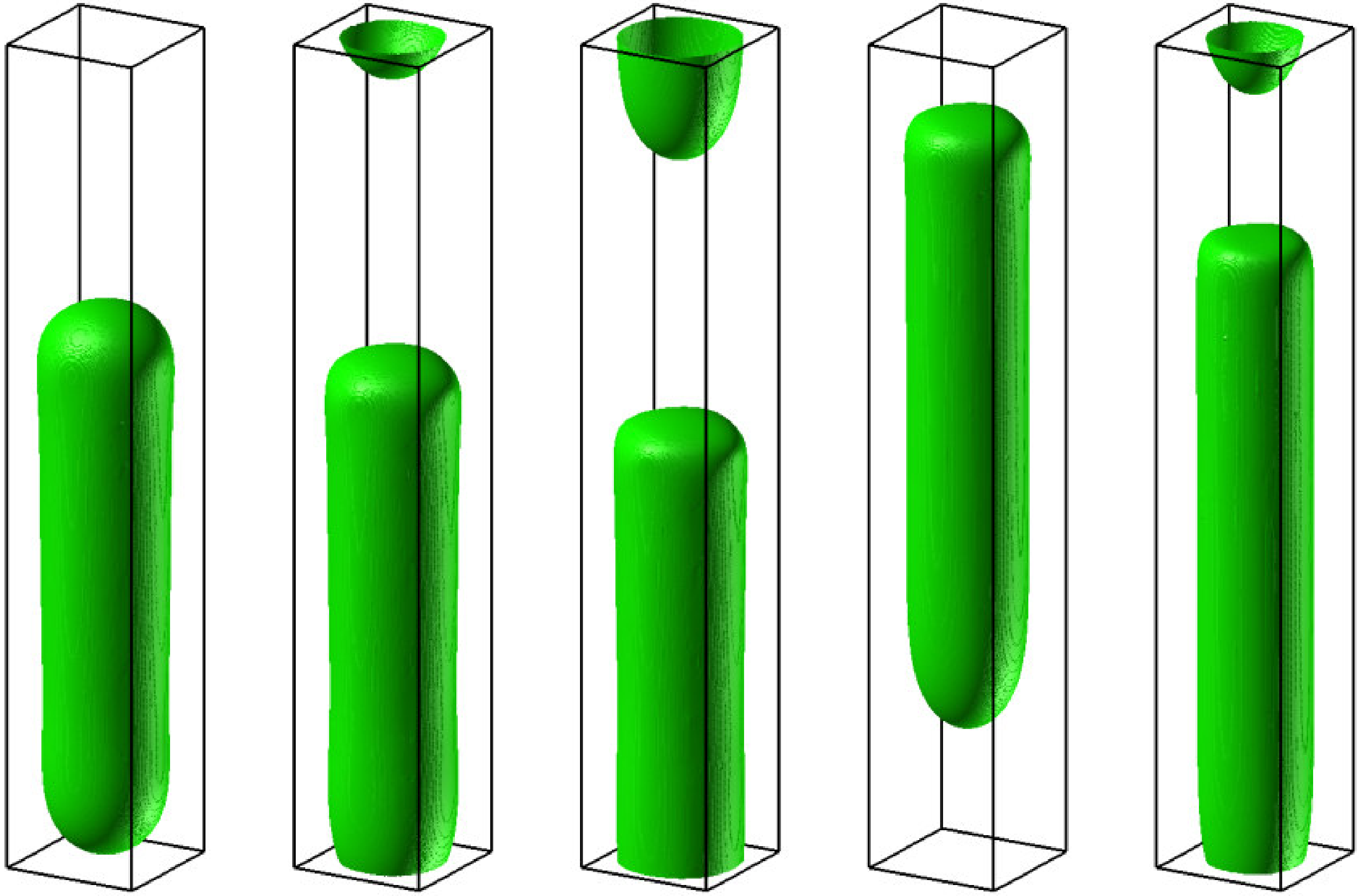
Steady bubble shape at different *Ca*

$$L_{\mathrm{uc}} = 6\,\mathrm{mm}$$
$$\varepsilon_{\mathrm{G}} = 0.4$$

$$\frac{Re}{Ca} = \frac{\sigma \rho_{\mathrm{L}} D_{\mathrm{h}}}{\mu_{\mathrm{L}}^2} \equiv La = 27.27$$

