Radiation transport and multiphase particle laden flows

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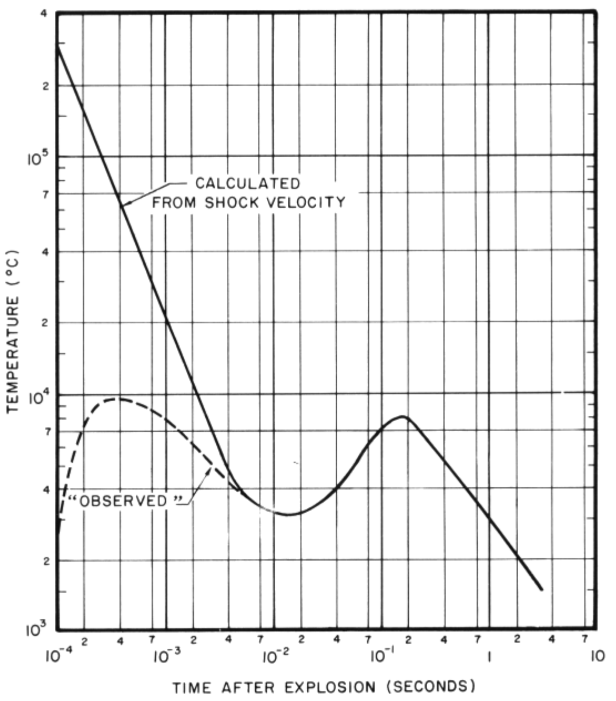
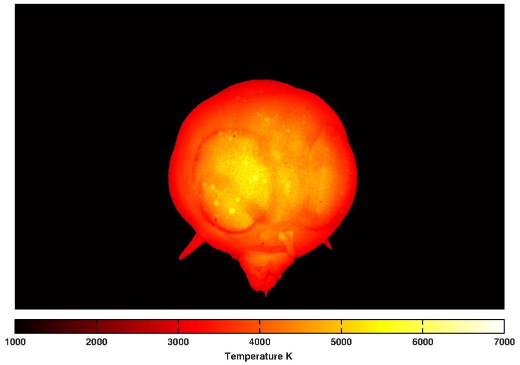
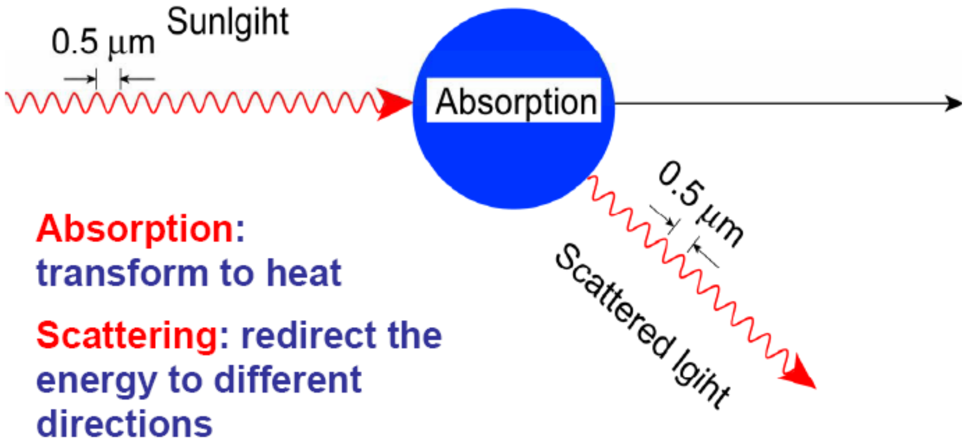
Challenge/Problem Needing the work

During early-time fireball development, environmental particles such as aerosols, dust or soil particles could be present in the atmosphere or entrained into the fireball





Variation of apparent fireball surface temperature with time in a 20-kiloton air burst (Glasstone & Dollan, 1977)



