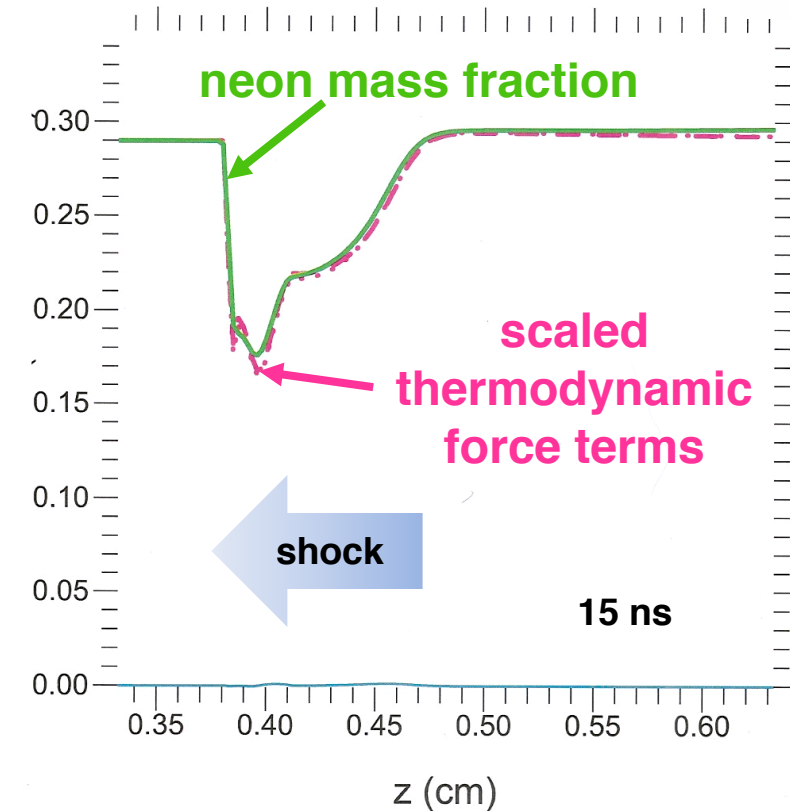# Species separation in shock waves: simple solution of a multispecies ion transport model

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Ion species mass flux is produced by gradients in concentration, pressure, temperature, and electric potential

- **The diffusive "drift" flux of ion species *j*, relative to the mass-averaged mean flow, is**

$$\vec{i} = \rho_j \left(\vec{u}_j - \vec{u} \right)$$

where u_j is mean velocity of species *j*; u is mass-averaged velocity of mean flow

- **Diffusive flux in a binary mixture is determined by gradients[1-3]:**

ion and electron thermodiffusion

$$\vec{i} = -\rho D \left(\boxed{\nabla c} + \boxed{k_P \nabla \log P_i} + \boxed{\frac{e k_E}{T_i} \nabla \Phi} + \boxed{k_T^{(i)} \nabla \log T_i} + \boxed{k_T^{(e)} \nabla \log T_e} \right)$$

concentration diffusion   **barodiffusion**   **electrodiffusion**

for density ρ, diffusivity *D*, mass fraction $c \equiv \rho_j/\rho$, ion pressure P_i, ion temperature T_i, electron temperature T_e, electric potential Φ

