Development of 3D Heat Transfer and Pyrolysis in FDS

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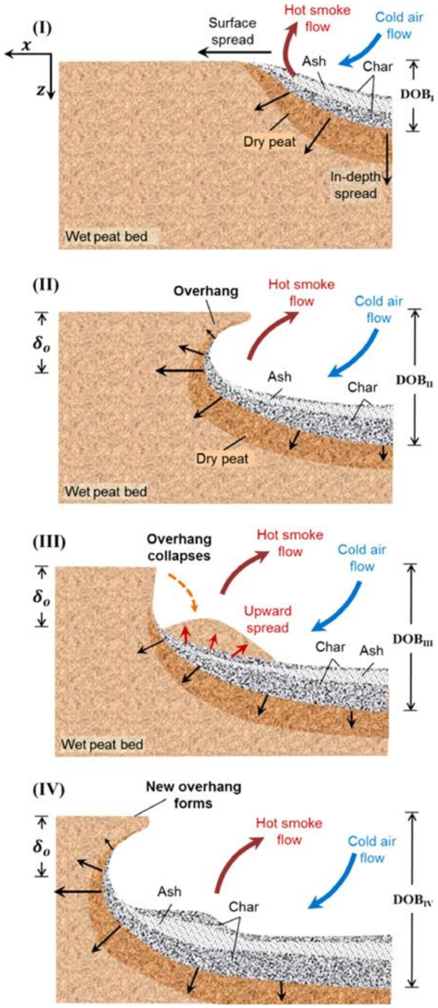
Background and Motivation

- Structural analysis
- Lateral and downward flame spread
- Smoldering combustion


Choe, 2017


Ohlemiller & Shields, 2008

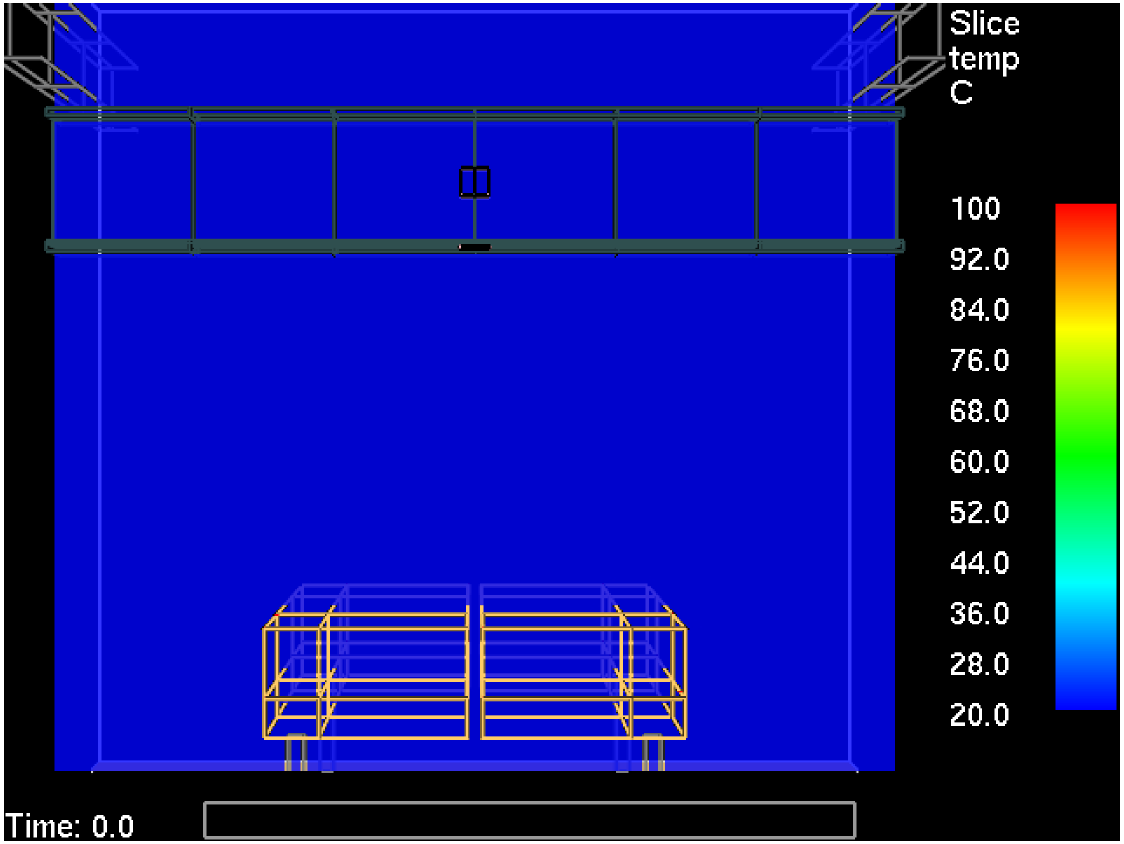


Huang et al., 2016

Previous Work

- Andreas Vischer, Aachen, 2009 thesis
- Volker Hohm and Matthias Siemon, Building Materials, Solid Construction and Fire Protection (iBMB) at Technische Universität Braunschweig
- Gpyro, Chris Lautenberger, Reax Engineering
- Thermakin, Stas Stoliarov, U. Maryland

Integration into FDS master



TEMPERATURE SLICE

Governing Equations

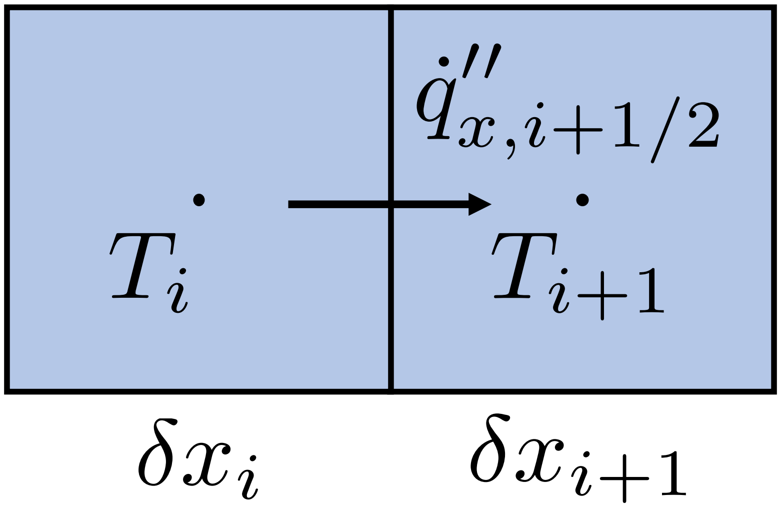
Local deformation affects heat flux

$$\rho_s c_s \frac{\mathrm{D}T}{\mathrm{D}t} = -\nabla \cdot \dot{\mathbf{q}}'' + \dot{q}'''$$

$$\frac{\mathrm{D}\rho_{s,\alpha}}{\mathrm{D}t} = \dot{m}_\alpha''' \,; \quad \alpha = 1, \ldots, N_m$$

