Numerical Simulation of Forward and Static Smoldering Combustion

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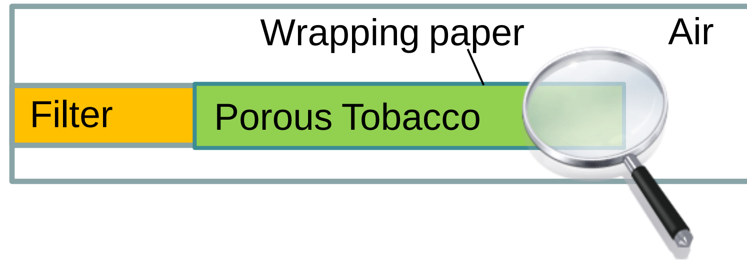
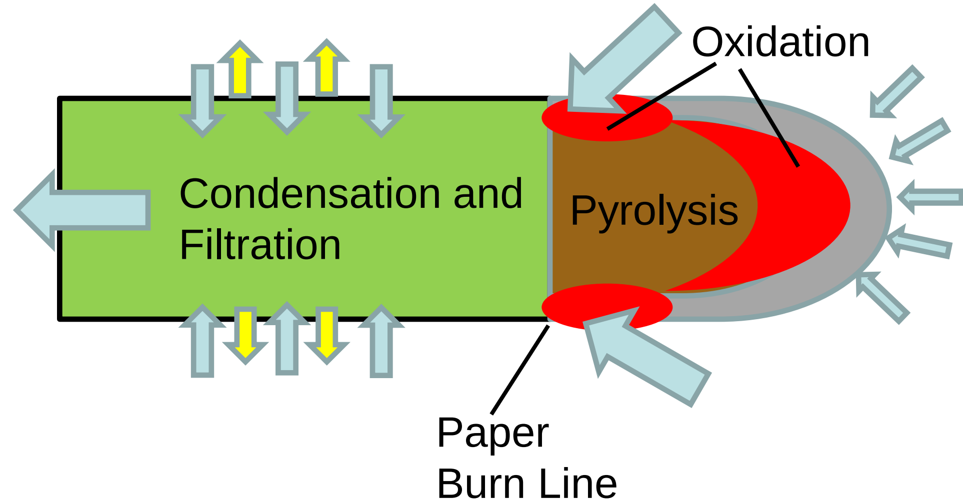
Outline

1. Introduction
2. Numerical Implementation in COMSOL
3. Results and Validation

Physics and Chemistry of Smoldering Combustion in a Cigarette

- Simulation domain encompasses tobacco rod, filter, paper and surrounding air
- Evaporation and pyrolysis zone exist ahead of oxidation zone due to pre-heating
- Transient problem due to alternation between natural smoldering and puffing
- Most air enters at paper burn line, radial advection and diffusion occur
- Local thermal equilibrium between gas and solid does not always hold
- Effective transport and thermo-physical properties depend on structure and change markedly with conversion (e.g. permeability, conductivity, diffusivities, etc.)





