Multi-scale modelling of molecular phenomena in plasma-assisted thin film deposition

Project Aim

This project aims to developing a comprehensive simulation model for the multi-scale hydrodynamics and physicochemistry of thin film deposition in an expanding thermal plasma jet reactor. The plasma jet, which is generated at near atmospheric pressure, supersonically expands into a near-vacuum environment. The challenge is to link continuum (CFD) gas flow simulations in the low Knudsen number regions, to molecular (DSMC) gas flow simulations in the high Knudsen number regions.

Progress

The earlier developed 2-dimensional steady-state hybrid Navier-Stokes/DSMC code has been extended to model transient flows. The applied Dirichlet-Dirichlet coupling in combination with domain overlap was found to hold significant advantages over flux based coupling methods published in literature, in that it much less sensitive to DSMC noise and allows for time step decoupling between the DSMC and NS solver.

Dissertations

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Scientific Publications

1. G. Abbate, B.J. Thijsse and C.R. Kleijn. Validation of a Hybrid Navier-Stokes/DSMC Method for Multiscale Transient and Steady-State Gas Flows International Journal on Multiscale Computational Engineering, 6(1), 2008, pp. 1-12.
2. G. Abbate, C.R.Kleijn, B.J.Thijsse, R.Engeln, M.C.M.van de Sanden, and D.C.Schram. The influence of rarefaction on the flow dynamics of a stationary supersonic hot gas expansion. Physical Review E, 77, 2008, article # 036703.
3. G. Abbate, B.J. Thijsse and C.R. Kleijn. "Multi-Scale Modelling of the 2-dimensional Flow Dynamics in a Stationary Supersonic Hot Gas Expansion" Lecture Notes in Computer Science 5102, pp. 251-260, 2008.

Projectleaders

CR Kleijn

Researchtheme

Complex dynamics of fluids
Mathematical and computational methods for fluid flow analysis

Participants

G Abbate

Cooperations

Prof.dr. B.J.Thijsse (TUD-WbMT)
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Funded

Delft Centre for Computational Science & Engineering
1st 100% 2nd - 3rd -

Start of the project

2004

Information

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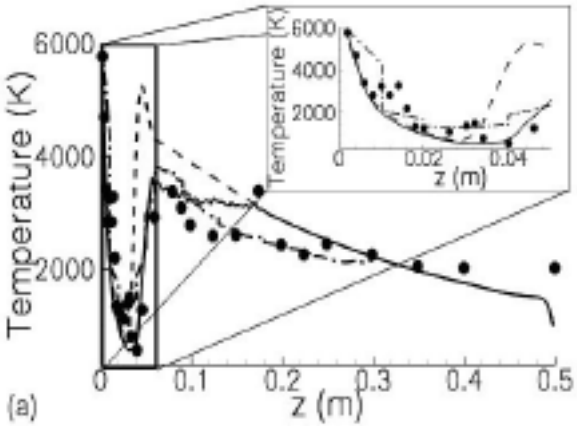

Temperature distribution along the axis of symmetry of a gas jet supersonically expanding from 0.6 bar into a 20 Pa environment.
Continuum CFD simulations (- -), DSMC simulations (-.-.), Hybrid DSMC/CFD simulations (——), Experiments (●)