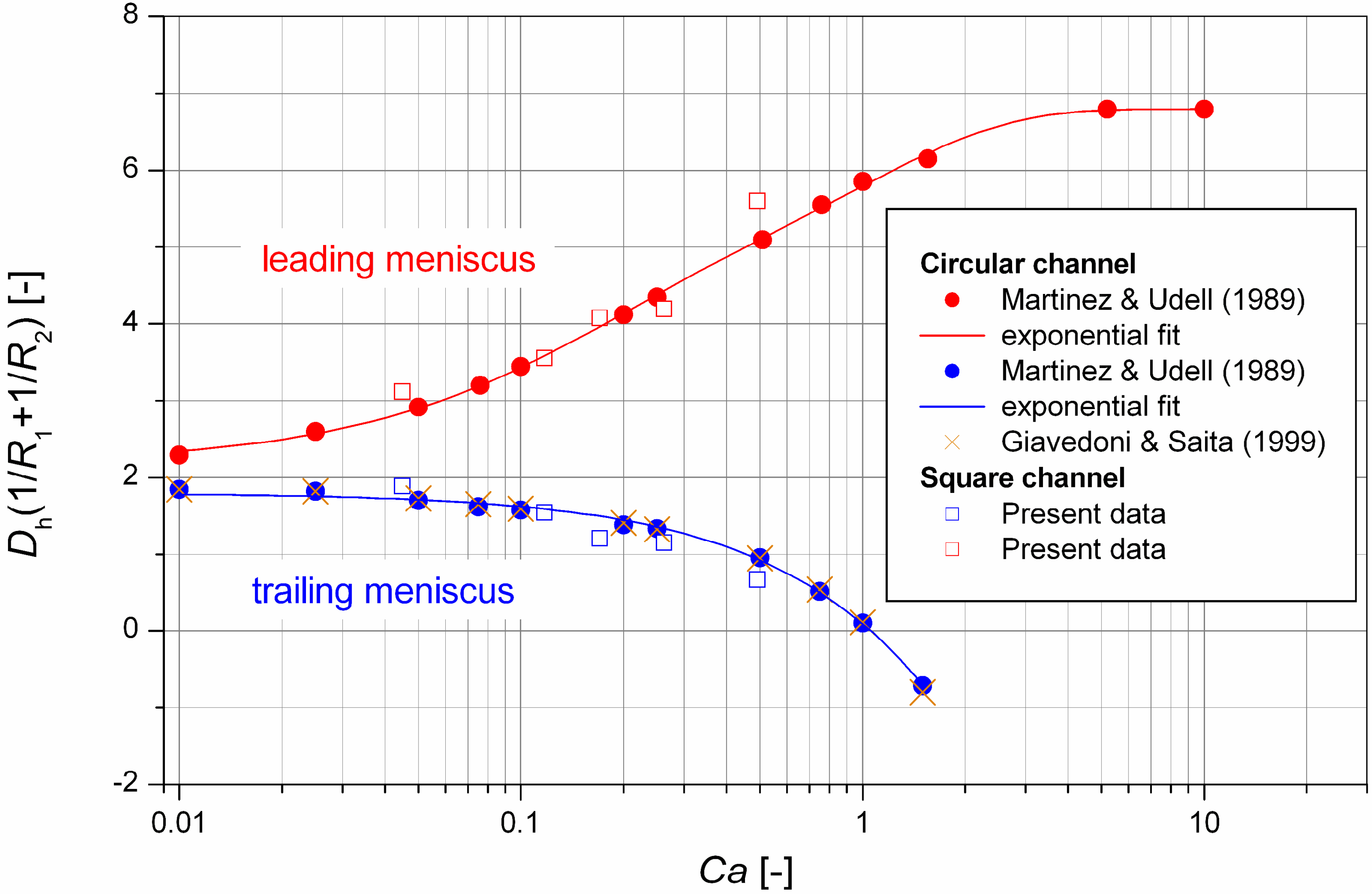
$$Ca \equiv \frac{\mu_{\mathrm{L}} U_{\mathrm{B}}}{\sigma}$$

$$Re \equiv \frac{\rho_{\mathrm{L}} D_{\mathrm{h}} U_{\mathrm{B}}}{\mu_{\mathrm{L}}}$$