Computing Heat Flux

Fourier's law: $\dot{\mathbf{q}}'' = -k\nabla T$



$$\dot{q}''_{x,i+1/2} = -k_{i+1/2}\frac{T_{i+1} - T_i}{\frac{1}{2}(\delta x_i + \delta x_{i+1})}$$

Input Parameters

HT3D=T invokes 2-way coupling with gas phase

```
&OBST XB=-.5,.5,-.5,.5,-.5,.5,
      HT3D=T,
      MATL_ID='STEEL',
      SURF_ID6='cold','adiabatic',
               'hot','adiabatic',
               'adiabatic','ht3d'/

&MATL ID            = 'STEEL'
      SPECIFIC_HEAT = 0.60
      CONDUCTIVITY  = 45.
      DENSITY       = 7850./

&SURF ID='ht3d', HT3D=T, COLOR='GREEN'/
&SURF ID='hot', TMP_FRONT=500, COLOR='RED'/
&SURF ID='cold', TMP_FRONT=20, COLOR='BLUE'/
&SURF ID='adiabatic', ADIABATIC=T, COLOR='GRAY'/
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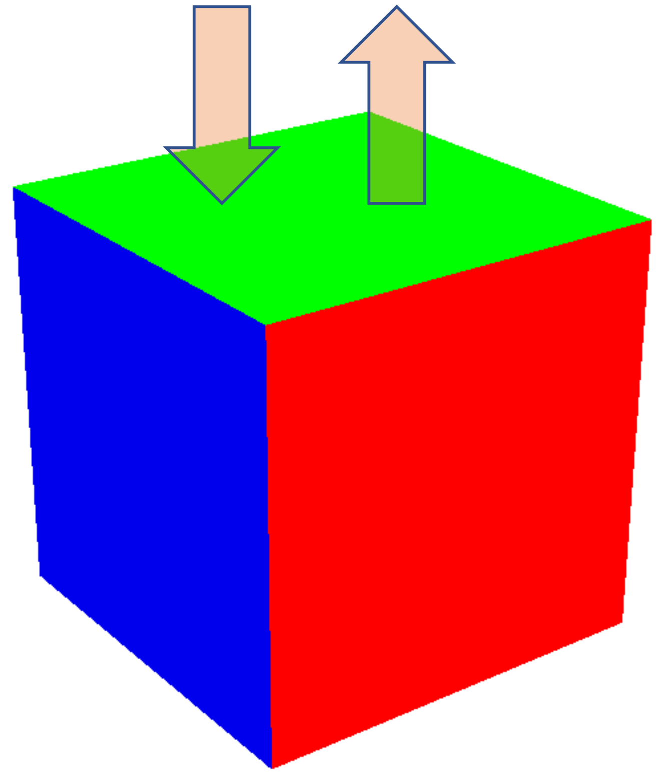
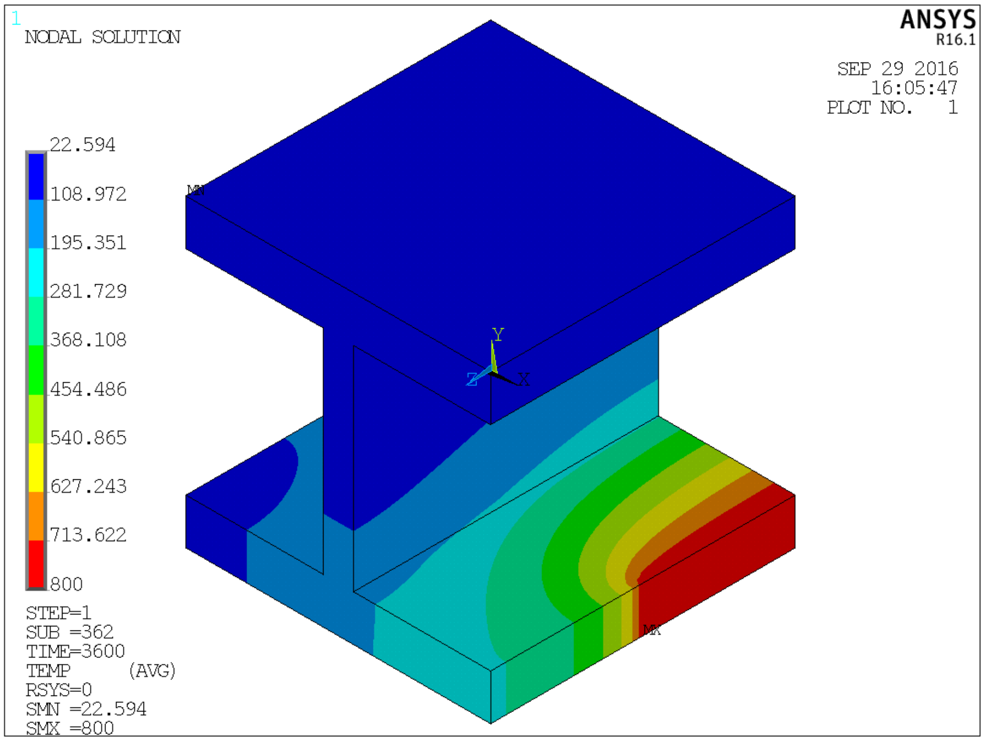
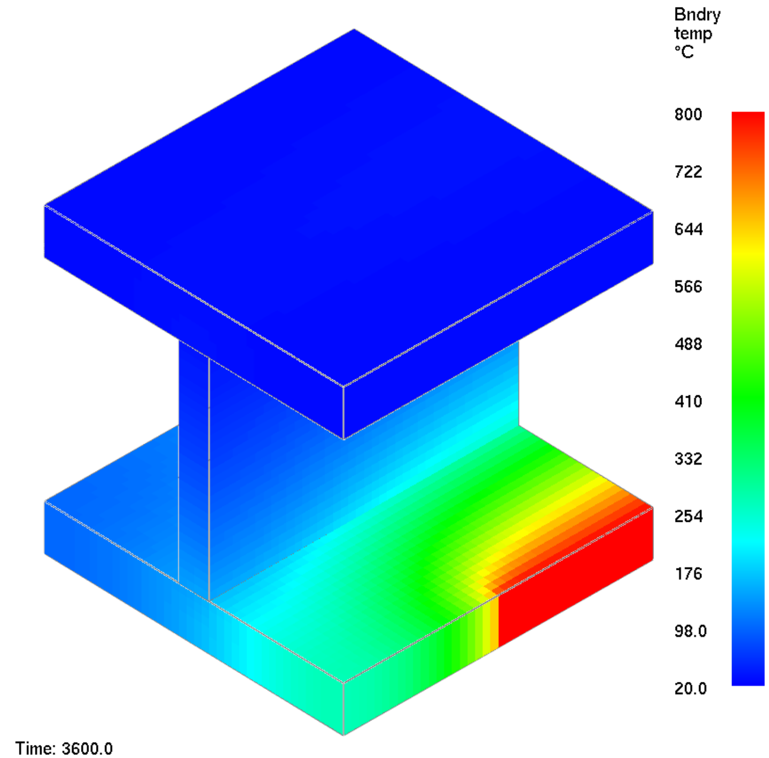


Heat Diffusion in Steel I-Beam

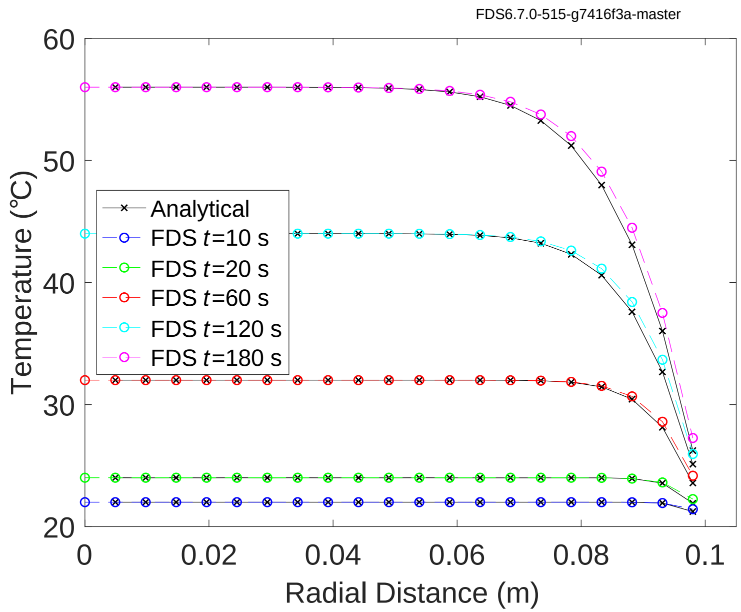


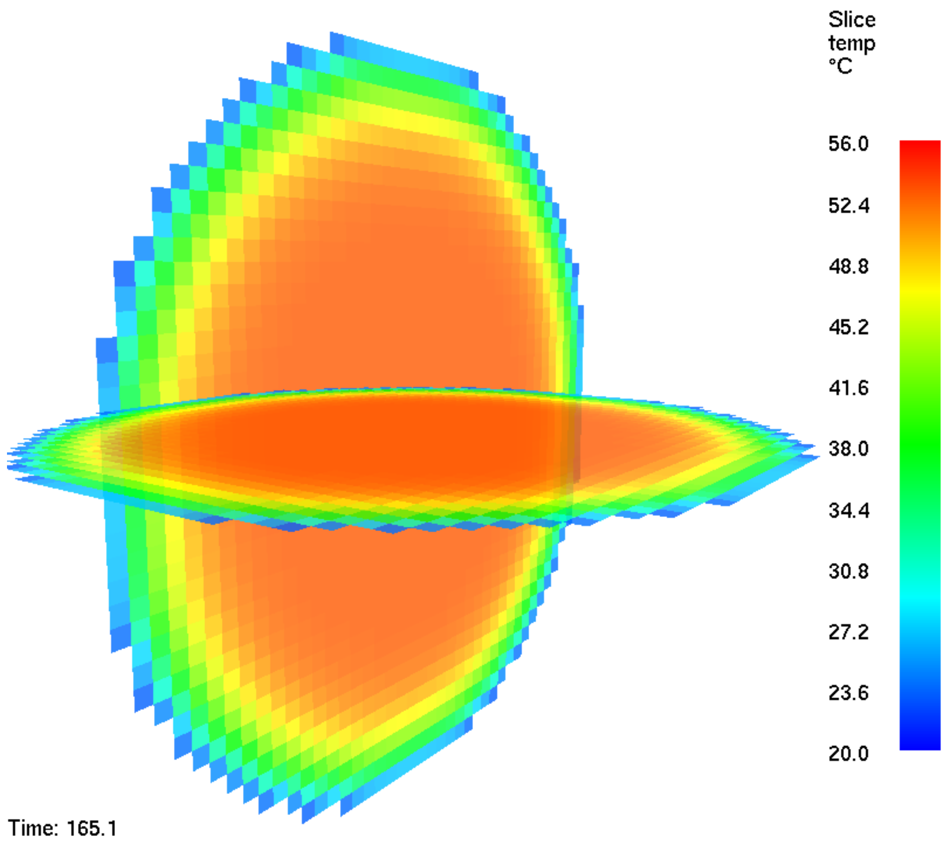


Any mention of commercial products within this paper is for information only; it does not imply recommendation or endorsement by NIST.

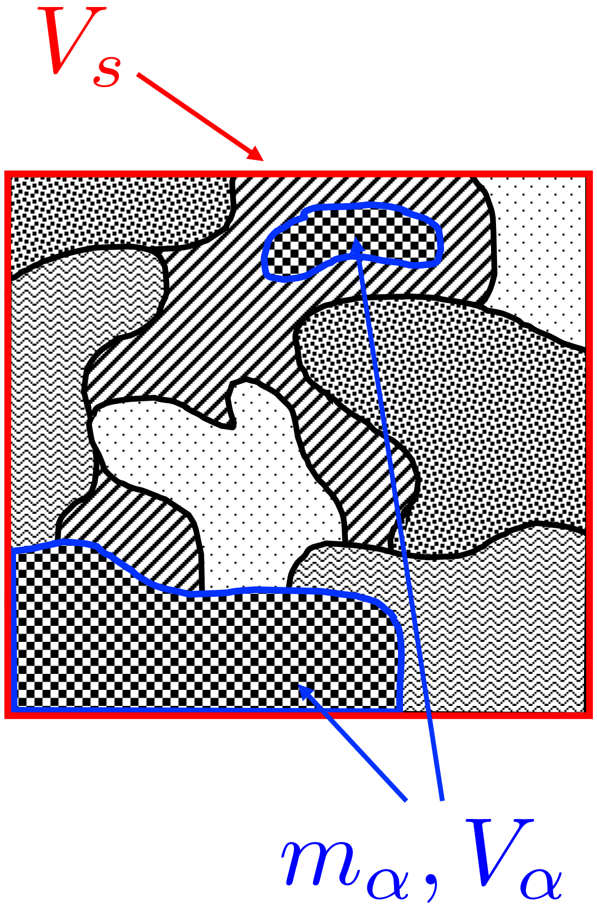
Internal Heating in Sphere

- Constant, uniform internal heat generation
- Constant, ambient surface temperature





Density Definitions



1. Material

$$\rho_\alpha \equiv \frac{m_\alpha}{V_\alpha}$$

2. Bulk

