Multicomponent Species Transport Models in Hydrodynamics Codes

Kinetics Physics in ICF Workshop 2016

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Outline

- Single-velocity, single-temperature continuum/hydrodynamic/ Navier-Stokes equations
  - small velocity and temperature differences
- Multicomponent Chapman-Enskog model for species diffusivity, viscosity, and thermal conductivity in plasmas
  - small departures from equilibrium
  - frictional forces balance interspecies forces
  - linear combinations of collision integrals
- Comparison with microphysics/ab initio data in binary mixtures

Basic Hydrodynamic Equations in Miranda use diffusion terms (shown w/o reactions or radiation)

transport terms:

- Species mass equation (ions):

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \bullet \left(\rho_\alpha \mathbf{u} + \mathbf{J}_\alpha \right) = 0, \quad \mathbf{J}_\alpha \equiv \rho_\alpha \left(\mathbf{u}_\alpha - \mathbf{u} \right)$$

species diffusion

- Momentum equation (mixture):

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \bullet \left(\rho \mathbf{u}\mathbf{u} + \boldsymbol{\tau} \right) = -\nabla p + \rho \mathbf{f}$$

viscous stress

- Internal energy equation (ion mixture):

$$\frac{\partial \rho e_i}{\partial t} + \nabla \bullet \left(\rho e_i \mathbf{u} + \mathbf{q}_i \right) + p_i \nabla \bullet \mathbf{u} = \boldsymbol{\tau}_i : \nabla \mathbf{u}$$

heat conduction

$$+ \gamma_{ei} (T_e - T_i)$$

temperature coupling

- (similarly for electron energy)

Individual species equations would feature coupling terms $K_{\alpha\beta}(u_\alpha - u_\beta)$ and $\gamma_{\alpha\beta}(T_\alpha - T_\beta)$.

Species mass flux, stress, heat flux are associated with diffusive transport coefficients

- Traditional down-gradient models

➢	$\mathbf{J}_\alpha \sim -\rho D \nabla y_\alpha$	Diffusivity	Fick's law
✓	$\boldsymbol{\tau} \sim \eta \left(\nabla \mathbf{u} + \nabla \mathbf{u}^\dagger - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right)$	Viscosity	Stokes' law
➢	$\mathbf{q} \sim -\kappa \nabla T$	Thermal conductivity	Fourier's law

- ➢ A more sophisticated diffusion model of coupled species mass and heat transport is used in Miranda
  - single ion temperature
  - no magnetic field
  - macroscopic charge neutrality (MHD)
  - special treatment of electron terms (Braginskii, Lee & More, …)

Coupled linear species mass and heat diffusion model for ions (Chapman & Cowling, Burgers)

- (2N-1) x (2N-1) matrix for diffusion of N ion species can be solved directly:

friction | cross | mass current

$$\begin{pmatrix} \overleftrightarrow{K} & \overleftrightarrow{C} \\ \overleftrightarrow{C}^{\dagger} & \overleftrightarrow{\Theta} \end{pmatrix} \bullet \begin{pmatrix} \vec{\mathbf{w}} \\ \vec{\mathbf{r}} \end{pmatrix} = \begin{pmatrix} \vec{\mathbf{d}}_p \\ \vec{\mathbf{d}}_T \end{pmatrix}$$

pressure+electric driver

thermal driver

cross | thermal | heat current

fluxes

$$\mathbf{J}_\alpha = \rho_\alpha \mathbf{w}_\alpha$$

$$\mathbf{q} = \sum_\alpha (n_\alpha k_B T_\alpha \mathbf{r}_\alpha + n_\alpha h_\alpha \mathbf{w}_\alpha)$$

✧ $\overleftrightarrow{K} \cdot \mathbf{w} = \vec{\mathbf{d}}_p$ corresponds to classic Stefan-Maxwell equations

✧ C matrix gives rise to thermodiffusion (Soret, Dufour) terms

There is no well defined diffusion coefficient for > 2 species.

Coupled linear species mass and heat diffusion model for ions (Chapman & Cowling, Burgers)

