Numerical investigations of gas-liquid flows in mini-channels for applications in chemical process engineering

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Abstract

In order to perform detailed numerical investigations of gas-liquid flows with deformable interfaces the in-house computer code TURBIT-VOF is developed at KIT. This contribution gives a concise overview about the mathematical and numerical foundation of the code and provides illustrations of its application in the field of chemical process engineering, where the flow of elongated gas bubbles moving within a continuous liquid phase through narrow channels is finding increasing technological and scientific interest. In the second part of the paper the performance of the TURBIT-VOF code on different hardware platforms available at KIT (NEC SX-8R, NEC SX-9, HP XC3000) is analyzed and conclusions for promising optimization and parallelization strategies are drawn.

1 Introduction

Operations in chemical process engineering that involve multiple phases (e.g. a gas and a liquid or two immiscible liquids) are traditionally performed in large devices (with typical dimension of one or several meters) such as stirred tank reactors, bubble columns or air lift reactors. Micro process engineering aims to perform these operations, where appropriate, in miniaturized devices (with typical dimension of 1 mm or below). The underlying goal is to achieve a "process intensification" by taking advantage of the large surface area to volume ratio and enhanced heat/mass transfer rates. In this context, ceramic monolith reactors (a block with hundreds of straight millimeter-sized rectangular channels) are a promising option for production of liquid fuels from syngas (a mixture of H_2 and CO) by Fischer-Tropsch synthesis [1]. To foster the understanding of the relevant flow phenomena and transport processes, here detailed numerical investigations of the flow of a regular sequence of elongated gas bubbles (Taylor bubbles) embedded in a continuous liquid phase within a single square mini-channel are performed.

2 Numerical method

The time-dependent three-dimensional computations are performed with the in-house computer code TURBIT-VOF developed at KIT. The code is written in Fortran and solves the Navier-Stokes equations with surface tension term in non-dimensional single field formulation for two incompressible Newtonian fluids with constant viscosity and coefficient of surface tension on a regular staggered Cartesian grid by a finite volume method. All spatial derivatives are approximated by central differences. Time integration is performed by an explicit third order Runge-Kutta method. A divergence free velocity field at the end of each time step is enforced by a projection method; the resulting Poisson equation is iteratively solved by the linear solver package LINSOL [2] developed at KIT. The dynamic evolution of the deformable gas-liquid interface is computed by a volume-of-fluid method with piecewise planar interface reconstruction. Thus, in each mesh cell where both phases coexist at a certain time step, the interface is locally approximated by a plane (whose location and orientation is "reconstructed"). For details about the governing equations and the numerical method we refer to [3].

3 Typical results

In performing a numerical simulation for a certain case, the transient evolution from the initial velocity field and bubble shape towards the fully developed flow of a bubble translating with constant velocity and steady shape (corresponding to a certain prescribed axial pressure drop) is computed in a sequence of jobs. Fig. 1 a) shows a sketch of the computational set-up. We consider a so-called unit cell, which consists of one gas bubble and one liquid slug. In axial (vertical) direction we apply periodic boundary conditions to mimic the influence of the trailing and leading bubbles. No-slip boundary conditions are used at the four lateral walls of the channel. As a result of a simulation, detailed data about the full three-dimensional and time-dependent phase distribution, velocity field and pressure field within both phases are obtained; see Fig. 1 b).

In a series of TURBIT-VOF simulations, the co-current downward flow of nitrogen bubbles in viscous squalane (which is a good solvent for Fischer-Tropsch products) within a vertical mini-channel was investigated. The inner dimensions of the square channel are 1 mm × 1 mm, which allows a direct comparison and validation with available experimental results. The axial length of the unit cell L_{uc} is up to 6 mm. In this case the (uniform) grid consists of 80 × 480 × 80 cubic mesh cells (about $3 \cdot 10^6$ mesh cells in total). In Fig. 2 the computed steady bubble shape is displayed for five different values of the capillary number $Ca = \mu_L U_B/\sigma$ and Reynolds number $Re = \rho_L D_h U_B/\mu_L$. Here, U_B is the bubble velocity, D_h the channel hydraulic diameter, σ the coefficient of surface tension, and μ_L and ρ_L are the liquid viscosity and density, respectively. Fig. 2 shows that with increase of Ca the rear and front meniscus of the bubble become more flat and pointed, respectively, in agreement with experiments [4].