$$\rho_{s,\alpha} \equiv \frac{m_\alpha}{V_s}$$

3. Total solid

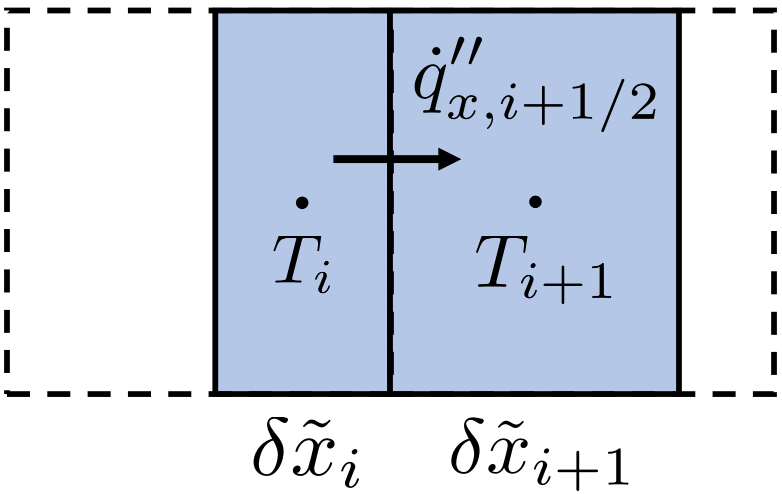
$$\rho_s \equiv \sum_\alpha \rho_{s,\alpha}$$

Modeling Deformation

- Changes in composition generally cause contraction or expansion of material
- Some challenges in 3D:
  1. Mechanical constitutive relation
  2. Advection term in conservation equations
  3. Moving boundaries
- Simple solution:
  1. Subgrid scale models of fluxes
  2. Burn away—remove solid cells as cell density goes to zero

Heat Flux with Local Deformation

- As material contracts (expands), distance between material points decreases (increases)



$$\dot{q}''_{x,i+1/2} = -k_{i+1/2}\,\frac{T_{i+1} - T_i}{\frac{1}{2}(\delta\tilde{x}_i + \delta\tilde{x}_{i+1})}$$

