Rebuilding of Rothe’s nozzle measurements with OpenFOAM software

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Abstract. In this paper the dsmcFoam solver is tested and validated for the three main solver functionalities of 1) free-stream boundary conditions, 2) kinetic intermolecular collision including internal degrees of freedom and 3) gas/surface interactions. The free-stream utility was improved such that a spatially uniform field of particles gets inserted now yielding reliable results for the cells located close to these patches. Implementation of the collision models were validated for two test cases (monatomic gas mixtures and diatomic gas) by observing the equilibration of both the kinetic and internal energies. It was found that the present code had good agreement to the independent codes of HAWK and SMILE as well as to results by G. Bird. The validation of the present codes treatment for the gas/surface interactions was evaluated using the benchmark case of Rothe’s nozzle measurements. Results show that the present version of dsmcFoam obtained good agreements for this case compared to the measurements of Rothe for density and temperature. It was also found that the Navier-Stokes solver of OpenFOAM produced reasonable results, even though the local Knudsen number of the flow exceeds the range of applicability for this method, Kn=0.1.

1. Introduction
Micro-electro mechanical systems (MEMS) become more common in our daily life and the area of their application is growing very fast. Design of MEMS and evaluation of their performance are mainly done using experimental methods. Obviously, an application of numerical methods can simplify and speed up development of new MEMS. Due to the small size of MEMS an inherent gas-flow can be in both continuum and transitional regimes despite a rather high working pressure. The continuum regime of gas flows are commonly and preferably simulated by the Navier-Stokes-Fourier (NSF) equations. However, experiments such as those performed by Arkilic et al. [7] and Colin [8] have shown that the conventional NSF equations may not produce accurate results for rarefied gas flows. It is normal practice to determine the rarefaction degree of gas flows by the Knudsen number (Kn). The Kn is the ratio of the average traveling distance of a molecule between successive collisions and the characteristic length scale of the flow. The NSF equations applied with continuous boundary conditions of velocity and temperature are commonly known to be valid up to a Knudsen number of 0.001 if no discontinuous boundary conditions are applied [9]. However, the applicability of the NSF equations can be extended to about 0.1 in case the discontinuous boundary conditions of velocity slip and temperature jump are applied [3]. A kinetic approach may therefore be necessary in order to simulate gas flows with Kn numbers higher than 0.1, for example, the direct simulation Monte Carlo (DSMC)
method [3]. The computational cost for this method, however, rapidly increases as the density increases. A suitable approach to obtain a relatively cheap method would be to combine the continuum and kinetic solvers to a hybrid method. However, it is important to obtain a clear understanding of the limits of either solver before the hybrid method can be applied.

According to G. Bird most DSMC programs are difficult to use and/or are not generally available. The main focus of this paper is to validate the DSMC solver (dsmcFoam) of the free and open CFD toolbox OpenFOAM version 2.0.1 by OpenCFD Ltd [2]. Some of the main attractive features of the dsmcFoam solver are that it is applicable for arbitrary 2D/3D geometries, it has parallel processing capacity, it utilizes a Maxellian distribution function for a free-stream flow patch, it incorporates the treatment of diffusive and specular wall reflection models and it applies the variable hard sphere model and a Larsen-Borgnakke internal energy redistribution model [12]. G. Bird considers dsmcFoam being an interesting new program initiative, but states definitive benchmark results are not yet available [13]. This work extends the validation of the dsmcFoam performed by Scanlon et al. [12] as the dsmcFoam solver is here validated for independent cases consisting of collision treatment, free-stream functionality and gas/wall interactions. The cell sizes of each case has been designed to approximately have five molecules in respect to time average in every cell. The DSMC test case of gas/wall interaction consists of the benchmark case of the Rothe nozzle [1] for which the compressible NSF solver of OpenFOAM (rhoCentralFoam) is also applied. Our aim is thus to validate both the NSF and dsmcFoam solvers of OpenFOAM against this well studied problem in order to further use it for MEMS applications.

2. Free-stream improvement of dsmcFoam

The free-stream utility is used to inject particles into the computational domain. This utility applies a Maxwellian velocity distribution function with prescribed values of density, velocity vector and temperature to inject a correct amount of particles at correct velocities. The injected particles move with their velocity and simulation time step. The validation of the free-stream utility was first considered when the Rothe nozzle case was simulated, where the default free-stream utility caused inaccurate pressure values for the cells closest to the inlet patch (about 10% lower than expected and varying with the time step size). A test case for the free-stream utility was thereafter designed which could clearly point out if molecules where inserted in an erroneous manner.

