Critical evaluation of CFD codes for interfacial simulation of bubble-train flow in a narrow channel

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Outline

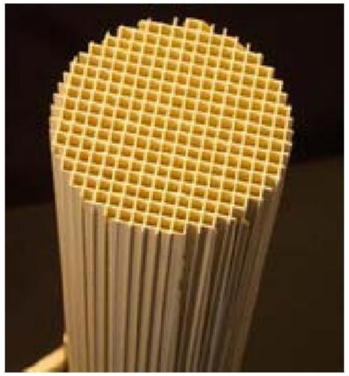
- Introduction and motivation
- Description of bubble train flow (BTF) test case
  - Governing equations and volume-of-fluid method
  - Computational setup
- Results of code-to-code comparison
  - Contributing codes: CFX, FLUENT, STAR-CD, TURBIT-VOF (in-house code)
- Conclusions

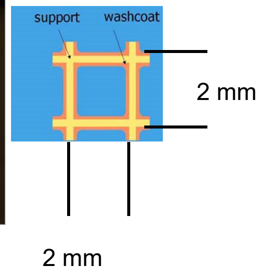
Introduction

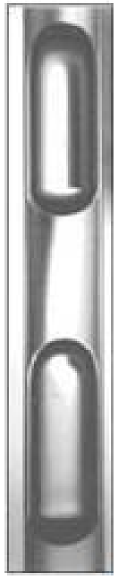
Process Intensification

Smaller
Cheaper
Safety
Skillful

Two Phase Flow
(Bubble Train Flow =BTF)







Industrial Advantages

Monolith Catalyst Reactors
-Enhance its mixing
Micro Bubble Reactors
-Provide Efficient mass transfer due to high İnterfacial area per unit volume

Optimal Conditions

Local
<u>Hydrodynamic</u>
Thermal and
Mass transfer
Phenomena

Experimental Studies

CFD alternative way

to get insight in <u>hydrodynamic</u> phenomena

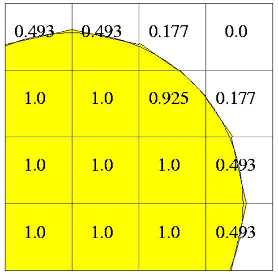
Goal of present study

- Evaluate commercial CFD codes for interfacial simulation of gas-liquid flows in small channels
  - STAR-CD 4.0
  - ANSYS CFX 10.0
  - FLUENT 6.2.16
- Perform simulations of bubble-train flow in a square mini-channel were surface tension forces are predominant
- Compare results with those of in-house code TURBIT-VOF which is already verified by experimental data* for BTF of silicon oil and air

*Thulasidas et al. Chem Eng Sci 52 (1995) 183-199

Governing Equations

- for f=1 the mesh cell is entirely filled with liquid (continuous phase)
- for f=0 it is entirely filled with gas
- for 0<f<1 both phases coexist



Based on f value, mixture density and viscosity and center-of-mass velocity can be defined

$$\mu_m \equiv f\mu_L + (1-f)\mu_G$$

$$\rho_m \equiv f\rho_L + (1-f)\rho_G$$

$$\mathbf{v}_m \equiv \frac{f\rho_L \mathbf{v}_L + (1-f)\rho_G \mathbf{v}_G}{\rho_m}$$

- Continuous liquid volume fraction conversation

$$\frac{\partial f}{\partial t} + \nabla \cdot f\mathbf{v}_m = 0$$

- Continuity or mass conservation

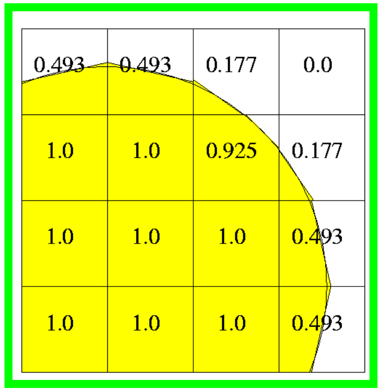
$$\nabla \cdot \mathbf{v}_m = 0$$

- Momentum Equation

$$\frac{\partial}{\partial t}(\rho_m \mathbf{v}_m) + \nabla \cdot \rho_m \mathbf{v}_m \mathbf{v}_m = -\nabla P + \nabla \cdot \mu_m \left(\nabla \mathbf{v}_m + (\nabla \mathbf{v}_m)^{\mathrm{T}}\right) + (\rho_m - \rho_L)\mathbf{g} - \mathbf{f}_{\mathrm{pd}} + \mathbf{f}_\sigma$$

“VOF-methods” in CFD codes

	TURBIT-VOF	FLUENT	STAR-CD	CFX
Time Integration Scheme	Explicit 3. order Runga-Kutta	1. order Implicit	1.order Implicit	1. order Imp 2. order Imp
Mesh Order	Staggered	Co-located	Co-located	Co-located
Options for Free Surface Problems	**VOF**, interface capturing by means of **-Reconstruct (EPIRA)**	**VOF**, interface capturing by means of **-Geo-reconstruct** **-Donor-acceptor** **-Euler-Explicit** **-Implicit**	**VOF**, interface capturing by means of **-HRIC** **-UD** high order schemes	Under **Homogeneous model** concept interface capturing by means of **high order schemes**



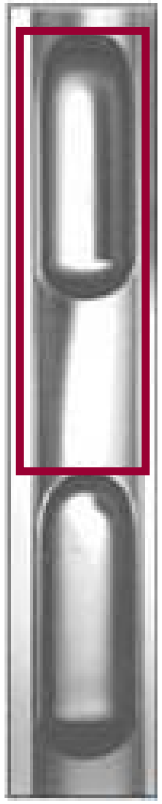
PLIC = Piecewise Linear Interface Calculation