… or ion diffusion can be solved in parts to extract standard thermal diffusion coefficients:

inverse diffusion **matrix**

thermodiffusivity

mass current

heat current

$$(\overleftrightarrow{K} - \overleftrightarrow{C} \cdot \overleftrightarrow{\Theta}^{-1} \cdot \overleftrightarrow{C}^{\dagger})\, \vec{\mathbf{w}} = \vec{\mathbf{d}}_p - \overleftrightarrow{C} \cdot \overleftrightarrow{\Theta}^{-1} \cdot \vec{\mathbf{d}}_T$$

$$\vec{\mathbf{r}} = \overleftrightarrow{\Theta}^{-1} \cdot \vec{\mathbf{d}}_T - \overleftrightarrow{\Theta}^{-1} \cdot \overleftrightarrow{C}^{\dagger} \cdot \vec{\mathbf{w}}$$

thermal conduction

Series of N x N matrix operations

fluxes

$$\mathbf{J}_\alpha = \rho_\alpha \mathbf{w}_\alpha$$

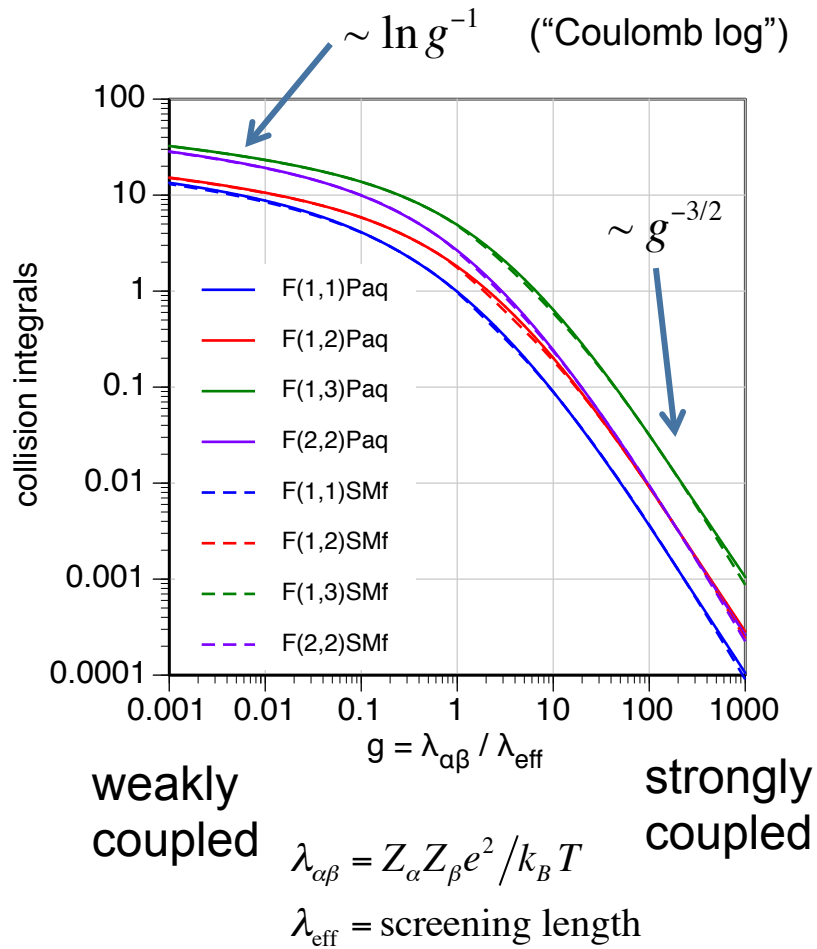
$$\mathbf{q} = \sum_\alpha (n_\alpha k_B T_\alpha \mathbf{r}_\alpha + n_\alpha h_\alpha \mathbf{w}_\alpha)$$

There is no well defined diffusion coefficient for > 2 species.

Matrix elements are linear combinations of binary collision integrals $\Omega^{(11)}$, $\Omega^{(12)}$, $\Omega^{(13)}$, $\Omega^{(22)}$

$$\frac{16}{3} n_\alpha n_\beta m_{\alpha\beta} \Omega_{\alpha\beta}^{(\ell m)} = \frac{8}{3} \frac{(\pi m_{\alpha\beta})^{1/2}}{(2k_B T)^{3/2}} n_\alpha n_\beta Z_\alpha^2 Z_\beta^2 e^4 F_{\alpha\beta}^{(\ell m)}$$

- For a given thermodynamic state and charge states (EOS), collision integrals are evaluated from Paquette cubic spline tables or Stanton-Murillo curve fits for screened Coulomb potentials
- In asymmetric mixtures, binary collisions can span the coupling range



$$\lambda_{\alpha\beta} = Z_\alpha Z_\beta e^2 / k_B T$$

$$\lambda_{eff} = \text{screening length}$$

The collision integrals do not in general behave like slowly varying ln Λ.