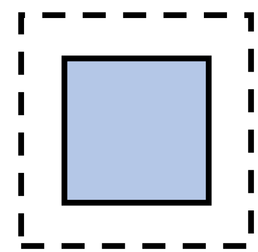
Local Material Deformation

$$\phi_s \equiv \frac{V_s}{V_{cell}} = \sum_\alpha \frac{V_\alpha}{V_{cell}} = \sum_\alpha \frac{m_\alpha/\rho_\alpha}{m_\alpha/\rho_{s,\alpha}} = \sum_\alpha \frac{\rho_{s,\alpha}}{\rho_\alpha}$$

Two simple models:

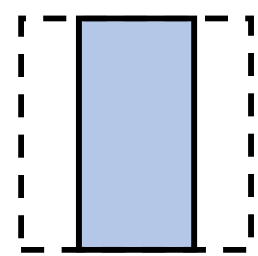
1. Isotropic: $\delta\tilde{x} = \phi_s^{1/D}\delta x$

   $\delta\tilde{y} = \phi_s^{1/D}\delta y$



2. Unidirectional: $\delta\tilde{x} = \phi_s \delta x$

   $\delta\tilde{y} = \delta y$

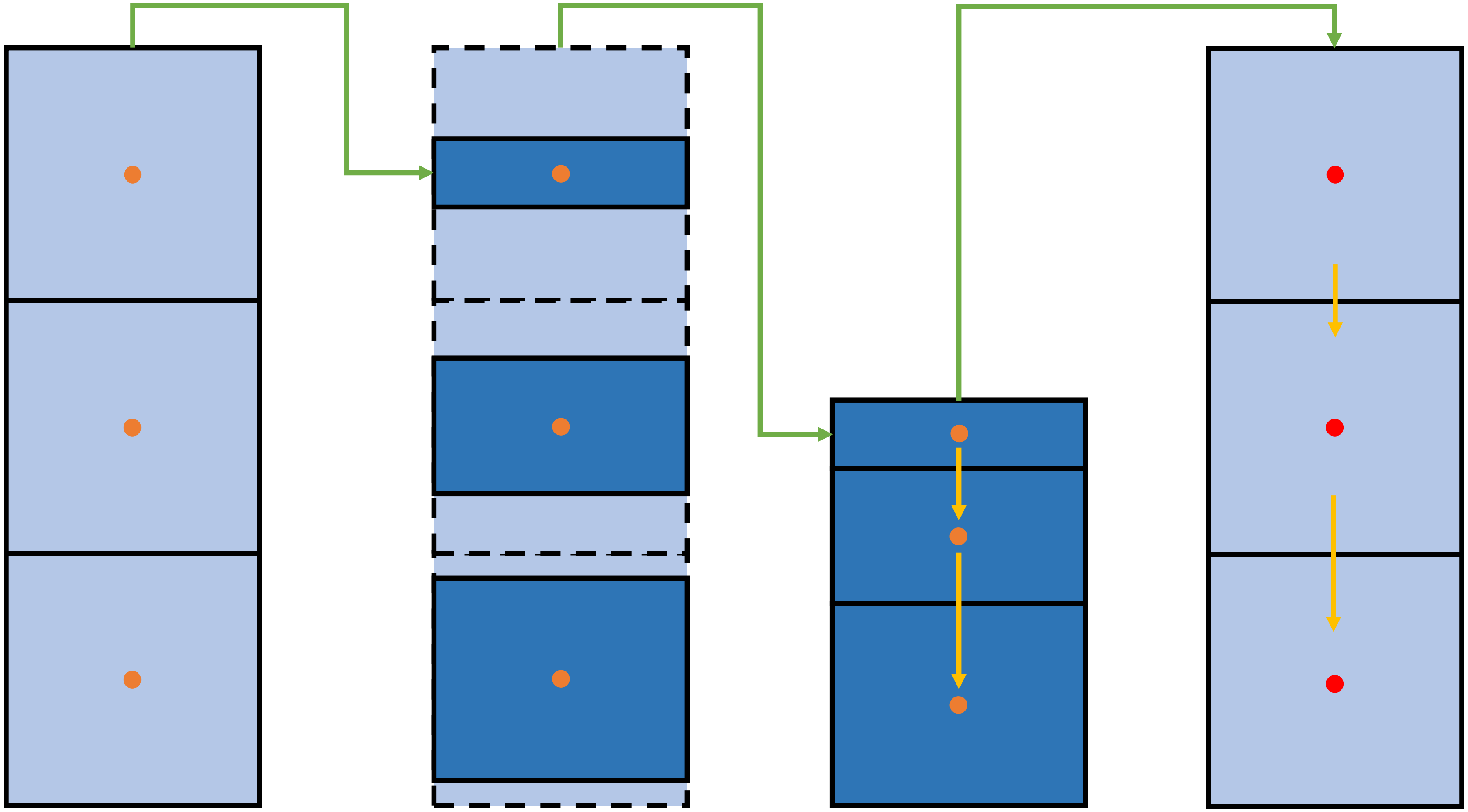


Compute new densities using old temperatures

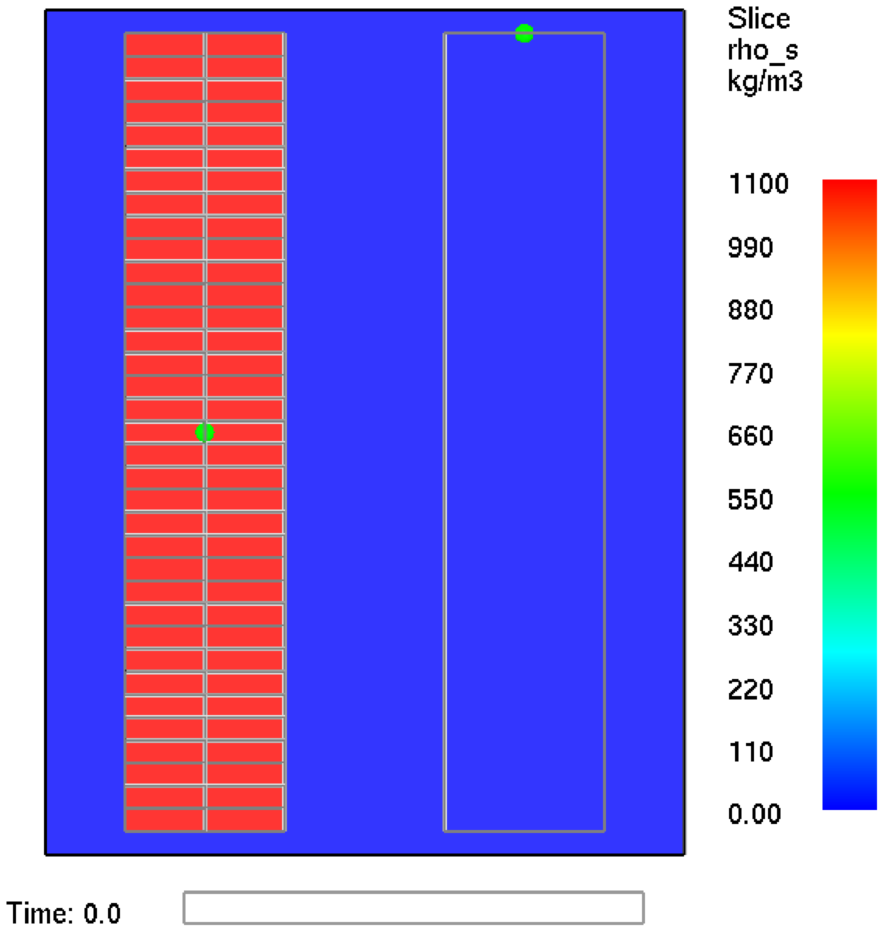