The test case for the free stream consists of a box with inlet on the left hand side and a vacuum on the opposing right hand side, see figure 1. The four remaining sides are set to reflect the particles specularly. The inlet patch is set to produce a free particle stream having a number density of \(2.4513 \times 10^{24} \text{ m}^{-3}\), a bulk velocity of 3000 m/s and a bulk temperature of 10 K. For this case every simulated particle represents \(4 \times 10^{10}\) molecules. The temperature is set low so that molecules obtain a low relative velocity to each other, which allow for the distribution of particles to be isolated and studied, only involve effects arising from the free-stream utility. The simulation box geometry is 0.1 m from inlet to outlet and have a square cross-section with side-width of 0.08 m. The box consists of 20 cells in the flow direction and 16 cells in the two other directions. The time step for this case is chosen to be 10 \(\mu\)s. The case is set not to treat collisions, since it is desired to isolate the phenomena of the insertion of DSMC particles.

In figure 1 (a) it is seen that particles of the conventional free stream utility are released in batches which flow down stream as blocks of particles moving towards the outlet. The free stream function is modified here such that the newly inserted molecules are moved with a step-fraction randomly chosen between zero and unity while all other molecules are moved with an initially full step fraction. This change of procedure causes a spatially correct uniformly distributed insertion of molecules at the inlet patches of the flow geometry. The result for the same test case using the modified free stream utility is shown in figure 1 (b). Here it is seen
that a more uniform distribution of molecules is present.

![Number density of particles in the periodic box](image)

**Figure 1.** Number density of particles in the periodic box. (a) Default free stream utility. (b) Improved free stream utility.

### 3. Collision treatment of dsmcFoam

Two validation cases of G. Bird [3] are chosen in order to validate collision treatment of the variable-hard-sphere model and the Larsen-Borgnakke model of dsmcFoam. The latter of the two models considers polyatomic molecules and thereby treats the interchange of translational energy and rotational energy (vibrational energy cannot be treated for dsmcFoam). In the first validation case only the variable hard sphere model is tested for a gas mixture consisting of 90% of argon molecules (number density \(1.647 \times 10^{19} \text{ m}^{-3}\)) and 10% of helium molecules (number density \(0.183 \times 10^{19} \text{ m}^{-3}\)). For these cases every simulated particle represents \(5 \times 10^{10}\) molecules. The helium molecules are initialized at a temperature of 500 K and the argon molecules are initialized at a temperature of 100 K. The temperature convergence is studied as a function of simulation time. The molecules are simulated in a cubic domain with specular reflecting walls. A comparison of these results is also made with the DSMC codes Hawk [4] and SMILE [5]. The results of this case are shown in figure 2.

![Temperature equilibrium of helium and argon gas species](image)

**Figure 2.** Temperature equilibrium of helium and argon gas species.

![Equilibration of translational (tr) and rotational (ro) temperatures](image)

**Figure 3.** Equilibration of translational (tr) and rotational (ro) temperatures.
It is seen in figure 2 that the three models have the same rate of convergence to the temperature of about 140 K which occurs approximately at a physical time of 0.004 seconds. In figure 3 it is seen that the translational and rotational temperatures of the dsmcFoam model converges to a temperature of 600 K at the physical time of about 0.004 seconds, in similarity to theoretical and DSMC results of G. Bird.

4. Rothe nozzle benchmark validation

The treatment of gas-wall interactions for dsmcFoam is validated using experimental nozzle flow data (Exp) obtained by Rothe [1]. The inlet radius of the converging cone has a height of about 8.3 mm and a half angle of 30 degrees. This is followed by a diverging cone with an exit radius of about 21 mm and a half angle of 20 degrees. The two cones are connected via a throat section with a radius, $r = 2.55$ mm. The longitudinal radii of curvature at the throat equals half of the throat radius. For this nozzle an air flow is present at the inlet and a vacuum condition at the outlet. The Reynolds number notation by Rothe [1], $B = \rho_0 (2H_0)^{1/2}/\mu_0$, is adopted in this investigation, where $H_0$, $\mu_0$ are the specific enthalpy and dynamic viscosity respectively in the stagnation chamber. In this paper the $B = 590$ case of Rothe is chosen to be simulated, with an applied inlet pressure of 473.86 Pa and a temperature of 300 K in agreement to [5].

