

Gas-Kinetic Simulation of Microdroplet-Gas Interaction

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Introduction

Most numerical approaches to handle gas-fluid interactions are based on continuum methods. A main disadvantage is the necessity of continuum assumptions including local thermodynamic equilibrium or limitations to quasi-steady conditions.

Within this project the interaction between gas flows and liquid nano-scale droplets will be simulated using the Direct Simulation Monte Carlo (DSMC) method [1]. DSMC approximates the gas flow from a microscopic point of view and discrete simulation particles allow for a treatment of non-equilibrium effects. Consequently, a comparison between DSMC and existing analytical results will be of fundamental interest to analyse the effects of equilibrium assumptions and flow unsteadiness.

In this work the used methods and tools are presented. The used models are described and the first results are presented and discussed.

Direct Simulation Monte Carlo

The gas phase is modelled by approximatively solving the Boltzmann equation (1) with the DSMC method where t is the time, \vec{v} the velocity, \vec{x} the spatial position, F the external forces and m the species mass.

$$\left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla_{\vec{x}} + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} \right) f(\vec{x}, \vec{v}, t) = \frac{\partial f}{\partial t} \Big|_{\text{Collision}} \quad (1)$$

The focus is to statistically reconstruct the particle distribution function $f(\vec{x}, \vec{v}, t)$ with N discrete particles distributed in space with

$$f(\vec{x}, \vec{v}, t) = \sum_{p=1}^N w_p \cdot \delta(\vec{x} - \vec{x}_p(t)) \cdot \delta(\vec{v} - \vec{v}_p(t)) \quad (2)$$

Where $w_p = N_{real}/N_{sim}$ is the weighting factor of the simulated particles, δ the delta function, $\vec{x}_p(t)$ and $\vec{v}_p(t)$ the time dependant particle position and particle velocity respectively. In contrast to Molecular Dynamics simulations the deterministic description of each microscopic particle state and interaction is not of interest. Movement and collision are decoupled in every simulation time step and collisions are solved statistically using phenomenological probability models and comparison to random numbers. Macroscopic values like number density and heat fluxes are then calculated from moments of the resulting sampled particle distribution, E.g., particle number density $n = \int f dv$ and heat flux $\dot{q}_i = \frac{m}{2} \int c^2 \cdot c_i \cdot f dc$ with the thermal velocity $c_i = v_i - u_i$.

Plasma Flow Solver PICLas

PICLas [2], a highly flexible tool for simulation of rarefied 3D plasma flows, is used for the shown simulations. PICLas is cooperatively developed by the Institute of Aerodynamics and Gasdynamics (IAG) and the Institute of Space Systems (IRS) at the University of Stuttgart. Figure 1 illustrates a representative simulation time step in PICLas, where the Particle in Cell (PIC) and DSMC method are coupled. Particle in Cell (PIC) calculates the interpolation of electromagnetic forces and DSMC the intermolecular collisions. Additionally other continuum based particle methods are in development to approximatively solve the total Boltzmann equation such as Fokker-Planck (FP), Bhatnagar-Gross-Krook (BGK) and Low-Difusion (LD).

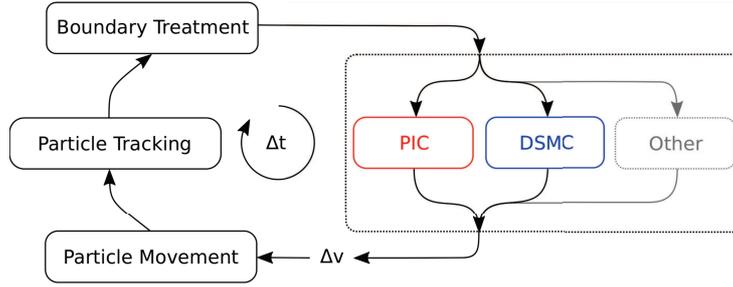


Figure 1. Scheme showing one simulation time step (Δt) of PICLas with the loadable solver modules

Liquid boundary

For the simulation of liquid boundaries a simple evaporation / condensation model is implemented. To calculate the number of evaporating particles ΔN per time step Δt from a liquid surface area A_{liq} the Hertz-Knudsen equation (3) is used. The saturation pressure p_s is defined by the Antoine equation (4) for a given liquid temperature T_{liq} with A , B and C being species specific parameters. Energies and velocities of evaporating particles are sampled from a Maxwell distribution at liquid temperature. For condensation every liquid species particle colliding with the liquid surface is removed and gas species particles are reflected applying diffuse scattering. This represents a condensation coefficient $\sigma_c=1$. The described implementation is tested by simulating a 3D domain with periodicity in x and y direction representing a quasi-1D test case of H_2O evaporation into pure O_2 gas as shown in figure 2. Furthermore, figure 3 shows the velocity distribution sampled in the vicinity of the liquid boundary for both species.