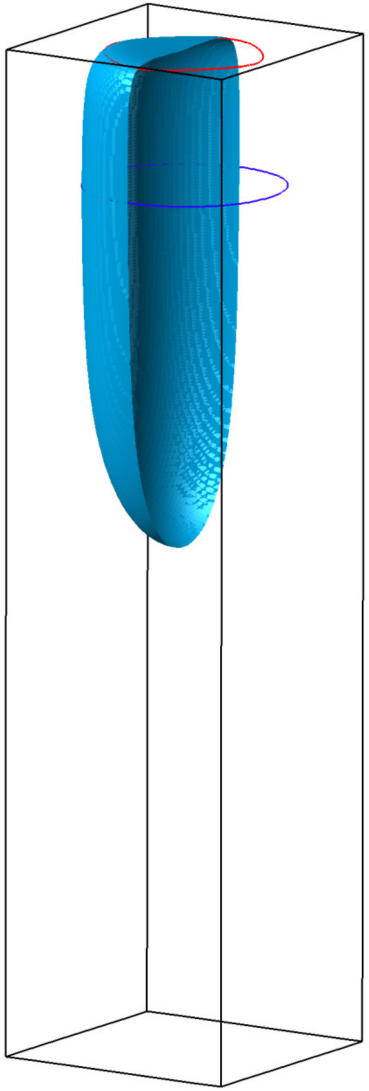


Ca =	0.045	0.12	0.17	0.26	0.49
Re =	1.22	3.19	4.64	7.16	13.4

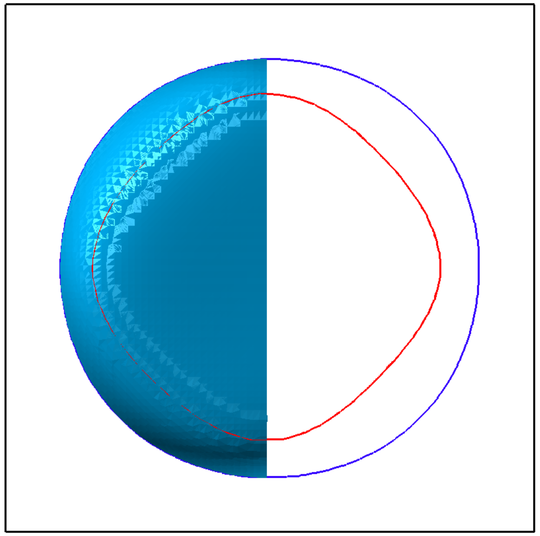
Front and rear curvature



Steady bubble shape for higher *Ca*



$$L_{uc} = 4\,\text{mm}, \quad \varepsilon_G = 0.2, \quad Ca = 0.65, \quad Re = 17.7$$