1. L.D. Landau and E.M. Lifshitz, *Fluid Mechanics*, §59 (1959)
2. G. Kagan and X.Z. Tang, Phys. Plasmas 19, 082709 (2012)
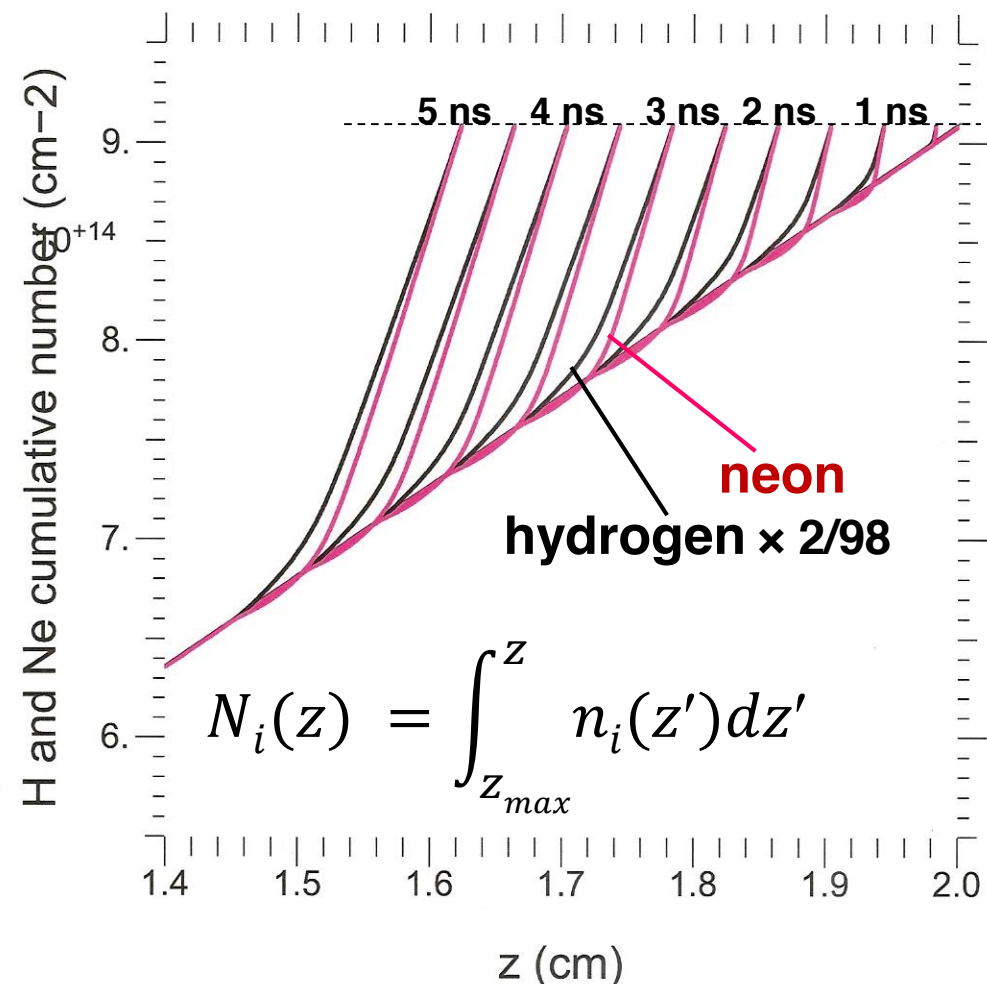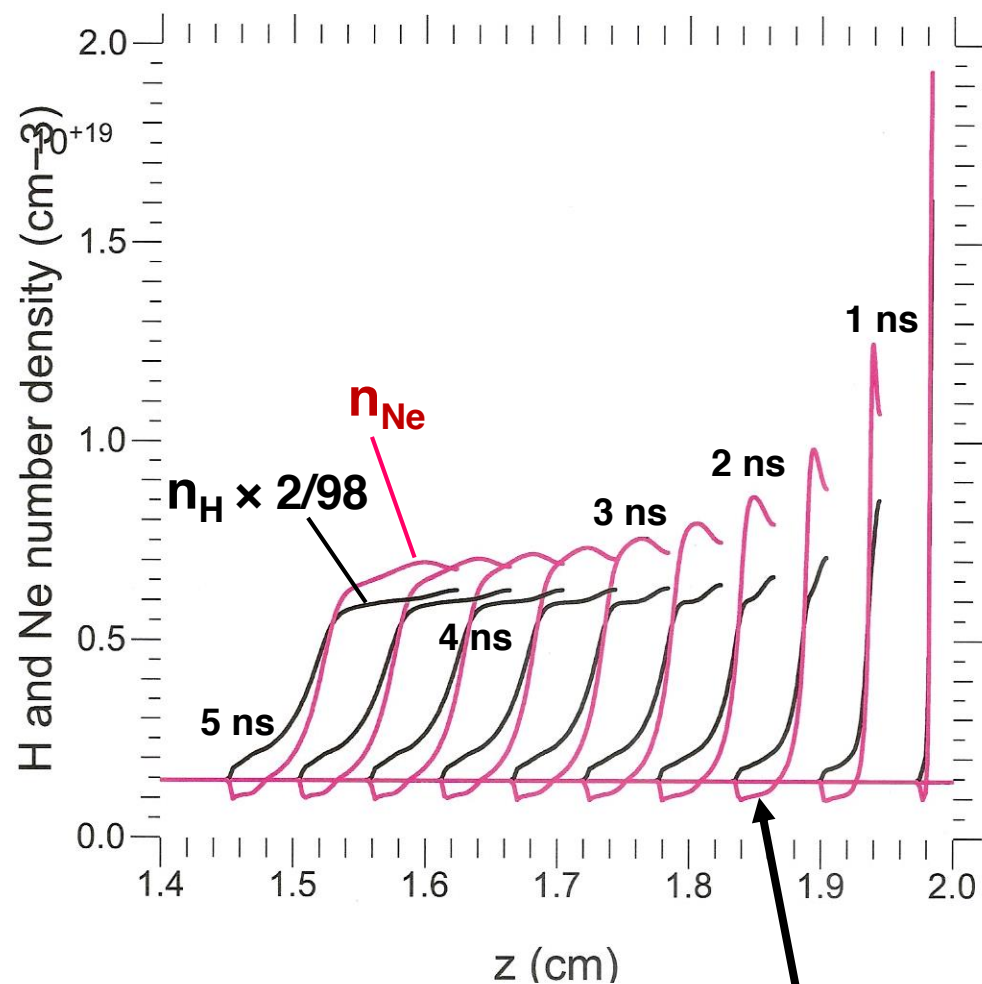3. G. Kagan and X.Z. Tang, Phys. Lett. A 378, 1531 (2014)