Schematic description of scattering and absorption of the sunlight

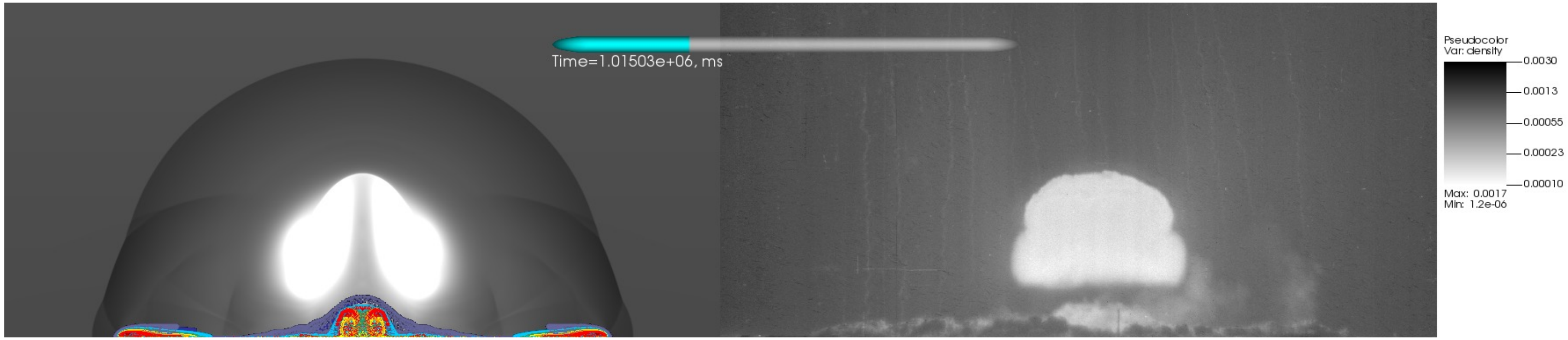
Rayleigh limit: $k_{0scat} \approx \lambda^{-4}$ and $k_{0abs} \approx \lambda^{-1}$

Question: How particles affect cooling, entrainment and radiation properties of the fireball?

Effort overview

➢ ***Previous work:***

Grable 15kT shot: Decoupled Radiation and Hydro effects. Introduced heated layer due to radiation effects that induces particle entrainment



(Kanarska et al., 2021 4th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling)

➢ ***Develop coupled approach for multiphase particle and radiation transport***

➢ ***Derive particle dependent opacity***

➢ ***V&V analytical solutions and nuclear shots***

➢ ***Study effects of particles on fireball cooling and entrainment***

Multiphase module

DEM multiphase model describes multiple multiphase species, including dense particles (Chinnaya, 2004). Both E-E and E-L approaches are available

Phase I

$$\frac{\partial \alpha_c}{\partial t} = -V^I \frac{\partial \alpha_c}{\partial x}$$

$$\frac{\partial \alpha_c \rho_c}{\partial t} + \frac{\partial \alpha_c \rho_c u_c}{\partial x} = 0$$

$$\frac{\partial \alpha_c \rho_c u_c}{\partial t} + \frac{\partial(\alpha_c \rho_c u_c^2 + \alpha_c P_c)}{\partial x} = P^I \frac{\partial \alpha_c}{\partial x} + F^I$$

$$\frac{\partial \alpha_c \rho_c E_c}{\partial t} + \frac{\partial(\alpha_c \rho_c u_c E_c + \alpha_c u_c P_c)}{\partial x} = P^I V^I \frac{\partial \alpha_c}{\partial x} + F^I V^I + Q^I$$