Solution for binary diffusion in a plasma is easier to diagnose

- Solution for binary (α,β) species mass flux:

electronic terms

$$\vec{\mathbf{J}}_\alpha = -\vec{\mathbf{J}}_\beta = -\frac{\rho D_{\alpha\beta}}{n_i k_B T_i}\frac{y_\alpha y_\beta}{x_\alpha x_\beta}\left(\underbrace{\nabla p_\alpha - y_\alpha \nabla p + z_\alpha \nabla p_e}\right. + k_{T\alpha}^{(i)} n_i k_B \nabla T_i + \left. k_{T\alpha}^{(e)} n_e k_B \nabla T_e\right)$$

interdiffusivity

thermodiffusion coefficients

- Barodiffusion and thermodiffusion can drive species separation in homogeneous mixtures

- For uniform total pressure, going from neutral to ionized increases the pressure driver in ideal fluids by an electronic "thermodynamic factor"

$$\Theta_e = \left(\langle Z\rangle + \langle Z^2\rangle\right)\Big/\left(\langle Z\rangle + \langle Z\rangle^2\right) \geq 1\ ,\ \ \langle Z^n\rangle = x_\alpha Z_\alpha^n + x_\beta Z_\beta^n$$

ion fractions

$$x_\alpha = \frac{n_\alpha}{n_\alpha + n_\beta}$$

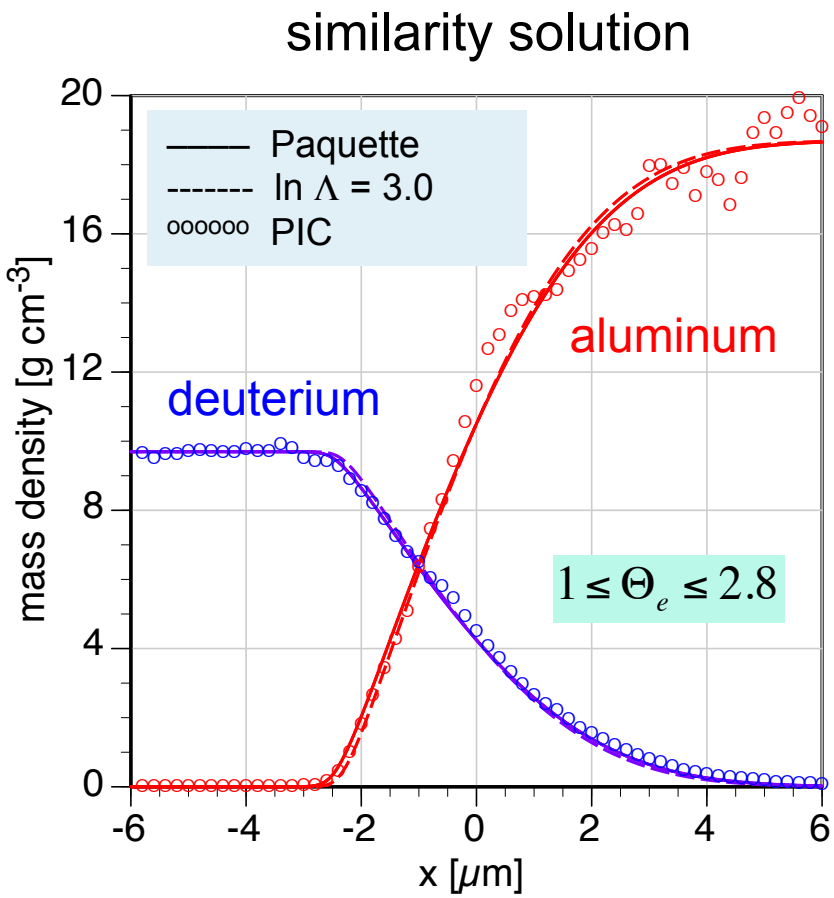
$$y_\alpha = \frac{n_\alpha m_\alpha}{n_\alpha m_\alpha + n_\beta m_\beta}$$

$$z_\alpha = \frac{n_\alpha Z_\alpha}{n_\alpha Z_\alpha + n_\beta Z_\beta}$$

There is no well defined diffusion coefficient for > 2 species.

Comparison with binary diffusion in ab initio calculations (Particle-In-Cell)

- PIC (LSP-Wilkes): Diffusion of D-Al interface in total pressure equilibrium
  - ✓ diffusion enhanced by ionization
  - ✓ rate of diffusion consistent with diffusivity model
- MD diffusivity and viscosity from weakly to moderately coupled homogeneous binary mixtures also agree well with the model, esp. using Stanton-Murillo λ_{eff}



Binary diffusion model gives good agreement with ab initio data.