Compute solid volumes using new densities

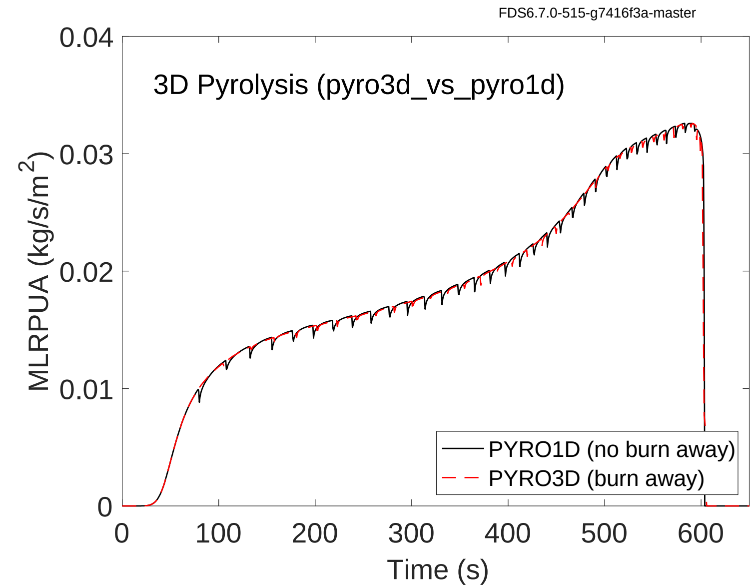
Compute heat fluxes on solid volumes

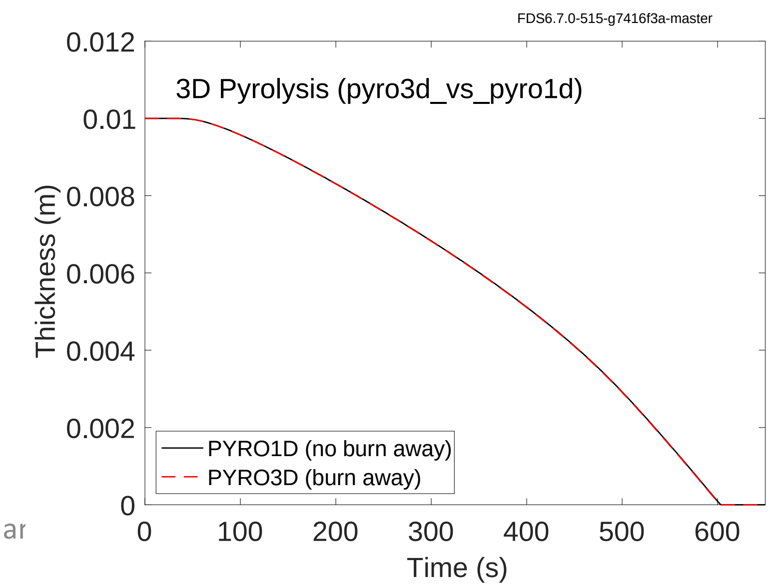
Compute new temperatures using heat fluxes



PMMA Slab: Mass Loss Rate and Thickness







Radiative Heat Transfer

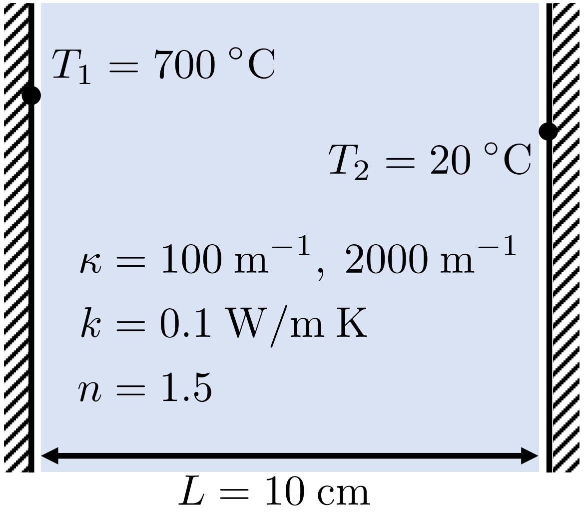
$$\dot{\mathbf{q}}'' = -(k + k_r)\nabla T$$

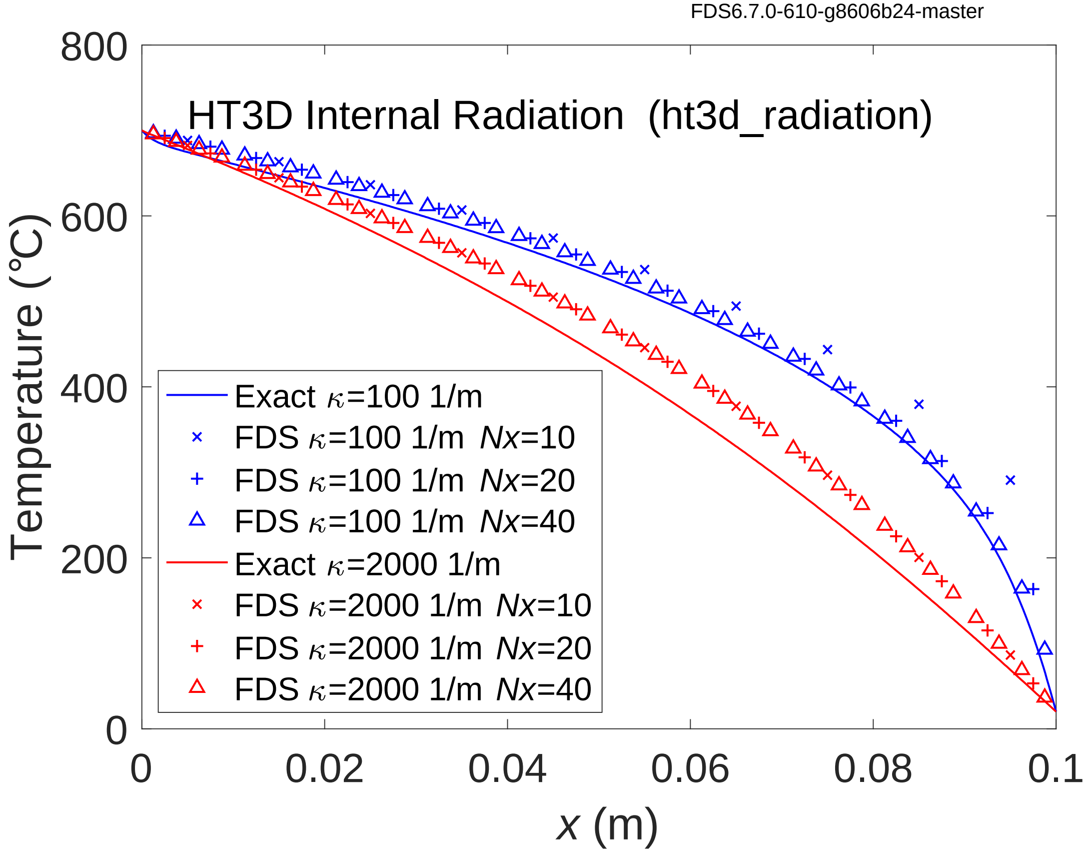
$$k_r = \frac{16 n_s^2 \sigma T^3}{3\kappa_s}$$

- Many problems are thermally thick
- Diffusion approximation is extremely efficient in 3D

Material	Absorption Coefficient (1/m)	Thermal Thickness for 1 cm slab
HDPE	1300	13
PMMA	2700	27
PA66	3920	39.2

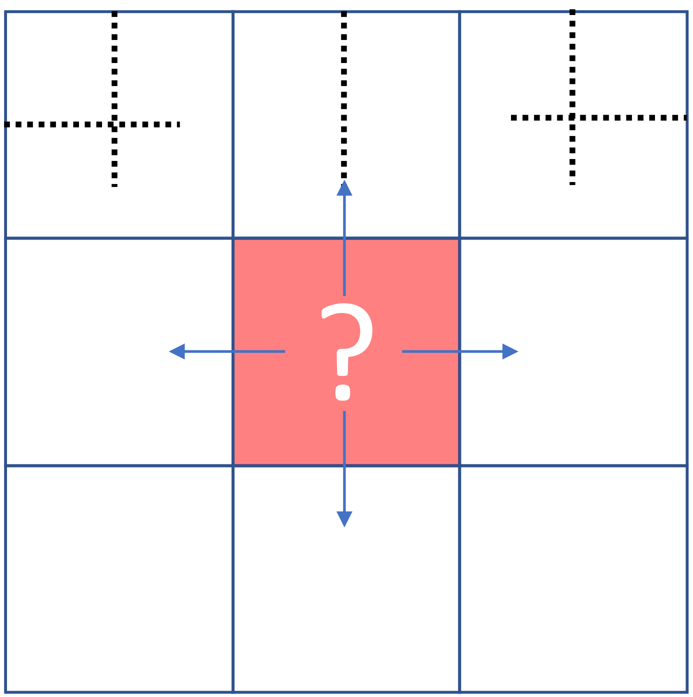
Radiation Verification