Phase II

$$\frac{\partial \alpha_d}{\partial t} = V^I \frac{\partial \alpha_c}{\partial x}$$

$$\frac{\partial \alpha_d \rho_d}{\partial t} + \frac{\partial \alpha_d \rho_d u_d}{\partial x} = 0$$

$$\frac{\partial \alpha_d \rho_d u_d}{\partial t} + \frac{\partial(\alpha_d \rho_d u_d^2 + \alpha_d P_d)}{\partial x} = -P^I \frac{\partial \alpha_c}{\partial x} - F^I$$

$$\frac{\partial \alpha_d \rho_d E_d}{\partial t} + \frac{\partial(\alpha_d \rho_d u_d E_d + \alpha_d u_d P_d)}{\partial x} = -P^I V^I \frac{\partial \alpha_c}{\partial x} - F^I V^I - Q^I$$

$$P_{c,d}^a = EOS(\ldots\ldots)$$

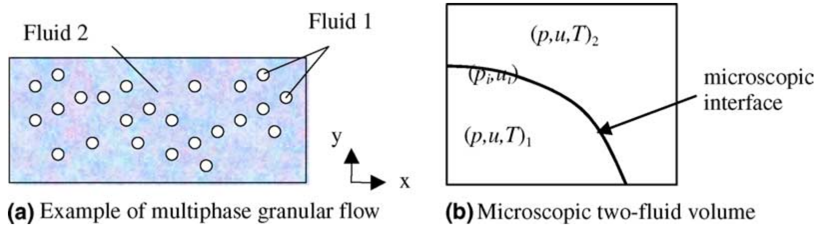
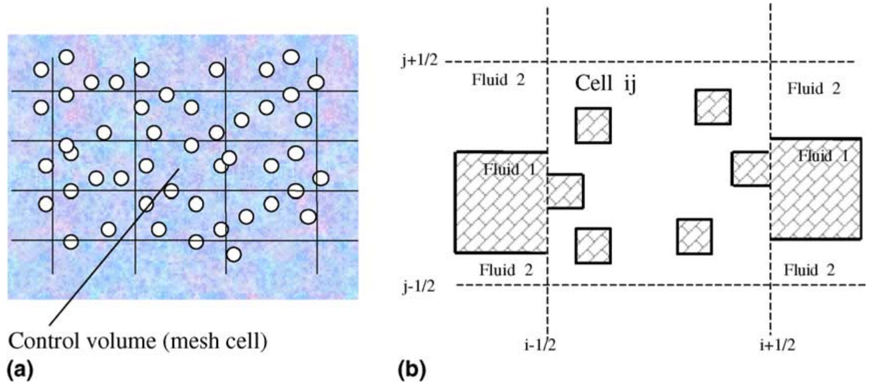


Fig. 2. Schematic representation of the two-phase control volume and interface control volume.



Chinnaya A., E. Daniel, and R. Saurel. 2004. *Modelling detonation waves in heterogeneous energetic materials. Journal of Computational Physics*, 196(2):490–538.

Multigroup Radiation Diffusion module

Multigroup Radiation Diffusion *model is based on Shestakov et al. (2013) multigroup equations*

$$\partial_t E + \nabla \cdot \boldsymbol{F} = \kappa[4\pi n^2 B_\nu(T) - v_g E]$$

$$\left(\frac{1}{v_g}\right) \partial_t \left(\frac{\boldsymbol{F}}{n^2}\right) + \nabla \cdot \left(\frac{v_g \bar{\bar{P}}}{n^2}\right) = -\kappa \frac{\boldsymbol{F}}{n^2}.$$

$$B_\nu(T) = \frac{2h_p \nu^3/c^2}{\exp\left(\frac{h_p \nu}{k_b T}\right) - 1}$$

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda} = v_p / \left(1 + \frac{\nu}{n}\frac{dn}{d\nu}\right)$$

Where $v_p = c/n$

Where the spectral energy density E, the flux $\boldsymbol{F}$, and the pressure tensor $\bar{\bar{P}}$ as

