Towards self-consistent diffusion models in plasmas used for deposition

Towards self-consistent diffusion models in plasmas used for deposition

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Introduction

In many plasma models Fick's law is used to describe the diffusive fluxes. Fick's law validity requires the presence of a dominant background gas. In that case all collisions are caused by a single species and the diffusive fluxes are decoupled. In plasmas used for chemical vapor deposition the gas inlet of O_2 and $SiCl_4$ can be strongly dissociated. The consequence is that Fick's law is expected to be inaccurate. More accurate results can be obtained by solving the Stefan-Maxwell equations. The solution procedure for these coupled system of equations can sometimes initiate numerical instabilities. These instabilities are investigated.

Theory

The mass balance is given by

$$\frac{\partial \rho y_i}{\partial t} + \nabla \cdot \rho y_i u_i + \nabla \cdot \rho y_i v_i = m_i \omega_i .$$

The diffusive velocities are given by

$$Fv = -d = -\nabla z + \frac{cE_{amb}}{p},$$

with z the pressure fractions, p the pressure and $c_i = n_i q_i$.
The friction matrix is given by

$$\boldsymbol{F} = \begin{bmatrix} \sum_{i\neq 1} f_{i1} & -f_{12} & -f_{13} \\ -f_{12} & \sum_{i\neq 2} f_{i2} & -f_{23} \\ -f_{13} & -f_{23} & \sum_{i\neq 3} f_{i3} \end{bmatrix} \text{ with } f_{ij} = \frac{z_i z_j}{D_{ij}}.$$

This matrix is singular. It can be regularized with

$$\tilde{F} = F + \alpha y y^T, \tilde{D} = D + 11^T/\alpha$$

with y the mass fractions. The mass fluxes can thus be obtained from $J = \rho y^T \tilde{D} \tilde{M} \nabla y - 11^T/\alpha$, with $\tilde{F}\tilde{D} = I$ and $\tilde{M}\nabla y = \nabla z$. When charged particles are present $\tilde{D}$ should be replaced with

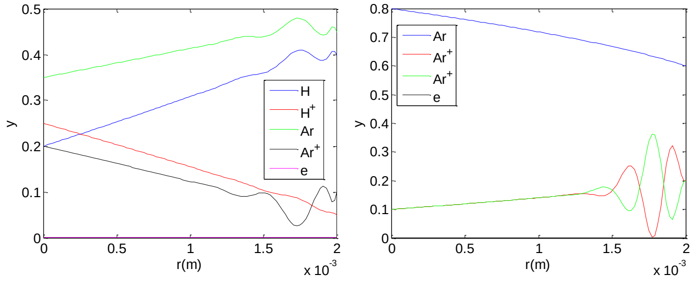
$$\hat{D} = D\left[I - \frac{Dcc^T D}{<c,Dc>}\right],$$

and $\gamma r r^T$ should be added to J with $r_i = q_i/m_i$.

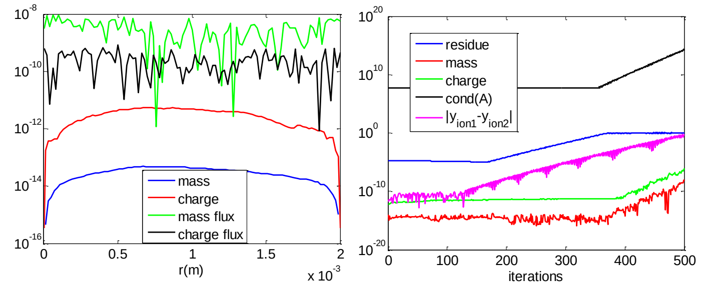
Instabilities

The system is simplified to $\nabla \cdot \rho y_i v_i = 0$ and Dirichlet (constant) boundary values are applied. Simulations using neutral mixtures or a single ion converge smoothly. This is not the case when multiple ions are present. Initially the simulation seems to converge. At some point the mass fractions of the ions start to oscillate. These oscillations can be prevented with underrelaxation. In 2D models this solution is too expensive and a different one is required.

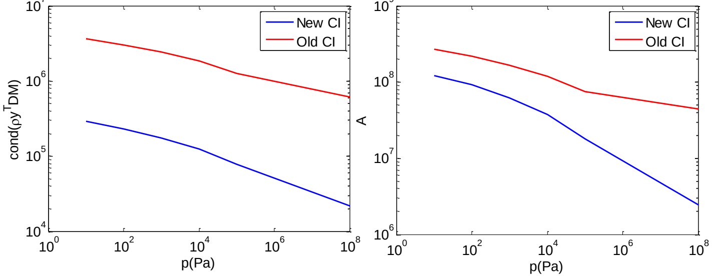
Diverging solutions



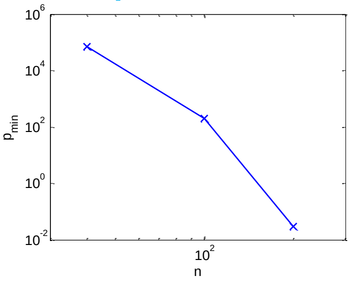
Numerical accuracy



Collision integrals and pressure



Grid points and alternative methods



Changing the interpolation method has no effect. Additionally a description using the mass fluxes, molar fractions or analytical reductions have the same stability problems.

Conclusion

The exact cause of the oscillation is not understood. Reducing the pressure increases the probability of instabilities. Besides the underrelaxation the number of grid points also influences the stability.