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Summary

The here presented work is dedicated to the development of a software analysis tool specialized for Taylor bubble flows in a wide range of applications and covering a variety of geometrical realizations. Accordingly, a higher order FEM based interface tracking simulation software has been designed which due to the underlying isoparametric discretization and interface aligned mesh construction allows a semi-implicit treatment of the surface tension force term. The such designed numerical framework guarantees only a negligible amount of mass loss rate resulting in suitability of the tool for long time-scale simulations. Exploiting these numerical advantages the software has been applied for the system of Coiled Flow Inverter (CFI) capillaries characterized by a range of coil diameters and Reynolds numbers for which the pseudo-periodic flowfield has been obtained and extracted for further mixing quantification studies by the help of particle tracking based analysis. In the framework of this postprocessing analysis such a suitable transformation of the results has been applied which reveals the most important features of the characteristic flow patterns and makes it possible to qualitatively but even quantitatively characterize the behavior of the established flow patterns. Therefore, such a combination of robust CFD techniques together with the respective process performance quantification makes this approach suitable for tailored process design.

Keywords: Interface tracking, Coiled flow inverter, Implicit treatment of surface tension, Mixing characterization

Introduction

Process intensification and process control belong to the main objectives of chemical engineering, which are only then approachable if the understanding of all relevant processes is available or accessible. Aside of experimental analysis CFD methods are well accepted frameworks serving for these purposes in a wide range of chemical engineering applications. However, in the field of multiphysics processes only those CFD techniques might contribute with reliable prediction possibilities which are equipped with the combination of suitable discretization methods and efficient numerical approaches. Typical example of such type of problems is related to Taylor bubble flows in curved capillaries which is subjected to multiphase flows with dynamically evolving interfaces and the presence of thin laminar film layers between the dispersed phase and the capillary wall. Pioneering works in this regards reach back to a steady, spatially periodical simulation framework presented by Kashid et al. (2007). A remarkable review of CFD methods used for individual Taylor bubble flows in more complex geometries have been provided by Wörner (2012). Axisymmetric simulations of straight capillaries with transport of species and chemical reactions have been provided by Yang et al (2017). The most recent work of Chatterjee et al (2021) demonstrated the formation (pinch off) of the bubbles and their respective transportation in straight and curved capillaries under wetting conditions by the use of contact angle boundary conditions at the triple phase contact lines. The most accurate simulation approach so far presented in the framework of Taylor bubble flows within curved capillaries has been so far presented by Gaddem et al (2021) who have utilized a suitable transformation method making it possible to resolve the bubble transportation under non-wetting conditions. Moreover, the transport of species and performance of chemical reactions have also been analyzed based on the computationally determined flowfields. Simulation attempts focusing on fully resolved (with interface aligned meshes) Taylor bubble flows in a large geometrical representation of CFIs have so far not been achieved and therefore it becomes the central focus of this work. The numerical framework has already been defined in the computational framework of single Taylor bubbles in Mierka et al (2021), which in the current work has been extended towards multiple bubbles in arbitrarily curved capillaries.

Numerical Methods

The mathematical model of this work is based on Mierka *et al.* (2021) which is related to a direct numerical simulation of the corresponding multiphase flow problem in a framework of an interface tracking approach implemented in the open source FEM package Featflow. This approach requires an instationary direct resolution of the g/l interface which is therefore always aligned with the computational mesh. The combination with the higher order Q_2/P_1 iso-parametric FEM

Table 1. Summary of the computationally considered cases. d – capillary diameter, D – coil diameter, P – pitch length of the coil, $\bar{v}$ – average velocity (Flowrate divided by cross-sectional area). “Geo” stands for the geometrical variants (see Figure 2), “OP” stands for the respective operation condition (flowrate).