Adapted from Baker, R R, *PECS*, 7, (1981), 135-153

Numerical Implementation in COMSOL

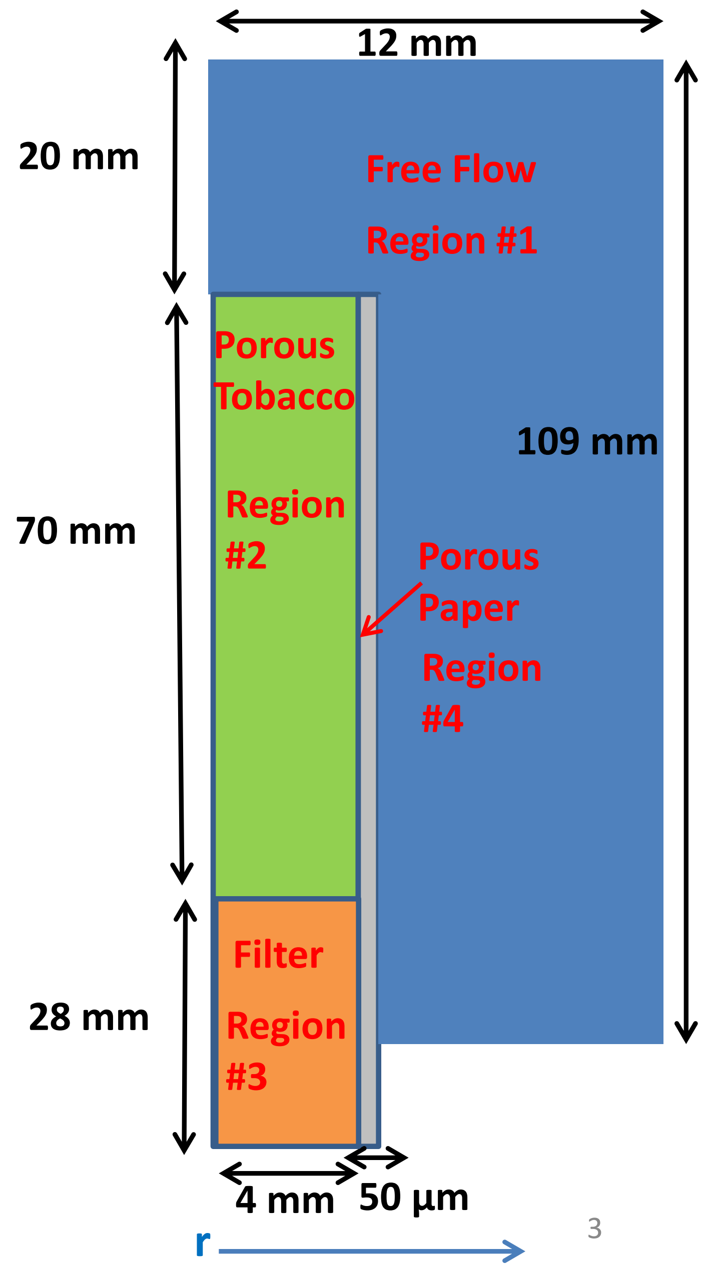
2-D axisymmetric domain employed

Physics interfaces used:

- (**Reaction Engineering**, synced with:)
- **Free and Porous Media Flow**: Regions 1,2,3,4 (Source term in Region 2 accounts for solid-to-gas reaction)
- **Transport of Concentrated Species**: Regions 1,2,3,4 (Source terms in Region 2 account for reactions)
- **Heat Transfer in Fluids**: Regions 1,2,3,4 (Source terms account for interphase heat transfer in Regions 2,3,4)

  and

- **Heat Transfer in Solids**: Regions 2,3,4 (Source terms account for heats of reaction and interphase heat transfer)
- **Domain ODEs**: Region 2 (for tobacco, char and moisture densities)
- **Domain ODE**: Region 4 (for paper permeability)



Numerical Implementation: Volume Averaged Conservation Equations

Mass Conservation:

$$\frac{\partial(\phi\rho)}{\partial t}+\nabla\circ(\phi\rho\mathbf{u})=\sum_j\sum_k \nu_{j,k}\Re_k \equiv Q$$

Gas Species Eq:

$$\phi\,\rho\left(\frac{\partial w_j}{\partial t}+\mathbf{u}\circ\nabla w_j\right)=-\nabla\circ\mathbf{J}_j+\sum_k \nu_{j,k}\Re_k - w_j Q$$

6 Major Gas Species included (O_2, CO, CO_2, N_2, H_2O and “Volatiles”)

Thermal Energy (Gas):

$$(\rho c_p)_{eff}\frac{\partial T_g}{\partial t}=\nabla\circ(k_{eff}\nabla T_g)-\sum_j(N_j\,c_{p,j})\circ\nabla T_g+h_{g-s}A_{g-s}(T_s-T_g)$$

Thermal Energy (Solid):

$$(\rho c_p)_{eff}\frac{\partial T_s}{\partial t}=\nabla\circ(k_{eff}\nabla T_s)+\sum_k(-\Delta h_r\Re_k)+h_{g-s}A_{g-s}(T_g-T_s)$$

Solid Species (char, volatile precursors):