A Hybrid Ion Viscosity Model is used in the hydrodynamics code

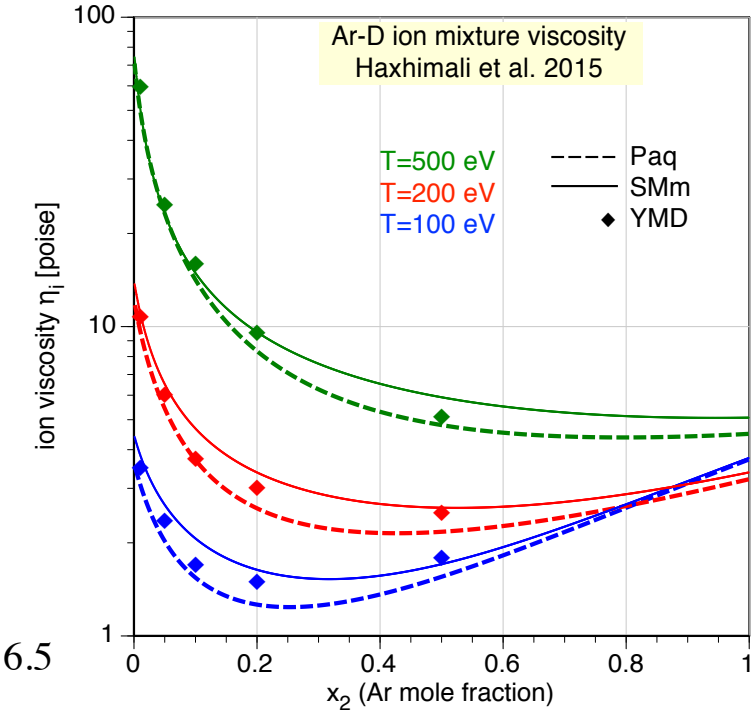
- Kinetic part from classical CE theory

$$\eta_i = \sum_\alpha \eta_\alpha \ , \ \frac{5}{3} n_\alpha k_B T_i = \eta_\alpha \sum_\beta \nu_{\alpha\beta} + \sum_\beta m_{\alpha\beta} \left(\frac{\eta_\alpha \nu_{\alpha\beta}}{m_\beta} - \frac{\eta_\beta \nu_{\beta\alpha}}{m_\alpha} \right) \left(\frac{10\Omega_{\alpha\beta}^{(11)}}{3\Omega_{\alpha\beta}^{(22)}} - 1 \right) \ , \ \nu_{\alpha\beta} = \frac{16 n_\beta m_{\alpha\beta}}{3 m_\alpha} \Omega_{\alpha\beta}^{(22)}$$

$$\eta_i \approx \frac{5}{3} \sum_\alpha n_\alpha k_B T_i \left\{ \sum_\beta \nu_{\alpha\beta} \right\}^{-1} \quad \text{(depends only on } \Omega_{\alpha\beta}^{(22)}\text{)}$$

- All N(N+1)/2 binary pairs of collisions need to be calculated
- Ad hoc blend of kinetic theory (weak coupling limit) to Murillo's (2008) Yukawa Viscosity Model (strong coupling limit)

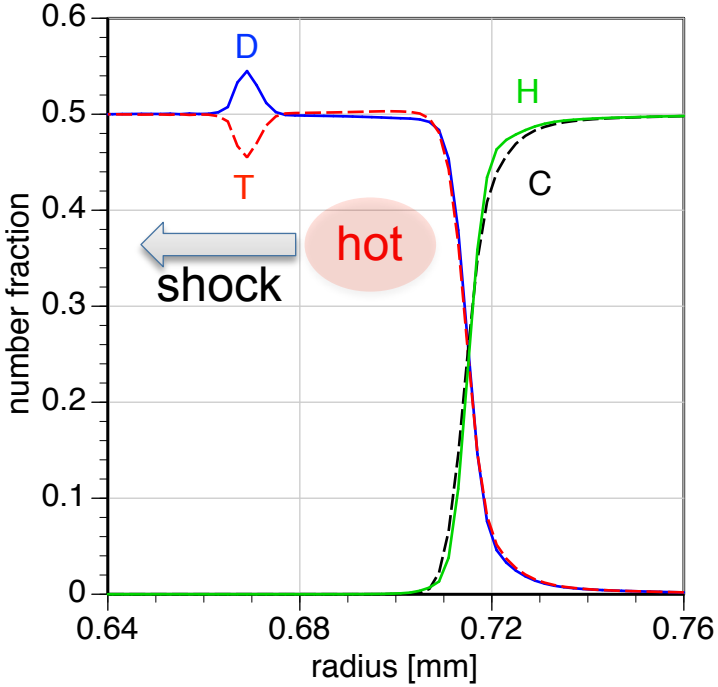
$$\Gamma_{12} \equiv \frac{Z_1 Z_2 e^2}{k_B T a_i} = 1.3 - 6.5$$