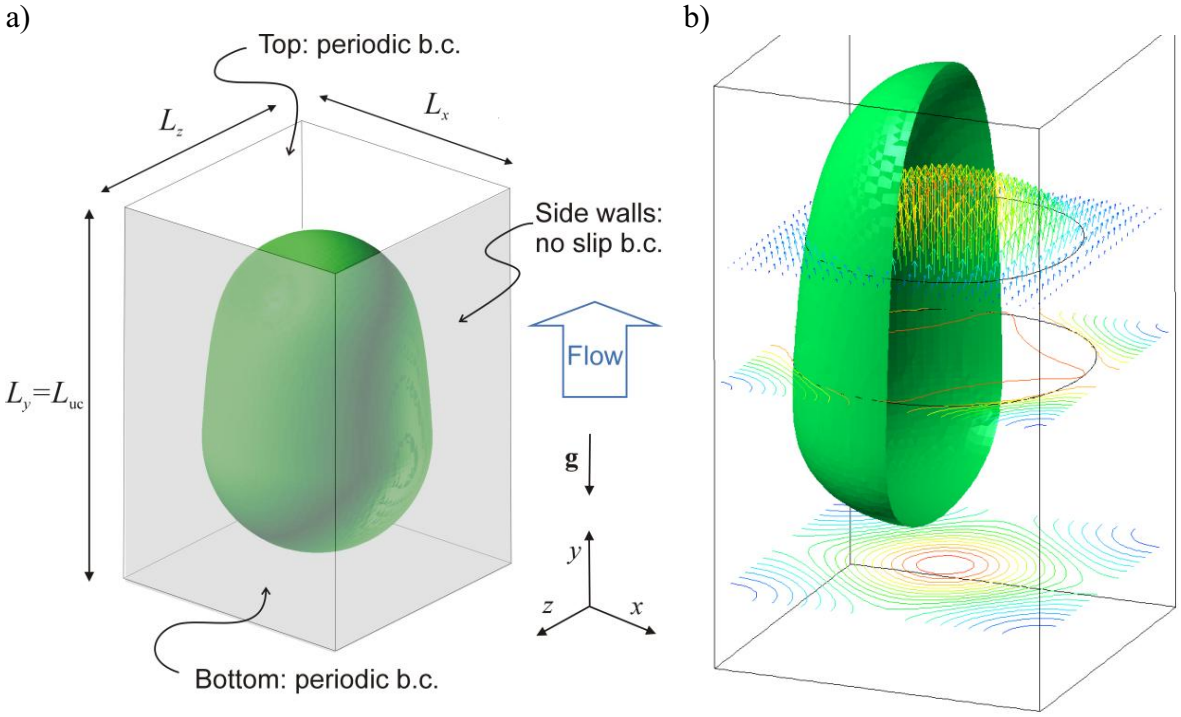

Fig. 1: a) Sketch of computational domain and coordinate system. b) Visualization of computed bubble shape (only half of the bubble is displayed). Also shown are the local velocity field (vectors) and the concentration field (contour lines) of a chemical species (which is transferred from the gas into the liquid phase) in different axial cross-sections

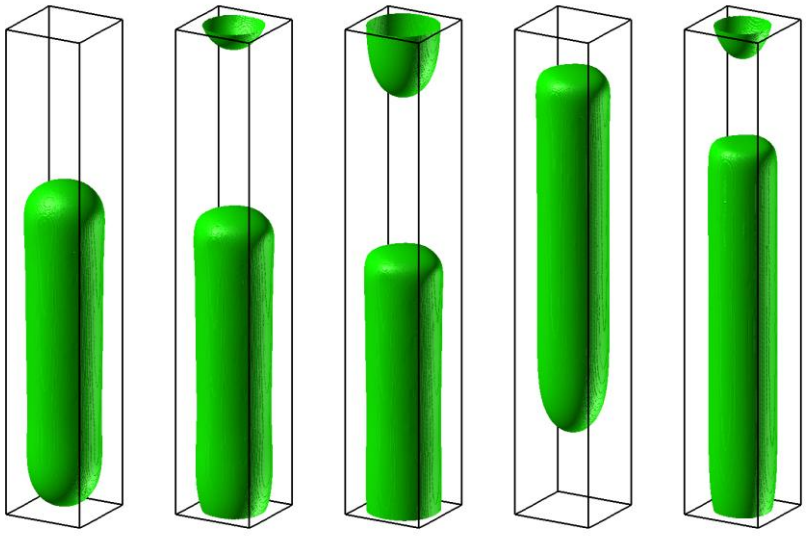

Fig. 2: Perspective view of computed steady bubble shape for L_{uc} = 6 mm for five different values of the capillary number. From left to right, the values of (*Ca; Re)* are (0.045; 1.22), (0.117; 3.19), (0.17; 4.64), (0.25; 6.81), (0.491; 13.4). The solid lines indicate the size of the computational domain. For further details about the simulations we refer to [4,7]

Additionally to the hydrodynamics, the transient interfacial mass transfer of a (passive) chemical species (initially dissolved in the gas phase only) into the continuous liquid phase can be simulated starting from hydrodynamically fully developed flow. Optionally, this mass transfer can be combined with a chemical reaction, which can be homogenous (i.e. occur in the liquid bulk phase) or heterogeneous (i.e. occur at the channel walls) [5,6].