$$\frac{d\rho_{solid,i}}{dt}=\sum_k \nu_{i,k}\Re_k$$

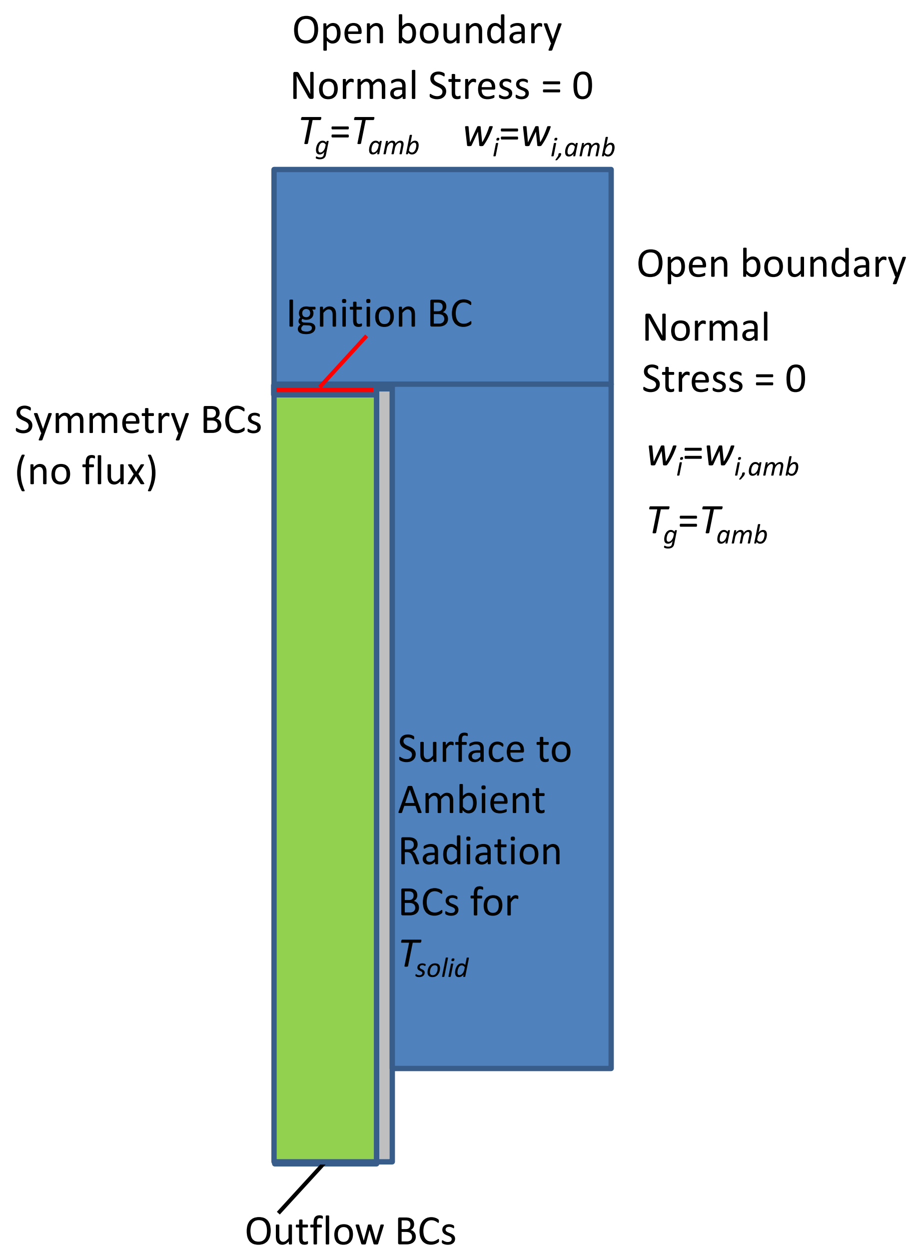
Momentum (porous rod):

$$\frac{\rho}{\phi}\left(\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\circ\nabla\frac{\mathbf{u}}{\phi}\right)=-\nabla p-\left(\frac{\mu}{\kappa}+\frac{Q}{\phi^2}\right)\mathbf{u}+\nabla\circ\left[\frac{1}{\phi}\left\{\mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\right)-\frac{2}{3}\mu(\nabla\circ\mathbf{u})\mathbf{I}\right\}\right]+\mathbf{F}$$

Momentum (free flow):

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\circ\nabla\mathbf{u}\right)=-\nabla p+\nabla\circ\left[\left\{\mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\right)-\frac{2}{3}\mu(\nabla\circ\mathbf{u})\mathbf{I}\right\}\right]+\mathbf{F}$$

Numerical Implementation in COMSOL



<u>Initial and Boundary Conditions</u>

- Atmospheric initial conditions with zero initial velocity are employed
- Puffing/smoldering transition via application of prescribed flow rate at outlet

