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Predicting Soot Formation and Emission in Wildland Fires with FIRETEC

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Rocky Mountain Research Station

Tall Timbers Research Station & Land Conservancy

Canada Natural Resources Canada Canadian Forest Service

U.S. AIR FORCE

Defense Threat Reduction Agency United States of America

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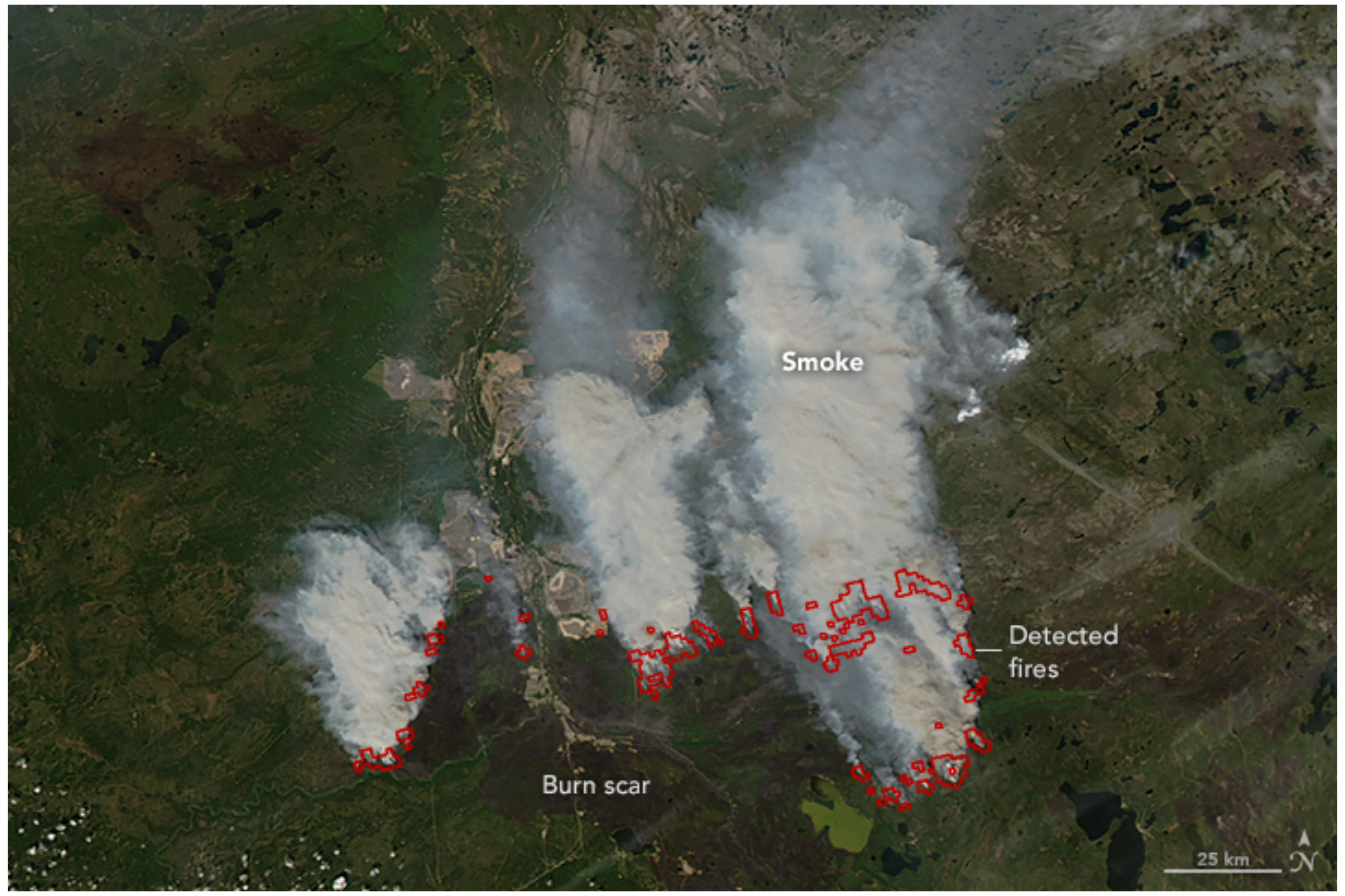
Motivation - Emissions



NASA earth observatory index, Fort McMurray Fire in Alberta, May 25, 2016
https://earthobservatory.nasa.gov/images/event/87986/fort-mcmurray-fire-in-alberta

- Wildland and urban fires are an issue of national security
- Smoke formation and dispersion a major health concern
- Forest Service to use prescribed fire as a fire management tool
- Use of prescribed fire comes with a responsibility for the smoke formed
- Current ‘state-of-the-art’ models use emission indexes
- These emission indexes feed into atmospheric models for plume evolutions

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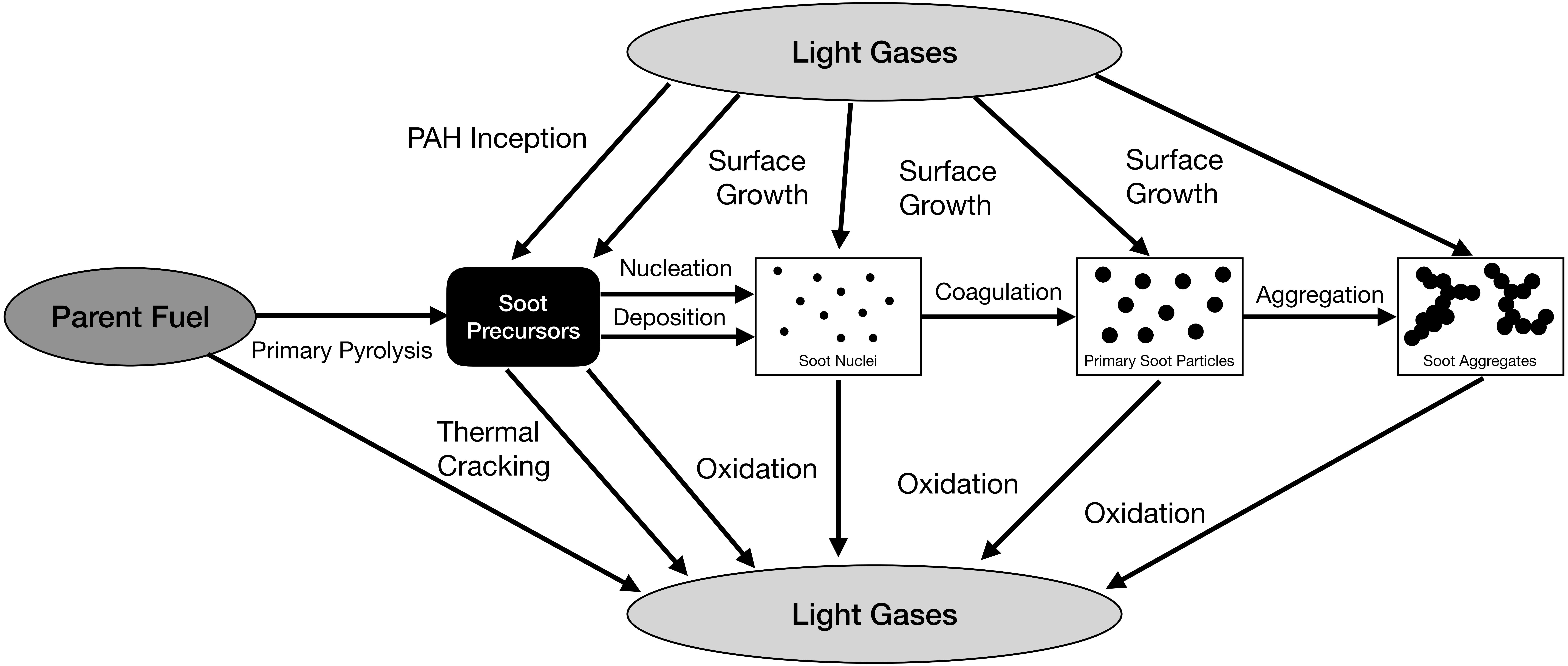
Soot Formation from Solid Fuels