	Geo1/OP1	Geo2/OP1	Geo2/OP2	Geo2/OP3	Geo3/OP1	Geo3/OP2	Geo3/OP3
$d\ [mm]$	1.6	1.6	1.6	1.6	1.6	1.6	1.6
$D\ [mm]$	6.0	12.0	12.0	12.0	24.0	24.0	24.0
$P\ [mm]$	3.0	3.0	3.0	3.0	6.0	6.0	6.0
$\bar{v}\ [cm \cdot s^{-1}]$	3.0	3.0	3.0	12.0	3.0	6.0	12.0

based discretization method allows a semi-implicit treatment of the surface tension $\mathbf{f}_{st}$ by taking advantage of the Laplace-Beltrami transformation:

$$\mathbf{f}_{st} = \int_\Gamma \sigma\left(\underline{\Delta}\ \mathbf{x}|_\Gamma\right) \cdot \mathbf{v}\ d\Gamma \tag{1}$$

Since the new interface position $(\mathbf{x}|_\Gamma)^{n+1}$ can be expressed as the function of the old interface position and the new velocity at the interface:

$$(\mathbf{x}|_\Gamma)^{n+1} = (\mathbf{x}|_\Gamma)^n + \mathbf{u}_\Gamma^{n+1}\Delta t \tag{2}$$

it allows us to represent the surface tension term in a semi-implicit manner guaranteeing a strong stability of the system. The general solution strategy is related to a direct numerical simulation (DNS) of the corresponding multiphase flow problem in a framework of an interface tracking approach, which requires an instationary direct resolution of the *g/l* interface by the computational mesh. The arising set of governing equations written in the generalized (single or multiphase) framework is as follows:

$$\rho(\mathbf{x})\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right] - \nabla \cdot (\mu(\mathbf{x})[\nabla \mathbf{u} + \nabla \mathbf{u}^T]) + \nabla p = \mathbf{f}_{st} \tag{3}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{4}$$

where $\rho(\mathbf{x})$ and $\mu(\mathbf{x})$ represent the density and viscosity of the given phase which, however, depends on (in case of application for a multiphase problem) the particular interface location Γ separating the liquid and the gas phase from each other.

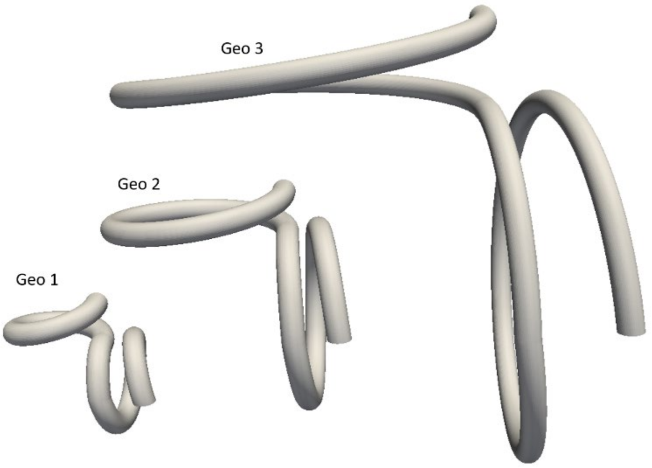

Figure 1. Visual representations of the 3 computationally considered geometrical CFI variants consisting of the inflow coil (2π), inverter bend ($\pi/4$) and outflow coil (2π).

