Hybrid Navier-Stokes/DSMC gas flow simulations in very low pressure thin film deposition

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Abstract. An adaptatively coupled continuum-DSMC approach for compressible, viscous flows has been developed. The continuum domain is described by the unsteady Navier-Stokes equations, solved using a finite volume formulation in compressible form to capture the shock. The molecular domain is solved by DSMC. The coupling procedure is an overlapped Schwarz method with Dirichlet-Dirichlet boundary conditions. The domains are determined automatically by computing the Kn number with respect to the local gradients length scale. The method has been applied to simulate a 1-D shock tube problem and a 2-D expanding jet in a low pressure chamber.

INTRODUCTION

In several applications we are faced with the challenge to model a gas flow undergoing a transition from the continuum to the rarefied flow regime. Examples include: flow around vehicles at high altitudes, particularly re-entry of vehicles in a planetary atmosphere [1], flow through microfluidic gas devices [2], small cold gas thruster nozzle and plume flows [3], and low pressure thin film deposition processes from expanding plasma or gas jets [4].
The main goal of our research, is to develop a comprehensive simulation model for the multi-scale physicochemistry of thin film deposition processes based on the application of an expanding thermal plasma. These processes are of great interest in micro-electronics, coating technology, manufacture of LCD (Liquid Crystal Display) screens etc. During the deposition processes a thermal plasma is generated at a relatively high pressure of 0.1-0.5 bar and then the plasma jet rapidly expands into a low pressure chamber at 10-100 Pa. For this reason the particles mean free path length increases and the gas flow regime changes from the continuum, via the transitional to the rarefied. To understand many intriguing hydrodynamic questions related to these expanding thermal plasma flows [4], it is sufficient to study the hydrodynamic behavior of an expanding gas jet under similar conditions, neglecting plasma effects.
It is always very complicated to describe this kind of flows; in the continuum regime ($Kn \ll 1$), the Navier-Stokes equations can be used to model the gas flow, whereas free molecular flow ($Kn \gg 1$) can be modelled using Molecular Dynamics models. For the intermediate Knudsen number ranges ($Kn = 0.01 - 10$), neither of the approaches is suitable. In this regime the best method to use is DSMC (Direct Simulation Monte Carlo), but, however, when the Knudsen number is less than ~ 0.05, its time and memory expenses become inadmissible.
Different solutions have been proposed to compute such flows. The most standard uses a continuum solver with analytical slip boundary conditions [5]. This method is suitable only in conditions where $Kn < 0.1$ and the precise formulation of the slip boundary conditions is strongly geometry dependent. For this reason, several hybrid continuum/molecular models have been proposed to couple continuum solvers to molecular methods, for instance: Molecular Dynamics (MD) and Navier-Stokes (N-S) equations [6], Boltzmann and N-S equations [7], Direct Simulation Monte Carlo (DSMC) technique and Stokes equations [2], DSMC and incompressible N-S equations [8], and DSMC and N-S equations [9].
In our case we considered, in the continuum regime, the compressible N-S equations and, in the transitional regime, DSMC because it is several order of magnitude more efficient than MD and the Boltzmann equations solvers. The coupling of the two models is reached through an overlapped Schwarz method [8] with Dirichlet-Dirichlet boundary conditions. It is an adaptative method in which, during the computations, the Kn number with respect to the local gradients is computed to determine and divide the CFD (Computational Fluid Dynamics) domain from the DSMC one.

THE HYBRID COUPLING METHOD

CFD Solver

The CFD code used is a 2-D, unsteady code based on a finite volume formulation in compressible form to capture the shock. It uses an explicit, second-order, flux-splitting, MUSCL scheme for the Navier-Stokes equations [10]. An explicit scheme was used because it is more accurate and even if it is more time expensive, the highest time expenses are supposed to come from the DSMC.
Because a high temperature flow has to be modelled, it was not possible to consider both viscosity and thermal conductivity constant, so a power-law temperature dependence was used for the viscosity μ and a model coming from kinetic gas theory for the thermal conductivity κ. The density was computed from the ideal gas law.

Molecular Algorithm: DSMC

We developed a 2-D DSMC code, based on the algorithm that has been described in more detail in [11].
For the implementation of inlet (outlet) boundary conditions, a "particle reservoirs" approach is used. A Maxwell-Boltzmann or a Chapmann-Enskog [12] velocity distributions can be used to generate molecules in those reservoirs.