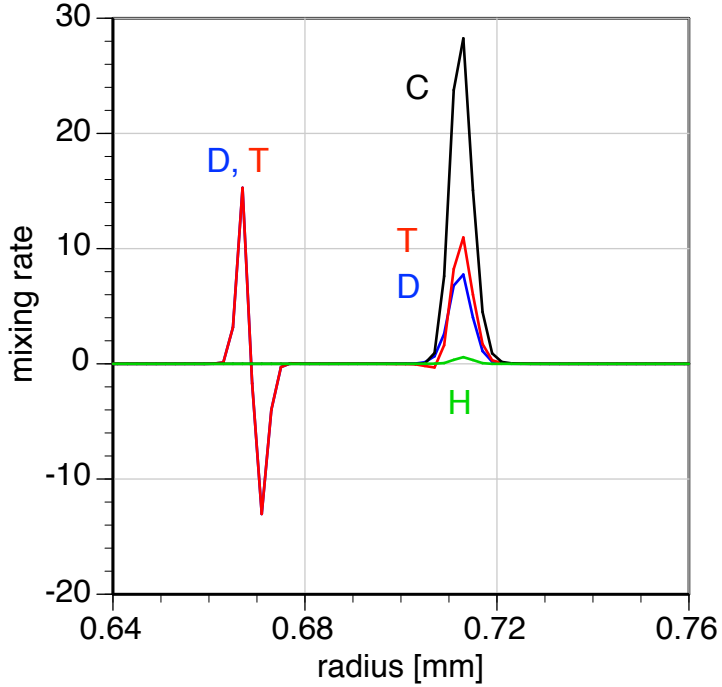
The hybrid model gives good agreement with weak to moderately coupled ab initio data.

A variety of baro- and thermo-diffusion effects arise in multicomponent mixtures

- Species separation in shock (mostly barodiffusion)



- Diffusion of H inhibited (baro+thermodiffusion)



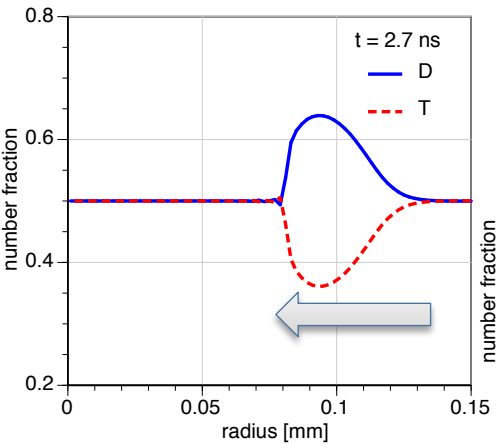
$$\frac{1}{2}\frac{d}{dt}\int \rho y_\alpha (1-y_\alpha)\,dV = \int (-\mathbf{J}_\alpha \cdot \nabla y_\alpha)\,dV$$

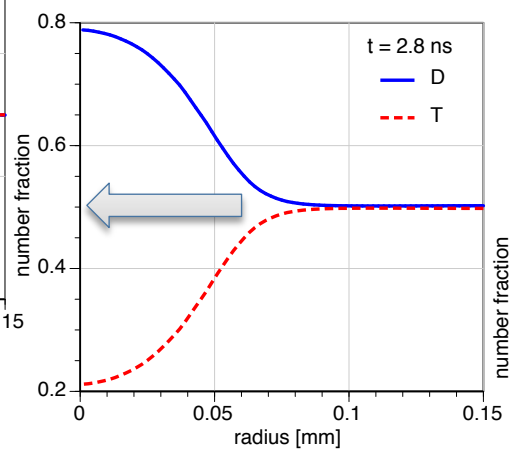
species mixing rate

Diffusion model gives species separation but inaccurate shock structure.

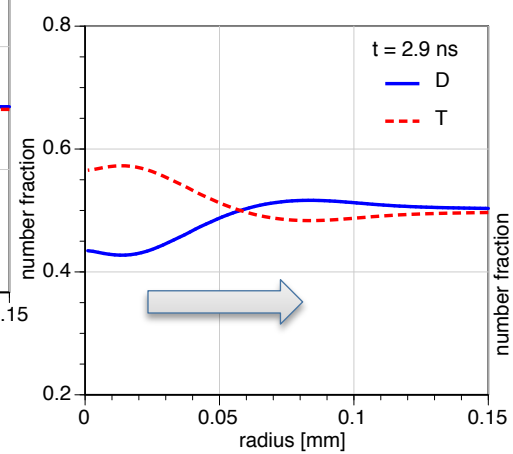
Barodiffusion: An excess of the heavy species is left behind a reflected shock

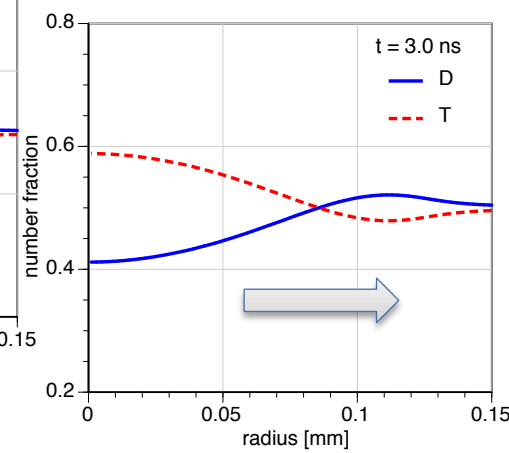
- Shock in D+T mixture, cf. PIC simulations in Bellei et al. 2014





- Diffusion (linear) approximations are invalid in strong shocks!