$$E = (1/v_g) \int_{4\pi} d\omega I,$$

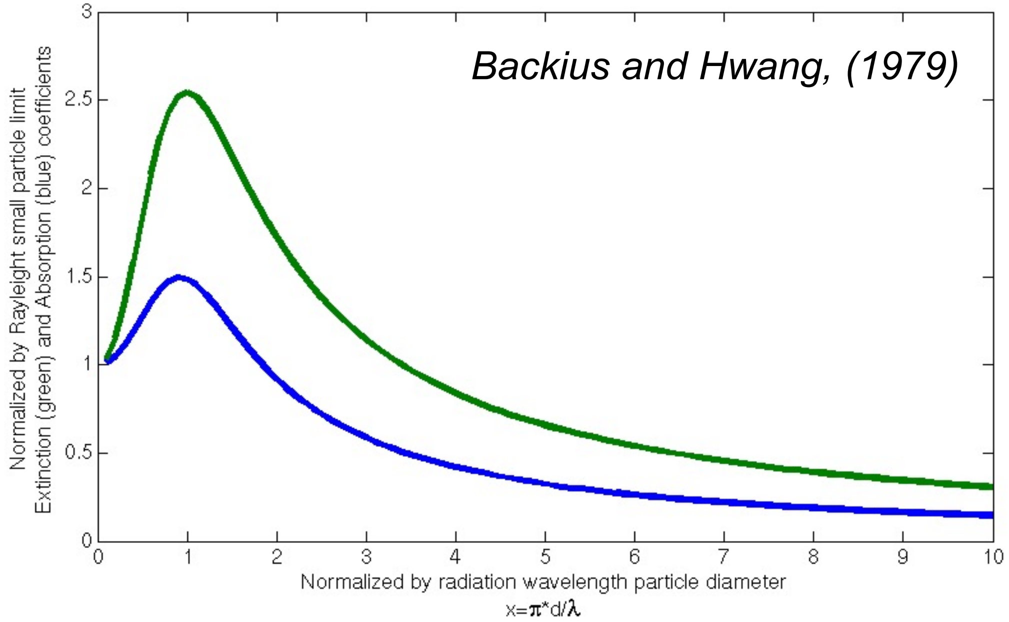
$$\boldsymbol{F} = \int_{4\pi} d\omega \boldsymbol{\Omega} I,$$

$$\bar{\bar{P}} = (1/v_g) \int_{4\pi} d\omega \boldsymbol{\Omega\Omega} I$$

Shestakov A. *et al. Multifrequency radiation diffusion equations for homogeneous, refractive, lossy media and their interface conditions*, Journal of Comp. Phys., 243, p. 293-304 (2013)

Particle size dependent opacity

- Opacity is usually calculated by using mass/volume average between materials in most Hydro codes.
- However, the particle size can affect radiation properties
- We develop a coupled multiphase/radiation approach to incorporate particle effects on radiation transport



*Extinction and absorption coefficients for different particles sizes as assembled in Backius and Hwang (1979). The example is shown for the material complex refractive index m = 1.0-1.0*i.*

$$k^{*\,-1.2} = [k_0^*(1 + 6.78k_0^{*2})]^{-1.2} + (3.09/k_0^{*0.1})^{-1.2}$$

$$k_{abs}{}^{*\,-1.6} = [k_0^*(1 + 2.30k_0^{*2})]^{-1.6} + (1.66/k_0^{*0.16})^{-1.6}$$

The Raleigh small particle limit of a nondimensional extinction coefficient can be derived as

$$k_0^*(\eta, \boldsymbol{m}) = -4\bar{x}\mathcal{J}\left(\frac{\boldsymbol{m}^2-1}{\boldsymbol{m}^2+2}\right) = -\left(\frac{24\bar{x}kn}{(\boldsymbol{n}^2-\boldsymbol{k}^2+2)^2+4\boldsymbol{n}^2\boldsymbol{k}^2}\right)$$

Coupled Multiphase and Radiation transport approach

Lagrange Hydro ALE step → Multigroup Radiation → Radiation Energy Deposition to Multiphase → Advance Multiphase

I *Solve Lagrange Hydro ALE equations*

II ***Derive particle size dependent opacity using Backius&Hwang (1979) approach***

III *Derive mixture opacity by doing mass fraction/volume fraction averaging between particle size dependent opacity and other materials in multiphase*

IV *Solve Multigroup diffusion equations (Shestakov et al., 2013)*

V ***After all Thermal/Radiation routines are done the energy is translated into the initial energy for each multiphase species. The energy between species are distributed based on the corresponding ρc_v, where ρ is the species density and c_v is the heat capacity.***