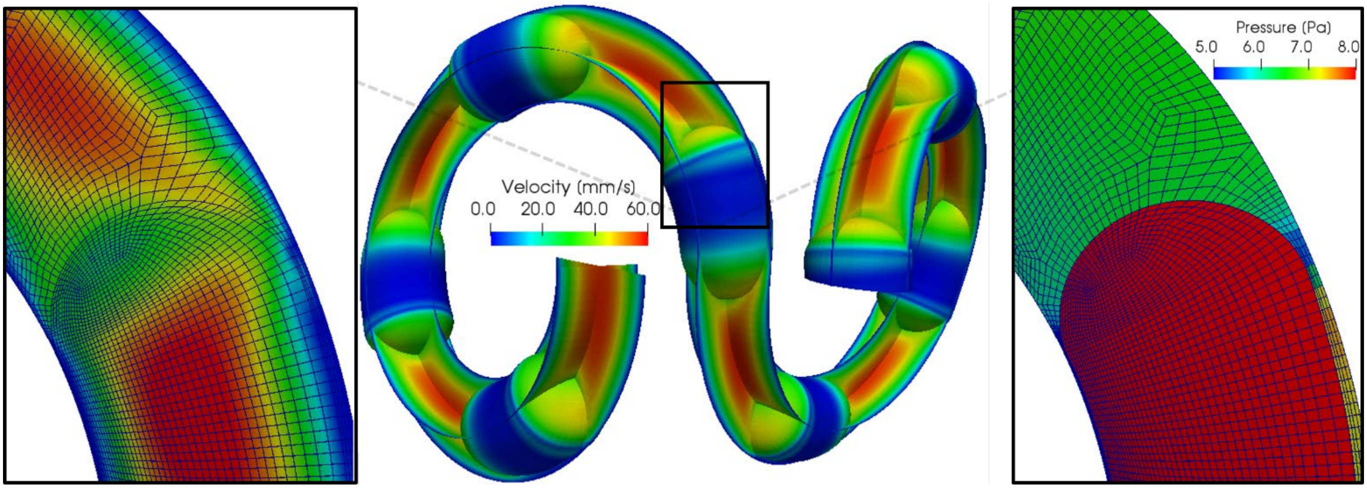

Figure 2: Typical simulation result of the CFI Taylor bubble for the geometry “Geo 1” showing the interface aligned mesh. The close-ups show the respective velocity distribution and the resolved pressure jumps on the respective sides of the interfaces. Note, that the irrelevant buffer regions located at the inflow and outflow of the geometry have been clipped away.

The technical realization of the CFI geometry is based on a transformation mechanism allowing to map arbitrary points from a "straight" capillary system into the curved one. All computational meshes have been created according to this transformation by merging as many identical single bubble/slug patches as the underlying geometry has required to be filled up. The corresponding mesh-deformation equation was also subjected to this decomposition strategy so that each (bubble/slug) mesh segment has been deformed only in its own compartment domain while sharing the mesh nodes with its neighboring compartment. The time-dependent displacement of the computational mesh, $\mathbf{d}$, has been computed by a simple mesh deformation equation:

$$\nabla \cdot (\nabla \mathbf{d} + (\nabla \mathbf{d})^T \ ) = 0 \qquad (5)$$

with tangential slip boundary conditions at the *g/l* interface and at the compartment walls of each individual slug section. The displacement transport equation has been discretized with the Q_1 element in the framework of FEM.

Table 2. Parameter list of physical properties of the gas (G) and liquid (L) phase used for the simulations.

ρ_L	[kg/m^3]	1000
μ_L	[Pa.s]	$1.12 \cdot 10^{-3}$
ρ_G	[kg/m^3]	1.2
μ_G	[Pa.s]	$1.80 \cdot 10^{-5}$
$\sigma_{L/G}$	[N/m]	$[2.50 \ - \ 20.0] \ \cdot 10^{-3}$

Results and Discussion

Several simulation cases (see Table 1) have been generated for a CFI of inner diameter of 1.6 mm, while covering a range of coil diameters (6 mm-24 mm) and a range of Re numbers (48-192). The simulation domain in each of these simulations has covered a full coil+bend+coil geometry (see Figure 2) so that the influence of the inverter bend between the coil segments could be investigated. All cases have been computed until a pseudo periodic condition by the help of additional (bubble/slug) buffer segments fed from the inflow side until two consecutive solutions have not differed more than the prescribed tolerance. The such obtained periodical solutions have been extracted for the subsequent mixing performance analysis by utilization of a (massless) particle tracing initialized by particle seeds in 4 quadrants of the first liquid slug as shown in Figure 3 and Figure 4. For the postprocessing of these particle tracing results the same transformation method has been utilized, however, this time in the inverse direction. The such transformed data made it possible to compare and characterize the dynamic particle distribution (z) in the angular direction (x) and along the length (y) of the capillary. Such a particle distribution reconstruction – referring to the geometrical representation shown in Figure 2 – for the 4 initial particle seeds is demonstrated in Figure 3. The reconstruction is clearly addressing the justification of the 90° bend which substantially contributes to enhanced mixing of the liquid slug.