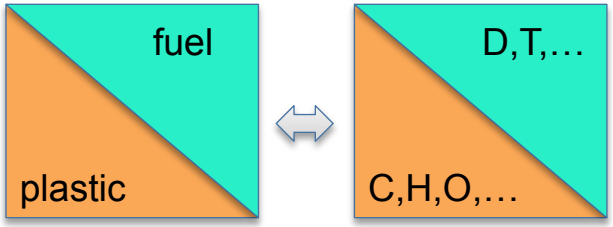


- Unlike MC, PIC, MD, no capability for
  - temperature separation and anisotropy
  - kinetic effects

Diffusion model gives species separation but inaccurate shock structure.

Summary

- The multicomponent ion diffusion model in Miranda hydro code requires calculation of all N(N+1)/2 binary collision terms
- No ad hoc mixing rules (for the kinetic theory part)
  - blend with OCP viscosity models for WDM
  - concoct hybrid models for conductivity, diffusion?
- Fair agreement for diffusivity & viscosity with microphysics simulations in weak to moderately coupled binary mixtures
  - lack of ion thermal conductivity or thermodiffusivity validation
  - lack of ternary, quaternary, etc. mixture validation
- Modeling issues:
  - treatment of diffusion of material groups
  - partially dissociated and ionized mixtures



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Extras

Species hydrodynamics equations are reduced to single-velocity, single-energy equations

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \bullet \left(\rho_\alpha \mathbf{u}_\alpha \right) = 0$$

$$\frac{\partial \rho_\alpha \mathbf{u}_\alpha}{\partial t} + \nabla \bullet \left(\rho_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha + \boldsymbol{\tau}_\alpha \right) = -\nabla p_\alpha + \rho_\alpha \mathbf{f}_\alpha + \sum_\beta \mathbf{F}_{\alpha\beta}$$

$$\frac{\partial \rho_\alpha e_\alpha}{\partial t} + \nabla \bullet \left(\rho_\alpha e_\alpha \mathbf{u}_\alpha + \mathbf{q}_\alpha \right) + p_\alpha \nabla \bullet \mathbf{u}_\alpha = \boldsymbol{\tau}_\alpha : \nabla \mathbf{u}_\alpha + \sum_\beta Q_{\alpha\beta}$$

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \bullet \left(\rho_\alpha \mathbf{u} + \mathbf{J}_\alpha \right) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \bullet \left(\rho \mathbf{u}\mathbf{u} + \boldsymbol{\tau} \right) = -\nabla p + \rho \mathbf{f}$$

$$\frac{\partial \rho e}{\partial t} + \nabla \bullet \left(\rho e \mathbf{u} + \mathbf{q} \right) + p \nabla \bullet \mathbf{u} = \boldsymbol{\tau} : \nabla \mathbf{u}$$

$$\rho \mathbf{u} = \sum_\alpha \rho_\alpha \mathbf{u}_\alpha$$

$$\rho e = \sum_\alpha \rho_\alpha e_\alpha$$

Individual species equations would feature coupling terms $K_{\alpha\beta}(u_\alpha - u_\beta)$ and $\gamma_{\alpha\beta}(T_\alpha - T_\beta)$.

Extras

Coupled species mass and heat diffusion model
Chapman-Enskog (Chapman & Cowling, Burgers)

- Friction & heat exchange terms balance interspecies forces

$$\sum_\beta K_{\alpha\beta}(\mathbf{w}_\alpha - \mathbf{w}_\beta) + \sum_\beta (C_{\alpha\beta}\mathbf{r}_\beta - C_{\beta\alpha}\mathbf{r}_\alpha) = -\nabla p_\alpha + y_\alpha \nabla p + n_\alpha e Z_\alpha \mathbf{E}$$

$$B_\alpha \mathbf{r}_\alpha - \sum_\beta A_{\alpha\beta}\mathbf{r}_\beta + \sum_\beta C_{\beta\alpha}(\mathbf{w}_\beta - \mathbf{w}_\alpha) = -n_\alpha k_B \nabla T_\alpha$$

$$T_{\alpha\in i} = T_i \ , \quad \mathbf{B} = \mathbf{0}$$

fluxes

$$\mathbf{J}_\alpha = \rho_\alpha \mathbf{w}_\alpha$$

$$\mathbf{q} = \sum_\alpha (n_\alpha k_B T_\alpha \mathbf{r}_\alpha + n_\alpha h_\alpha \mathbf{w}_\alpha)$$