SLIC = Simple Line Interface Calculation

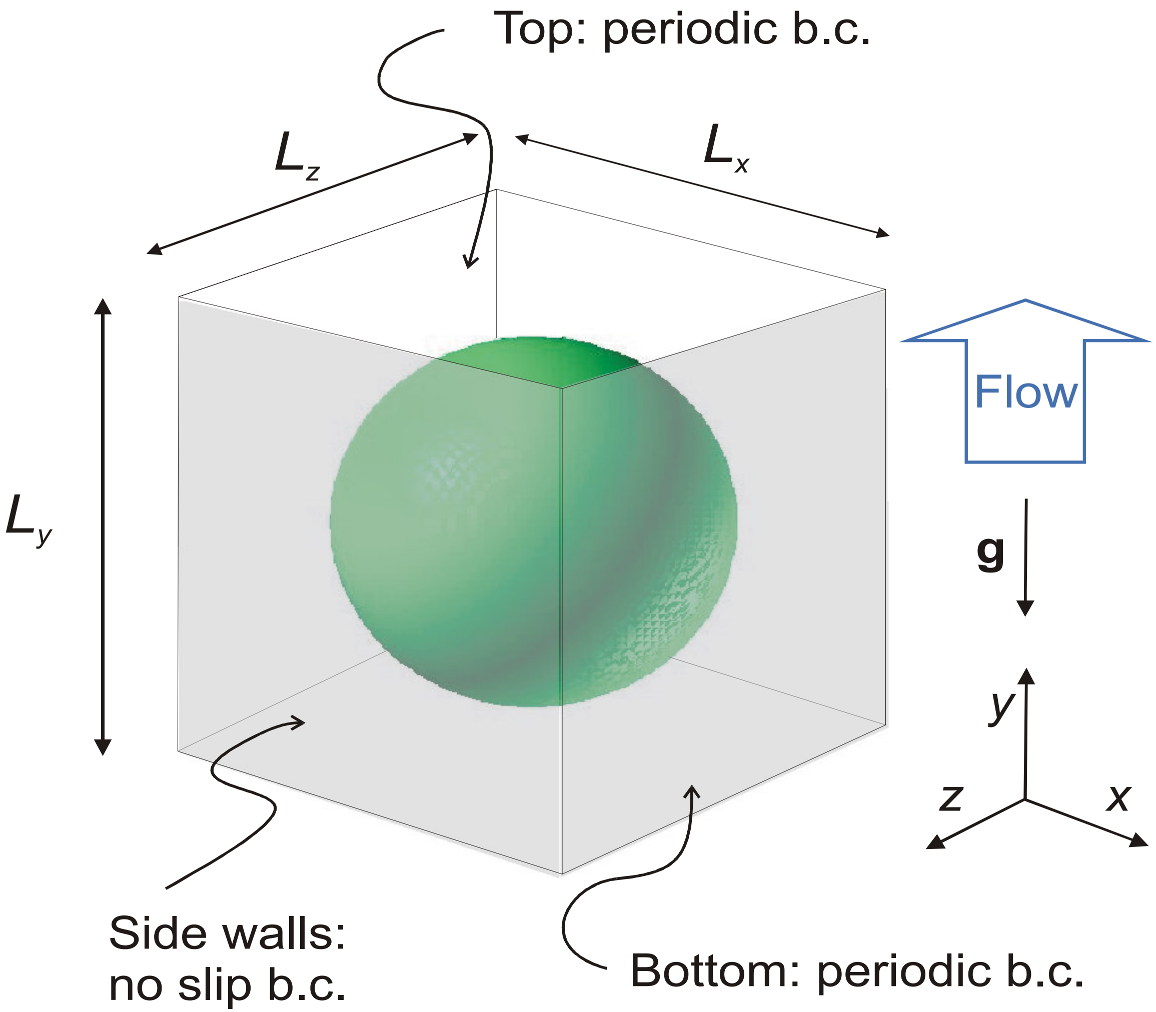
Problem of difference scheme methods for *f*-equation:

Artificial smearing of interface by numerical diffusion

Numerical Setup for TURBIT-VOF, CFX and STAR-CD



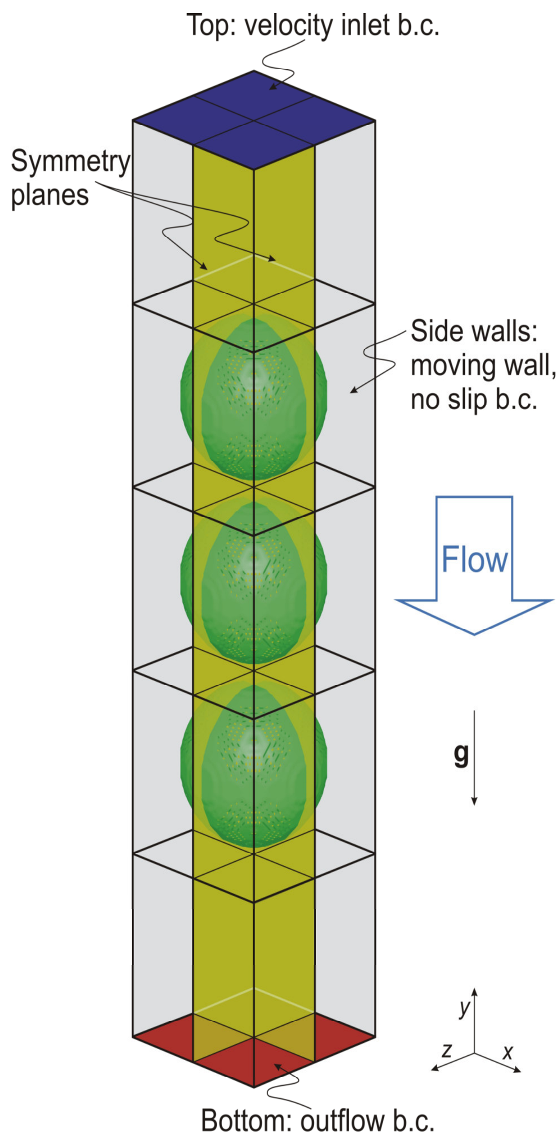
- Consideration of one unit cell in fixed frame of reference
- Use of periodic boundary conditions at top and bottom
- $L_x = L_y = L_z$ = 2 mm



Ghidersa, Wörner, Cacuci: Chem. Eng. J. 101 (2003) 285-294

Numerical setup for FLUENT

- FLUENT does not allow to use VOF method in combination with periodic boundary conditions
- Therefore simulations are performed in moving frame of reference
- Domain: 1 mm × 10 mm × 1 mm
- Downward wall velocity corresponds to terminal bubble velocity of TURBIT-VOF



Test Conditions

Physical properties

- Silicon oil $\rho_L = 957 kg/m^3$ $\mu_L = 0.048 Pa.s$
- Gas $\rho_G = 11.7 kg/m^3$ $\mu_L = 1.85\times10^{-5} Pa.s$
- Surface tension $\sigma = 0.02218 N/m$