<u>Mesh and Elements Details:</u>

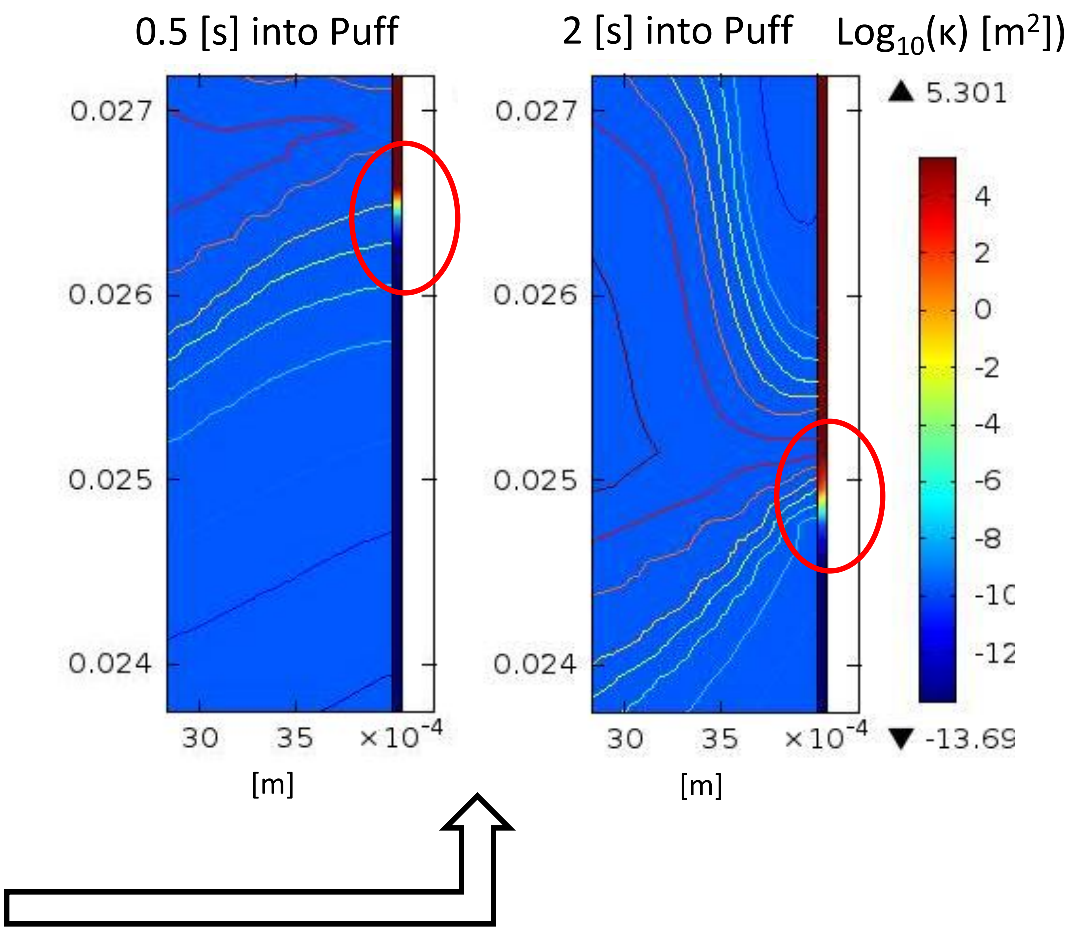
- Non-uniform **mapped** mesh (*thin* paper!) elements for porous regions
- Free quad elements in free flow region
- Most elements linear, although 2^{nd} order shape functions used for some variables

<u>Solver Settings:</u>

- Time dependent BDF solver
- Newton's Method at each time step
- Employed either <u>Direct MUMPS</u> solver or Iterative GMRES with Multigrid Preconditioner and Vanka pre- and post-smoothers

Numerical Implementation in COMSOL: Sub-models

- Properties calculated dynamically as function of temperature, porosity, etc.
- Diffusion is calculated using the Maxwell-Stefan approach for multi-component diffusion, accounts for porous medium
- Temperature dependent thermal conductivities and viscosity of gas mixture are incorporated, effective thermal conductivities for *each* phase
- Pyrolysis reactions: 4-precursor model
- Solid conductivity accounts for contribution of shred-to-shred radiation
- Solid-to-gas heat transfer coefficient
- Tobacco permeability increases 3 orders of magnitude with conversion
- Paper burns @ 723 K and permeability increases by 20 orders of magnitude



Riley D, et al., PhysicoChemical Hydrodynamics*, 7, (1986), 255-279*

Muramatsu M et al., *Beitr. Tabakforsch*, 11, (1981), 79-86

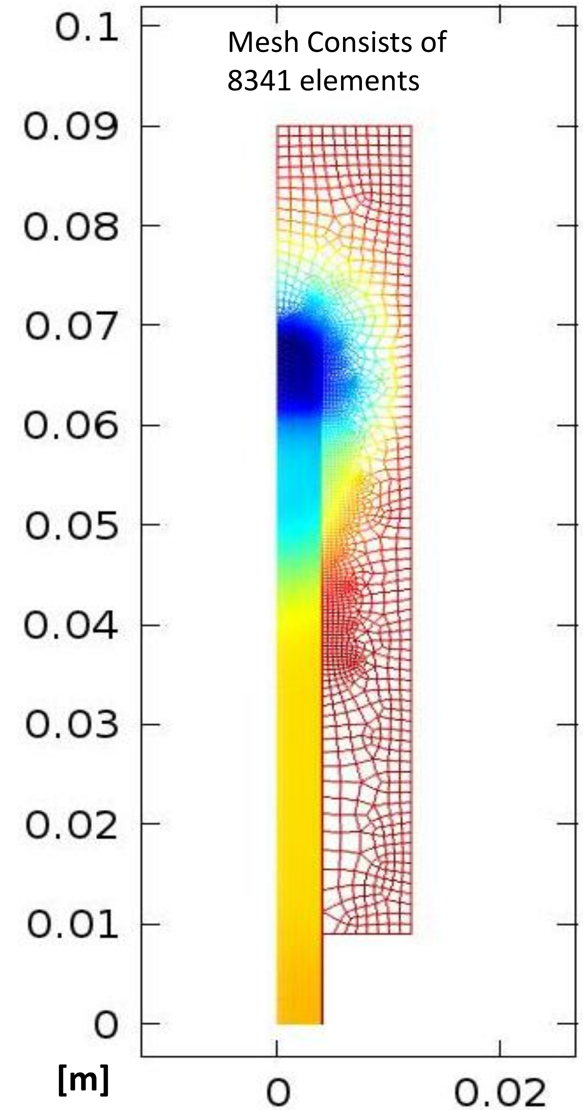
Saidi et al., *App. Math. Mod.,* 31 (2007) 1970-1996