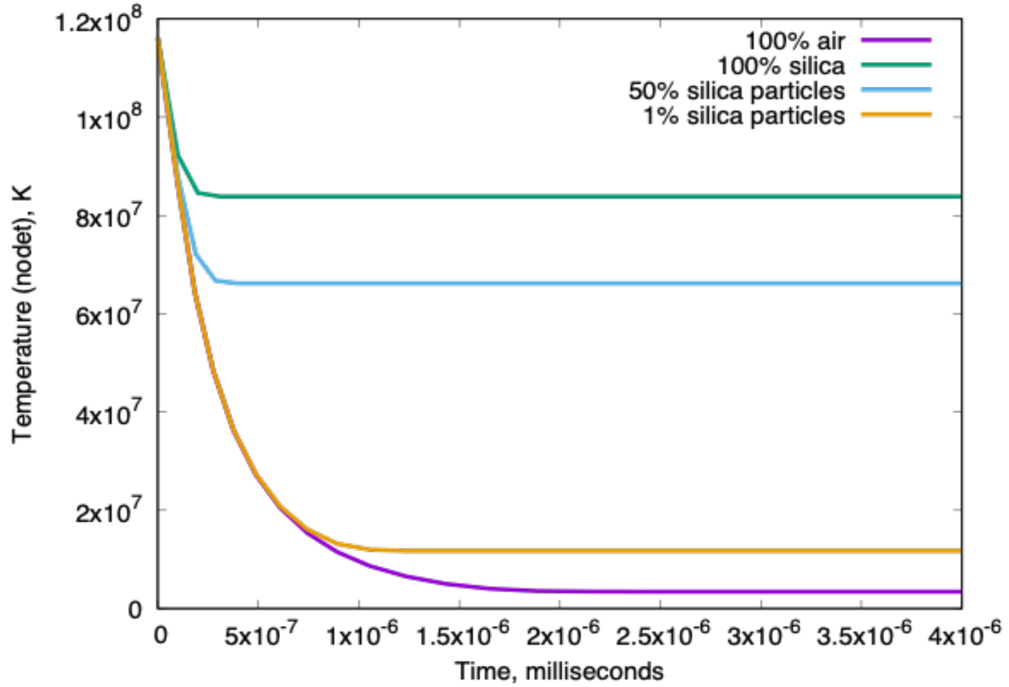
VI *Advance Multiphase module using DEM algorithm (Chinnaya et al., 2004)*

V&V studies

0D simulation showing energy balance is achieved between the matter energy and the radiation energy. Matter energy is initialized with a temperature of 1e4 eV, with no radiation energy. According to a simple energy balance the final temperature can be found using:

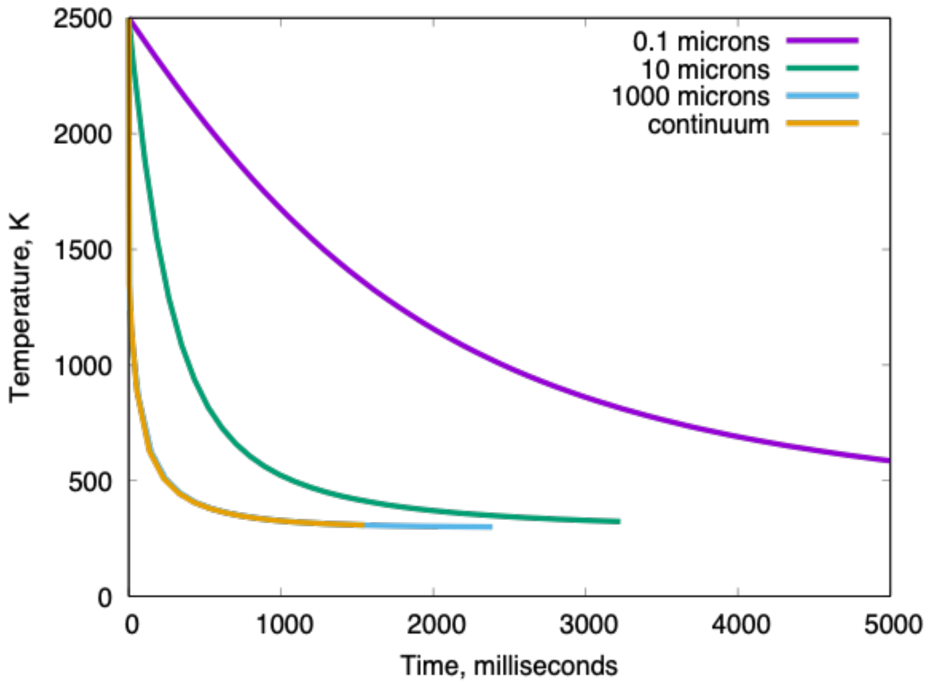
$$0 = -\rho c_v T_0 + aT^4 + \rho c_v T$$