I've performed 1D planar simulations of a shock wave traveling through a hydrogen-neon gas mixture (e.g., Hans Rinderknecht's shock tube) using the Zimmerman-Paquette-Kagan-Zhdanov ("ZPKZ") ion transport model*
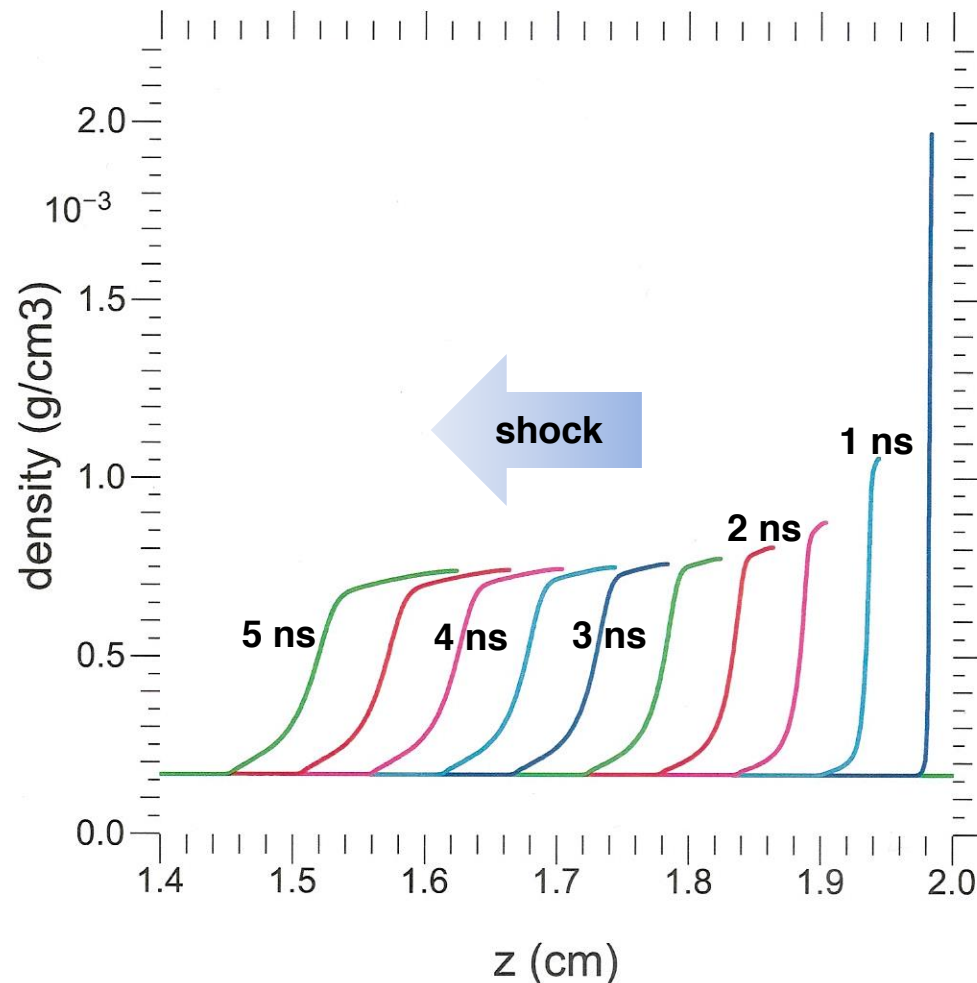
- Gas composition is 98% H, 2% Ne by atom ($\rightarrow$ 29% by mass)