Numerical Implementation in COMSOL: Validation

- In order to **validate simulation,** we must use *identical* conditions and properties as experiments…
- Employed full-size cigarette and extended domain radially to twice the cigarette radius
- Incorporated paper permeability used in experiments and used paper's O_2 diffusivity given by Riley 1986
- Employed full Puff/Smolder cycles for ISO Regime:

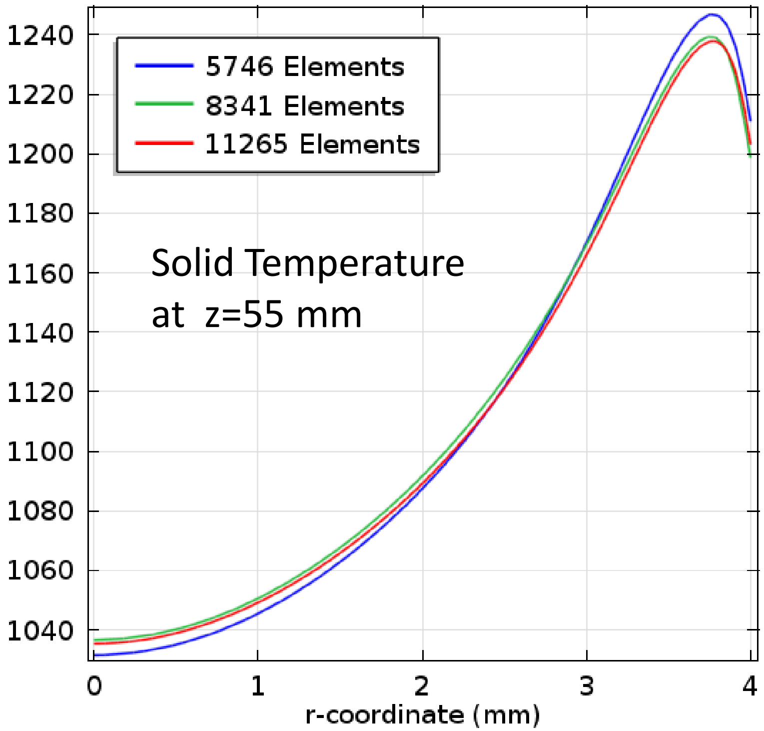
  -**Puff volume: 35 cc/ 2 sec**
  -**Smoldering interval: 58 sec**

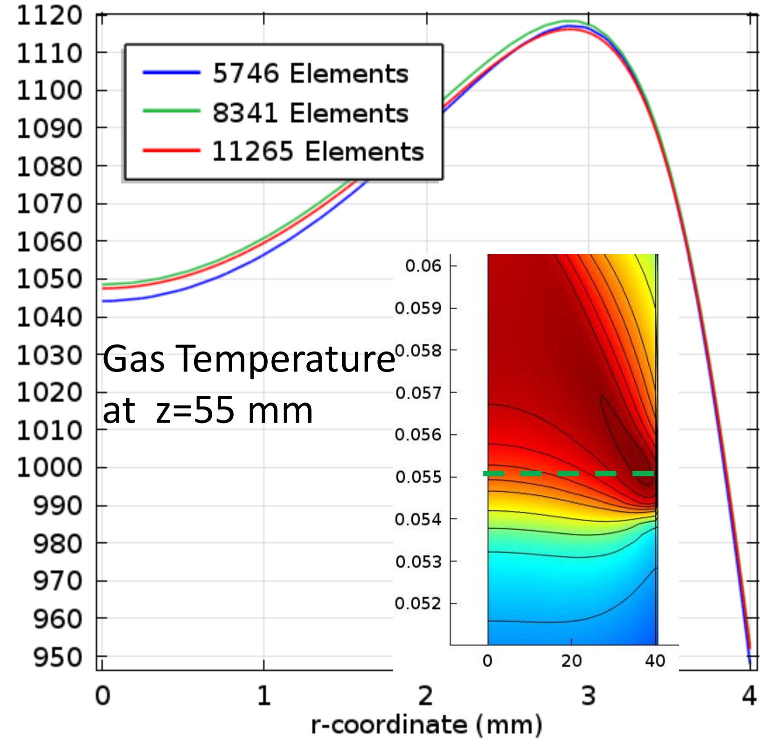
- Similar to experiment, 9 mm of cigarette is covered by smoking machine
- Still some unknown parameters, use same sub-models as literature (Saidi et al. 2007)

