

秘密★长期

A multi-component hydrodynamic plasma model for resolving mesoscopic disequilibria

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Outline

- I. Motivation
- **II. Model formulation**
- **III.Verification and validation**
- **IV.Application**
- V. Conclusion



• Multi-material and nonlinear hydrodynamic instability and mixing is significant to ICF





High explosive

- HMX/Void grain mix
- Reactant/product atomic mix

Temperature~keV plasma transport (viscosity/mass diffusion) impact mix development ^[1,2]

Diffusion (velocity disequilibrium) is a dominant mixing mechanism in gas-filled capsule

3 [1] A.B. Zylstra, PRE, 2018. [2] Vold E, POP, 2022.



• The ion temperature separation affects mixing development and fusion reaction

Grain mix MARBLE exp^[1]



Atomic: reaction in ion temperature diseq.

- **OMEGA:** D³He exp. ^[2]
- SG: Obtained evidence for temperaure separation betweem Dion T-ion (~4keV)

In Eulerian framework ion-temp. equilibrium causes non-physical oscillation at material interface



4 [1] Haines B.M., et al., NC, 2020. [2] Rinderknecht H.G., et al., PRL, 2015. [3] **Zhang C**., et al., JCP, 2022.



- Traditional ICF codes (xRAGE/HYDRA/LARED-S etc.) rely on one-fluid equilibrium hydrodynamic equations
- Equilibrium models fail to capture mechanical/thermal disequilibrium between different ion species

Traditional models

Baer-Nunziato model not applicable

- Only grain mix
- Ion-electron equilibrium



Two-fluid model not applicable

• Only atomic mix

New model

Muti-component disequilibrium model

Requirements:

I. Physical components

Viscosity, heat conduction, ion-electron temp. diseq., ion-ion mechanical/thermal diseq.

- II. 1st & 2nd law of thermodynamics
- III. Reduction to classical models
- IV. Unified formulation for atomic and grain mix



We obtain the HED-BN model by means of moment- and spatial- averaging of the BGK model. The 14eqn HED-BN model is then reduced by asymptotic analysis with some relaxation times as perturbation parameter. The reduced models can deal with velocity/temperature diseq. between ion-electron and different ion species.





□ Key step 1: derivation of the HED-BN model by moment- and spatial- averaging of the BGK model.

 $\frac{\partial f_r}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_r = \Omega_r[\mathbf{f}] \qquad r = lk, \ l:ion/electron, \ k:component index$ \mathbf{u}_{iI} \mathbf{u}_{i1} \mathbf{u}_{i2} electron u_{e2} \mathbf{u}_{e1} \mathbf{u}_{eI} **Spatial coordinate** $\Omega_{lk} = \Omega_{lk,lk} + \sum X_{l'j} \Omega_{lj,l'j} + X_{lk'} \Omega_{lk,lk'} + \mathbf{n} \cdot \nabla X_{lk'} \Omega_{lk,lk'}^A$ i=k.k'Same comp. Same comp. diff. comp. diff. comp. ion-ion ion-elec ion-ion ion-ion elec-elec elec-elec elec-elec Volume col. Surface col. (atomic mix) (grain mix)



□ Key step 1: derivation of the HED-BN model by moment- and spatial- averaging of the BGK model.

Why do we need two electron temperatures?

- For describing sub-grid temperature distribution
- Maintain neutrality





□ Key step 1: derivation of the HED-BN model by moment- and spatial- averaging of the BGK model.



14 equations



□ Key step 2: Evaluate ICF mechanical/thermal relaxation times and determine the perturbation parameter for asymptotic analysis.