- Initial gas density = 0.167 mg/cm^3

- In simulation, shock wave is generated by motion of right-hand boundary ("piston")
  - Piston moves from right to left
  - Piston accelerates from 0 km/s to 800 km/s over 0.6 ns
  - Resulting shock wave travels at ~1070 km/s = 1.07 mm/ns

- Radiation transport plays no role, as determined by switching it on and off

- Shock structure is dominated by physical viscosity

* N. Hoffman, G. Zimmerman et al., Phys. Plasmas 22, 052707 (2015); G. Kagan and X.Z. Tang, Phys. Lett. A 378, 1531 (2014); C. Paquette, C. Pelletier, G. Fontaine, G. Michaud, Ap. J. Suppl. Series 61, 177 (1986); V. M. Zhdanov, *Transport Processes in Multicomponent Plasma*, Taylor and Francis, New York, 2002

Neon shock front lags behind hydrogen shock front

Left panel: H and Ne number density (cm−3) vs z (cm). Curves labeled n_{Ne}, $n_H \times 2/98$, with time labels 1 ns, 2 ns, 3 ns, 4 ns, 5 ns.

Right panel: H and Ne cumulative number (cm−2) vs z (cm). Time labels 5 ns, 4 ns, 3 ns, 2 ns, 1 ns. Labels: neon, hydrogen × 2/98.

Total number of ions is conserved

$$N_i(z) = \int_{z_{max}}^{z} n_i(z')dz'$$

Is it really plausible that Ne density drops at head of shock? Artifact of Navier-Stokes approximation[1]?

1. F. S. Sherman, JFM 8, 465 (1960)

hne017

Compare *simulations* to *analytic solution* for species separation in planar steady shock wave

- **Consider binary mixture: light species + heavy species**

- **Conservation of mass for light species:**

$$\rho \frac{\partial c}{\partial t} + \rho \vec{u} \cdot \nabla c + \vec{\nabla} \cdot \vec{i} = 0$$

  - **Mass fraction c of light species varies because of drift flux i of light species**

- **In shock frame, flow is in steady state:**

$$\rho u \frac{dc}{dx} + \frac{di}{dx} = 0$$

- **Integrate, since ρu = constant = $\rho_+ u_+$ in planar flow:**

$$\rho_+ u_+ \left[c(x) - c_+ \right] = -i(x)$$

- **…which is a nonlinear ODE for light-species concentration:**

$$\frac{dc(x)}{dx} - \frac{\rho_+ u_+}{\rho(x) D(c(x))} \left[c(x) - c_+ \right] = -k_P(c(x)) \frac{d \log P_i}{dx} - \frac{e k_E(c(x))}{T_i} \frac{d\Phi}{dx} - k_T^{(i)}(c(x)) \frac{d \log T_i}{dx} - k_T^{(e)}(c(x)) \frac{d \log T_e}{dx}$$

"+"("–") indicates values in unshocked (shocked) material

Ignore nonlinearities by using mean values for diffusivity and slowly varying diffusion ratios

- **Replace actual nonlinear ODE with approximate linear ODE:**

$$\frac{dc(x)}{dx} - \frac{\rho_+ u_+}{\overline{\rho}\overline{D}}\left[c(x) - c_+\right] = -\overline{k}_P \frac{d\log P_i}{dx} - \frac{e\overline{k}_E}{T_i}\frac{d\Phi}{dx} - \overline{k}_T^{(i)}\frac{d\log T_i}{dx} - \overline{k}_T^{(e)}\frac{d\log T_e}{dx}$$

- **Express the log gradient of quantity Q (= P, T_i, T_e, ρ) as**

$$\frac{d\log Q}{dx} = \frac{1}{L_i}\frac{\Delta Q}{\overline{Q}}S_Q(x) \quad \textbf{where} \quad \Delta Q \equiv Q_- - Q_+ \quad \textbf{and} \quad \overline{Q} \equiv \tfrac{1}{2}\left(Q_- + Q_+\right)$$

  where L_i is the shock width and S_Q is a shape function

- **Use ambipolar approximation:** $e\dfrac{d\Phi}{dx} = \dfrac{e}{en_e}\dfrac{dP_e}{dx} \approx \dfrac{T_e}{n_e}\dfrac{dn_e}{dx} \approx \dfrac{T_e}{Zn_i}\dfrac{Zdn_i}{dx} \approx T_e\dfrac{d\log\rho}{dx}$