*where a = 4*sigma/c, sigma is the Stefan Boltzman constant, and c is the speed of light.*



I

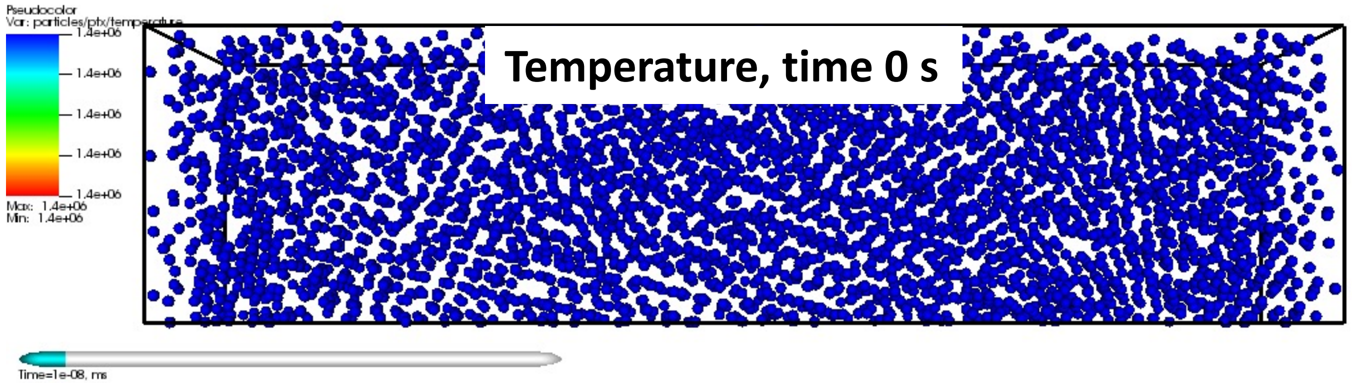
1D simulation showing evolution of the temperatures for the radiation cooling of the silica/air mixture. 50% volume fraction of silica in all cases. New particle size dependent opacity is tested with 16 groups (Multigroup diffusion model) and 3 particle sizes. For the large enough particles (1000 microns) the continuum representation of opacity (by mass average) provides asymptotic case for our particle size dependent opacity