The simulation geometry and mesh for the dsmcFoam solver are illustrated in figure 4, for which the results are compared with results obtained by the DSMC solver SMILE [5] and the NSF solver of OpenFOAM (NSF-OF). The geometry consists of an axisymmetric two degree wedge of the real nozzle. Although the nozzle geometry is given by Rothe [1] it is important to apply inlet and outlet domains to include certain upstream and downstream effects of the nozzle domain. Upstream of the converging cone a 10 mm long inlet domain is introduced with the free-stream path applied on the left hand side, see figure 4. Downstream of the diverging cone a vacuum chamber is applied with a height of about 29 mm and a length of about 25 mm.

Investigations has been performed by Ivanov et al. [5] concerning sensitivity of these inlet and outlet conditions, based on which the dimensions of the inlet domain and the outlet domains are chosen similarly here. With a similar shape of inlet domain Ivanov et al. found that there was no significant affect dependent on whether the insertion of particles was performed having an (on average) radially uniform velocity profile or a parabolic velocity profile. Due to this reasoning molecules are inserted in this investigation with a flat velocity profile. The mesh is structured except for the converging cone section which is unstructured. The standard mesh of this case consists of 68 017 cells, where only one cell layer is placed in the symmetry direction. The side planes of the wedge are simulated as symmetry-planes by applying specular reflecting surfaces. The dsmcFoam simulation of the Rothe nozzle uses the free stream utility at the inlet and outlet of the nozzle. Collisions are treated by a variable hard sphere model with the extension of Larssen-Borgnakke method for exchanging translational and rotational energy. The temperature of the Rothe nozzle is sufficiently low for vibrational energy to be negligible. Hence the variable hard sphere model with Larssen-Borgnakke translational/rotational energy exchange treatment is considered adequate. The walls of the nozzle scatter reflected molecules according the the fully diffuse Maxwellian distribution of a temperature of 300 K. It should be noted that the SMILE solver treating wall collisions as adiabatic. The NSF was applied with the Maxwellian velocity slip [10] (slip) or both Maxwellian velocity slip and the Smoluchowski temperature jump [11], here referred to as discontinuous boundary conditions (D-BC). The case is run in parallel on four processors divided as illustrated in figure 4. The hardware used is a cluster computer with 16 cpu nodes of 2.34 Ghz AMD opteron processors with 62.95GB RAM memory. For the steady state case to equilibrate takes about a week and averaging of the properties takes also about one week. The NSF solver is run on a single machine.
Figure 4. Nozzle mesh for dsmeFoam, where inl., outl. and w. refer to inlet, outlet and wall respectively. Mesh is a two degree axisymmetric wedge of real nozzle. The processors domains are indicated by numbers in red circles.

The dsmeFoam solver simulates nitrogen gas according to the variable hard sphere model having the parameters shown in Table 1. In the simulation for the B=590 case every dsme particle represents $5 \times 10^8$ real molecules.

| property                  | value                              |
|---------------------------|------------------------------------|
| mass                      | $46.5 \times 10^{-27}$ [kg/m$^{-3}$]|
| $d_{ref}$                 | $4.17 \times 10^{-10}$ [m]         |
| internal degrees of freedom | 2 [-]                             |
| $\omega$                  | 0.74 [-]                           |
| $T_{ref}$                 | 273 [K]                            |
| relaxation collision number | 5.0 [-]                           |

4.1. results

The Knudsen number is calculated for the B=590 case using the dsmeFoam solver. The Kn number is calculated as the ratio of the mean free path, $\lambda$, to the characteristic length scale of the case, $L$. The mean free path for the nitrogen gas is calculated for the variable hard sphere model as follows:

$$\lambda = \frac{1}{\sqrt{2n\pi d_{ref}^2 \left( \frac{T_{ref}}{T} \right)^{\omega-0.5}}}.$$

where $n$, $d_{ref}$ and $T_{ref}$ are the number density, reference diameter and temperature respectively for the gas and $\omega$ is the exponent that relates viscosity to temperature i.e. $\mu \propto T^\omega$ [3]. The length scale is calculated as follows:

$$L = \frac{\Phi}{\partial \Phi/\partial x_i}.$$
In (2) the parameter $\Phi$ is a macroscopic property of the flow e.g. density, bulk velocity or temperature. The Knudsen number is mapped for the $B=590$ case by modifying the post processing utility `dsmcFieldsCalc` of OpenFOAM. In figure 5 the local Knudsen number is illustrated by using the calculated number density in (1) and temperature in (2).