Conclusions

The developed highly accurate multiphase flow model has proven its robustness by its application on the CFI geometry in a wide range of flow parameters so to reveal the influence of the individual parameters on the mixing efficiency of gas/liquid capillary slug flow. The here developed transformation method has played a key role in the construction of the periodical fluid domain as well as in the postprocessing analysis focused on flow mixing characterization and parameter comparison.

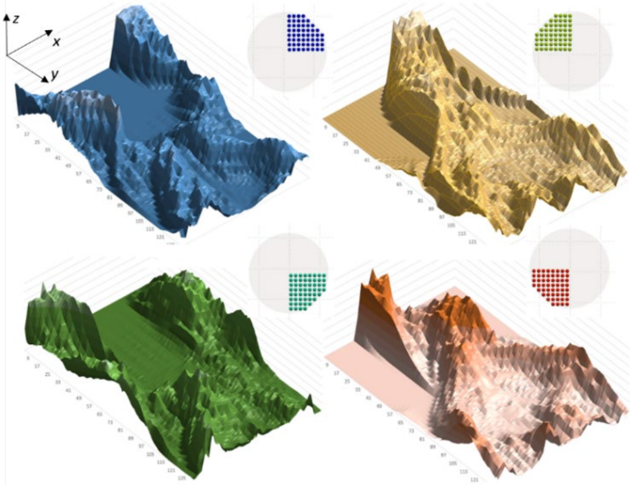

Figure 3: Mixing visualization via particle probability distribution (z) in angular (x) and axial direction (y) of capillary for the particle seeds initialized in the respective capillary quadrants.

Acknowledgements

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References

Kashid M.N., Agar D.W., Turek S., 2007. CFD modelling of mass transfer with and without chemical reaction in the liquid/liquid slug flow microreactor, Chem. Eng. Sci. 62.

Wörner, M., 2012. Numerical modeling of multiphase flows in microfluidics and micro process engineering: a review of methods and applications. Microfl. Nanofl. 12.

Yang L., Nieves-Remacha M.J., Jensen K.F., 2017. Simulations and analysis of multiphase transport and reaction in segmented flow microreactors, Chem. Eng. Sci. 169.

Chatterjee S., Ghanta K.Ch., Hens A., 2021. Study of multiphase flow inside straight and spiral microchannel and effect of two phase flow on Dean's vortices, Chem. Eng. Res. and Des. 165.

Gaddem M.R., Ookawara S., Nigam K.D.P., Yoshikawa S., Matsumoto H., 2021. Numerical modeling of segmented flow in coiled flow inverter: Hydrodynamics and mass transfer studies, Chem. Eng. Sci. 234, 116400.

Mierka, O., Turek, S., 2021. Numerical Simulation Techniques for the Efficient and Accurate Treatment of Local Fluidic Transport Processes Together with Chemical Reactions. In: Schlüter, M., Bothe, D., Herres-Pawlis, S., Nieken, U. (Eds.) Reactive Bubbly Flows. Fluid Mechanics and Its Applications, Springer Cham.