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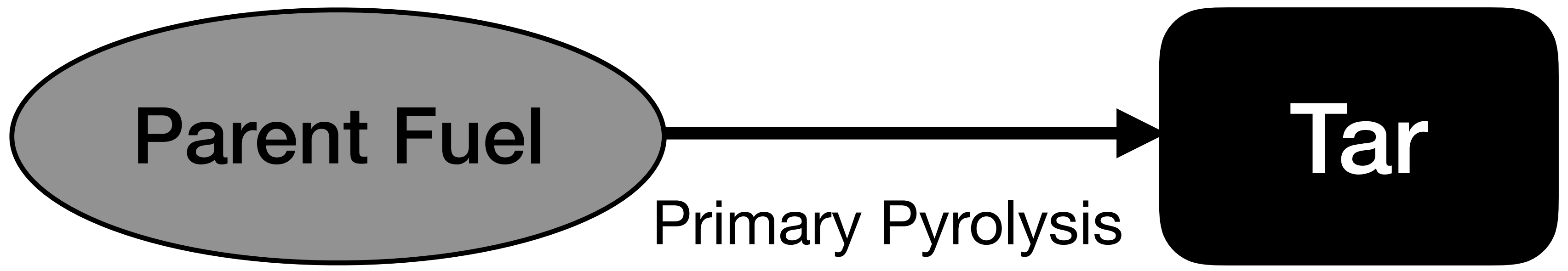
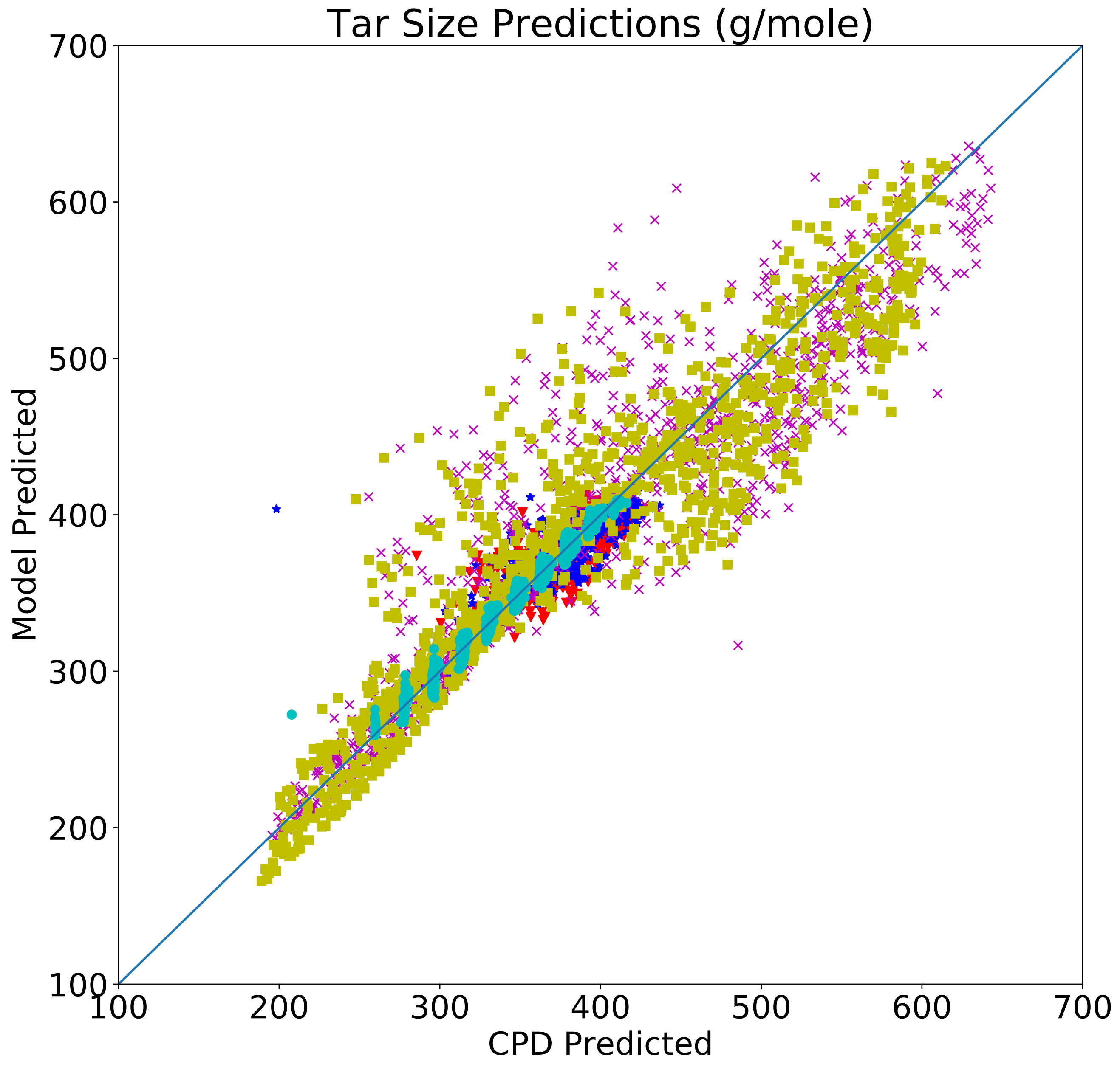
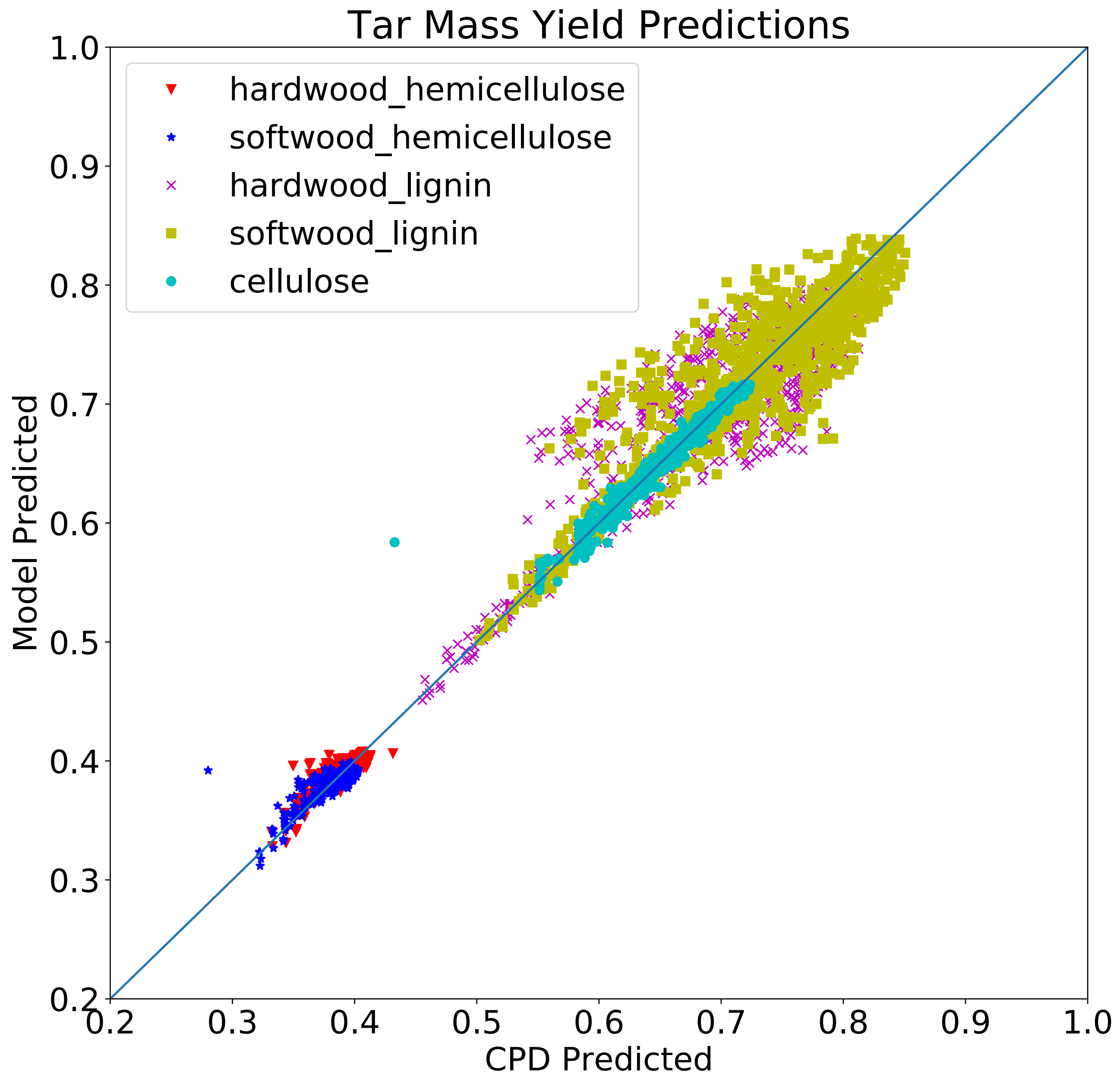
Previously Developed Model

