Efficient solvers for advection diffusion reaction equations

Project Aim

Development of efficient solvers for chemical vapour deposition reactors. The large system of non-linear coupled partial differential equations is very stiff. So efficient time discretization methods are developed. The resulting non-linear systems should be solved very efficiently in order to compute the solution within a reasonable time.

Progress

Nowadays, many generally applicable simulation codes are available for computational fluid dynamics. However, most of these codes are unsuited for the simulation of chemically reacting flows. This is due to the numerical stiffness of the coupled systems of advection-diffusion-reaction equations that occur. Currently, we try to solve the system by the Euler backward method, which implies that nonlinear systems have to be solved for each time step. It appears that in some situations the Newton-Raphson method only converges if very small time steps are used. After using the Projected Newton-Raphson method we get good convergence results. We are able to solve 17 species on a 3dimensional geometry with a grid of 50x50x50 grid points in a reasonable time (some hours CPU time). Applications are chemical vapor deposition machines and solid oxide fuel cells.

Dissertations

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Scientific Publications

1. S. van Veldhuizen and C. Vuik and C.R. Kleijn, Comparison of ODE Methods or Laminar Reacting Gas Flow Simulations Num. Meth. Part. Diff. Eq., 24, pp. 1037-1054, 2008.

Project leaders
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Research theme
Complex dynamics of fluids

Participants
C Vuik, S van Veldhuizen, CR Kleijn

Cooperations
TUD/TNW/MSP, TNO Science and Industry, CWI

Funded
DCSE, TNO Science and Industry
1st 90% 2nd - 3rd 10%

Start of the project
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