Gas void fraction

$$\varepsilon = \frac{V_{Gas}}{V_{UnitCell}}$$

Case 1: Buoyancy driven flow

$(\rho_G - \rho_L)g = 9273.4 N/m^3$

High gas void fraction $\varepsilon \approx 33\%$ (H) , Low gas void fraction $\varepsilon \approx 30\%$ (L)

$Ca = \mu_L U_B / \sigma = 0.065$ $Re_B = \rho_L D_h U_B / \sigma = 1.205$

Case 2: Pressure driven flow

$(\rho_G - \rho_L)g = 9273.4 N/m^3$

High gas void fraction $\varepsilon \approx 33\%$ (H)

$\Delta p = -18 Pa$

$Ca = 0.204$ $Re_B = 3.75$

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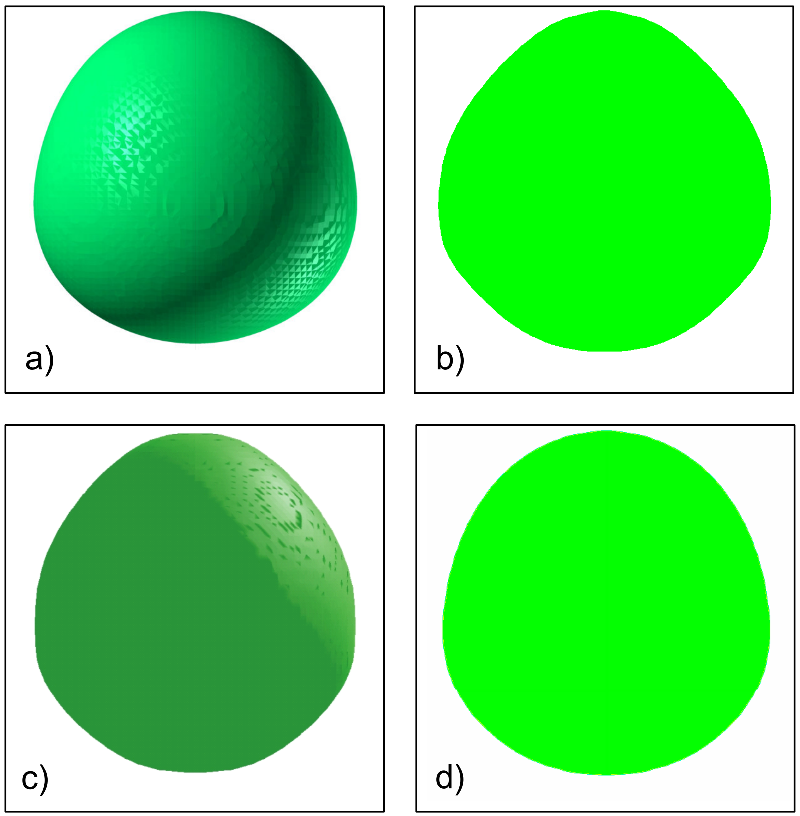
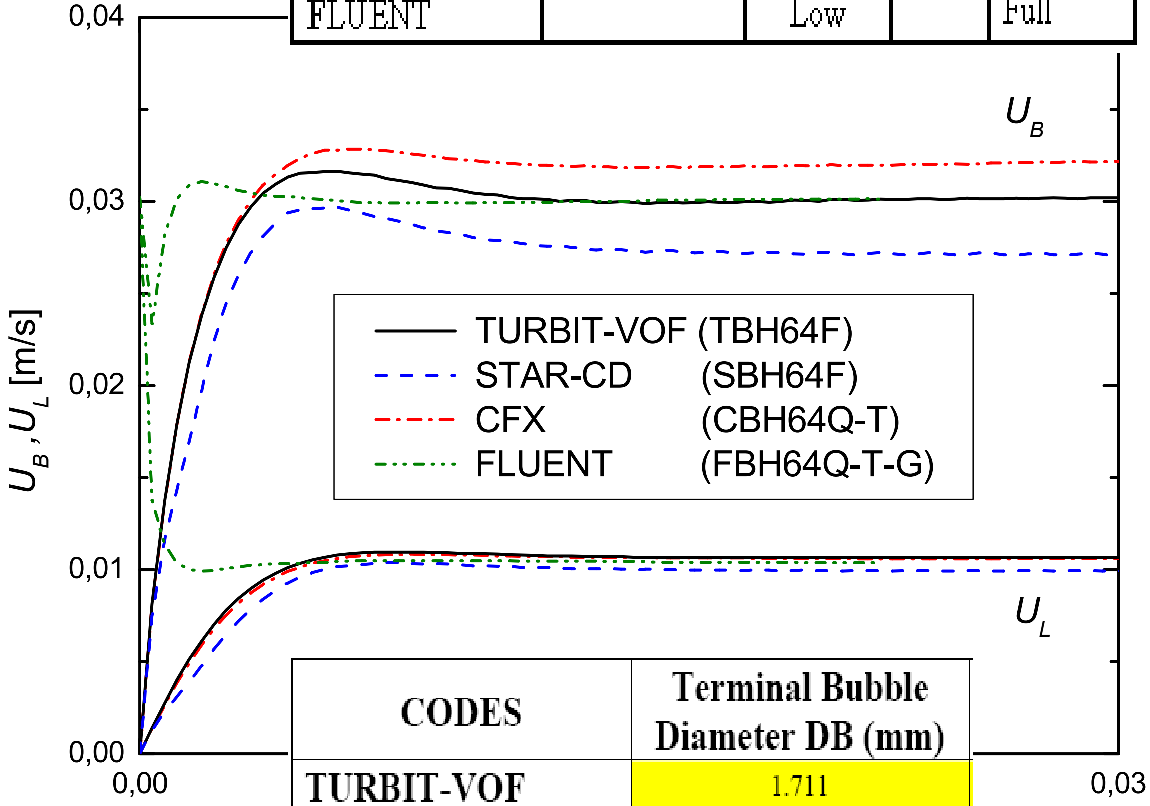
Case 1: Buoyancy driven flow

TURBIT-VOF STAR-CD



FLUENT CFX

TURBIT-VOF	B Buoyancy	H High	48 64 128	Q Quarter
STAR-CD				
CFX		L Low		F Full
FLUENT				