"enthalpy diffusion"

- Center-of-mass constraint $\sum_\alpha \rho_\alpha \mathbf{w}_\alpha = 0$
- Macroscopic charge neutrality, current $\sum_\alpha n_\alpha Z_\alpha = 0$, $\sum_\alpha n_\alpha Z_\alpha e \mathbf{w}_\alpha = \mathbf{j}$
- Electron terms are treated separately (Lee & More, Braginskii), and electric field eliminated in terms of ∇p_e using $m_e \ll m_i$

Extras

Friction coefficients, 1st approximation (Chapman & Cowling, Burgers)

- Matrix elements are linear combinations of collision integrals

$$A_{\alpha\beta} = \frac{2}{5} K_{\alpha\beta} \frac{m_\alpha m_\beta}{(m_\alpha + m_\beta)^2} \left(3 + z'_{\alpha\beta} - \frac{4}{5} z''_{\alpha\beta} \right)$$

$$B_\alpha = \frac{2}{5} \sum_\beta \frac{K_{\alpha\beta}}{(m_\alpha + m_\beta)^2} \left(3m_\alpha^2 + m_\beta^2 z'_{\alpha\beta} + \frac{4}{5} m_\alpha m_\beta z''_{\alpha\beta} \right)$$

$$C_{\alpha\beta} = K_{\alpha\beta} \frac{m_\alpha z_{\alpha\beta}}{(m_\alpha + m_\beta)}$$

$$\boxed{K_{\alpha\beta} = \frac{16}{3} n_\alpha n_\beta m_{\alpha\beta} \Omega_{\alpha\beta}^{(11)}}$$

$$z_{\alpha\beta} = 1 - \frac{2}{5} \frac{\Omega_{\alpha\beta}^{(12)}}{\Omega_{\alpha\beta}^{(11)}}$$

$$z'_{\alpha\beta} = \frac{5}{2} - 2 \left(\frac{\Omega_{\alpha\beta}^{(12)}}{\Omega_{\alpha\beta}^{(11)}} - \frac{\Omega_{\alpha\beta}^{(13)}}{5\Omega_{\alpha\beta}^{(11)}} \right)$$

$$z''_{\alpha\beta} = \frac{\Omega_{\alpha\beta}^{(22)}}{\Omega_{\alpha\beta}^{(11)}}$$

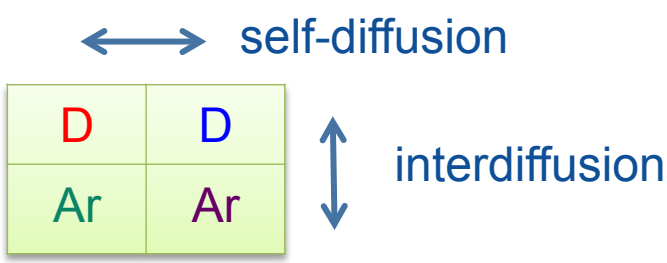
$$m_{\alpha\beta} \equiv \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}$$

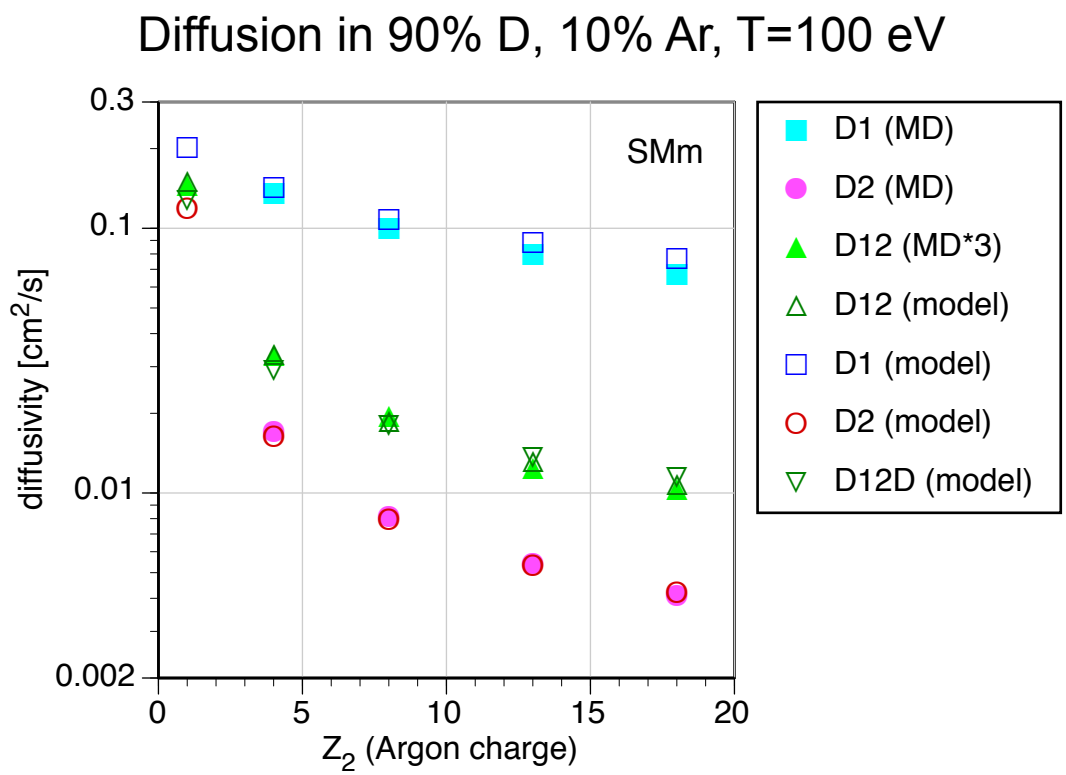
- For N species, N(N+1)/2 binary pairs of each collision integral must be calculated; these are also used for viscosity