$$\frac{\Delta N}{\Delta t} = \sigma_c A_{liq} \frac{p_s}{(2\pi m k_B T_{liq})^{1/2}} \quad (3)$$

$$\log_{10}(p_s) = A - \frac{B}{C - T_{liq}} \quad (4)$$

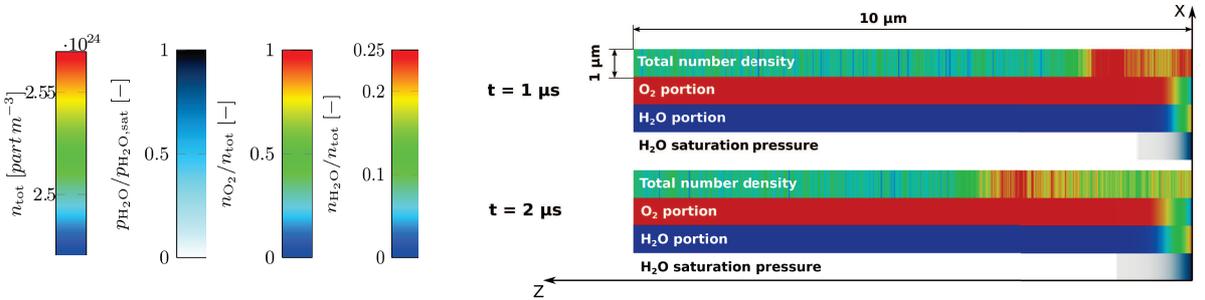


Figure 2. Simulation of liquid evaporation with liquid boundary at $z = 0 \mu\text{m}$. Domain is symmetric in x and y direction with an open boundary at $z = 10 \mu\text{m}$. Initial values: $p_\infty = 10\,000 \text{ Pa}$, $T_{O_2} = T_{H_2O} = 293 \text{ K}$.

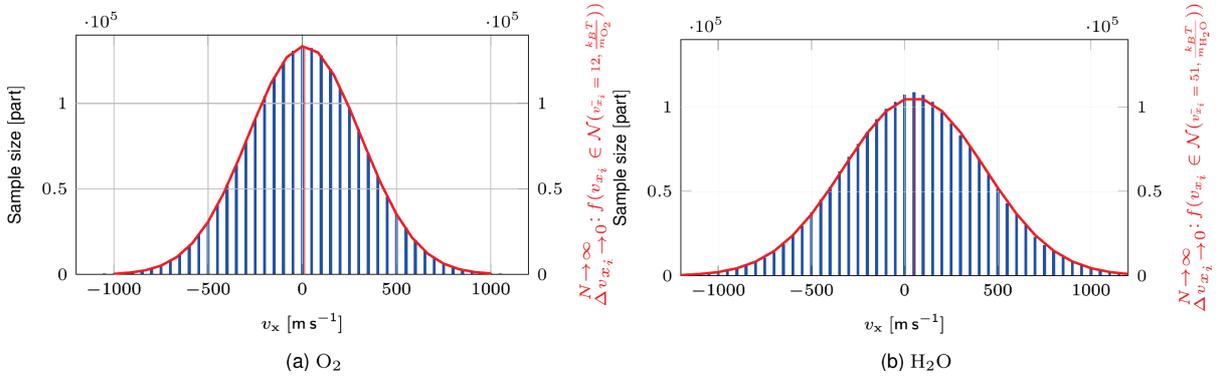


Figure 3. Plots showing comparison of sampled (blue bars) particle velocity distribution (z -component) to calculated (red line) distribution for infinite particle numbers at liquid boundary within $\Delta z = 1 \mu\text{m}$.

Simulation of evaporating droplet

To investigate influences of microscopic effects of droplet evaporation a 3D simulation setup of a flow around an evaporating droplet was constructed. Due to the physical constraints of DSMC for this density region, the number of simulated particles is quite high. To reduce computational effort the computational domain was reduced to a $\frac{1}{4}$ sphere. Table 1 shows chosen parameters for the simulation and figure 4 shows a 2D slice showing a density result.

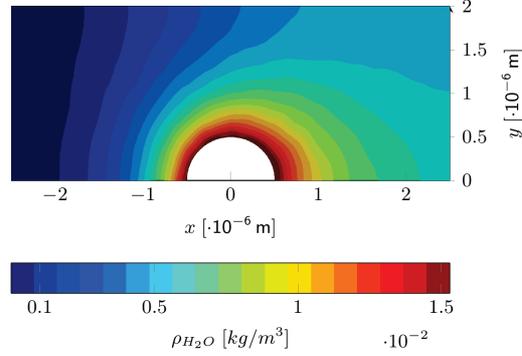


Figure 4. Vapor density around an evaporating H_2O droplet in a O_2 flow for given parameters at t sample simulated with a $\frac{1}{4}$ sphere 3D domain.