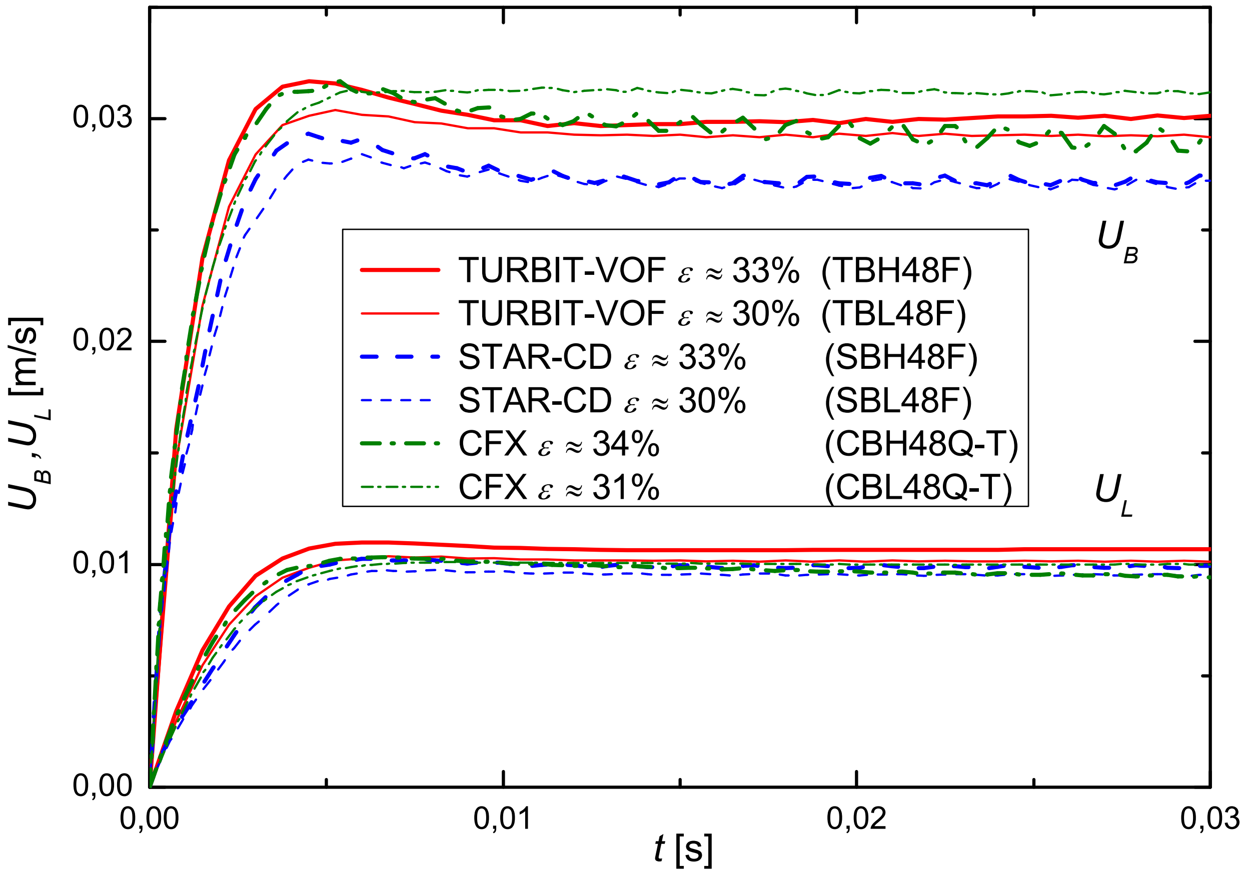


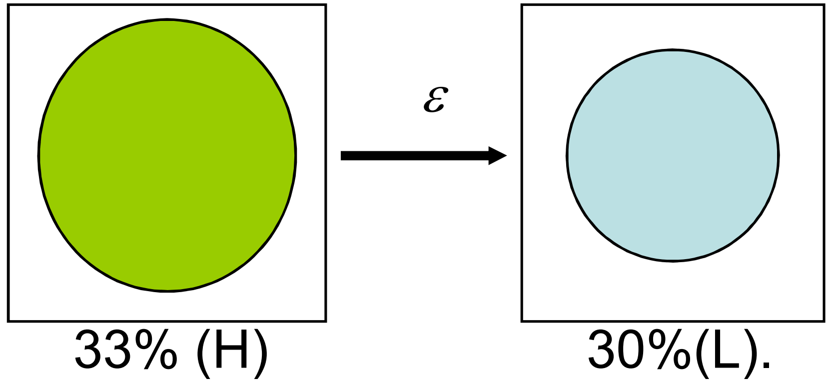
CODES	Terminal Bubble Diameter DB (mm)
TURBIT-VOF	1.711
STAR-CD	1.756
CFX	1.704
FLUENT	1.709