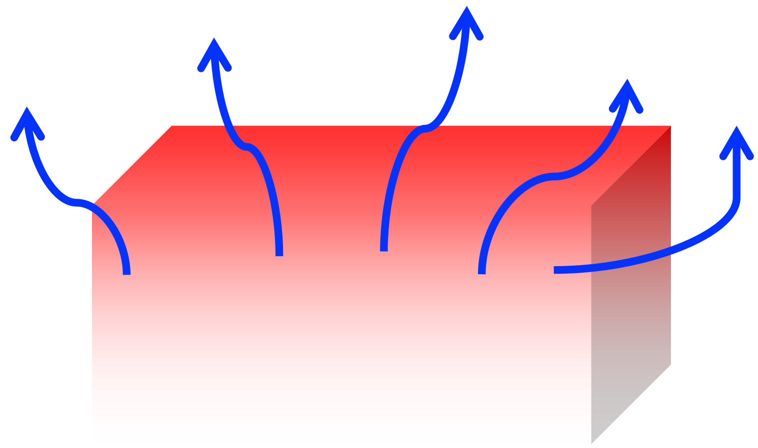




Exact solution from Modest, Radiative Heat Transfer, 2nd Edition.

Pyrolysis Gas Transport





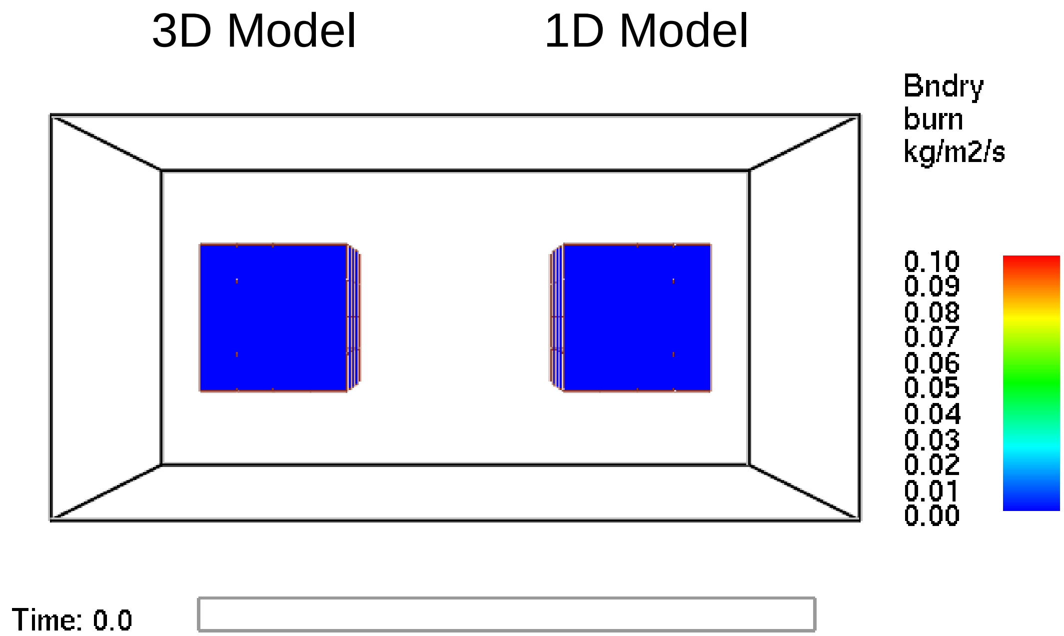
$$\frac{\partial \rho_{\mathrm{g},\alpha}}{\partial t} = -\nabla \cdot \mathbf{j} + \dot{m}'''_{\mathrm{g},\alpha}$$

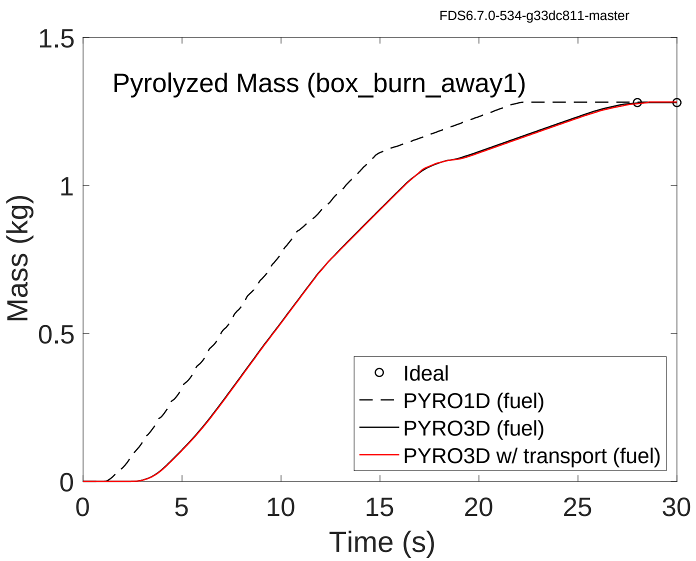
$$j_x = -D_\alpha \frac{\partial \rho_{\mathrm{g},\alpha}}{\partial \tilde{x}}$$

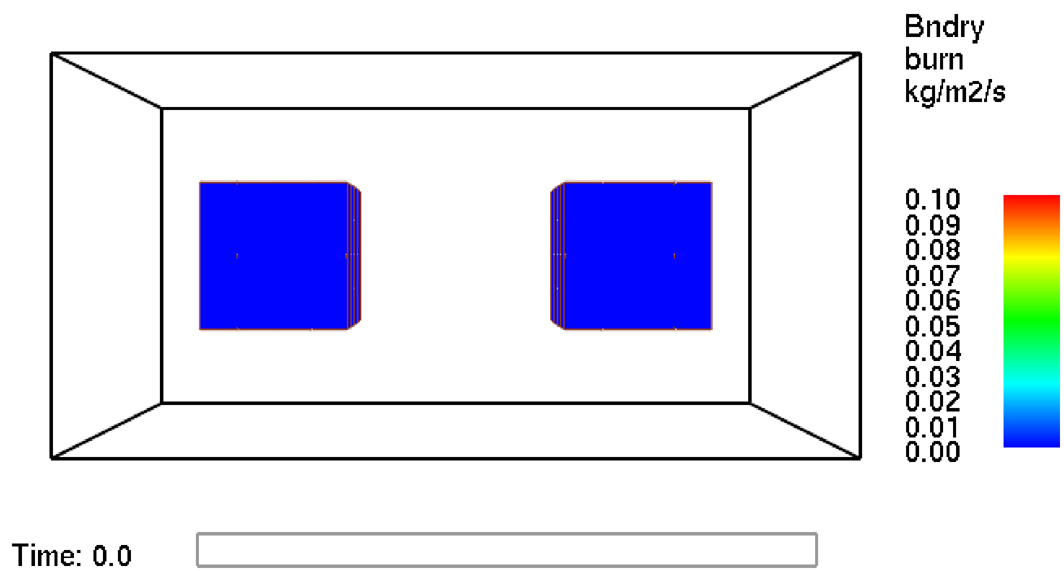
$$\rho_{g,F} = \begin{cases} 0 & \text{if } g \text{ is fuel} \\ \rho Y_{g,F} & \text{if } g \text{ is oxidizer} \end{cases}$$

Burn Away

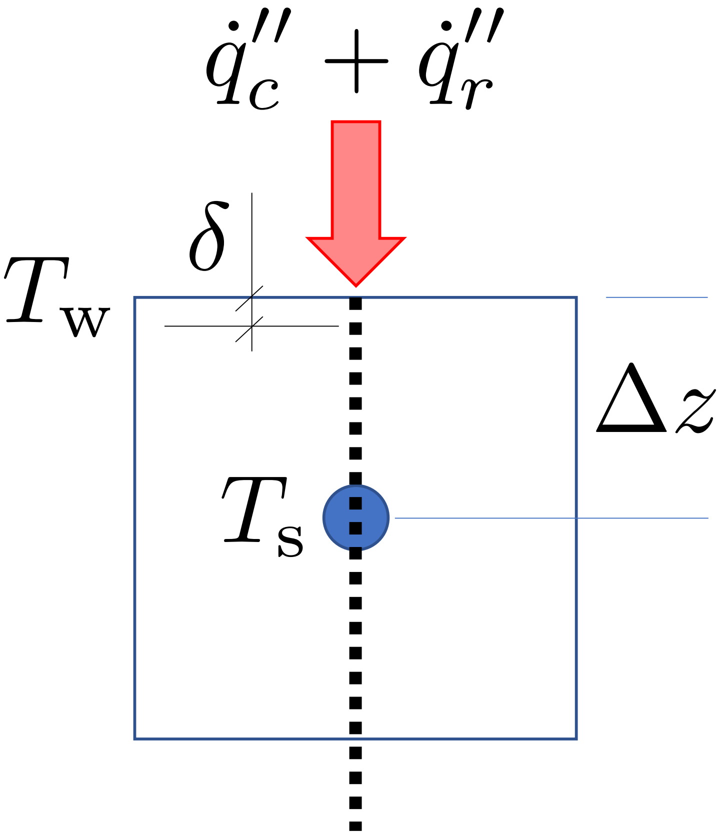
- 40 cm cubes
- Low density “foam”
- Compartment walls at 1100 °C







Solid Sub-Surface Heat Flux Model



$$\delta = \sqrt{\frac{\tau \; k_{\rm s}}{\rho_{\rm s} c_{\rm s}}}$$

$$\dot{q}_{\rm c}'' + \dot{q}_{\rm r}'' = -k_{\rm s} \frac{T_{\rm w} - T_{\rm s}}{\delta}$$

Closing remarks

- Development of an efficient 3D pyrolysis model is needed for reliable predictions of flame spread (work in progress)
- Subgrid-scale models of heat and mass fluxes were used to account for local deformation
- The resultant model has been verified and tested for several scenarios
- Next steps:
    - Anisotropy
    - Thin obstructions (coupling with 1D model?)
    - Porous media flow

Acknowledgements

- FDS development team
- Simo Hostikka, Deepak Paudel