4 Code performance on different hardware platforms

The current hardware platform for production jobs with TURBIT-VOF is the vector computer system NEC SX-8R at the Steinbuch Center for Computing (SCC) located at KIT Campus North. The code is compiled with the sxf90 compiler and an option that ensures double precision representation of all REAL variables. The computations are performed on a single processor since the code is not yet parallelized. The CPU time per mesh cell and time step for running a certain case is typically in the range $60 - 100$ µs. In a transient simulation usually a few 10 000 time steps are computed; this corresponds to a total CPU time of one or several month. As a first step toward the intended optimization of the code, a flow trace analysis is performed by running one of the cases displayed in Fig. 2 for 10 time steps. The results of the flow trace analysis are listed in Table 1. Only those subroutines are included in Table 1 who require at least 1% of the total CPU time. As can be seen, about 75.1 % of the CPU time is consumed by program unit linin2, which includes the calls to the LINSOL solver package for solution of the pressure Poisson equation. The column "Vectorization Optimization Ratio" in Table 1 shows a value close to 100 % for this program unit, indicating excellent vectorization. The other five program units listed in Table 1 belong to the interface reconstruction algorithm EPIRA (exact plane interface reconstruction algorithm) [3,8]. The intersection between the plane which represents the interface and the cubical mesh cell is a polygon, with either 3, 4, 5 or 6 edges. The procedure to determine the number of edges and the location and orientation of each polygon involves a distinction

Program unit	**Frequency**	**Exclusive time**		**Vect. Opt. Ratio**	**Remark**
	[-]	[s]	[%]	[%]	
linin2	10	2499.7	75.1	99.37	Solution of Poisson equation
volume	13165932	181.1	5.4	47.16	Interface reconstruction
wsepbe	103814562	168.5	5.1	0.00	Interface reconstruction
wsepir	415258248	160.7	4.8	0.00	Interface reconstruction
wsbkor	10802207	39.0	1.2	0.00	Interface reconstruction
wsepia	1590	34.4	1.0	0.00	Interface reconstruction

Table 1: Results of flow trace analysis on NEC SX-8 for 10 time steps

between a large number of different cases. As a consequence, the EPIRA algorithm includes many `IF` statements and is thus hard to vectorize. Therefore, for most of these subroutines (with exception of the function volume) the Vectorization Optimization Ratio is zero. Overall, the code reaches a performance of about 4 GFLOPS on SX-8.

Recently the installation at SCC was upgraded by a SX-9, NECs most recent vector system. Since the LINSOL package is not available yet on SX-9, first test runs of TURBIT-VOF on SX-9 are performed using the LINSOL binary compiled on SX-8. The total CPU time for 10 time steps on a 80 × 480 × 80 mesh is reduced from 3327.4 s on SX-8 to 2422.6 s on SX-9, i.e. is about 27.2 % lower on SX-9 than on SX-8. The CPU time of the six program units listed in Table 1 on SX-8 and SX-9 is compared in Fig. 3 a). As can be seen, the vector code (i.e. linin2) is about 65 % faster on SX-9 than on SX-8. On the other hand, scalar code (the program units corresponding to the interface reconstruction) is more than 100 % slower on SX-9 than on SX-8. As a consequence, LINSOL requires only about 35.8 % of the total CPU time on SX-9 instead of the 75.1 % on SX-8, see Fig. 3 b).

The SCC at KIT Campus South operates the distributed memory parallel computer HP XC3000 (abbreviated hc3) which consists of SMP nodes with 64 bit Xeon processors from Intel. On hc3, the TURBIT-VOF code is compiled with the Intel compiler (version 10.1.022) with three different optimization options (-g = no optimization, -O2, and -O3). In Fig. 4 the CPU time on a single hc3 node is compared to that on SX-8 and SX-9. It is evident that the CPU time on hc3 is more than three times larger than on SX-8. Interestingly, the optimization level has only a very small effect on the overall CPU time. The reason is that on hc3 about 97 % of the CPU time is needed by the LINSOL library, which is not affected by the optimization option.