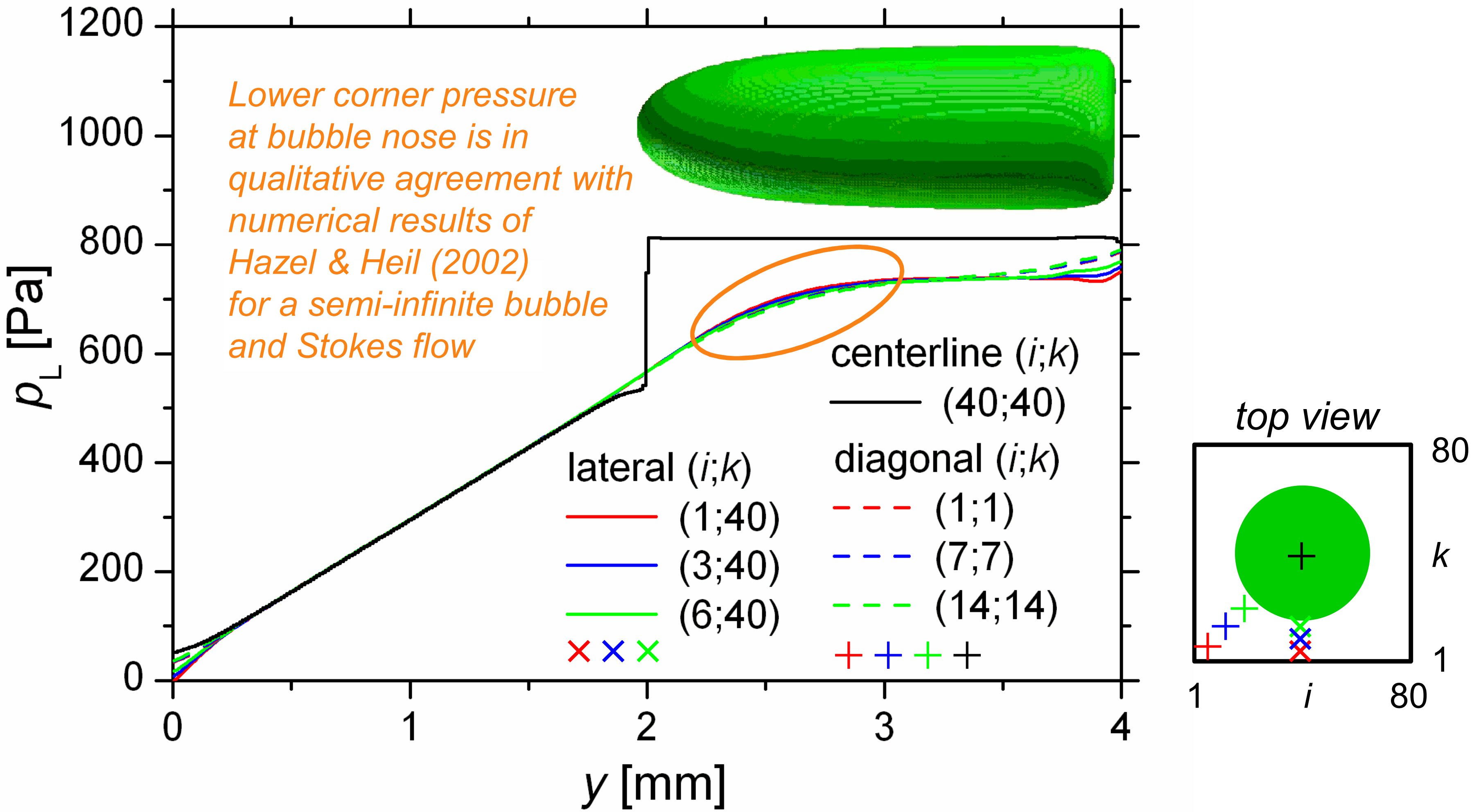


Bubble front and bubble body are axisymmetric, bubble rear is not!