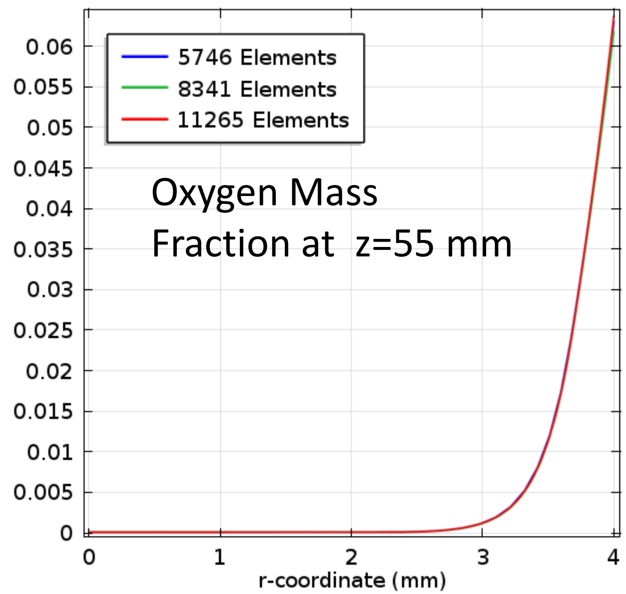


Baker, R R, *High Temp. Science,* 7 (1975) 236-247
Baker, R R, *Beitr. Tabakforsch*, 11, (1981), 1-17
Riley D, et al., PhysicoChemical Hydrodynamics*, 7, (1986), 255-279*