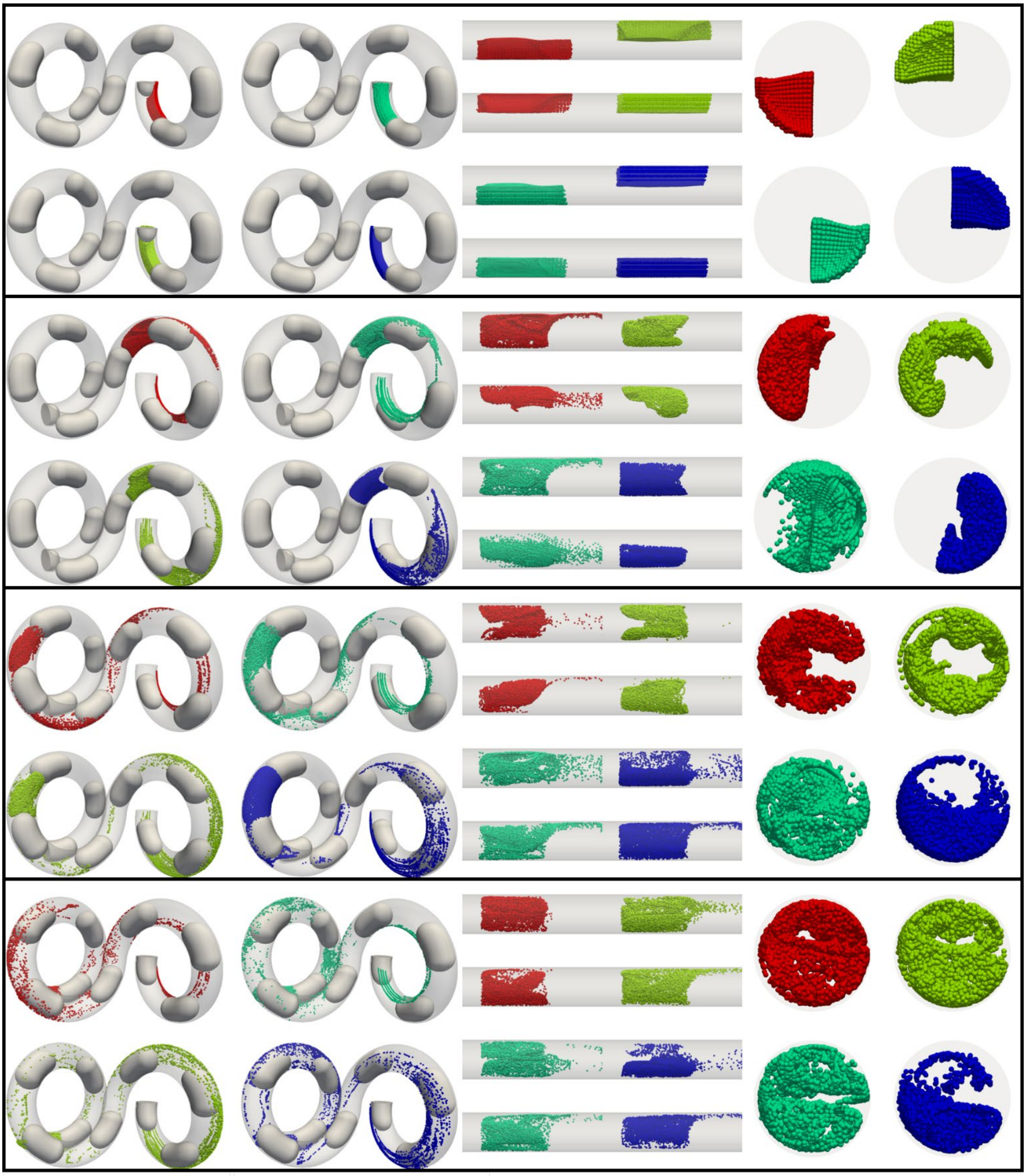

Figure 4. Mixing analysis simulation with the use of particle tracing method. Leftmost sequence shows the particle dynamics in the real geometry. Middle and Right sequences show the particle dynamics in the “backtransformed” geometry in the axial and cross-sectional direction by following the initially seeded liquid slug segment. The evolution of the particle distribution is visualized in the top-to-bottom direction.