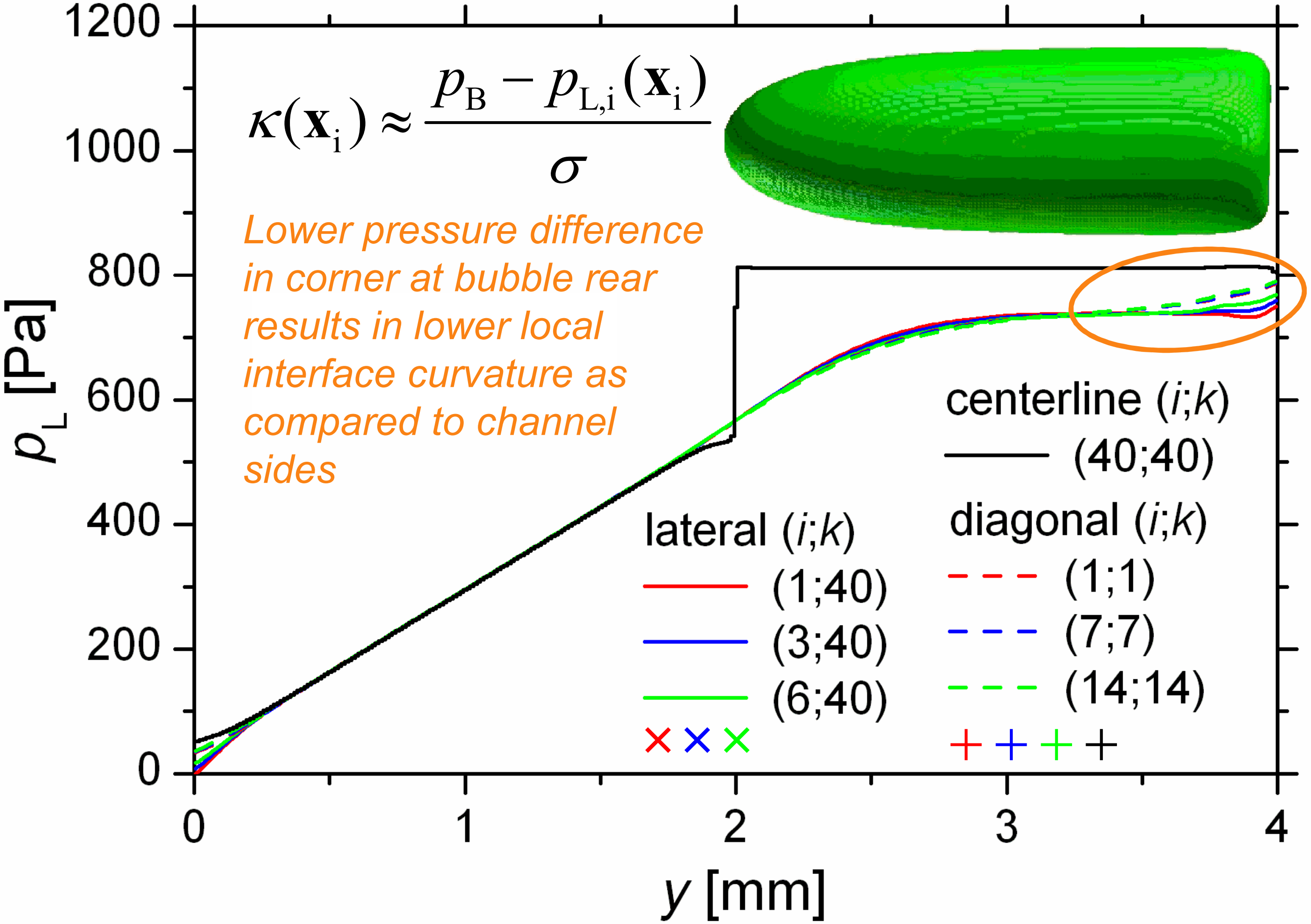
- Approximate relation for the local interface curvature κ at a point $\mathbf{x}_i$ located on the interface

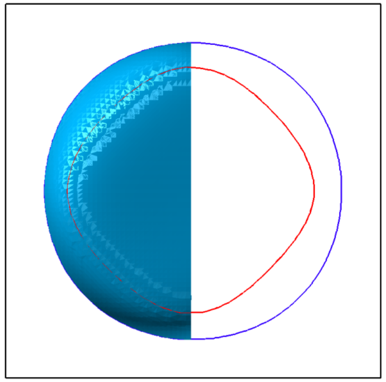
$$\kappa(\mathbf{x}_i) \approx \frac{p_B - p_{L,i}(\mathbf{x}_i)}{\sigma}$$