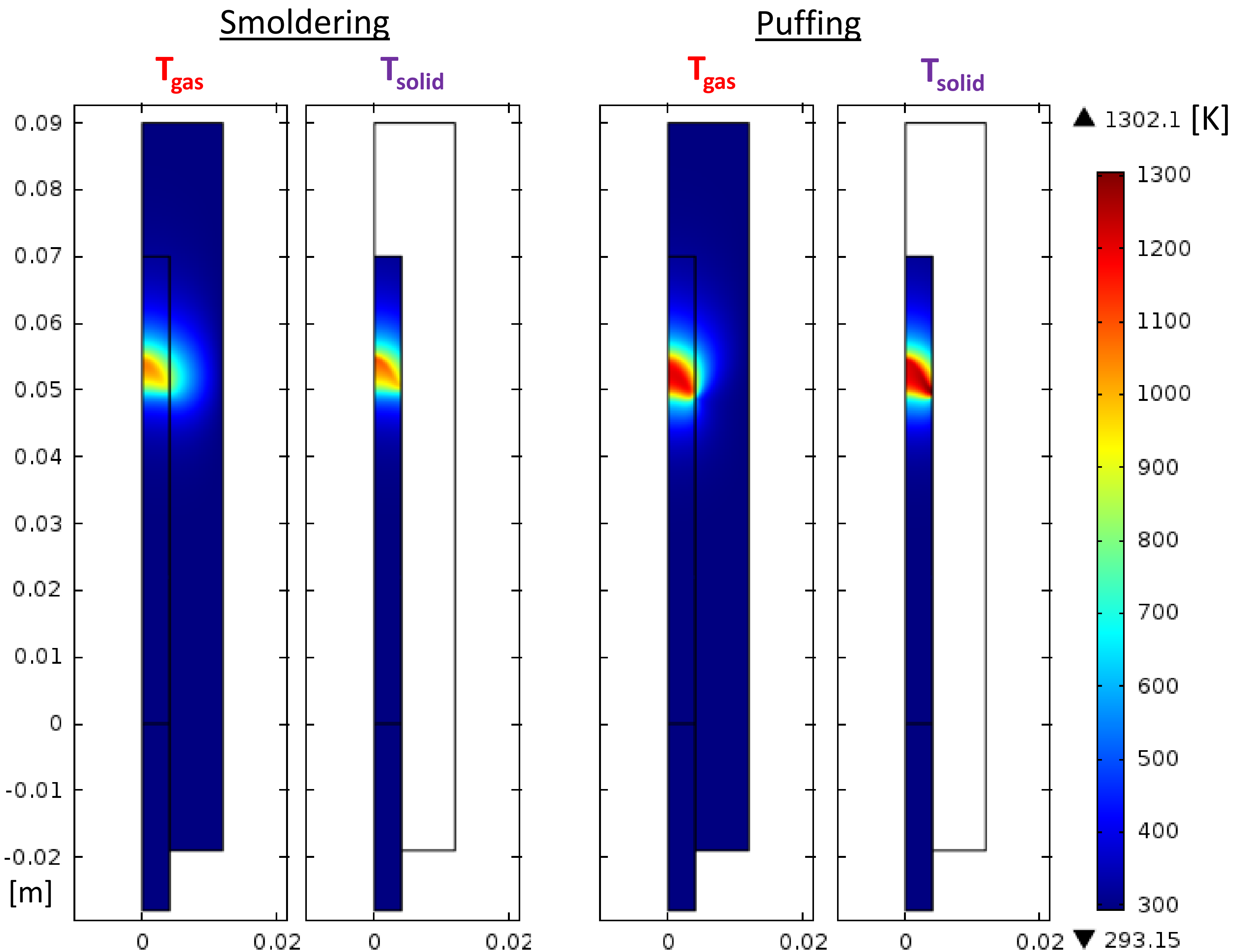
Mesh Refinement



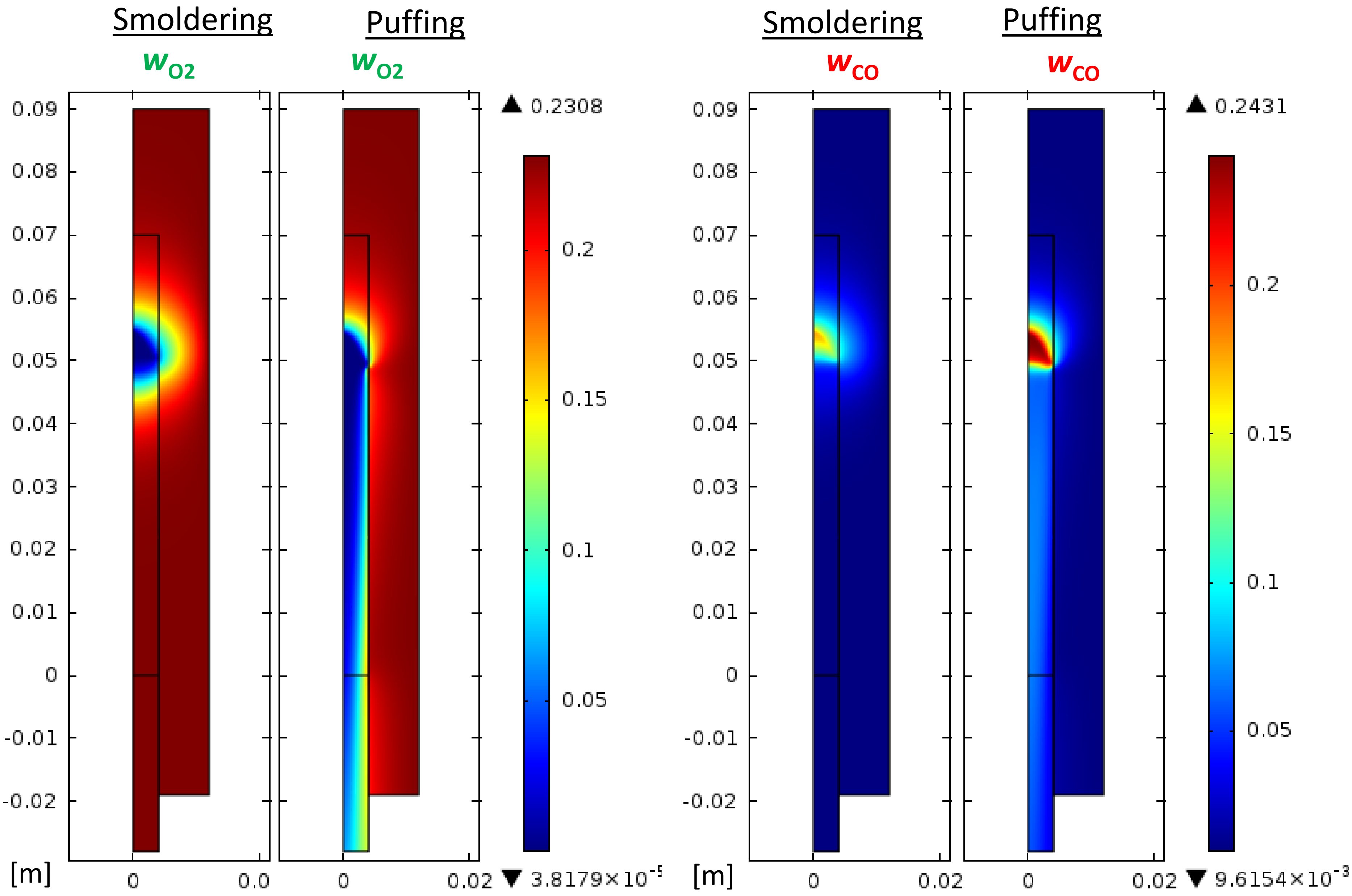