- How much is produced?
- What size?
- Chemistry?







- Developed an easy-to-evaluate surrogate model
- Calibrated thousands of executions of the CPDbio model
- Evaluates based on the fundamental components of biomass, pressure, gas temperature
- Chemistry is represented by breaking tar into benzene, toluene, naphthalene, and phenol-like molecules

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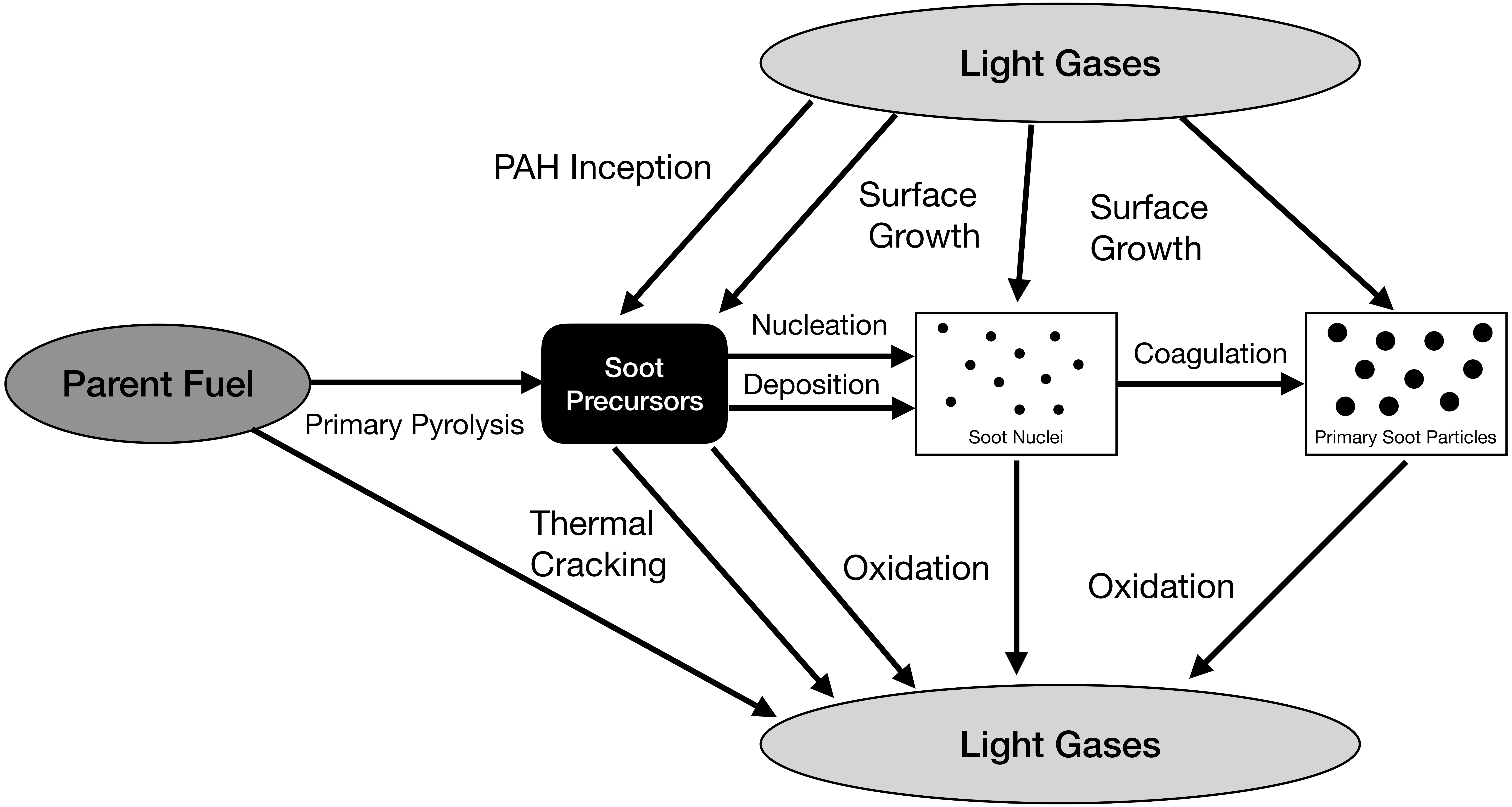
Soot Formation from Solid Fuels



Resolves:

1 Tar
2 Soot

Tar Number Density

$$\frac{dN_{tar}}{dt} = r_{TI} - r_{SN} - r_{TD} + r_{TS}$$

Soot Number Density

$$\frac{dN_{soot}}{dt} = r_{SN} - r_{SC}$$

Soot Mass Density

$$\frac{dM_{soot}}{dt} = r_{SN} + r_{TD} + r_{SS}$$

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FIRETEC

- Landscape-scale LES model
- First developed in 1997 by Rod Linn @ LANL
- CFD (grid size 2x2m)
- Coupled with HIGRAD, an atmospheric turbulence model
- Requires HPC resources
- Well validated, published, and cited in the Fire community
- Not open-source