For FLUENT pressure drop is output and its value is -0.7 Pa

For other codes periodic pressure is input and its value is -0 Pa

Influence of gas holdup

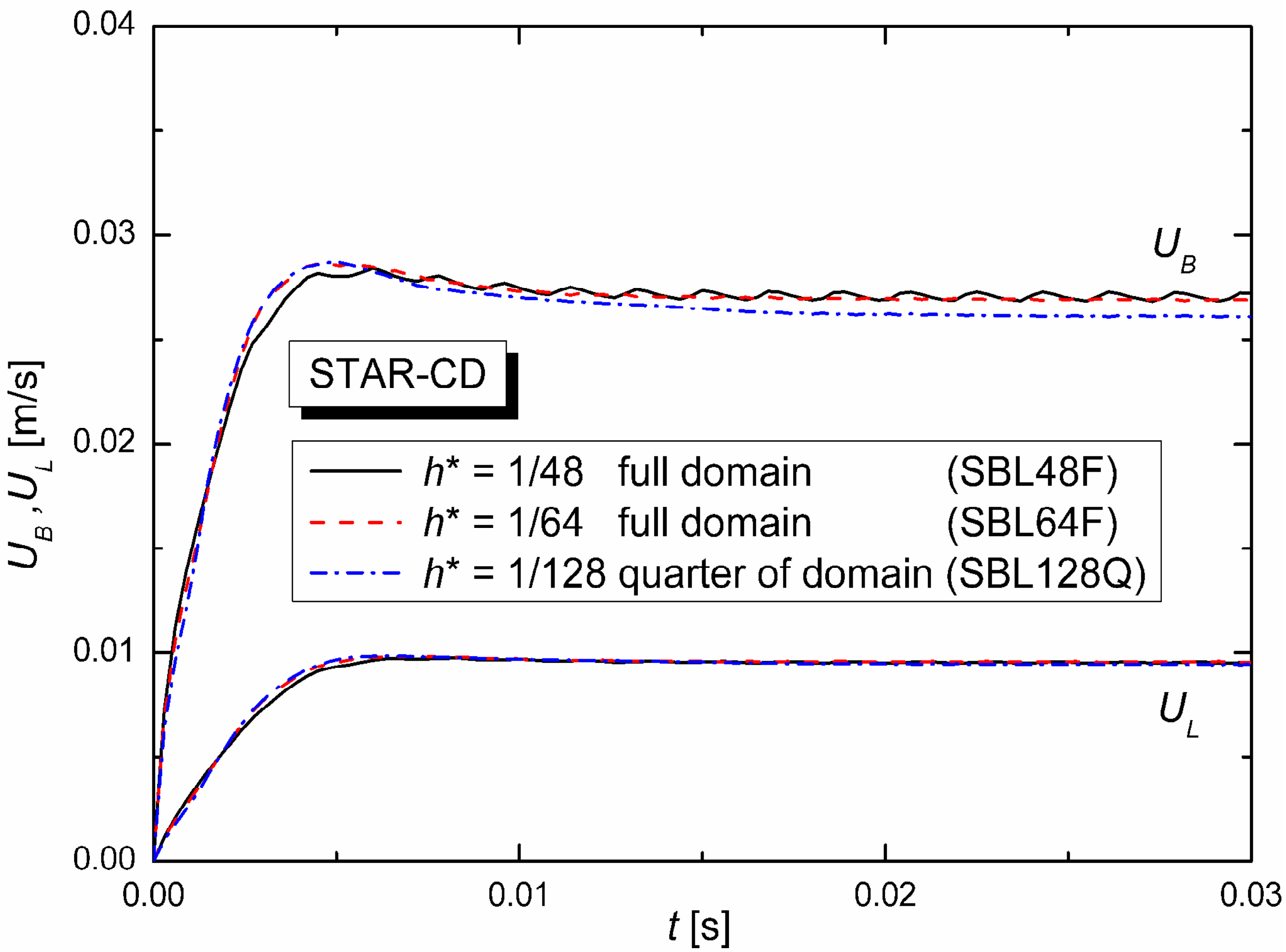




Due to decreasing initial void fraction, terminal bubble velocity should decrease.

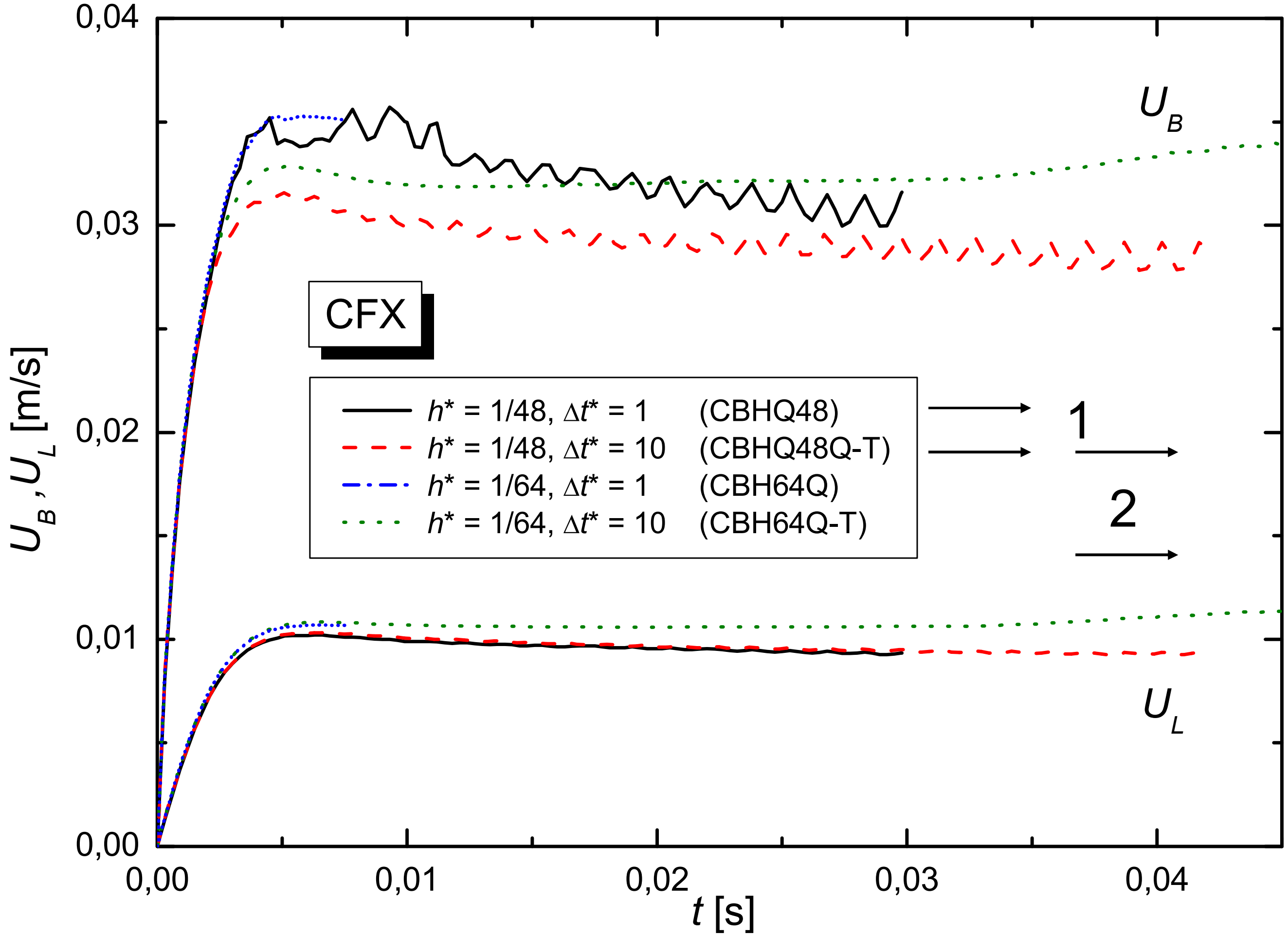
STAR-CD: bubble terminal velocity is almost the same for low and high void fraction
CFX: low void fraction results in higher bubble velocity than high void fraction (unphysical)