- **Then linear ODE is**

$$L_i\frac{d\Delta c(x)}{dx} - \frac{\rho_+ u_+ L_i}{\overline{\rho}\overline{D}}\Delta c(x) \approx -\left[\overline{k}_P \frac{\Delta P_i}{\overline{P}_i}S_P(x) + \overline{k}_E \frac{T_e}{T_i}\frac{\Delta\rho}{\overline{\rho}}S_\rho(x) + \overline{k}_T^{(i)}\frac{\Delta T_i}{\overline{T}_i}S_{Ti}(x) + \overline{k}_T^{(e)}\frac{\Delta T_e}{\overline{T}_e}S_{Te}(x)\right] = -F(x)$$

Linear ODE is solved using an integrating factor

- **Change to dimensionless independent variable** $q \equiv x/L_i$: $\dfrac{d\Delta c(q)}{dq} - A\Delta c(q) = -F(q)$

  where $A \equiv \dfrac{\rho_+ u_+ L_i}{\overline{\rho}\overline{D}}$ **and** $c(q) \equiv c(q) \quad c_+$

- **Solution is found with integrating factor** $\exp(Aq)$:

$$\Delta c(q) = -\exp(Aq)\int \exp(-Aq)F(q)dq$$

$$= \frac{F(q)}{A} - \frac{\exp(Aq)}{A}\int \exp(-Aq)\frac{dF(q)}{dq}dq \quad \textbf{(integrate by parts)}$$

$$= \frac{F(q)}{A} - \sum_{n=1}^{\infty}\frac{1}{(-A)^{n+1}}\frac{d^n F(q)}{dq^n} \quad \textbf{(repeated integration by parts)}$$