Schwarz Coupling

Two different strategies have been developed and implemented for coupling the Navier-Stokes based CFD code to the DSMC code: One for steady state flow simulation, the other for unsteady flow simulations. Both will be described below.

Steady Formulation

The hybrid coupling method proposed is based on the Schwarz method [8] and it consists of two stages.
The first stage is a prediction stage, where the unsteady N-S equations are integrated in time on the entire domain Ω until a steady state is reached. From this steady state solution, local Kn numbers with respect to the local gradients length scales [13] are computed according to

$$Kn_Q = \frac{\lambda}{Q} | \bigtriangledown Q |$$

where Q is a flow property (density, temperature etc.); The values of Kn_Q are used to split Ω in the subdomains Ω_{DSMC} ($Kn > Kn_{split}$), where the flow field will be evaluated using the DSMC technique, and Ω_{CFD} ($Kn < Kn_{split}$), where N-S equation will be solved. For Kn_{split} a value of 0.05 was used. Between the DSMC and CFD regions an overlap region is considered, where the flow is computed with both the DSMC and the CFD solver.
In the second stage, DSMC and CFD are run in their respective subdomains with their own time steps (Δt_{DSMC} and Δt_{CFD}, respectively), until a steady state is reached. First DSMC is applied; molecules are allocated in the DSMC subdomain according to the density, velocity and temperature obtained from the initial CFD solution. A Maxwell-Boltzmann or a Chapmann-Enskog distributions can be chosen to create molecules. It is important to say that the grid is automatically refined in the DSMC region in order to respect the DSMC requirements. The boundary conditions to the DSMC region comes from the solution in the CFD region. As described in the previous section for the inlet (outlet) boundary, outside the overlapping region some "particle reservoirs" are considered. In these cells molecules are created according to density, velocity, temperature and their gradients of the solution in the CFD region, with a Maxwell-Boltzmann or a Chapmann-Enskog distributions. After running the DSMC, the N-S equations are solved in the CFD region. The initial and boundary conditions comes from the solution in the DSMC region averaged over the CFD cells.
Once a steady state solution has been obtained in both the DSMC and N-S region, the local Kn_Q numbers are re-evaluated and a new boundary between the two regions is computed. This second stage is iterated until in the overlapping region DSMC and CFD solutions differ less than a prescribed value.

We made an extensive study of the influence of various coupling parameters, such as the size of the overlap region ($4-59$ mean free path lengths) and the amount of averaging applied to the reduce DSMC noise (averaging over 5, 30 and 50 repeated runs). The influence of these parameters on the final solution was found to be small.

Unsteady Formulation

In the unsteady formulation, the described coupling method is re-iterated every coupling time step $\Delta t_{coupling} >> \Delta t_{DSMC}, \Delta t_{CFD}$, starting on the solution at the previous time step. As expected, it was found to be necessary to keep the Courant number (based on the coupling time step, the molecules most probable velocity, and the CFD grid cell size) below one, in order to avoid instabilities in the solution.
In the second stage, every coupling step, the program compares the predicted DSMC region with the one of the previous step. In the cells that still belong to the DSMC region, we consider the same molecules of the previous time step whose properties were recorded. Molecules that are in the cells that no longer belong to the DSMC region are deleted. In cells that have changed from being a CFD cell into being a DSMC cell, new molecules are created with a Maxwell-Boltzmann or a Chapmann-Enskog distribution, according to the density, velocity and temperature of the CFD solution at the previous time step.
At the end of the every coupling step molecule properties are recorded to set the initial conditions in the DSMC region for the next coupling step.

RESULTS

1-D Shock-Tube Problem

The unsteady coupling method was applied to the unsteady shock tube test case (fig.1).

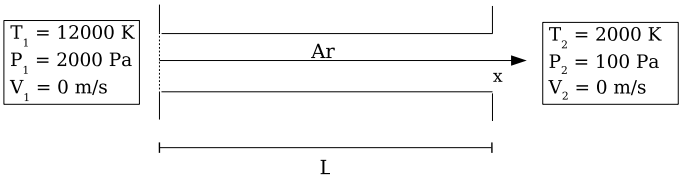

FIGURE 1. Shock tube test case.

