Numerical Discretisation = Navier Stokes + Transport Equations

- Stationary solvent flow with velocity \( \vec{u} \), pressure \( p \), dynamic viscosity \( \eta \) and density \( \rho \) inside the flow cell is governed by the incompressible Navier-Stokes equations

\[
-\eta \Delta \vec{u} + \rho \vec{u} \cdot \nabla \vec{u} + \nabla p = 0 \quad \text{in} \; \Omega, \quad \nabla \cdot \vec{u} = 0 \quad \text{in} \; \Omega
\]

- Divergence-constraint: crucial for mass conservation → use divergence-free finite element methods (Scott-Vogelius FEM, novel modified nonconforming Crouzeix-Raviart FEM [4]).
- Less expensive (non-divergence-free) Taylor-Hood FEM gives comparable results [2, 3].

- Species transport with concentration \( c \), diffusion coefficient \( D \):

\[
\nabla \cdot (-D \nabla c + \vec{c} \cdot \vec{u}) = s \quad \text{in} \; \Omega \quad \text{and} \quad c = c_{inlet} \quad \text{at} \; \text{inlet}
\]

discretised by an exponentially fitted volume method with Voronoi cells as control volumes. On every \( \partial K_L \cap \partial L \) set

\[
u_{KL} = \int_{\partial K_L} \vec{u} \cdot \hat{n}_L - \hat{n}_K ds/|\sigma_{KL}|
\]

Find \( c_K \in B(\epsilon) \) with \( |\epsilon_K - c_{inlet}| \) such that

\[
\sum_{L \text{ neighbour of } K} \frac{|\sigma_{KL}|}{|\hat{n}_L - \hat{n}_K|} \cdot g(\epsilon_K, c_L, u_{KL}) = |K| \cdot s_K \quad \text{for all} \; K \in K_0 \setminus K_0
\]

where \( g(\epsilon_K, c_L, u_{KL}) = D \left( B(u_{KL}) \right) - B(-u_{KL}/D) c_L \) with \( B(z) = z/(1-e^{-z}) \).

Detection of \( O_2 \) diffusion coefficients in various solvents

- Experiment:
  - Detection of relation between mass flow and mass spectrometric current by independent experiment
  - Detection of mass spectrometric current \( i \) from \( O_2 \) diffusing through the membrane of the measurement chamber for flow rates \( u = 0.1 \ldots 80 \text{mm}^3/s \)

- Interpretation:
  - Detection of inlet concentration from lowest flow rate under the assumption that no \( O_2 \) remains in the outlet (strongly diffusion dominated case)
  - Levenberg-Marquardt fit of diffusion coefficient \( D \) using coupled flow+transport simulation as forward solver
  - Detection of working chamber height (uncertain due to experimental construction) based on known solvents \( (O_2/H_2O, [1]) \)
  - Use fit procedure with known cell height to detect diffusion coefficient for new solvents

References


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