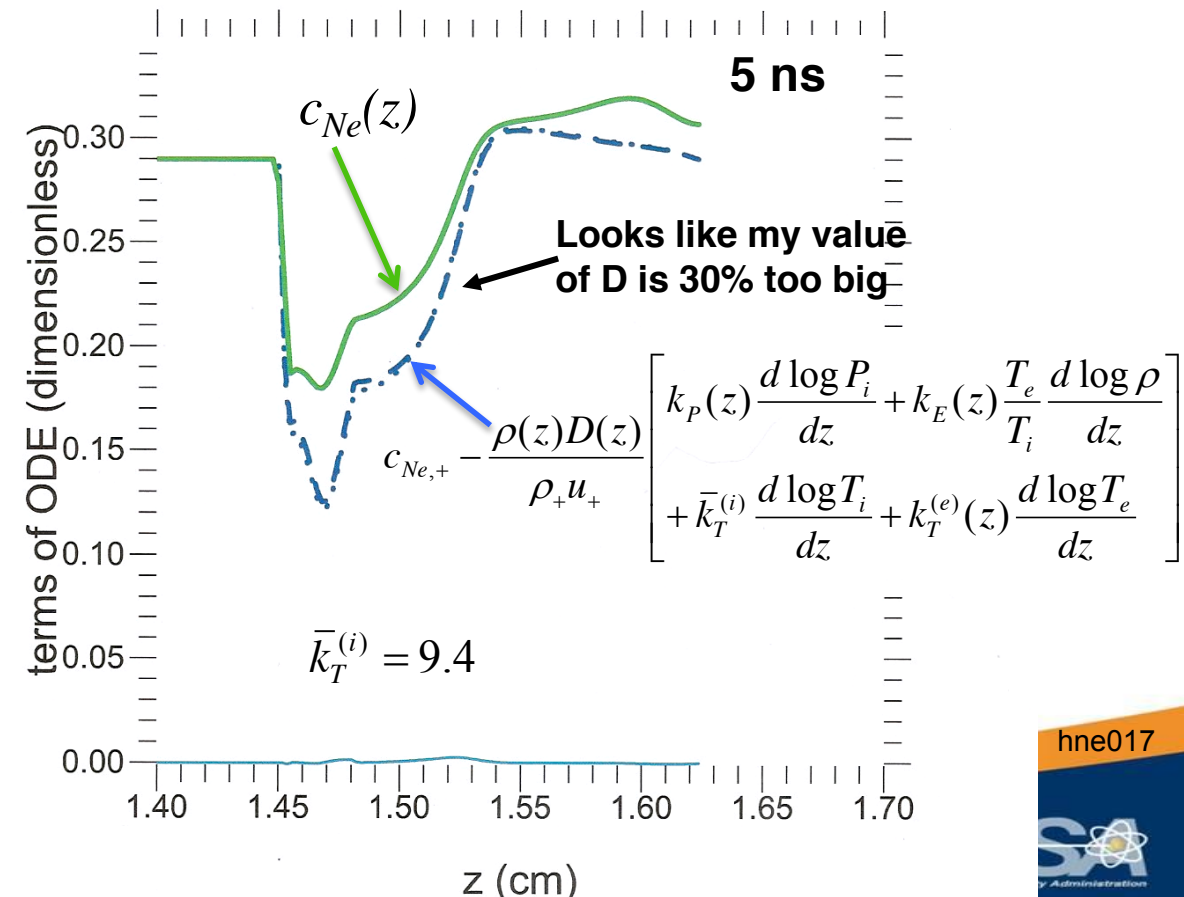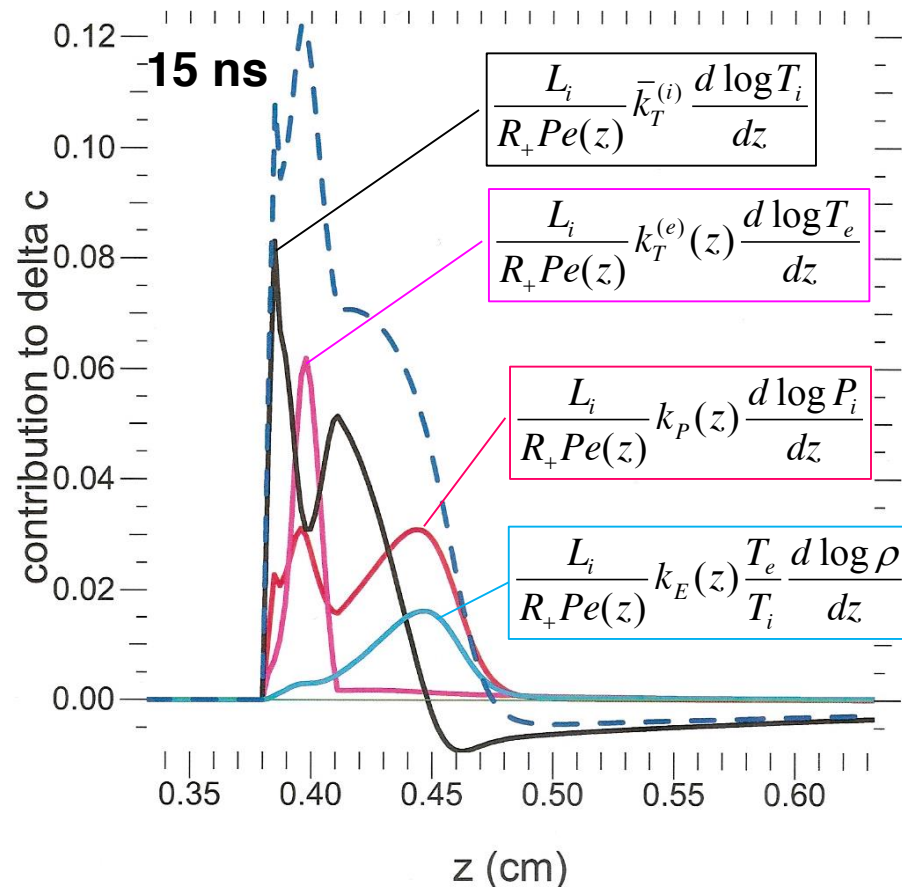- **In limit of large** A, $\Delta c(q) = F(q)/A$ **; i.e., species separation replicates force terms**
  - **Equivalent to neglecting** $d\Delta c(q)/dq$ **wrt** $A\Delta c(q)$ **in ODE**

Species separation in shock is governed by Péclet number Pe

- **Definition of dimensionless parameter A:** $A \equiv \dfrac{\rho_+ u_+ L_i}{\overline{\rho}\,\overline{D}} = \dfrac{\rho_+ v_s L_i}{\overline{\rho}\,\overline{D}}$

  - **Upstream fluid velocity in shock frame $u_+ = v_s$, shock velocity in lab frame**

- **Define** $Pe \equiv \dfrac{v_s L_i}{\overline{D}}$ **where L_i is shock width and $\overline{D}$ is mean diffusivity in shock**