![Figure 5. Kn number contours for $B=590$ case.](image)

From figure 5 the applicability of the NSF equation can be prematurely evaluated. Since the NSF equations should be applicable for Kn numbers up to $10^{-3}$ it is reasonable to assume this method is applicable from the inlet to the throat of the nozzle, but erroneous further downstream. With discontinuous boundary conditions the NSF method should be applicable up to Knudsen numbers of about 0.1. For the nozzle case it is not clear how far downstream this method is applicable since the wall region and axial part of the domain has higher Kn than the rest of the cross sectional domain.

In the left part of figure 6 the centerline profile of mass density is displayed throughout the nozzle. It can be seen that slightly downstream from the throat the NSF-OF solver deviates slightly from the experimental data. Downstream of the throat all of the solvers are considered to produce reasonable results. In the right part of figure 6 the radial profile of the density is displayed scaled by the axial value. It can be seen that the results of the dsmcFoam and the SMILE solvers agree well with the experimental data. It should also be noted that for the density profiles the adiabatic wall method produced similar results as for the thermal wall.
In figure 7 the rotational temperature is displayed. In the left part of figure 7 the centerline profile of temperature is displayed throughout the nozzle. It can be seen here that all the solvers produce reasonable results till an axial position of about 0.03 m after which the NSF-OF with slip and NSF-OF with D-BC has significantly lower temperature that the experimental data. In the right part of figure 7 the radial profile of the density is displayed scaled by the axial value. Here it can be seen that all the solvers are scattered from the experimental data. It is of particular interest to note that the dsmcFoam with thermal wall wall does not manage to capture the correct temperature jump at the wall. However the NSF-OF with D-BC manages to capture the validation temperature at the wall the best being about 15 K above.
Figure 7. Left, temperature profile in axial direction, experimental error-bars from [1]. Right, temperature profile in radial direction at axial position 0.0477 m.

In figure 8 the Mach number profiles are displayed for the dsmcFoam, NSF-OF with D-BC and SMILE solvers for the B=590 case. It can be seen that all the Mach number contours are in reasonable agreement, with the largest discrepancy for the NSF-OF solver with D-BC which has a slightly lower Ma number throughout the domain compared to the DSMC solvers.

Figure 8. Ma number contours for B=590 case. Contours from left to right are: 1, 1.5, 2, 2.5, 3 and 3.5

In figure 9 the density profiles are displayed for the dsmcFoam, NSF-OF with D-BC and SMILE solvers for the B=590 case. It can be seen that all the solvers agree reasonably well except for the for the 0.005 profile of the NSF-OF with D-BC at the axial position.
In figure 10 the temperature profiles are displayed for the dsmcFoam, NSF-OF with D-BC and SMILE solvers for the B=590 case. Here it can be seen that both DSMC solvers produce similar results for the 0.8, 0.6, 0.4 and 0.3 contours within the nozzle. However the dsmcFoam model produces a higher temperature than SMILE in the axial domain as can be seen for the 0.25 contour. It can also be seen that the NSF-OF with D-BC only agrees with the results of the DSMC solvers for the 0.8, 0.6 and 0.4 contours.
5. Discussion and conclusions
The free stream utility of dsmcFoam is improved in such a way that a uniform molecular field gets inserted at the free-stream patches. The collision treatment of dsmcFoam is validated where the variable hard sphere model show very good agreement with results of the alternative DSMC solvers HAWK [4] and SMILE [5]. The Larsen-Borgnakke treatment method for exchanging translational and rotational energy is validated with very good agreement to both theoretical and numerical results of G. Bird [3]. The dsmcFoam solver with corrected of free stream utility gave Rothe nozzle case good cell value results close to the inlet patch, which was not the case for the default free-stream utility. The dsmcFoam solver also in general showed to produce good results for the benchmark case of the Rothe nozzle [1] in comparison to the experimental results of Rothe and the numerical results of SMILE. Also the NSF solver of OpenFOAM is validated here both with and without discontinuous boundary conditions and show good results for large sections of the diverging cone of the Rothe’s nozzle case. However, close to the vacuum patch the rarefaction degree of the flow becomes too great for the NSF solver to produce accurate results for which other solvers are necessary. Further work will be devoted to implement adiabatic wall conditions for the dsmcFoam solver when applied to Rothe’s nozzle case. Further work will also be devoted to investigate the dsmcFoam and NSF solvers applicability for lower gas pressures of Rothe’s nozzle case such as the measurement results having Reynolds numbers of 260 and 110.

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