Extras

Comparison with binary diffusion in ab initio calculations (Yukawa Molecular Dynamics)

- Diffusion and viscosity coefficients (Green-Kubo) from homogeneous D-Ar mixtures (Haxhimali et al.)
- Self-diffusivity in mixture from quaternary solutions





- Tests of Darken relation $D_{12} \sim x_2 D_1 + x_1 D_2$

$$\Gamma_{12} \equiv \frac{Z_1 Z_2 e^2}{k_B T a_i} = 0.5 - 9.0$$

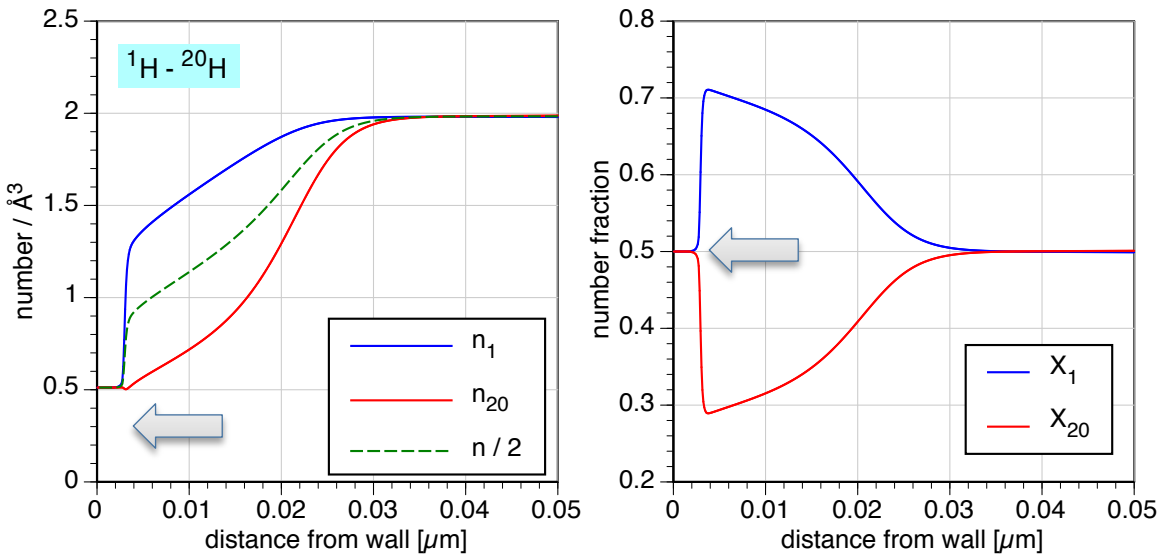
Binary diffusion model gives good agreement with ab initio data.

Extras

Species separation is observed in shocks due to baro- and thermo-diffusion

- Species separation in shocks
  - Observed in MC simulations (Bird) and lab exp'ts in neutral mixtures
  - Observed in PIC (Bellei) and MD (MacKay) in plasma mixtures
  - Single-temperature description *cannot* capture detailed shock structure like **temperature separation, anisotropy**, and **kinetic effects**
  - Diffusion (linear) approximations are invalid in strong shocks!

- Steady M=10 shock
- Z=1, T_e=1eV
- Ion shocks are observed to be much broader in ab initio simulations



Diffusion model gives species separation but inaccurate shock structure.

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