For grain mix evaluate with continuum mechanics



For atomic mix evaluate with coulomb collision

• Relaxation rate of mean velocities (Braginskii,1965)

$$\nu_{k/k'} = \frac{n_{k'}m_{kk'}}{m_k} \frac{4\sqrt{2\pi}\Lambda_{kk'}Z_kZ_{k'}e^4}{3\sqrt{m_{kk'}}(k_BT)^{3/2}}$$

• Relaxation rate of temperatures (Huba,2014)

$$\nu_{k/k'}^{T} = 1.8 \times 10^{-19} \frac{(m_k m_{k'})^{1/2} Z_k^2 Z_{k'}^2 n_{k'} \Lambda_{kk'}}{(m_k T_{k'} + m_{k'} T_k)^{3/2}}$$

- Mechanical relax. time (density, wave speed, grain size)
- Temperature relax. time (density, heat conuctivity, grain size)



□ Key step 2: Evaluate ICF mechanical/thermal relaxation times and determine the perturbation parameter for asymptotic analysis.



 Relax times in grain mix: thermal >> mechanical(velocity, pressure) (L=1µm, T<1keV, ~ 3 orders)

• Ion-elec. and ion-ion temperature relax time maybe of the same order 1keV, 0.1g/cc, $\tau_{ie}/\tau_{ii}=8$ (CD) $\tau_{ie}/\tau_{ii}=3$ (AlD)

$$\frac{\partial \mathbf{V}}{\partial t} = -\left(\frac{m_e n_e}{m_i n_i \tau_e} + \frac{1}{\tau_e}\right) \mathbf{V} \qquad \frac{\partial \delta T}{\partial t} = -2\left(\frac{m_e n_e}{m_i n_i \tau_e} + \frac{m_e}{m_i \tau_e}\right) \delta T$$

elec-ion relaxation times : mean velocity << temperature

Perturbations: mechanical relaxation time in grain mix, ion-elec. mean velocity relaxation time in atomic mix



□ Key step 3: By asymptotic analysis of the 14-eqn HED-BN model, one obtains the following approximations

◆ At the material interface, electron pressure relaxation rate >> ion pressure relaxation rate

$$O\left(\frac{\mu_p^{e1/e2}}{\mu_p^{i1/i2}}\right) \sim O\left(\sqrt{\frac{\rho_{ik}}{\rho_{ek}}}\right)$$

• Ion-electron momentum exchange is reduced to be a gradient term from a relaxation term $\alpha_k \mathbf{R}_{ik} \approx -\nabla \cdot \left(\alpha_{ik} \overline{\overline{P}}_{ek}\right) + \overline{\overline{P}}_{eI} \cdot \nabla \left(\alpha_{ik}\right) + \mathbf{M}_{ek}$

◆ The volume fraction equations for ions and electrons are reduced to be the same equation



□ Key step 4: By introducing an effective pressure relaxation to the atomic mix, we obtain a unified formulation for both grain and atomic mix

□ The effective unified model can be reduced to the classical two-fluid model





Volume fraction undefined \rightarrow **Pressure fraction** α_k^*

Atomic mix

Volume fraction $\alpha_r = \frac{1}{V} \int_V X_r dV$

Pressure relaxation \rightarrow **variation of** α_r

Pressure relaxation undefined \rightarrow Effective pressure relaxation

$$\frac{\partial p_{lk}^*}{\partial t} = \zeta_{lk}^* \left(p_{lk'}^* - p_{lk}^* \right), \quad \sum_k \zeta_{lk}^* \to \infty$$



□ Key step 5: Reduce multi-velocity to sing-velocity model with closure relation

- Neglect second-order terms of diffusion velocity w_k
- Close w_k with the Fick's law

$$\begin{array}{ll} \text{Grain mix} & \mathcal{O}\!\left(|\mathbf{w}_k|^2\right) \sim \mathcal{O}\!\left(\tau_u^2\right) \\ \text{Atomic mix} & \mathcal{O}\!\left(|\mathbf{w}_k|^2\right) \sim \mathcal{O}\!\left(\text{Kn}^2\right) \end{array}$$

• Diffusion velocity makes a non-negligible contribution to mixture momentum equation (especially for compressible flows)

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot \left(\rho \boldsymbol{u} \boldsymbol{u} - \sum \alpha_k \overline{\overline{T}}_{ak} \right) = \underbrace{\sum \boldsymbol{\nabla} \cdot \left(\alpha_k \overline{\overline{T}}_{wk} \right)}_{k}$$