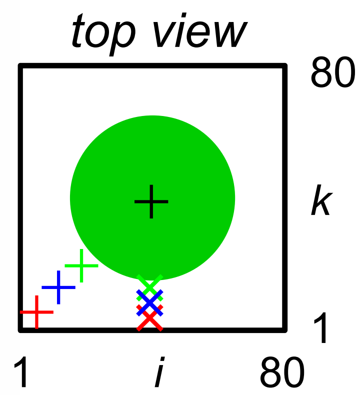
Axial profiles of liquid pressure



Axial profiles of liquid pressure

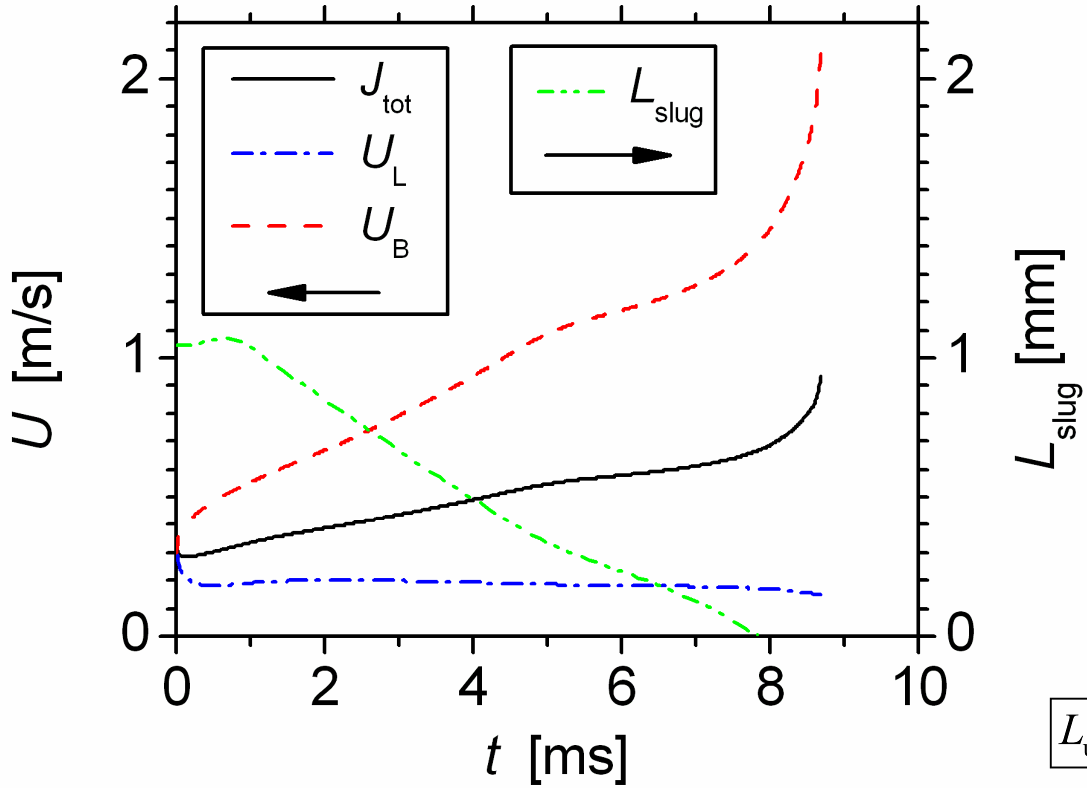






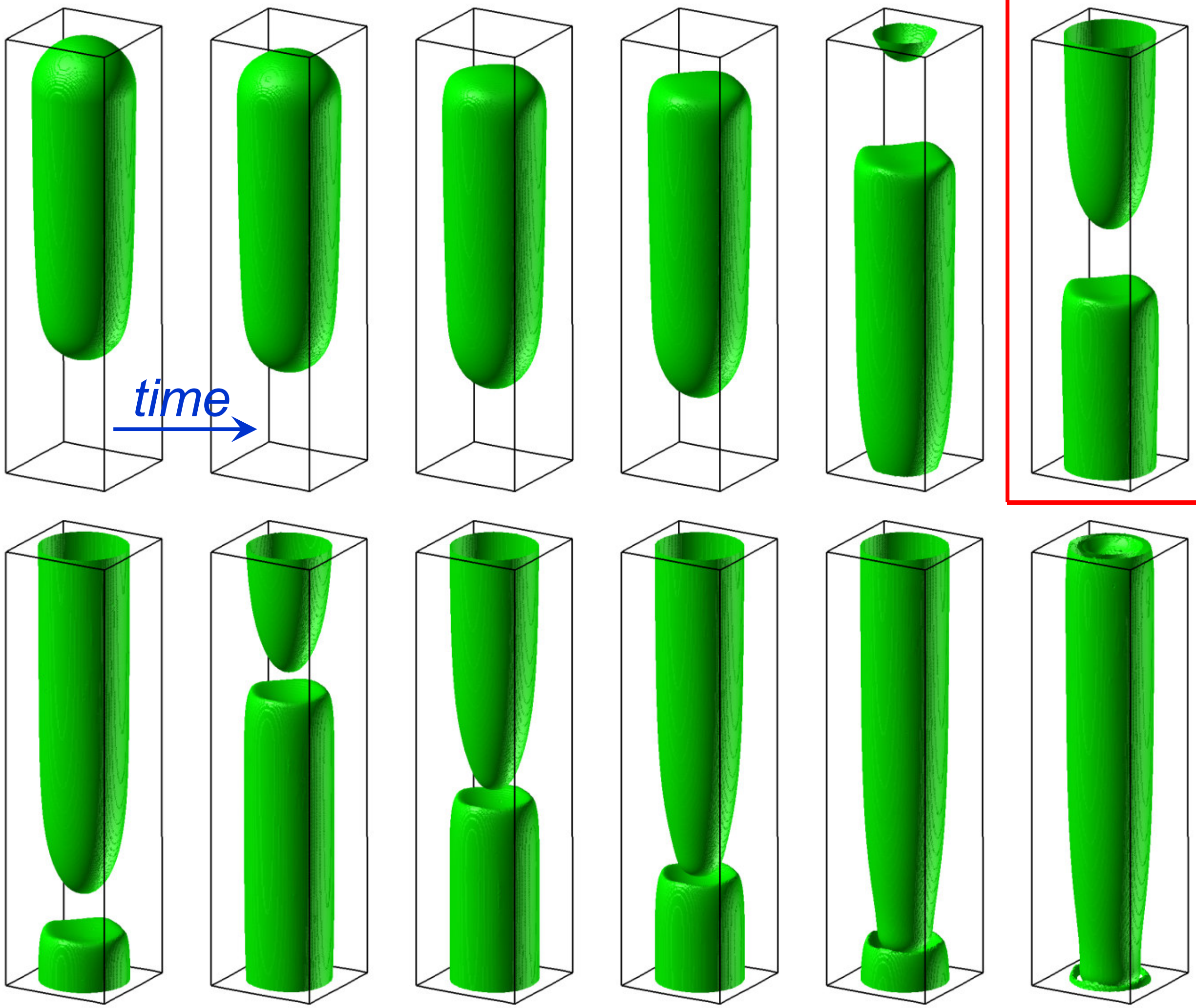
Transition to annular flow

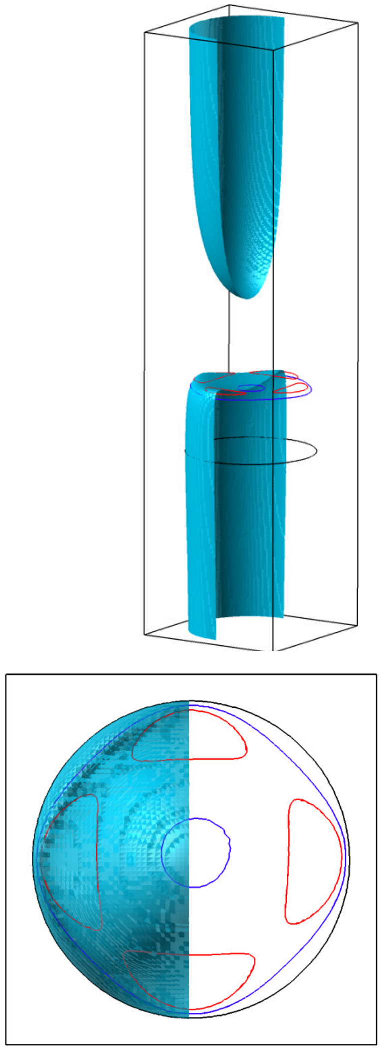
- For large prescribed pressure drop no steady bubble velocity rise is obtained
- The liquid slug length decreases and becomes zero



$L_{uc} = 4\,\mathrm{mm}, \quad \varepsilon_G = 0.4$

Transition to annular flow





L_{uc} = 4 mm, ε_G = 0.4

Conclusions

- The curvature of the front (rear) meniscus at the channel axis increases (decreases) with increase of the capillary number
- The values of the non-dimensional front/rear curvature in a square channel are similar to those in a circular channel
- At high values of the capillary number we find a novel bubble shape regime, not reported in literature so far, where the bubble nose and body are axisymmetric, while the bubble rear is not; instead the rear meniscus shows a symmetry with respect to the channel mid-planes and diagonals
- This shape of the rear meniscus has its origin in substantial variations of the liquid pressure in cross-sections at the bubble rear; the large pressure differences are presumably caused by inertial effects along curved streamlines
- Can this shape be confirmed by experiments? What is the range of (Ca, Re) where this novel shape may exist?