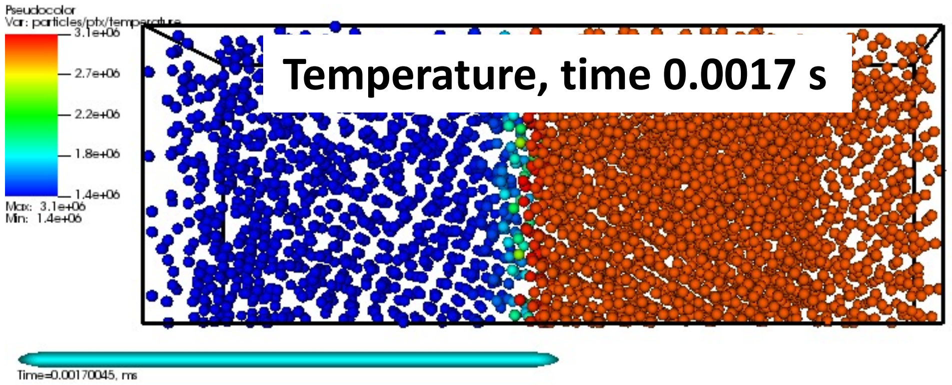


II

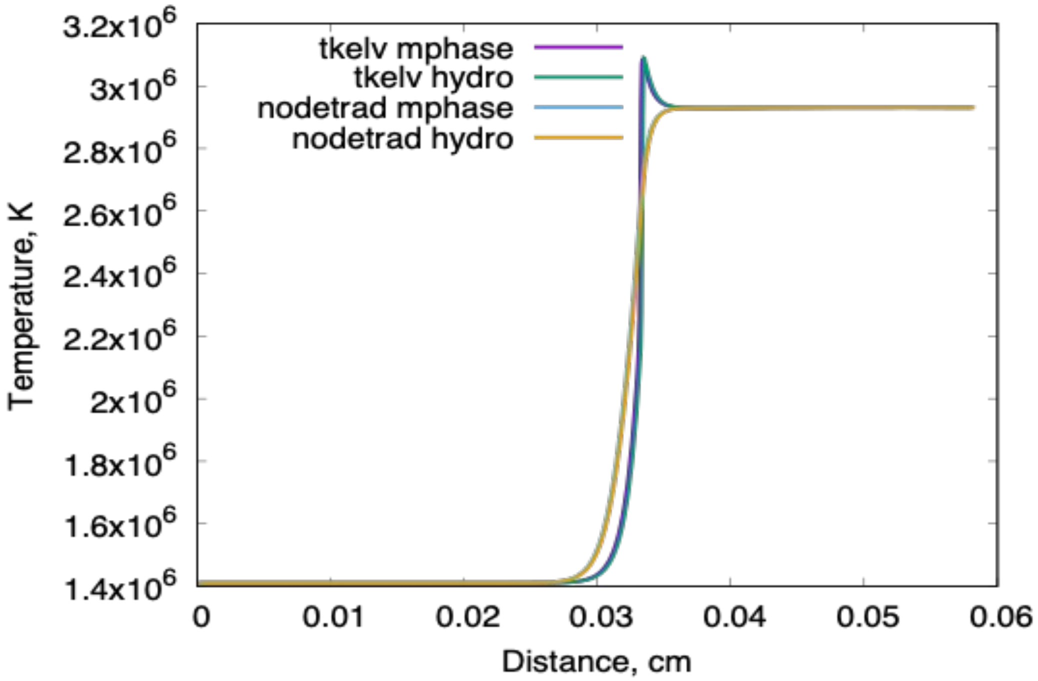
V&V studies (cont'd)