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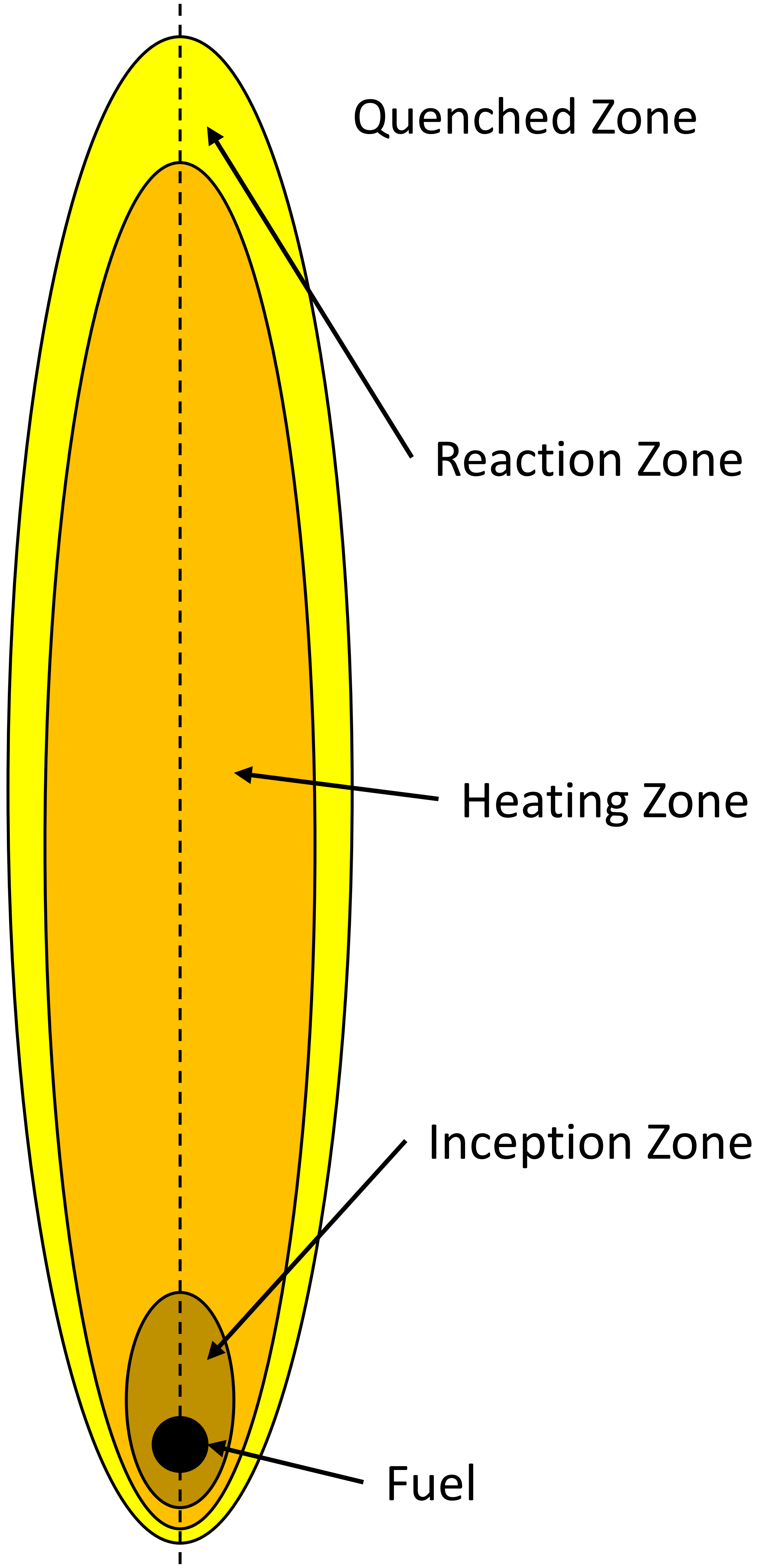
FIRETEC-Smoke Model - Concept



- How do we capture soot formation and emission on a 2 meter grid?
- Zonal model
- Each cell is partitioned into different zones of a flame
- At each timestep we assume a pseudo-steady state
- We take an average (centerline) evolution of soot particles
- This is a working model

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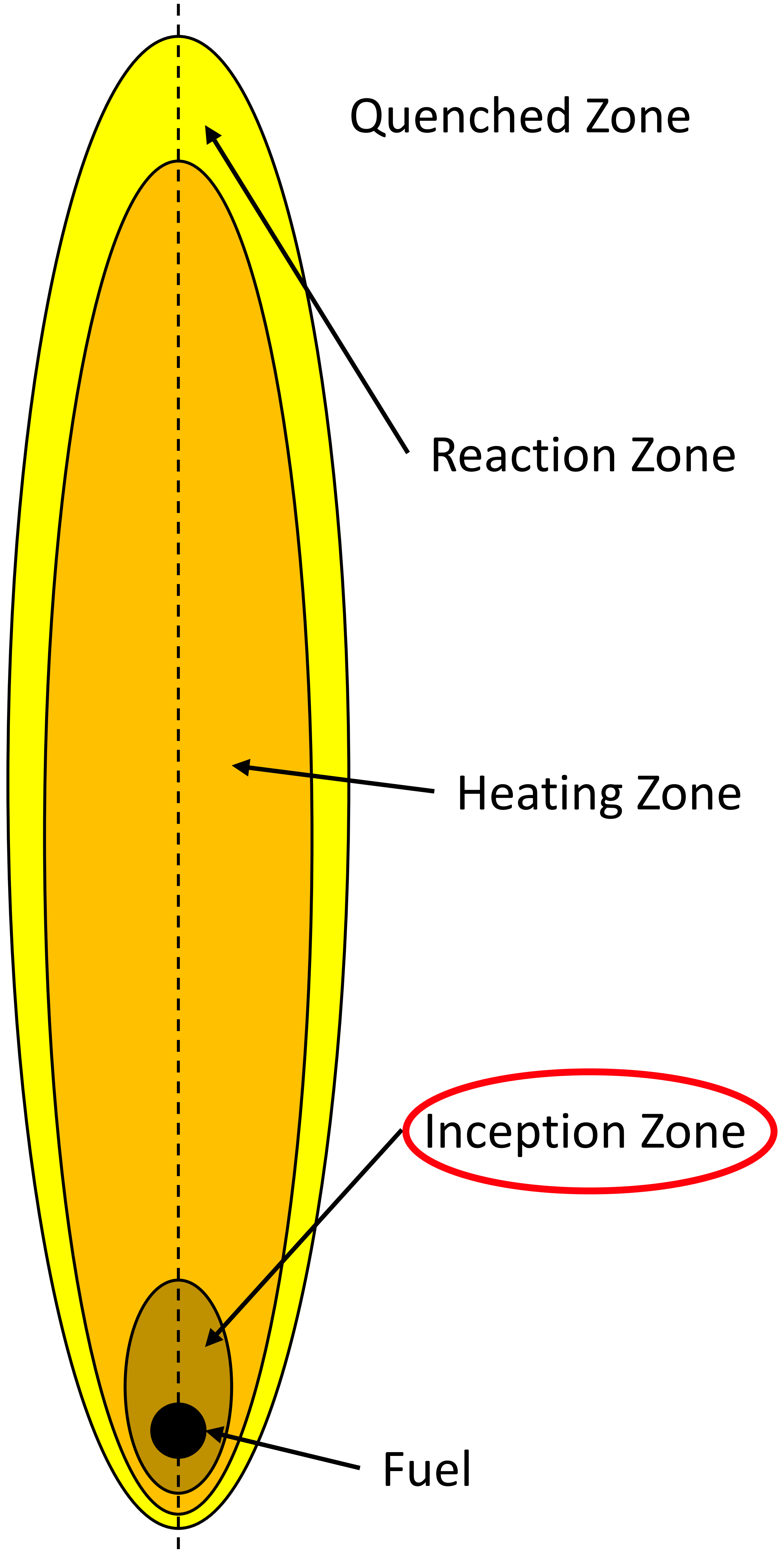
Inception Zone



- Primary pyrolysis occurs giving off tar molecules
- Tar molecules nucleate or thermally crack

$$\frac{dN_{tar}}{dt} = r_{TI} - r_{TC}\left(N_{tar}\right) - r_{SN}\left(N_{tar}^2\right)$$

- Assuming a pseudo-steady state at constant temperature
- Solve for the instantaneous concentration of tar

$$N_{tar} = \frac{-r_{TC} + \sqrt{r_{TC}^2 + 4r_{TI}r_{SN}}}{2r_{SN}}$$

- Compute rates of soot nucleation and thermal cracking to find the ratio of tar molecules converting to soot particles