The code models the flow field inside an $L = 0.5m$ long tube linking two tanks of the same fluid (Argon), but in different thermo-fluid-dynamic conditions. A membrane at the interface between the first tank and the tube divides the two regions where the fluid is in different conditions. At the instant $t = 0$ the membrane breaks and the fluid can flow from one region to the other. For the test, we suppose that in both tanks the fluid is initially at rest; in the left tank it is at a pressure $P_1 = 2000Pa$ and at a temperature $T_1 = 12000K$, while in the right tank it is at a pressure $P_2 = 100Pa$ and at a temperature $T_2 = 2000K$.
Inside the tube, we suppose that the flow is fully 1-D. Upstream (left) from the shock, the gas has a high temperature and relatively high pressure, and gradient length scales are small. Downstream (right) from the shock, both temperature and pressure are much lower, and gradient length scales are large. As a result, the local Knudsen number Kn_Q is high upstream from the shock, and low downstream of it. In the hybrid DSMC-CFD approach, DSMC is therefore applied upstream, and CFD is applied downstream. The continuum grid is composed by 100 cells in the x direction and 1 cell in the y direction, while the code automatically refines the mesh in the DSMC region to fulfill its requirements. In the DSMC region molecules were created with the Chapman-Enskog distribution. It was demonstrated, in fact, that in a hybrid DSMC/CFD method a Chapman-Enskog distribution is required when the viscous fluxes are taken into account, while a simple Maxwellian distribution is adequate when the continuum region is well approximated by the Euler equations [9]. The particle cross section was evaluated using the VSS model because it is more accurate than VHS to model viscous effect. The coupling time step is $\Delta t_{coupling} = 2.0 \times 10^{-6} sec.$ and the ensemble averages of the DSMC solution to reduce the scattering were made on 30 repeated runs. In addition to the hybrid approach, the problem was also solved using CFD only and DSMC only (which was feasible because of the 1-D nature of the

problem). The latter is considered to be the most accurate. In fig.2 the pressure inside the tube after $3.0 \times 10^{-5} sec.$, evaluated with the hybrid (Schwarz coupling) method is compared with the results of the full DSMC simulation and the full CFD simulation.

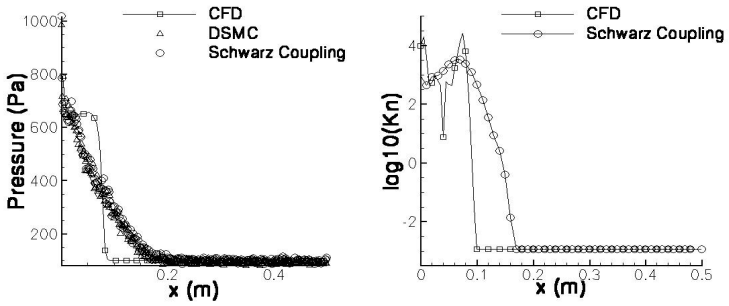

FIGURE 2. Pressure and Kn number in the tube after $3.0 \times 10^{-5} sec.$.

In the same picture also local Knudsen number Kn_Q, computed using the hybrid method, is compared with the full CFD simulation.
From the results shown in fig.2, it is clear that the full CFD approach fails due to the high values of the local Kn number caused by the shock presence. The full CFD approach predicts a shock thickness less than 1 cm, which is unrealistic considering the fact that the mean free path near the shock is of the order of several centimeters. In the full DSMC approach, therefore, the shock is smeared over almost 20 cm. The results obtained with the hybrid approach are virtually identical to those obtained with the full DSMC solver, but they were obtained in less than one fifth of the CPU time.

2-D Expanding Jet in the Low Pressure Deposition Chamber

The steady-state coupling method was applied to a steady state expanding neutral gas jet in a low pressure deposition chamber (fig.3).

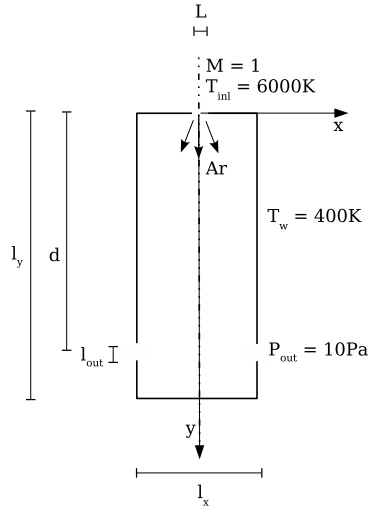

FIGURE 3. Expanding jet in a low pressure deposition chamber test case.