  - **Péclet number Pe expresses ratio of advective transport to diffusive transport**

- **Bulk flow time across shock $\tau = L_i/v_s$, so** $Pe = \dfrac{L_i^2}{\overline{D}\,\tau}$ **= (shock width/diffusion distance)²**

- **So** $A = \dfrac{\rho_+}{\overline{\rho}} Pe$ **$\approx Pe$ for weak shock, $\approx$ 0.4 Pe for strong shock in γ = 5/3 gas**
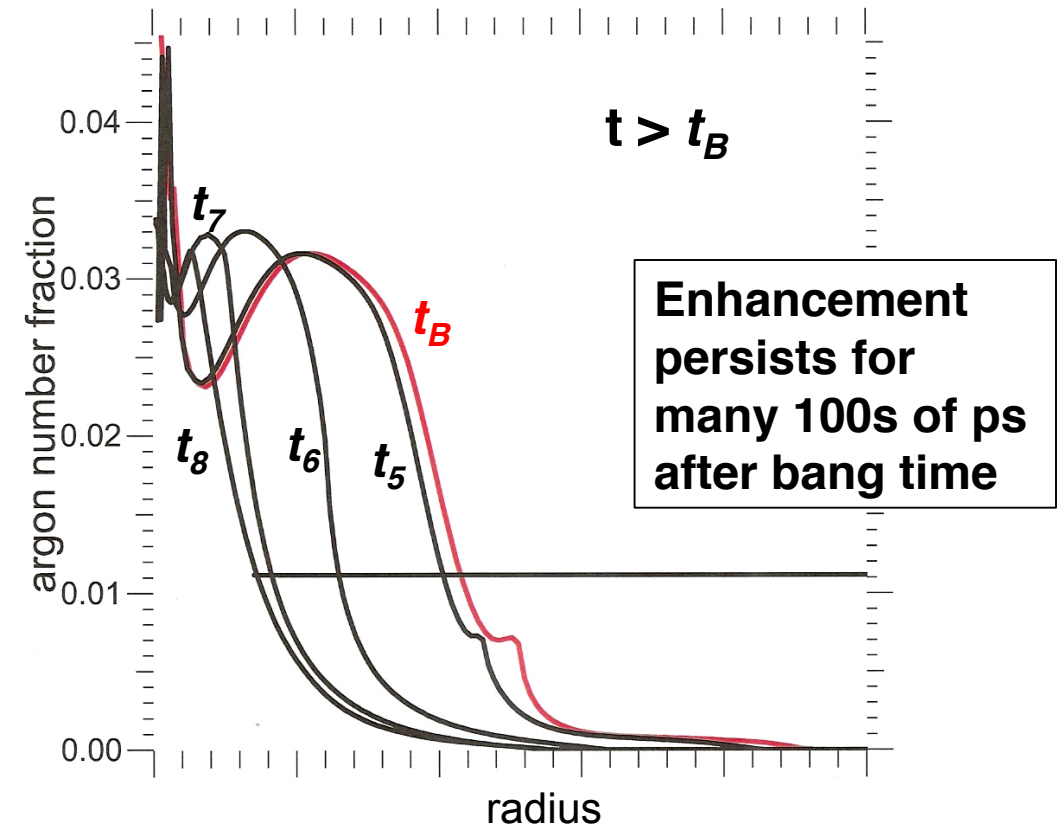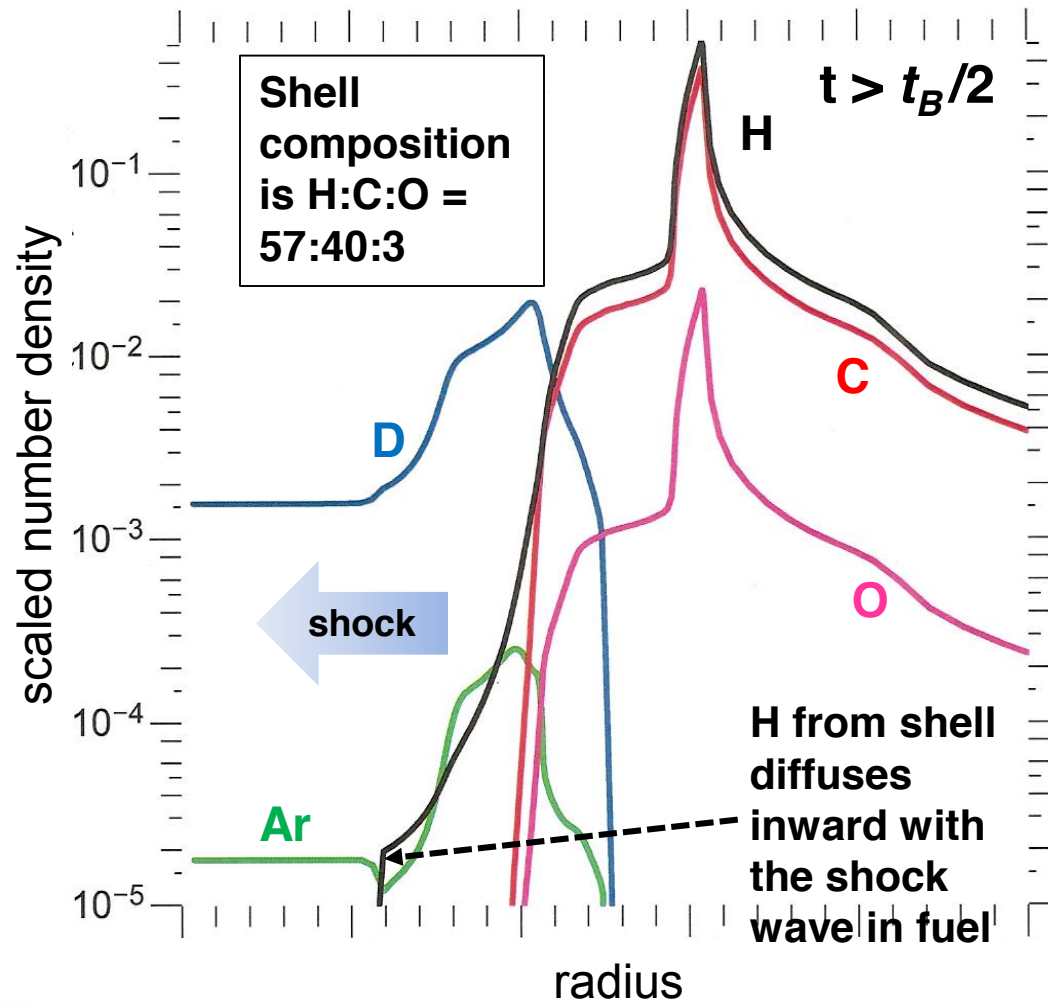
For large Pe, species separation is a replica of diffusive forces