$$N_{soot} = \frac{r_{SN}}{8r_{SN}r_{TC}} \qquad M_{soot} = 8m_{tar}N_{soot}$$

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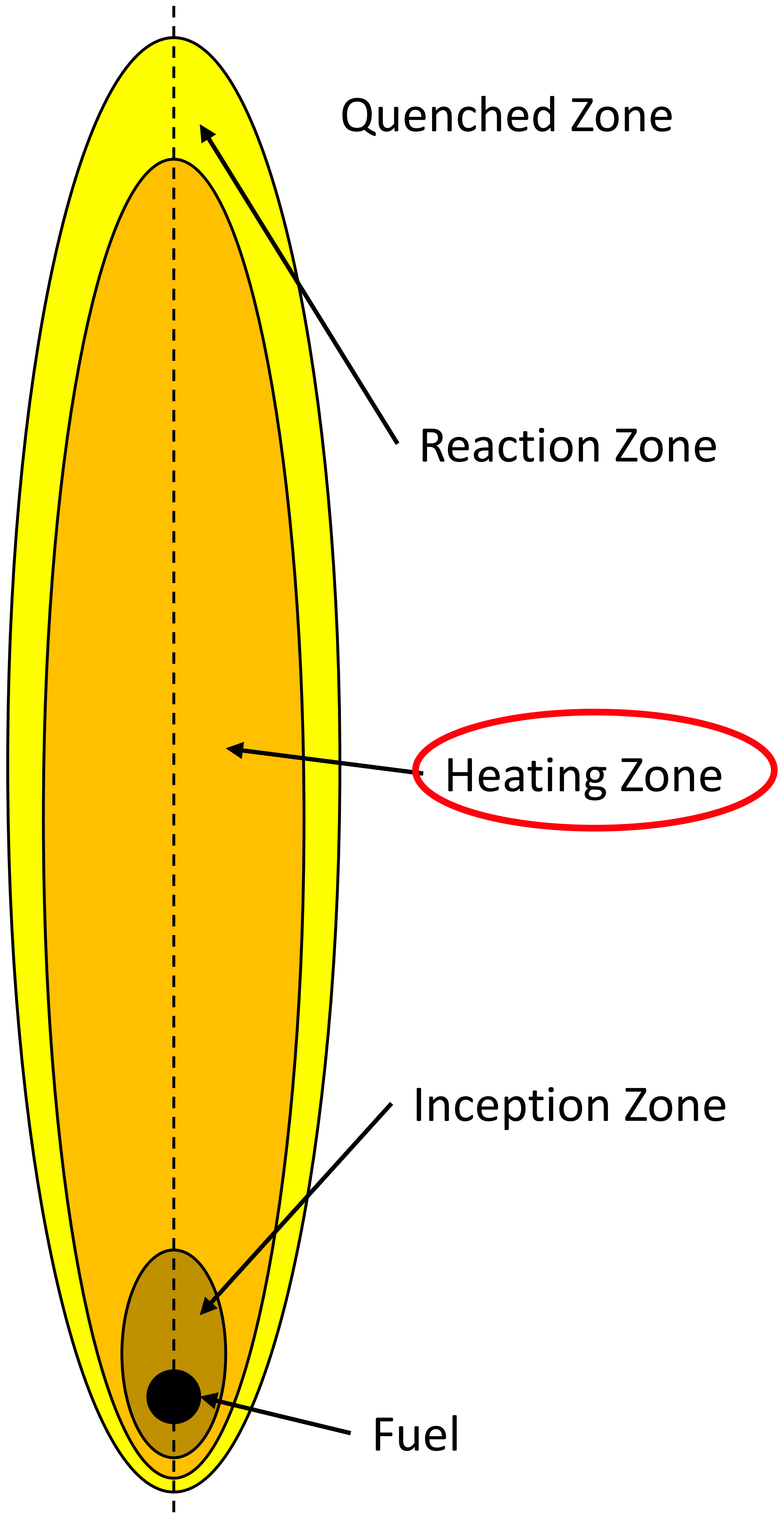
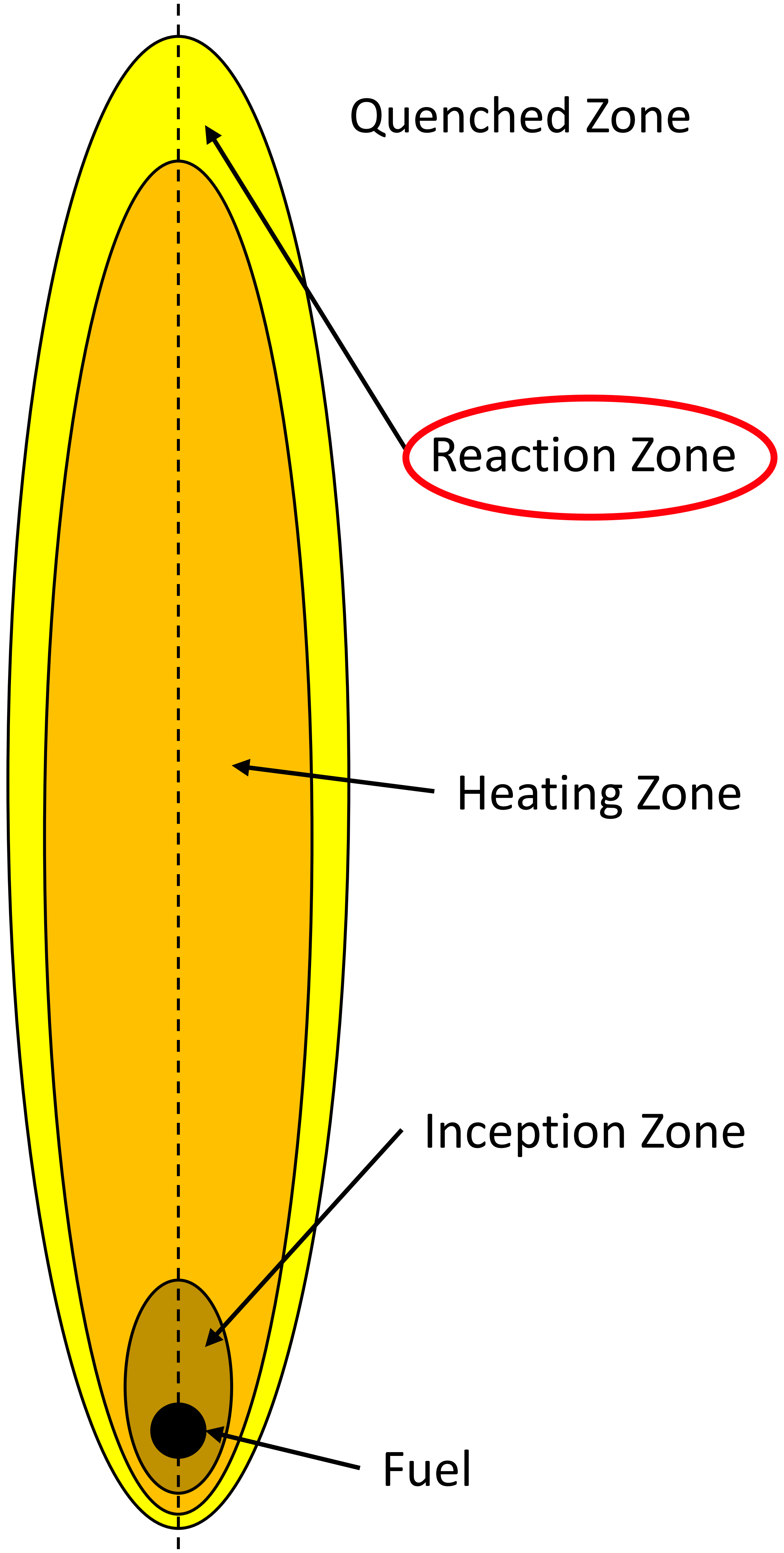
Heating Zone



- Size of heating zone determined by computing a FSD (Zhou 2002) and volume of flame (determined by oxygen depletion in cell)
- Particle residence time computed from heating zone size and gas velocity
- Soot particles coagulate in a free molecular regime
- Surface growth reactions through HACA

Zhou X., Mahalingam S., “A flame surface density based model for large eddy simulation of turbulent non premixed combustion,” *Physics of Fluids*, 2002, 14, L77-L80

Reaction Zone



- Thickness of reaction zone computed (Bilger 1976)
- Particle residence time computed from reaction zone thickness and gas velocity
- Soot oxidize according to a surface oxidation model
- Concentration of emitted particles compared to concentration of generated tar molecules to compute to number of emitted particles

Bilger R.W., "Reaction zone thickness and formation of nitric oxide in turbulent diffusion flames," *Combustion and Flame,* 1976, 26, 115-123