Grid refinement study for STAR-CD



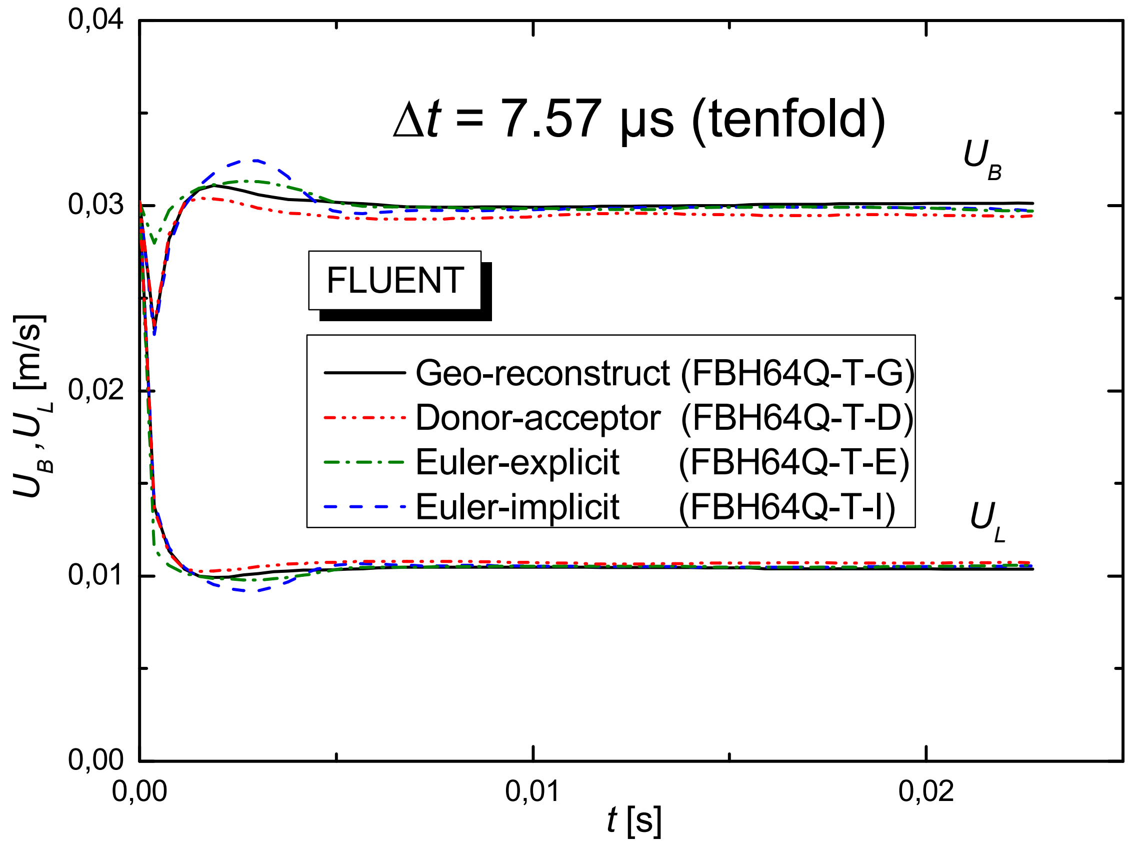
- Results do slightly depend on mesh size
- Refining the grid results in stronger underestimation of bubble velocity as compared to FLUENT and TURBIT-VOF

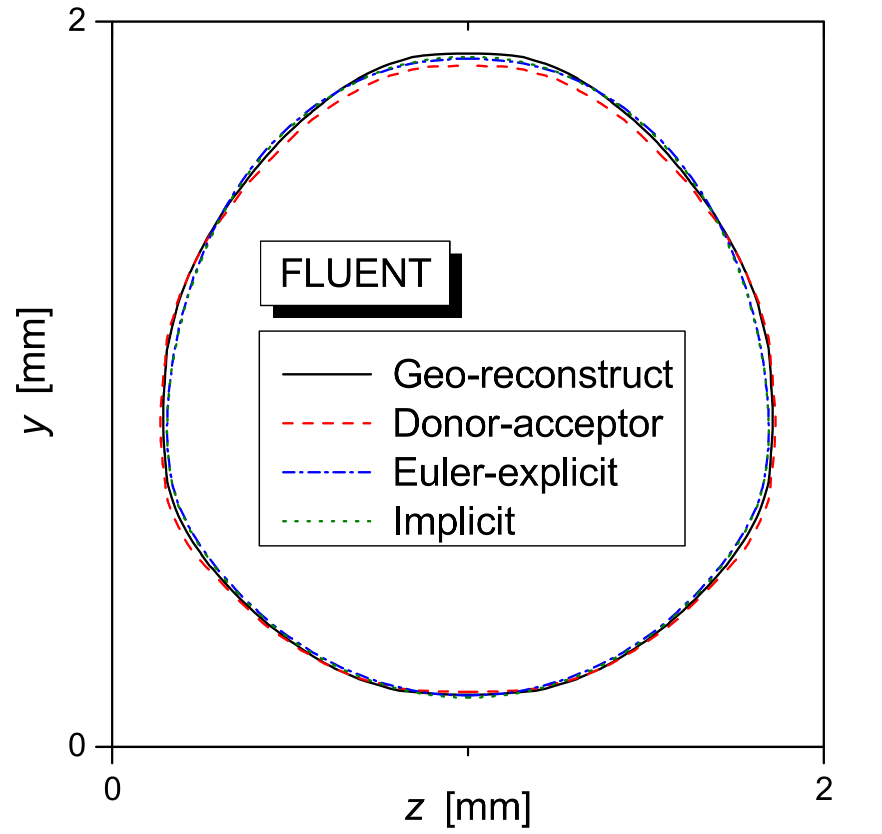
Grid and time step study for CFX



- Results depend on time step width (for same Δx)
- Results depend on mesh size (for same Δt)