Table 1. Parameters used for simulation of droplet evaporation. 3D quarter sphere chosen as computational domain.

Parameter		Dimension	Value
v_x	Flow velocity	$[m\ s^{-1}]$	10
T_{O_2}	Gas temperature	[K]	293
$T_{droplet}$	Droplet temperature	[K]	293
ρ_{O_2}	Gas density	$[kg\ m^{-3}]$	1.165
d	Droplet diameter	$[\mu m]$	1
Kn_d	Knudsen number (reference length $L = d$)	[-]	0.05
t_{sample}	Sampling time interval	$[\cdot 10^{-6}\ s]$	1
Δt	Simulation time step	$[\cdot 10^{-11}\ s]$	1

Influences of droplet size on drag coefficient

Simulations using droplet sizes from table 2 were performed for a solid and evaporating sphere using the previous setup of a $\frac{1}{4}$ sphere. Additionally, the drag forces F_d on the sphere in x direction were sampled.

Figure 5 shows the results of the drag coefficient calculated from respective simulation results with equation (6). Those results are compared to an analytic equation (5) for the drag coefficient at low Reynolds numbers [3]. The results match for the higher Reynolds number case. However, for the lower Reynolds number case the simulated drag coefficient seems to be underpredicted by the simulation. The reason might be continuum breakdown effects indicated by higher Knudsen numbers of 0.05 for this case as shown in table 2. However, to further investigate this behaviour additional simulations have to be conducted.

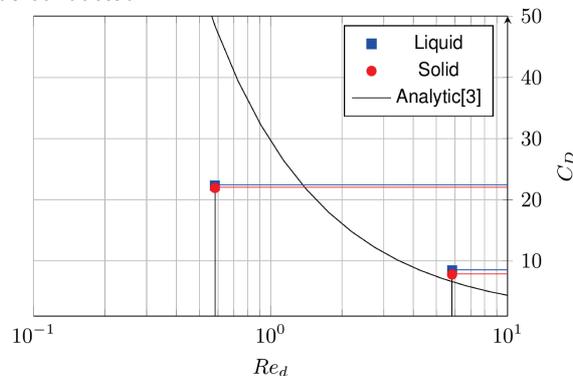


Figure 5. Drag coefficient for evaporating and solid sphere simulated with PICLAs and analytic values for respective Reynolds and Knudsen number values given in table 2.

$$C_d = C_0 \left[1 + \left(\frac{\bar{\delta}_0}{Re_d} \right)^{1/2} \right]^2 \quad C_0 \bar{\delta}_0 = 24, \quad \bar{\delta}_0 = 9.06 \quad (5)$$

$$C_d^{\text{sim}} \equiv \frac{2F_d}{\rho_\infty u_\infty^2 A_{ref}} \quad A_{ref} = \pi \left(\frac{d}{2} \right)^2 \quad (6)$$

Table 2. Resulting Reynolds and Knudsen numbers for respective diameters of simulated droplets.

Parameter	Dimension	Set 1	Set 2
d	Droplet diameter	1	10
Re_d	Reynolds number (reference length $L = d$)	0.5825	5.825
Kn_d	Knudsen number (reference length $L = d$)	0.05	0.005

Nomenclature

f	particle distribution function [-]
x	position / distance [m]
t	time [s]
F	force [N]
d	diameter [m]
A	surface area[m ²]
T	temperature [K]
m	mass [kg]
w_p	weighting factor of particle p [-]
N_i	particle number of i [part]
\dot{q}	heat flux [W m ⁻²]
c	thermal velocity [m s ⁻¹]
v	total velocity [m s ⁻¹]
u	drift velocity [m s ⁻¹]
ρ	density [kg m ⁻³]
p	pressure [Pa]
Re_d	Reynolds number for reference length d [-]
Kn_d	Knudsen number for reference length d [-]
σ_c	condensation coefficient [-]
k_B	Boltzmann constant [J K ⁻¹]

References

- [1] Bird, G. A., Molecular Gas Dynamics and Direct Simulation of Gas Flows, Oxford Science Publications 42, 1994.
- [2] Munz, C.-D. et al., Coupled particle-in-cell and direct simulation monte carlo method for simulating reactive plasma flows, Comptes Rendus Mécanique 342 (10) 662–670 (2014).
- [3] F. F. Abraham, Functional dependence of drag coefficient of a sphere on reynolds number, The Physics of Fluids 13 (8) 2194–2195 (1970).