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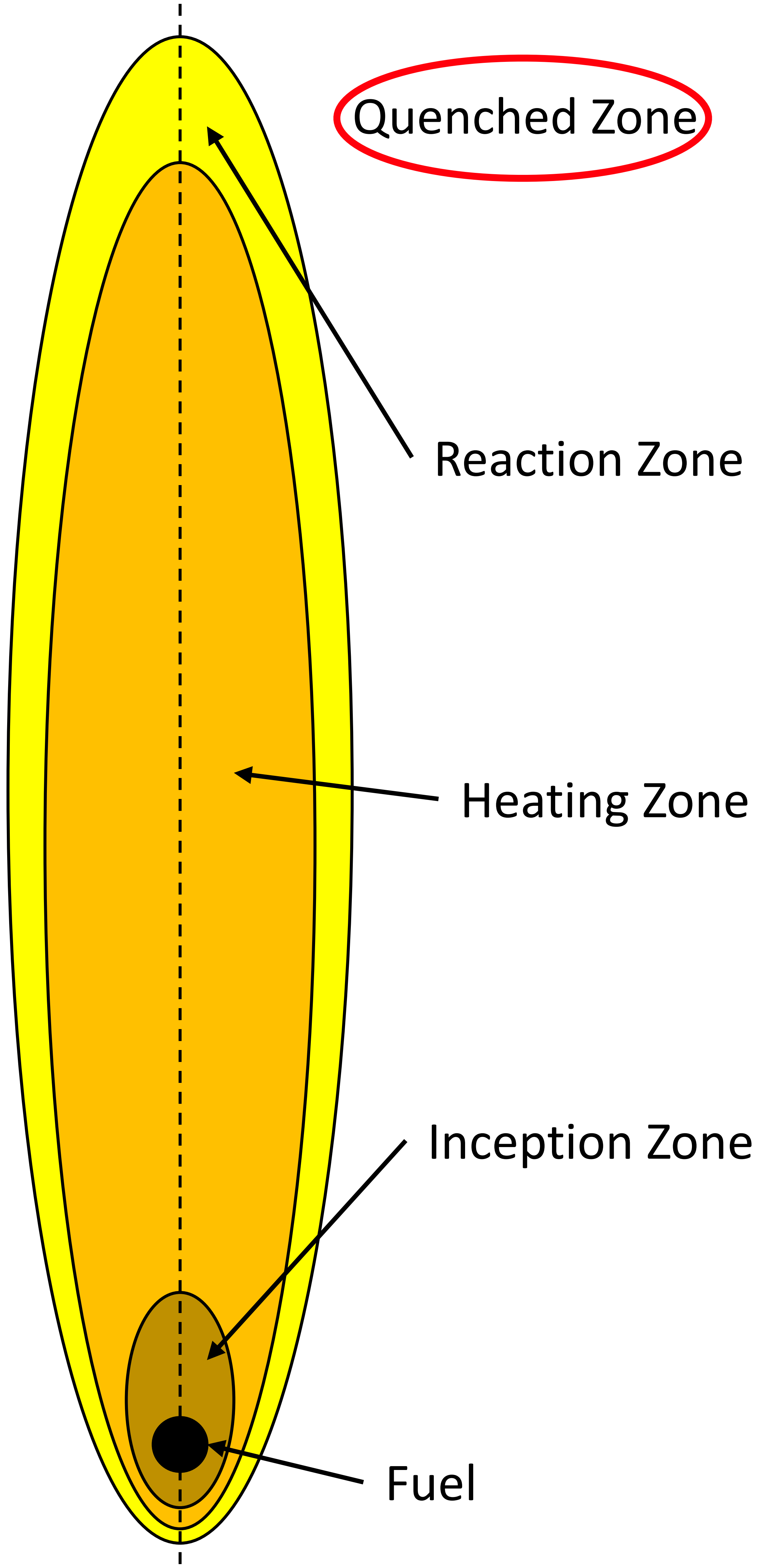
Quenched Zone



- Everything that is not on fire
- Continued particle coagulation in a continuum regime
- Particle settling
- Plume dynamics to be added here

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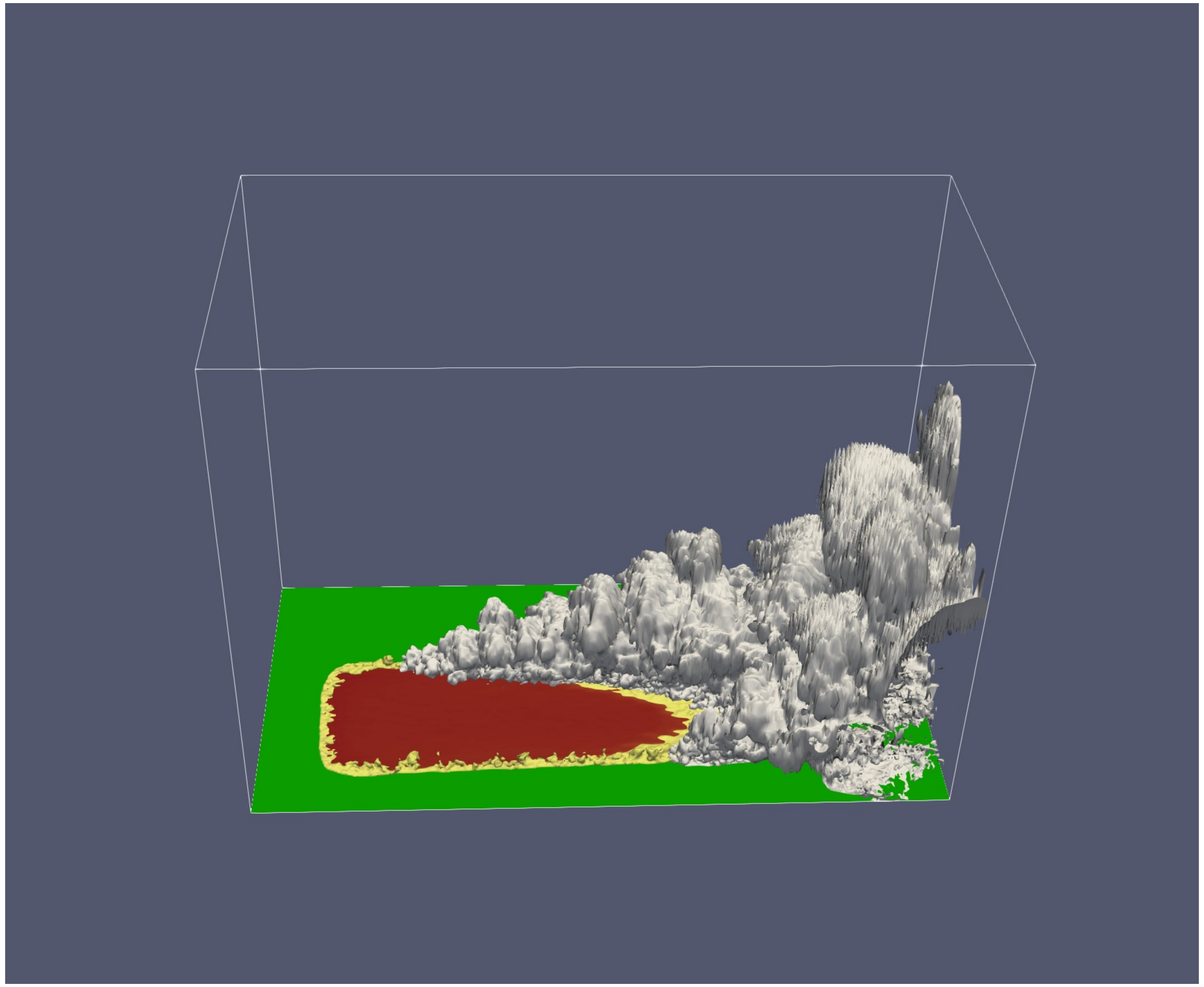
Results



Moderate Wind - Grassfire

- 200 x 150 x 300 m domain
- 2 x 2 m gridsize
- 6 m/s winds
- 1/7 power law wind profile
- Fire-line ignition
- 1 kg/m^3 grassland fuel-load
- 0.25 micron average emitted particle size