Thank you for your attention

Theoretical analysis of curvature

- Dynamic boundary condition normal to the interface

$$\boxed{p_{\mathrm{L,i}} - p_{\mathrm{G,i}} + \tau^{\perp}_{\mathrm{L,i}} - \tau^{\perp}_{\mathrm{G,i}} = \sigma\kappa}$$

$$\tau^{\perp}_{\mathrm{L,i}} = \mu_{\mathrm{L}} \left(\nabla \mathbf{v}_{\mathrm{L}} + (\nabla \mathbf{v}_{\mathrm{L}})^{\mathrm{T}} \right) : \mathbf{n}_{\mathrm{i}} \mathbf{n}_{\mathrm{i}}$$

$$\tau^{\perp}_{\mathrm{G,i}} = \mu_{\mathrm{G}} \left(\nabla \mathbf{v}_{\mathrm{G}} + (\nabla \mathbf{v}_{\mathrm{G}})^{\mathrm{T}} \right) : \mathbf{n}_{\mathrm{i}} \mathbf{n}_{\mathrm{i}}$$

- Assumptions: $p_{\mathrm{G,i}} = p_{\mathrm{B}} = const.,\quad \mu_{\mathrm{G}} / \mu_{\mathrm{L}} = 0.0006 \Rightarrow \tau^{\perp}_{\mathrm{G,i}} \approx 0$
- Non-dimensional interface curvature

$$\boxed{K \equiv \kappa D_{\mathrm{h}} \approx \frac{D_{\mathrm{h}}}{\sigma} \left(p_{\mathrm{L,i}} - p_{\mathrm{B}} + \tau^{\perp}_{\mathrm{L,i}} \right)}$$

- At front and rear stagnation point:

$$\tau^{\perp}_{\mathrm{L,tip/rear}} = \mu_{\mathrm{L}} \left(\nabla \mathbf{v}_{\mathrm{L}} + (\nabla \mathbf{v}_{\mathrm{L}})^{\mathrm{T}} \right) \Big|_{\mathrm{tip/rear}} : \mathbf{e}_{\mathrm{y}} \mathbf{e}_{\mathrm{y}} = 2\mu_{\mathrm{L}} \left. \frac{\partial v_{\mathrm{L}}}{\partial y} \right|_{\mathrm{tip/rear}}$$

Theoretical analysis of curvature

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- At front and rear stagnation point:

$$\left.\frac{\partial v_\mathrm{L}}{\partial y}\right|_\mathrm{tip} \approx -\left.\frac{\partial v_\mathrm{L}}{\partial y}\right|_\mathrm{rear} \approx \frac{U_\mathrm{L,cl} - U_\mathrm{B}}{L_\mathrm{nvbl,tip/rear}} \qquad U_\mathrm{L,cl} = C_\square J_\mathrm{tot} = 2.0962 J_\mathrm{tot}$$

$$K_\mathrm{tip} \approx \frac{D_\mathrm{h}(p_\mathrm{B} - p_\mathrm{L,tip})}{\sigma} + \frac{2D_\mathrm{h}}{L_\mathrm{nvbl,tip}} Ca \left(\frac{C_\square}{\psi} - 1\right) \qquad \psi \equiv \frac{U_\mathrm{B}}{J_\mathrm{tot}}$$

$$K_\mathrm{rear} \approx \frac{D_\mathrm{h}(p_\mathrm{B} - p_\mathrm{L,rear})}{\sigma} - \frac{2D_\mathrm{h}}{L_\mathrm{nvbl,rear}} Ca \left(\frac{C_\square}{\psi} - 1\right)$$

$$\boxed{K_\mathrm{tip} - K_\mathrm{rear} \approx \frac{D_\mathrm{h}(p_\mathrm{L,rear} - p_\mathrm{L,tip})}{\sigma} + 2Ca\left(\frac{C_\square}{\psi} - 1\right)\left(\frac{D_\mathrm{h}}{L_\mathrm{bl,tip}} + \frac{D_\mathrm{h}}{L_\mathrm{bl,rear}}\right)}$$

Axial profiles of axial velocity