An Argon jet at a temperature of $T_{inl} = 6000K$ and Mach number $M = 1$ is injected, through a slot of $L = 0.032m$ wide, in a chamber of dimensions $l_x = 0.32m$ in x direction and $l_y = 0.8m$ in y direction. The pressure inside the

chamber is kept at a value of $P_{out} = 10Pa$ by a pump connected to it through two slots of $l_{out} = 0.04m$ wide disposed on the lateral sides symmetrically with respect to the chamber vertical axis at a distance $d = 0.6m$ from the top. The walls of the chamber are cooled at a temperature $T_w = 400K$. Inside the chamber we suppose the flow to be 2-D, and because of the geometric symmetry with respect to the vertical axis only half of the flow field was simulated. The continuum grid is composed by 50 cells in the x direction and 160 cell in the y direction while the code automatically refines the mesh in the DSMC region to fullfill its requirements. In the DSMC region, molecules were created with the Chapman-Enskog distribution and the particle cross section was evaluated using the VSS model. Fig.4 shows the Knudsen number in the chamber, respectively evaluated with reference to the inlet dimension (Kn_L) and to the local temperature gradient length scale (Kn_T); Again, as in the case of the shock tube, there are various counteracting effects influencing the local Knudsen number: As a result of the decrease in pressure, the mean free path increases from the inlet to the exit of he chamber. As a result of the cooling of the gas, the opposite effect occurs. And finally, smaller local gradient length scales are present near the inlet than in the rest of the chamber. The overall effect is that (local) Knudsen numbers are high near the inlet, and low in the rest of the chamber. In the right-hand side of Fig.4, the resulting division between the DSMC, CFD and overlapping regions is shown.

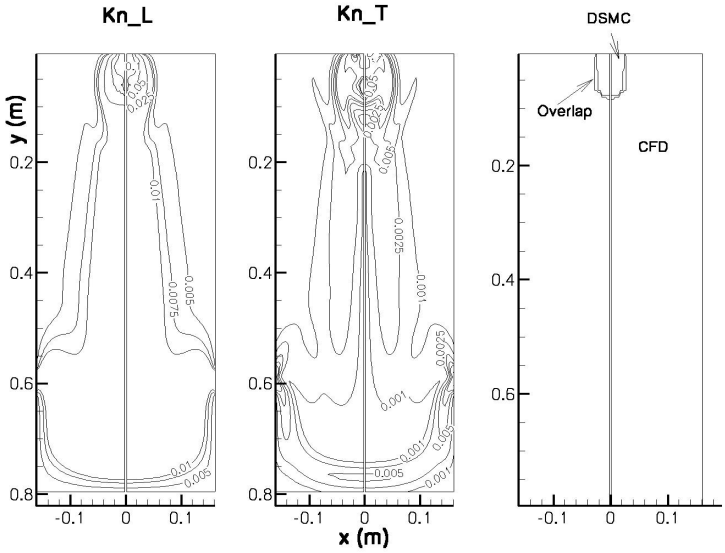

FIGURE 4. Kn number and CFD/DSMC domains splitting

In fig.5 the velocity and temperature fields inside the chamber, evaluated with the hybrid (Schwarz coupling) method, is compared with the results of a full CFD simulation. It is evident that the DSMC region influences the flow field and its effects are present in a region wider then the DSMC and overlapping regions alone. Far away from the DSMC region, however, the full CFD and the hybrid method give the very similar results.

CONCLUSIONS

A hybrid continuum-rarefied flow simulation method has been developed to couple a Navier-Stokes description of a continuum flow field with a DSMC description of a rarefied one. The coupling between the continuum and molecular subdomains is achieved by an overlapped Schwarz method, and has been implemented both for steady state and transient flows. Continuum subdomain boundary conditions are imposed on the molecular subdomain via particle reservoirs based on a Maxwell-Boltzmann or a Chapman-Enskog velocity distribution. The molecular subdomain boundary conditions are imposed on the continuum subdomain using simple averaging. The subdomains are determined automatically by computing the Kn number with respect to the local gradients length scale on a preliminary Navier-Stokes solution.

The method has been applied to a shock tube and to a 2-D expanding jet in a low pressure deposition chamber problems showing its capability of predicting the flow field even where a CFD solver fails.