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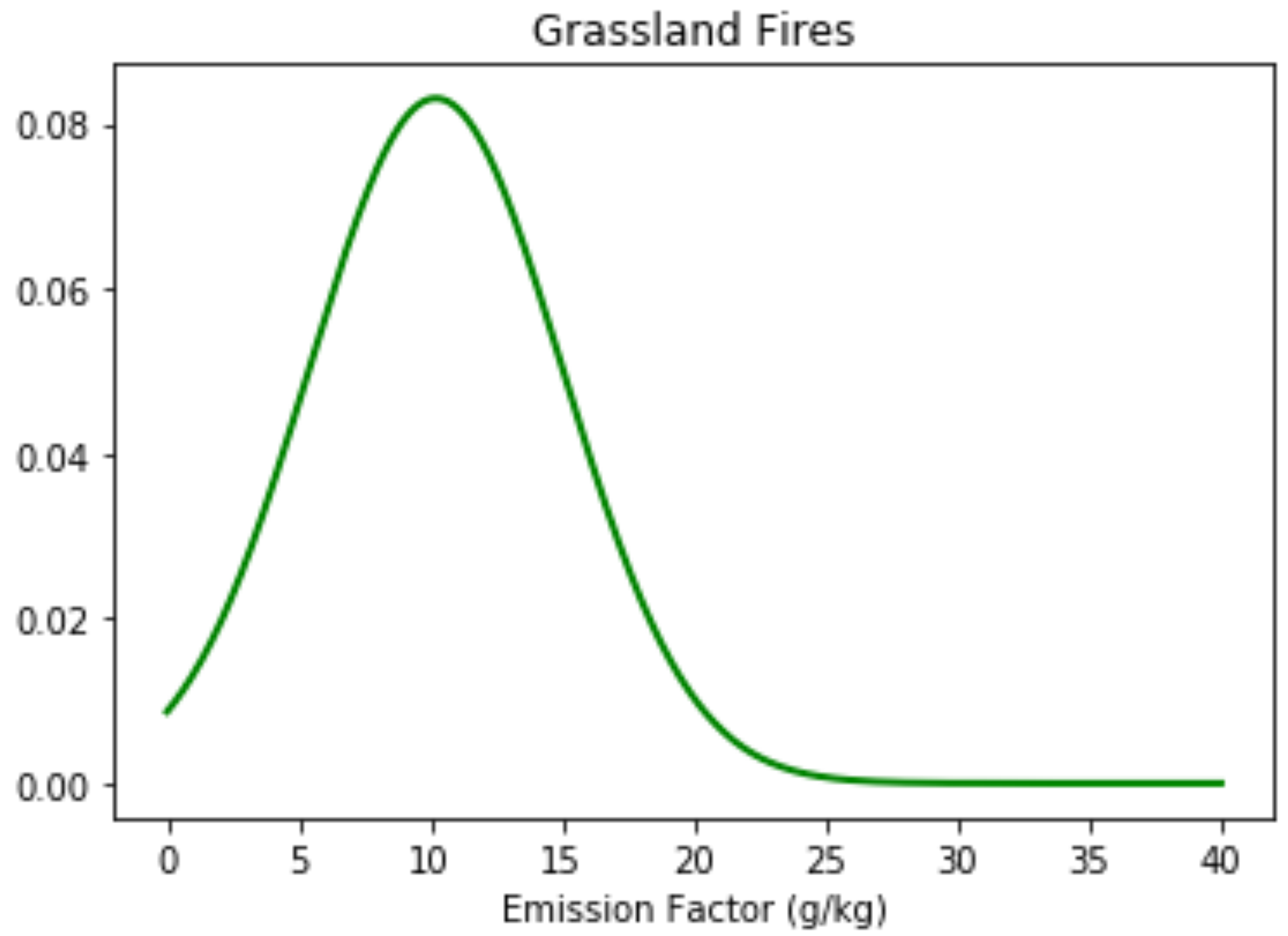
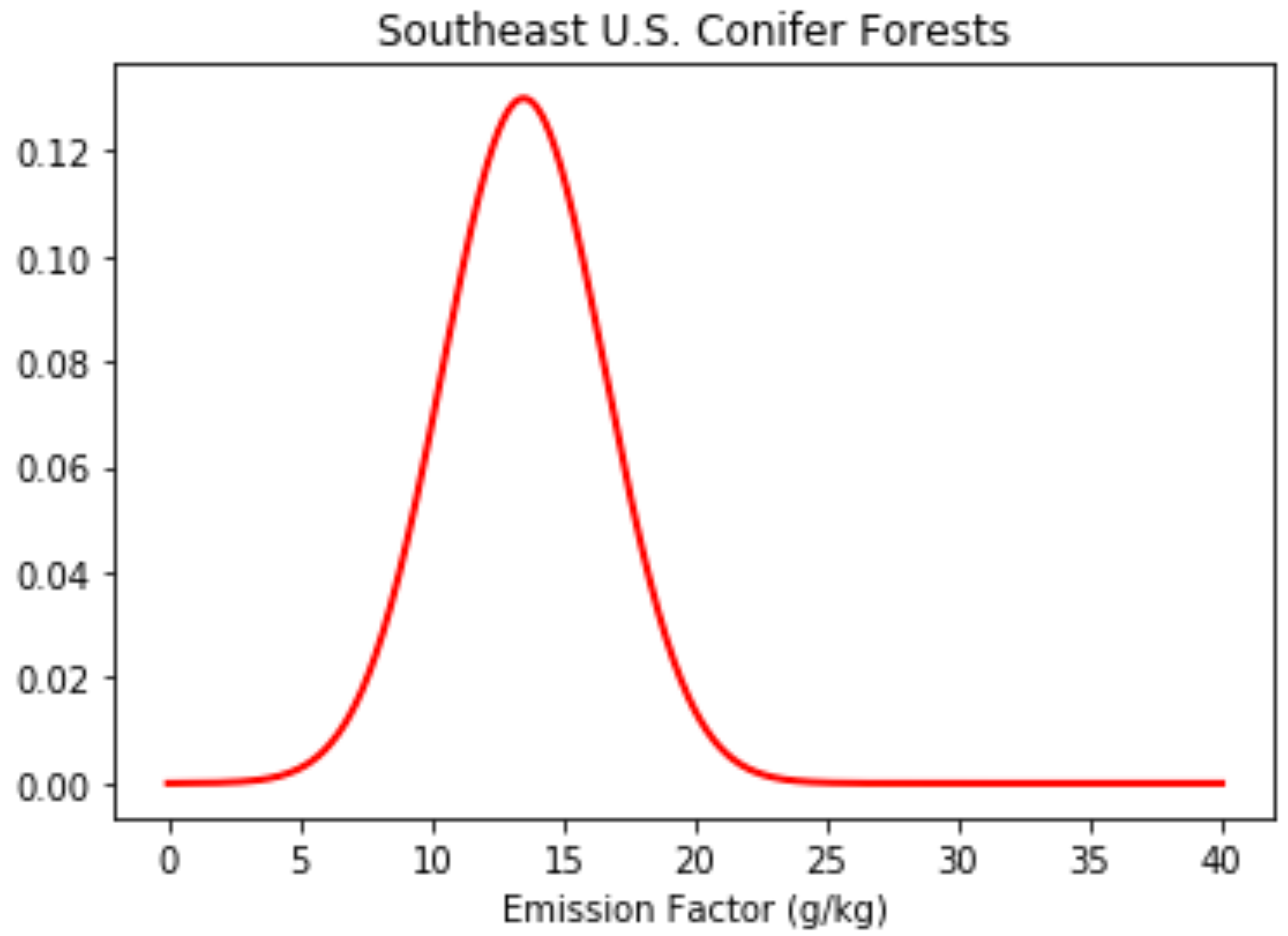
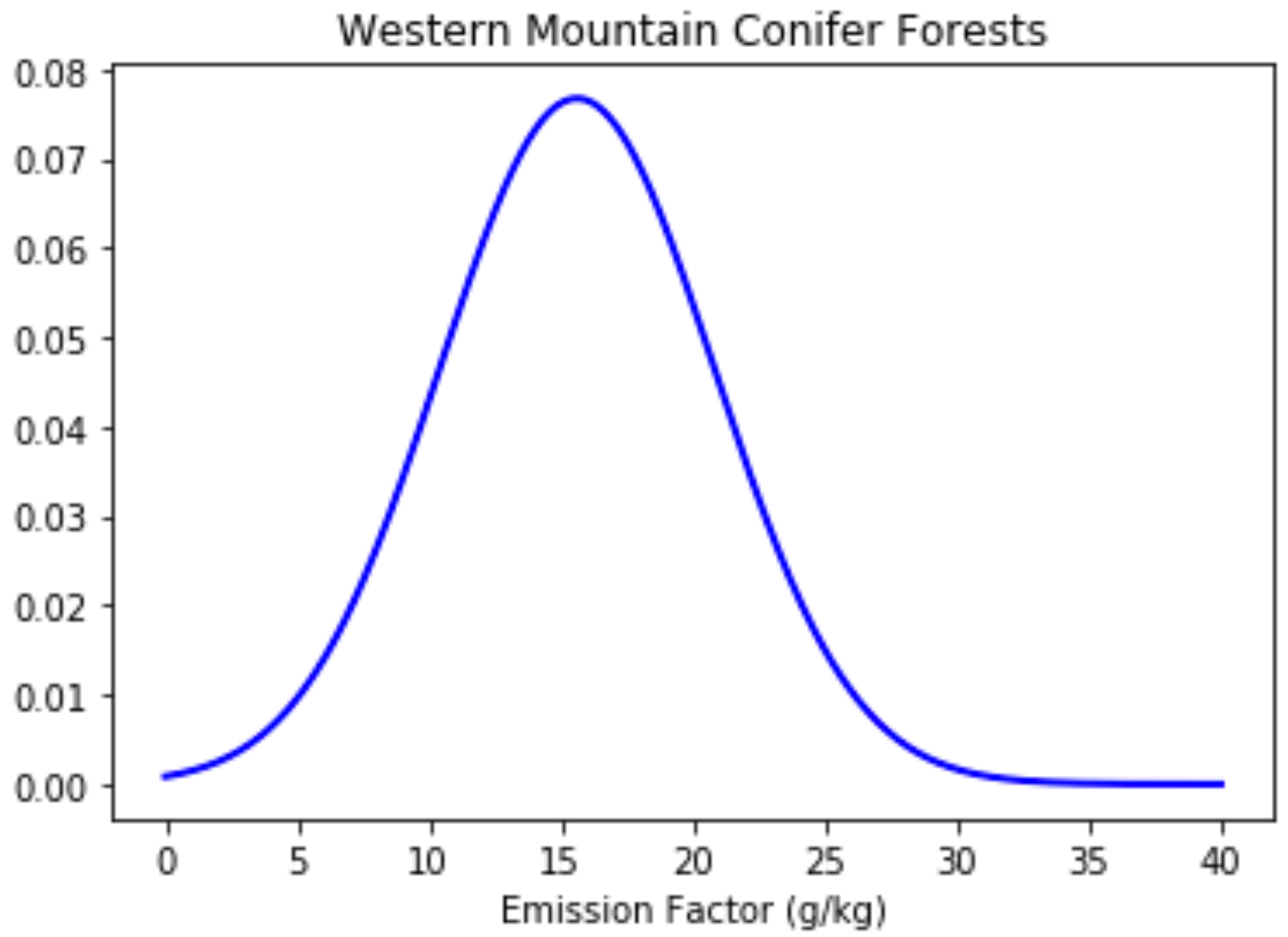
Comparisons to Experimental Measurements