• Neglecting the diffusion velocity contribution violates 2nd law





Different levels of relaxations lead to a hierarchy of disequilibrium models

Model	Ion eqns	Elec. eqns	Assumptions	Wave speeds
Nine-eqn	7	2	Ions in full diseq.	$u_1, u_1, u_2, u_2, u_I, u_1 \pm a_1, u_2 \pm a_2, a_k^2 = a_{ik}^2 + (a'_{ek})^2$
Eight-eqn	6	2	+ Ion velocities eq.	$u(6 \text{ times}), u \pm \sqrt{y_1 a_1^2 + y_2 a_2^2}$
Six-eqn	5	1	+ Ion/elec. mechanical eq.	u(4 times), $u \pm \sqrt{\frac{1}{\rho(\alpha_1/A_1 + \alpha_2/A_2)}},$ $A_k = \rho_k \left(a_{ik}^2 + (a'_{ek})^2\right)$
Five-eqn	4	1	+ Ion/elec. mechanical and thermal eq.	$u(3 \text{ times}),$ $u \pm \sqrt{\gamma_i p_i / \rho + a_e^2},$ $\gamma_i = \frac{\sum y_k C_{vik}(\gamma_{ik} - 1)}{\sum y_k C_{vik}} + 1$
Four-eqn	3	1	+ Ion/elec. mechanical, thermal and compressibility eq.	$u,u,u\pm\sqrt{a_i^2+(a_e')^2}$

• Hyperbolic, disequilibrium, thermodynamically compatible, reduction to classical models



II Model formulation : examples

- ◆ Reduce to **Baer-Nunziato model** if neglect electron
- Reduce to Zeldovich model for single fluid
- ♦ Repects 2nd law

9 equations, 2 velocities, 4 pressures, 4 temperatures



II Model formulation : examples

an model **8-e**

eqn model

$$\frac{\partial \alpha_k \rho_{ik}}{\partial t} + \nabla \cdot (\alpha_k \rho_{ik} \mathbf{u}) = -\nabla \cdot (\alpha_k \rho_{ik} \mathbf{w}_k),$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + \sum \alpha_k \overline{\overline{P}}_{ak}) = -\nabla \cdot (\sum \alpha_k \overline{\overline{P}}_{wk}),$$

$$\frac{\partial \alpha_k \rho_{ik} \varepsilon_{ik}}{\partial t} + \nabla \cdot (\alpha_k \rho_{ik} \varepsilon_{ik} \mathbf{u}) + \alpha_k p_{ik} \nabla \cdot \mathbf{u} = -p_{iI} \mathcal{P}_{ik} - \nabla \cdot (\alpha_k \rho_{ik} \varepsilon_{ik} \mathbf{w}_k) - \alpha_k p_{ik} \nabla \cdot \mathbf{w}_k + \mathcal{G}_{ik},$$

$$\frac{\partial \alpha_k \rho_{ek} \varepsilon'_{ek}}{\partial t} + \nabla \cdot (\alpha_k \rho_{ik} \varepsilon'_{ek} \mathbf{u}) + \alpha_k p_{ek} \nabla \cdot \mathbf{u} = -p_{eI} \mathcal{P}_{ek} - \nabla \cdot (\alpha_k \rho_{ik} \varepsilon'_{ek} \mathbf{w}_k) - \alpha_k p_{ek} \nabla \cdot \mathbf{w}_k + \mathcal{G}_{ek},$$

$$\frac{\partial \alpha_k}{\partial t} + \mathbf{u} \cdot \nabla \alpha_k = \mathcal{P}_k.$$