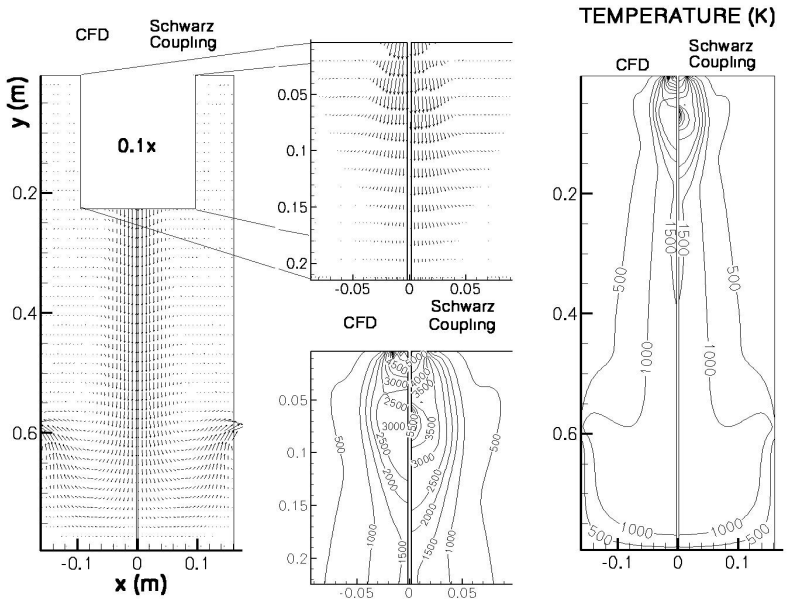

FIGURE 5. Velocity and temperature fields in the deposition chamber

ACKNOWLEDGMENTS

We thank Prof. D.C.Schram and M.C.M. Van de Sanden for a lot of usefull discussions and the DCSE (Delft Centre for Computational Science and Engineering) for financial support.

REFERENCES

1. F.Sharipov, Hypersonic flow of rarefied gas near the brazilian satellite during its re-entry into atmosphere, Brazilian Journal of Physics, vol.33, no.2, June 2003
2. O.Aktas, N.R.Aluru, A combined Continuum/DSMC technique for multiscale analysis of microfluidic filters, Journal of Computational Physics 178, 342–372 (2002)
3. C.Cai, I.D.Boyd, 3D simulation of Plume flows from a cluster of plasma thrusters, 36th AIAA Plasmadynamics and Laser Conference, 6-9 June 2005, Toronto, Ontario, Canada, AIAA-2005-4662
4. M.C.M.van de Sanden, R.J.Severens RJ, J.W.A.M.Gielen et al. (1996), Deposition of a-Si:H and a-C:H using an expanding thermal arc plasma, Plasma sources Science and Technology 5 (2): 268–274
5. B.Alder, Highly discretized dynamics, Physica A 240 (1997) 193-195
6. N.G.Hadjiconstantinou, Hybrid Atomistic-Continuum formulations and moving contact-line problem, Journal Computational Physics 154, 245–265 (1999)
7. P.Le Tallec, F.Mallinger, Coupling Boltzmann and Navier-Stokes Equations by half fluxes, Journal Computational Physics 136, 51–67 (1997)
8. H.S.Wijesinghe, N.G. Hadijconstantinou, A hybrid Continuum-Atomistic scheme for Viscous, incompressible gaseous flow, 2002
9. A.L.Garcia, J.B.Bell, W.Y.Crutchfield, B.J.Alder, Adaptative mesh and algorithm refinement using Direct Simulation Monte Carlo, Journal of Computational Physics 154, 134-155 (1999)
10. S.Y.Chou, D.Baganoff, Kinetic flux-vector splitting for the Navier-Stokes equations, Journal Computational Physics 130, 217–230 (1997)
11. G.A.Bird, Molecular gas dynamics and Direct Simulation Monte Carlo, Claredon Press Oxford Science, 1998
12. A.L.Garcia, B.J.Alder, Generation of the Chapman-Enskog distribution, Journal Computational Physics 140, 66–70 (1998)
13. Wen-Lan Wang, I.D.Boyd, Continuum Breakdown in Hypersonic Viscous Flows, 40^{th} AIAA Aerospace Sciences Meeting and Exhibit, January 14-17, 2002, Reno, NV