Field Measurements (Urbanski, 2008)







FIRETEC Matrix Simulations

Standard Fuel Map

- Semi-dry grassland
- Flat
- Predicted emission factor (45-90 g/kg)

Eglin Air Force Base (Florida) Fuel Map

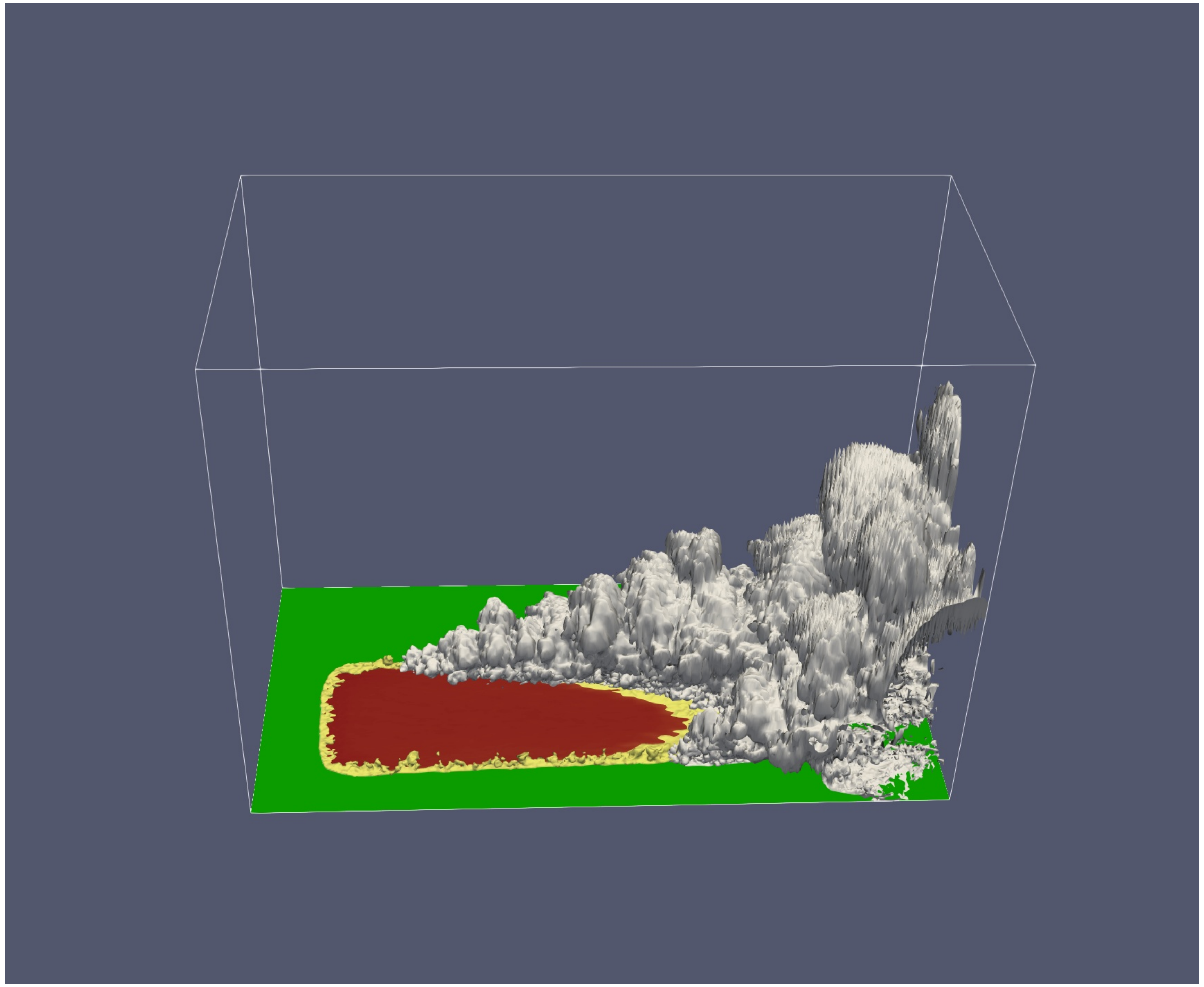
- Humid south conifer forests
- Flat
- Long-leaf pine and oak trees
- Predicted emission factor (60-110 g/kg)

Flagstaff Mountain Forest Service Center

- Semi-dry pine forests
- Flat
- Ponderosa pine trees
- Needle and grass understory
- Predicted emission factor (85-120 g/kg)

Urbanski S., Hao W., Baker S.,"Chemical Composition of Wildland Fire Emissions," *Developments in Environmental Science,* 2008, 79-107

Future Work



- Bring down the emissions
  - Explore particle shape during oxidation
  - Reaction layer thickness
  - Air entrainment
- Finish comparison matrix studies
- Explore emission-structure correlations
- Reduce emissions

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