5-eqn model

$$\frac{\partial \alpha_k \rho_{ik}}{\partial t} + \nabla \cdot (\alpha_k \rho_{ik} \mathbf{u}) = -\nabla \cdot (\alpha_k \rho_{ik} \mathbf{w}_k),$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + \sum \alpha_k \overline{P}_{ak}) = \nabla \cdot \left(\sum \alpha_k \overline{P}_{wk}\right),$$

$$\frac{\partial \rho \varepsilon_i}{\partial t} + \nabla \cdot (\rho \varepsilon_i \mathbf{u}) + p_i \nabla \cdot \mathbf{u} = -\nabla \cdot \left(\sum \alpha_k \rho_{ik} \varepsilon_{ik} \mathbf{w}_k\right) - \sum \alpha_k p_{ik} \nabla \cdot \mathbf{w}_k + \mathcal{G}_i,$$

$$\frac{\partial \rho \varepsilon'_e}{\partial t} + \nabla \cdot (\rho \varepsilon'_e \mathbf{u}) + p_e \nabla \cdot \mathbf{u} = -\nabla \cdot \left(\sum \alpha_k \rho_{ik} \varepsilon'_{ek} \mathbf{w}_k\right) - \sum \alpha_k p_{ek} \nabla \cdot \mathbf{w}_k + \mathcal{G}_e.$$

5 equations, **1** velocities, 2 pressures, 2 temperatures



II Model formulation : numerical methods

□ The proposed model is a hyperbolic-parabolic-relaxation system solved by the fractional step method

Hyperbolic

- 5th order Spatial reconstruction MLP
- Free of spurious oscillations
- Volume fraction positivity $(N \ge 3)$
- Interface-sharpening

Parabolic

• **Explicit** method LIM

(V.T. Zhukov, Mat. Model. 22 (2010).)

Relaxation

• Efficient fixed-point iteration

- 1. Zhang C., et al, JCP, 2022; Zhang C., et al, JCP, 2023.
- 2. Menshov I., Zhang C., 2021, WCCM-ECCOMAS.
- 3. Zhang C., et al., J. Sci. Comput., 83(31) (2020).
- 4. Zhang C., et al., Comput. & Fluids. 236(2022)105311.







□ Heat conduction, mass diffusion, viscosity, and LIM efficiency













22 [1] Sangam, et al., JCP, 444 (2021) 110565. [2] Clérouin, et al. EPL, 89(1998). [3]Paquette, et al. Astrophys. J. Supples



RTI at ICF deceleration stage



[1] Vold E., et al., POP, 2021.



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□ Numerical results in spherical geometry



The plasma diffusion affects the RTI
 development (characteristic wavelength = 10μm)

RT growth rate (Vold E., POP2020)

$$\omega = \left[\left(\frac{Agk}{(1+bkL_D)} + ((\gamma+aD)k^2)^2 \right)^{1/2} - (\gamma+aD)k^2 \right]$$



□ The simulation results agree with exp. results for the laser-ablation of HMX target



Cao Z., Chu G., Ma X., et al. Visualizing pore collapse in explosive using X-ray picosecond tracking imaging, PRL, under review.



Our disequilibrium model has numerical advantage over traditional one-fluid model





IV Application (1): disequilibria in grain mix

□ Ablation shock hits the grain mixture (Characteristic length = 10µm, temperature separation = 1MK, velocity separation = 10km/s)





IV Application (2): disequilibria in atomic mix

□ Our model resolves temperatures of different ion species and electrons in atomic mix of ICF





SC = shock convergence

IV Application (3): Effect of temperature relax. on RTI

- **D** Temperature relaxation slows down the development of RTI
- **Using one-fluid model may underestimate perturbation development**



D Temperature relaxation alters the acceleration at the interface



IV Application (4): Interpenetration mix in hohlraum

 The laser-ablated Au bubble and Helium interpenetration due to velocity disequilibrium. The resulting mix zone is as long as 300µm, leading to energy loss.







Conclusion

- We have proposed a multi-component disequilibrium model
- It resolves temperatures and velocities of different ion/electron species
- It has a unified formulation for atomic/grain mix
- It has numerical advantages in convergence and is free of spurious oscillations

The model has been used to evaluate the disequilibria in atomic/grain mix of ICF

- The temperature separation between ion species is as large as 3keV after shock convergence
- Temperature relaxation slows down RTI development
- Velocity disequilibrium causes serious inter-penetration mixing between Au and He in hohlraum (~300µm)