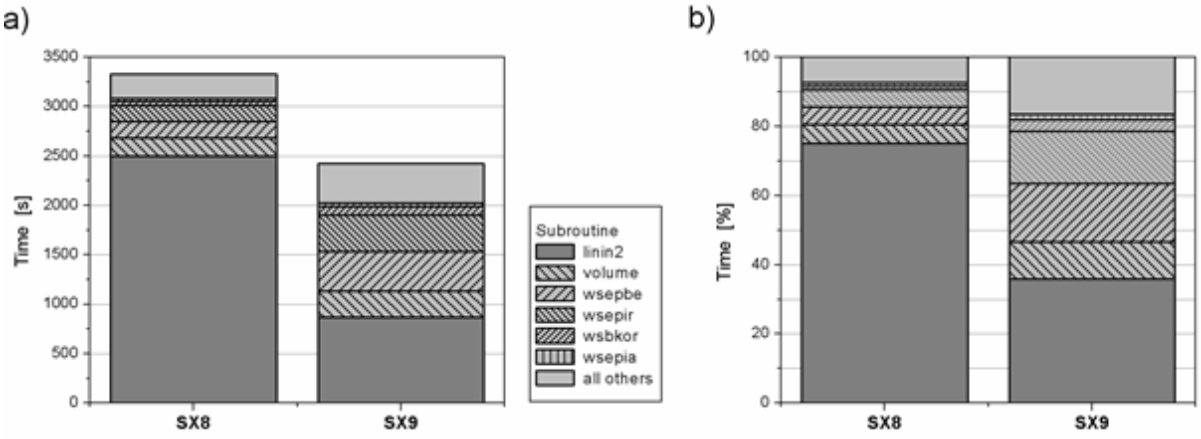

Fig. 3: Comparison of CPU time of different program units on SX-8 and SX-9: a) absolute CPU time (seconds); b) relative CPU time in percent of total CPU time

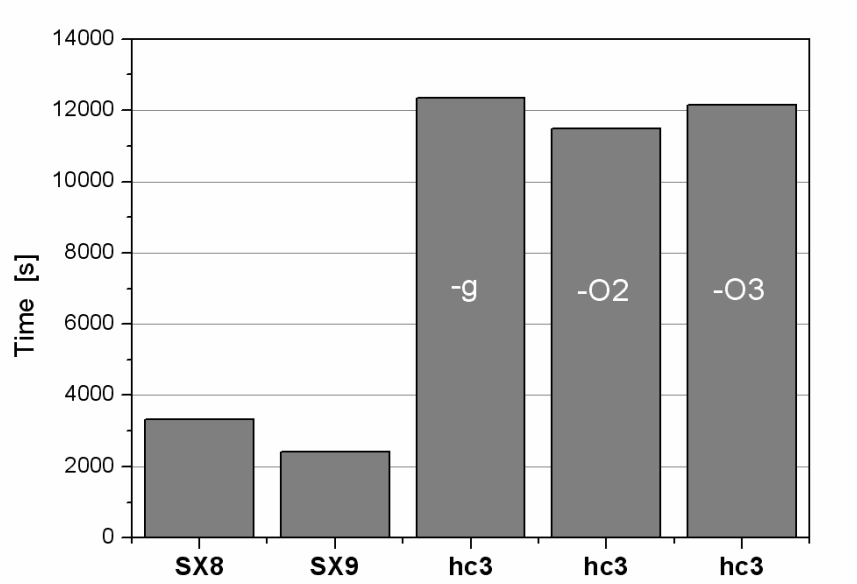

Fig. 4: Comparison of CPU time on SX-8, SX-9 and hc3 (with three different optimization options).

5 Conclusions

The analysis of the performance of the TURBIT-VOF code on different hardware platforms allows the identification of different strategies for possible optimization and parallelization. As on SX-8 about 75 % of the CPU time is required by LINSOL, the most meaningful optimization is to speed up the solution of the pressure Poisson equation. In this context, testing of three measures is suggested by SCC (H. Häfner): i) testing of different solvers available within the LINSOL package, ii) testing of a weaker residuum criterion (currently 10^{-8}), and iii) pre-conditioning. To improve the performance of the code on SX-9, an optimization and (if possible) vectorization of the yet not vectorizable interface reconstruction subroutines is mandatory. As concerns the hc3 machine, running the TURBIT-VOF code on a single node is not meaningful due to the very large CPU time of such a job. The wall clock time can probably drastically be reduced by running a parallel version of LINSOL on a certain number of processors. A promising strategy could thus be to run the unparallelized TURBIT-VOF code on a single hc3 node, but branch to multiple processors when LINSOL is called (a parallel version of LINSOL is available). After solution of the pressure Poisson equation the execution of the TURBIT-VOF code is continued on a single node again. In the near future we intend to test several of the mentioned optimization steps in cooperation with SCC SimLab Energy.

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