Lowrie problem** (Lowrie&Edwards, 2007) with particles* ***III



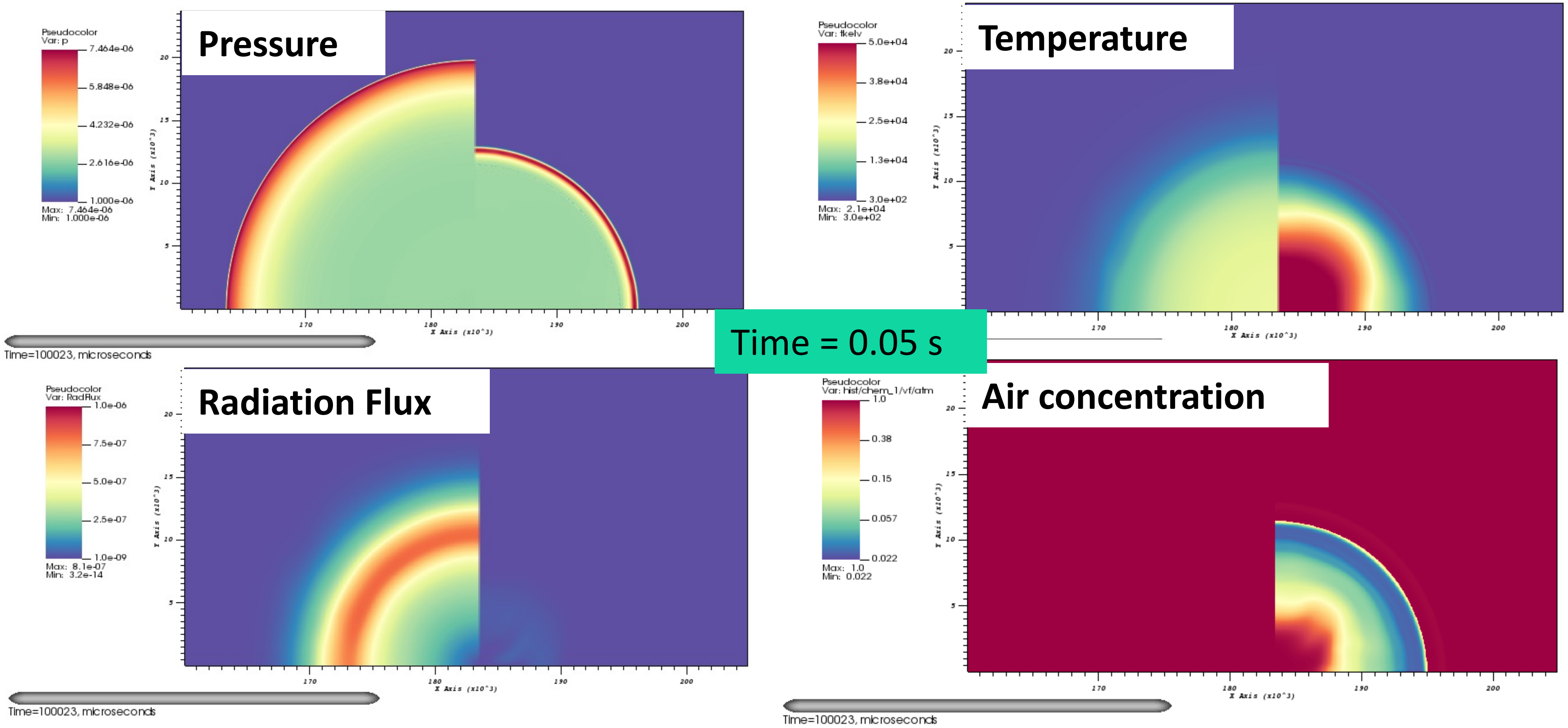


Multiphase/thermal/radiation solver with Lagrange particles (diameter 2.6 microns, volume fraction 0.01)



Comparison between pure hydro/thermal/radiation solver and multiphase/thermal/radiation solver. The cell centered temperature tkelv and radiation temperature nodetrad at 0.00140011 ms are shown.

Question 1: How particles affect cooling, entrainment and radiation properties of the fireball?



Y_0 = 11 kT, T_0 = 3.0e^{6}K, P0 = 100 Mbar, R = 60 cm, 51 groups, frequency 0.1 - 1e5 erg

Left: pure air (no particles)

Right: aerosol/dust particles in the atmosphere (0.1 microns, 1% volume)

Presence of the dust/aerosol particles may lead to substantial decrease of the radiation flux out from the fireball and, as a result, higher fireball temperatures in addition to slow down and weakening of the blast wave

Conclusions

- *Developed an improved coupled model for multiphase treatments of environmental materials/particles/chemical species including radiation effects*
- *We implemented particle size dependent opacity*
- *V&V studies*
- *Studied how particles affect cooling, entrainment and radiation properties of the fireball using hot sphere problem with background atmospheric aerosol/dust particles present (10 microns, 1% volume fraction)*
- *The cooling rate and radiation fluxes differ substantially in the presence of dust/aerosol particles, leading to the higher fireball temperatures in the presence of dust/aerosols.*
- *This emphasizes the importance of the environmental particles effects on the fireball cooling rates (thus associated chemistry and compositions)*

Acknowledgments

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