- **In limit of large Pe, $c(z) = c_+(z) + F(z)/R_+(z)Pe(z)$ where $Pe(z) = u_+L_i/D(z)$ and $R_+(z)$ is (compression)$^{-1}$, i.e., ratio of unshocked density to density**

15 ns

$$\frac{L_i}{R_+Pe(z)}\bar{k}_T^{(i)}\frac{d\log T_i}{dz}$$

$$\frac{L_i}{R_+Pe(z)}k_T^{(e)}(z)\frac{d\log T_e}{dz}$$

$$\frac{L_i}{R_+Pe(z)}k_P(z)\frac{d\log P_i}{dz}$$

$$\frac{L_i}{R_+Pe(z)}k_E(z)\frac{T_e}{T_i}\frac{d\log\rho}{dz}$$

contribution to delta c

z (cm)

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5 ns

$c_{Ne}(z)$

Looks like my value of D is 30% too big

$$c_{Ne,+} - \frac{\rho(z)D(z)}{\rho_+u_+}\left[k_P(z)\frac{d\log P_i}{dz} + k_E(z)\frac{T_e}{T_i}\frac{d\log\rho}{dz} + \bar{k}_T^{(i)}\frac{d\log T_i}{dz} + k_T^{(e)}(z)\frac{d\log T_e}{dz}\right]$$

$$\bar{k}_T^{(i)} = 9.4$$

terms of ODE (dimensionless)

z (cm)

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ZPKZ model shows a strong (~3X), persistent enhancement of argon concentration in core of IonSepMMI capsule following shock arrival

Shell composition is H:C:O = 57:40:3

$t > t_B/2$

H

C

O

D

shock

Ar

H from shell diffuses inward with the shock wave in fuel

scaled number density

radius

$t > t_B$

argon number fraction

t_7

t_B

t_8 t_6 t_5

Enhancement persists for many 100s of ps after bang time

radius

- **Enhancement is a result of ion thermodiffusion**
  - Simulations with ion thermodiffusion turned off show no such effect