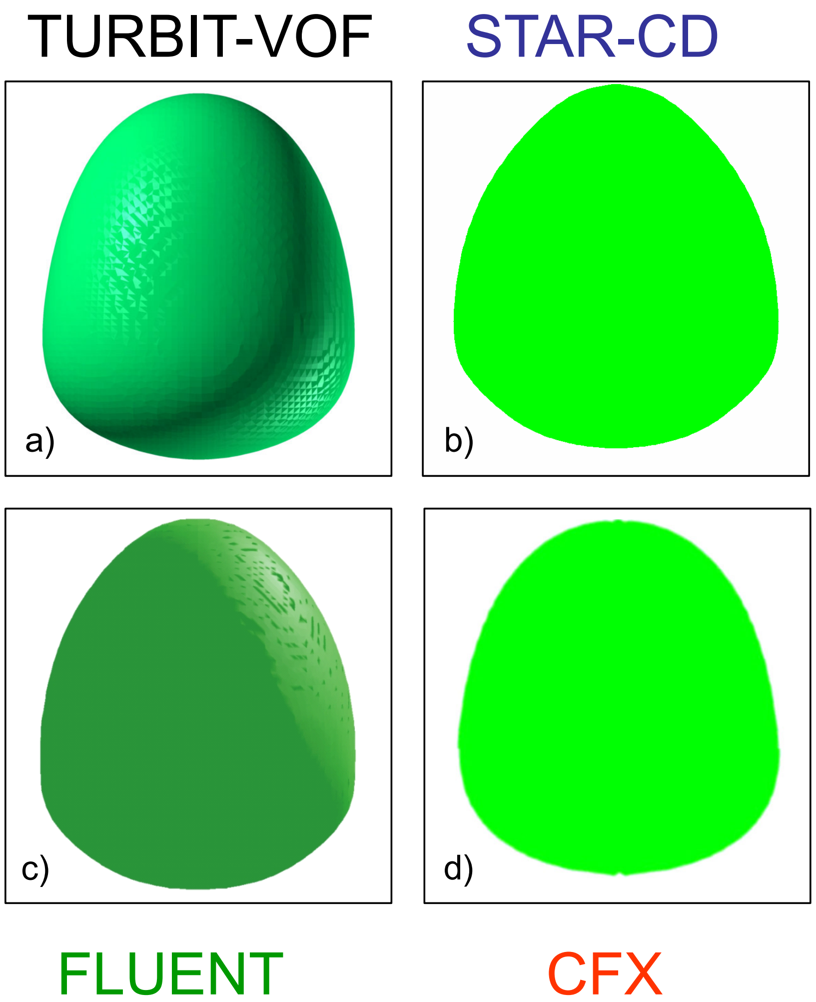
Different VOF methods in FLUENT



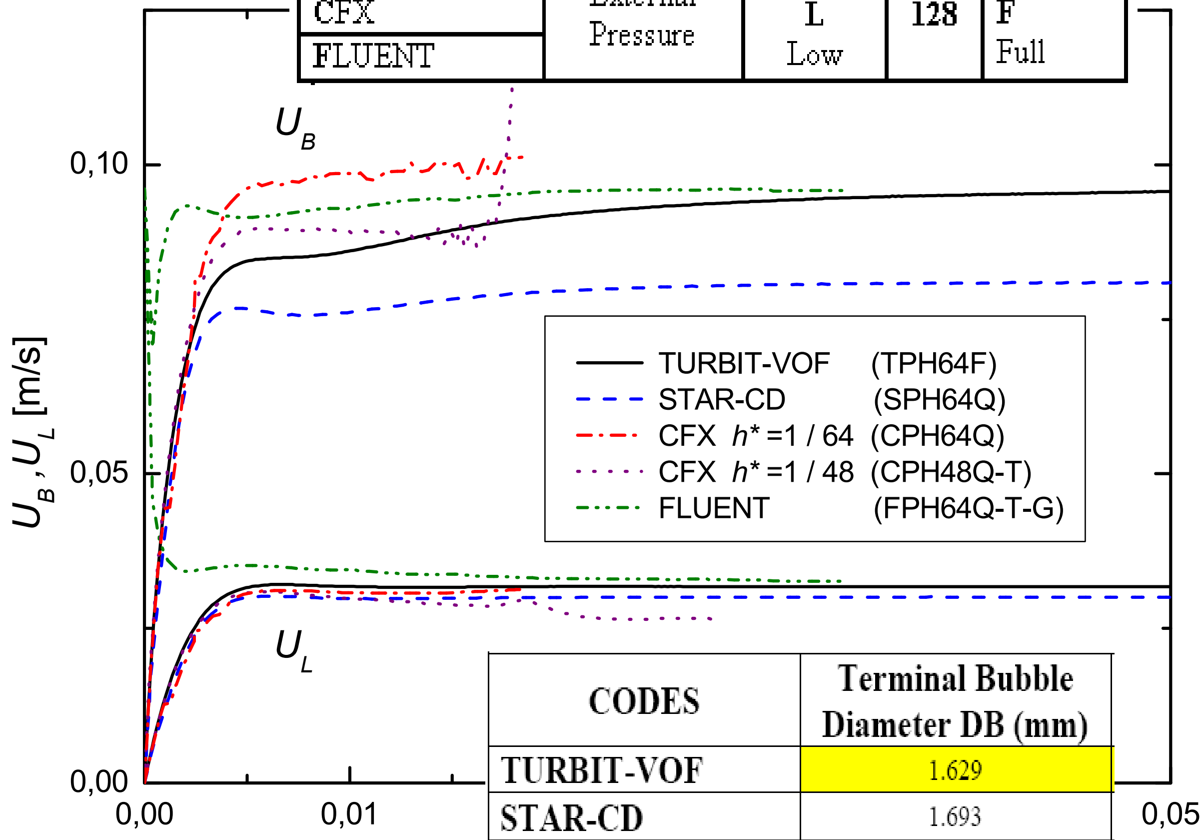


- „Geo-reconstruct" scheme is almost independent from Δx und Δt

Case 2: pressure driven flow



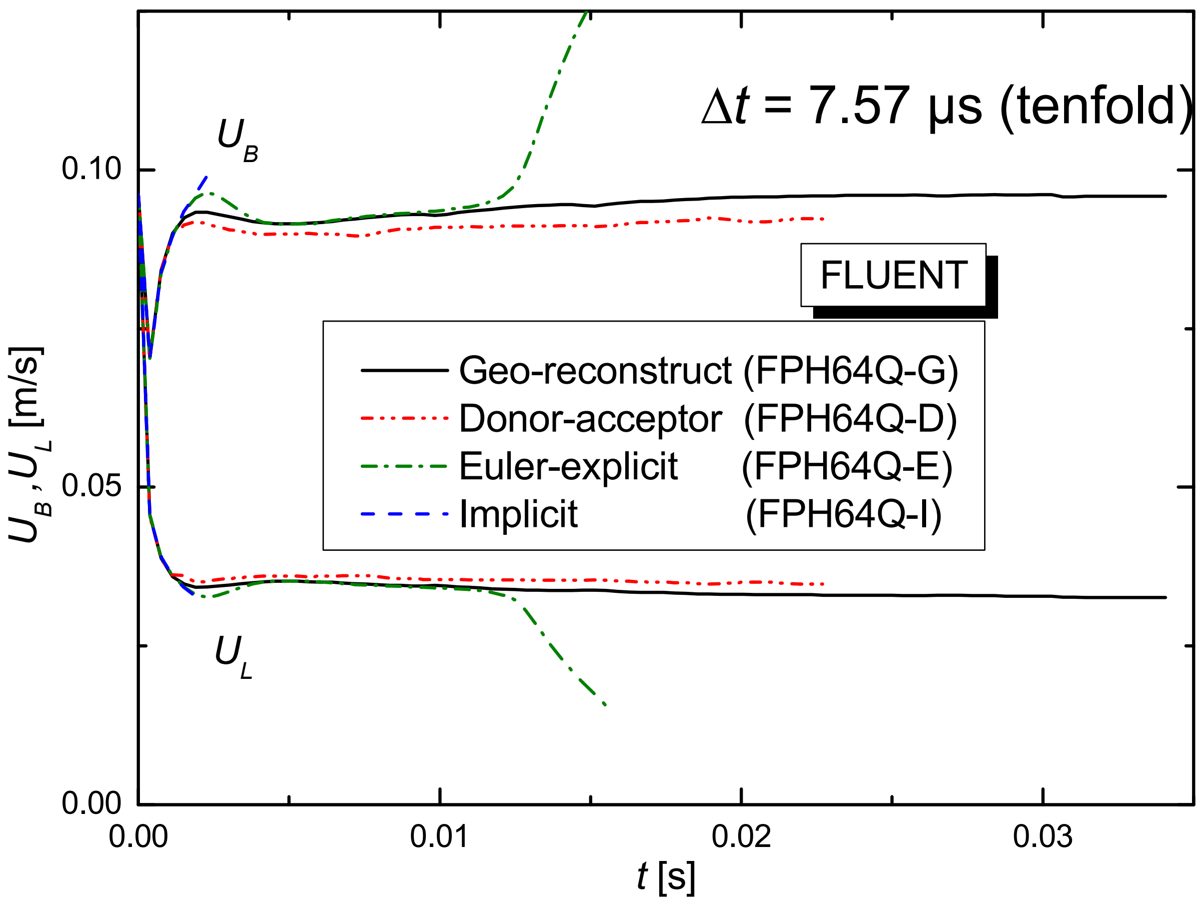
TURBIT-VOF STAR-CD	**P** Buoyancy& External Pressure	**H** High	**48** **64** **128**	**Q** Quarter
CFX FLUENT		**L** Low		**F** Full

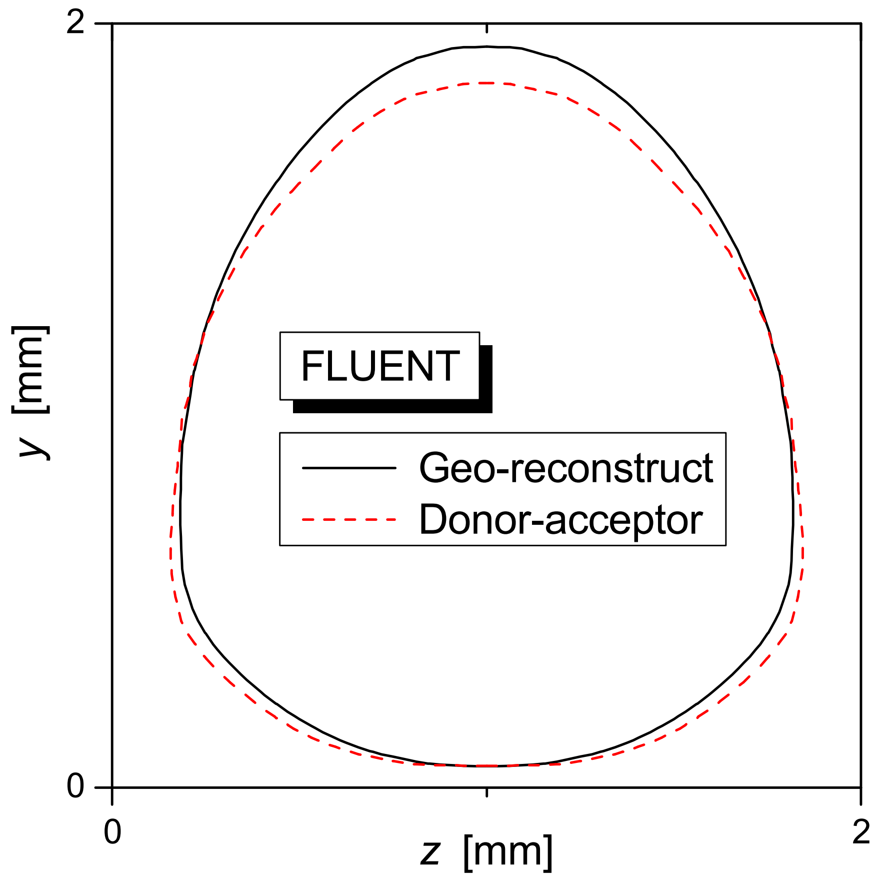


CODES	Terminal Bubble Diameter DB (mm)
TURBIT-VOF	1.629
STAR-CD	1.693
CFX	1.641
FLUENT	1.634

For FLUENT Periodic pressure is output and its value is -21.5 Pa
For rest of codes Periodic pressure is input and its value is -18 Pa

Different VOF methods in FLUENT





- Only VOF methods with reconstruction result in "bubble train flow"

Conclusions

- VOF methods based on piecewise linear interface reconstruction (PLIC) give consistent results
- Difference scheme methods have deficiencies
  - unphysical results for decrease of gas holdup (CFX,STAR-CD)
  - strong influence time step width (CFX)
  - influence of grid size (CFX, STAR-CD)
  - numerical diffusion may lead to artificial coalescence (all codes)
- For the commercial CFD codes the recommended PLIC reconstruction scheme is only available in FLUENT

For more information see paper in

“International Journal for Numerical Methods in Fluids“

(in press, but already available online)

Thanks for your attention…