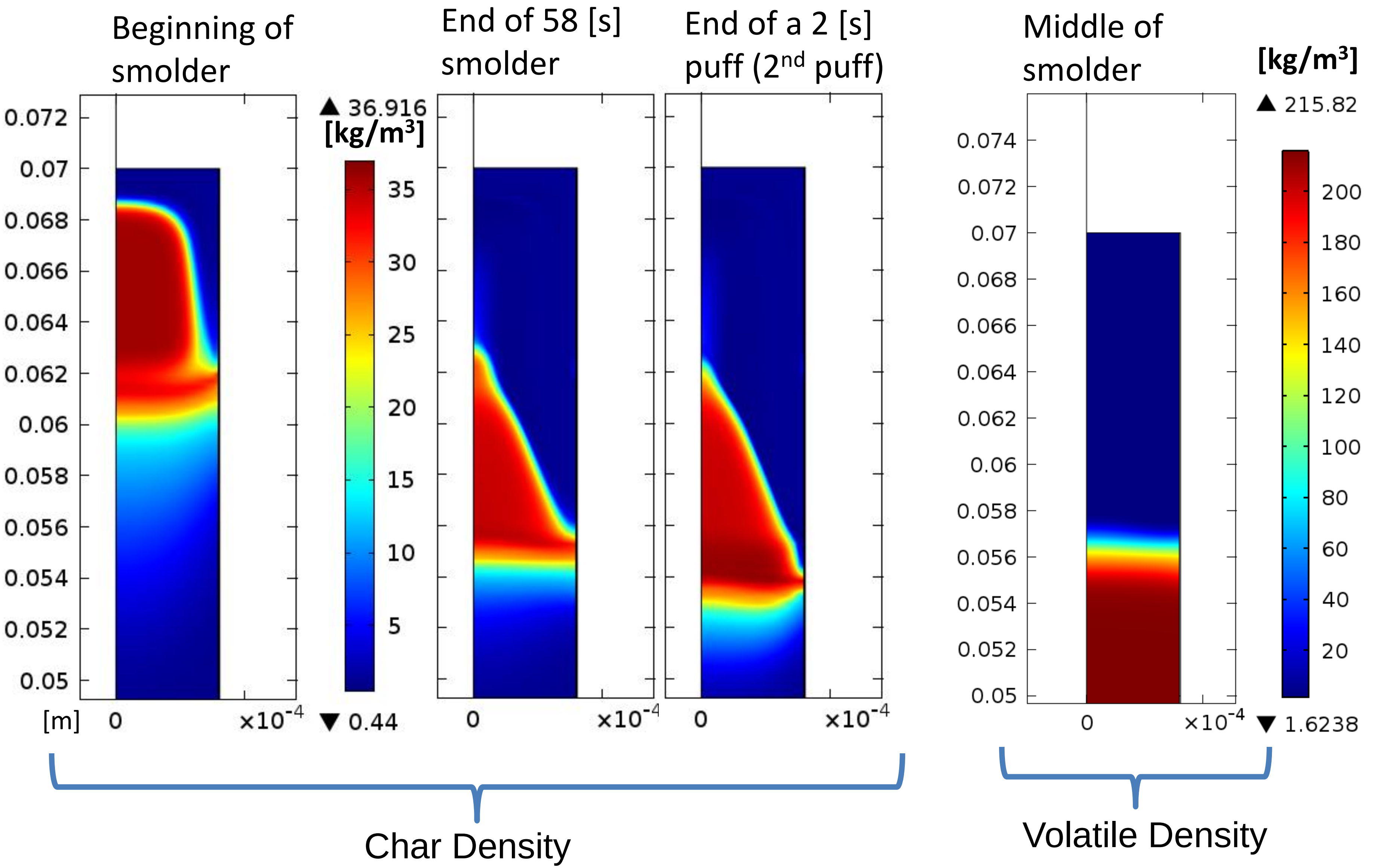
Full Temperature Profiles



Mass Fraction Profiles

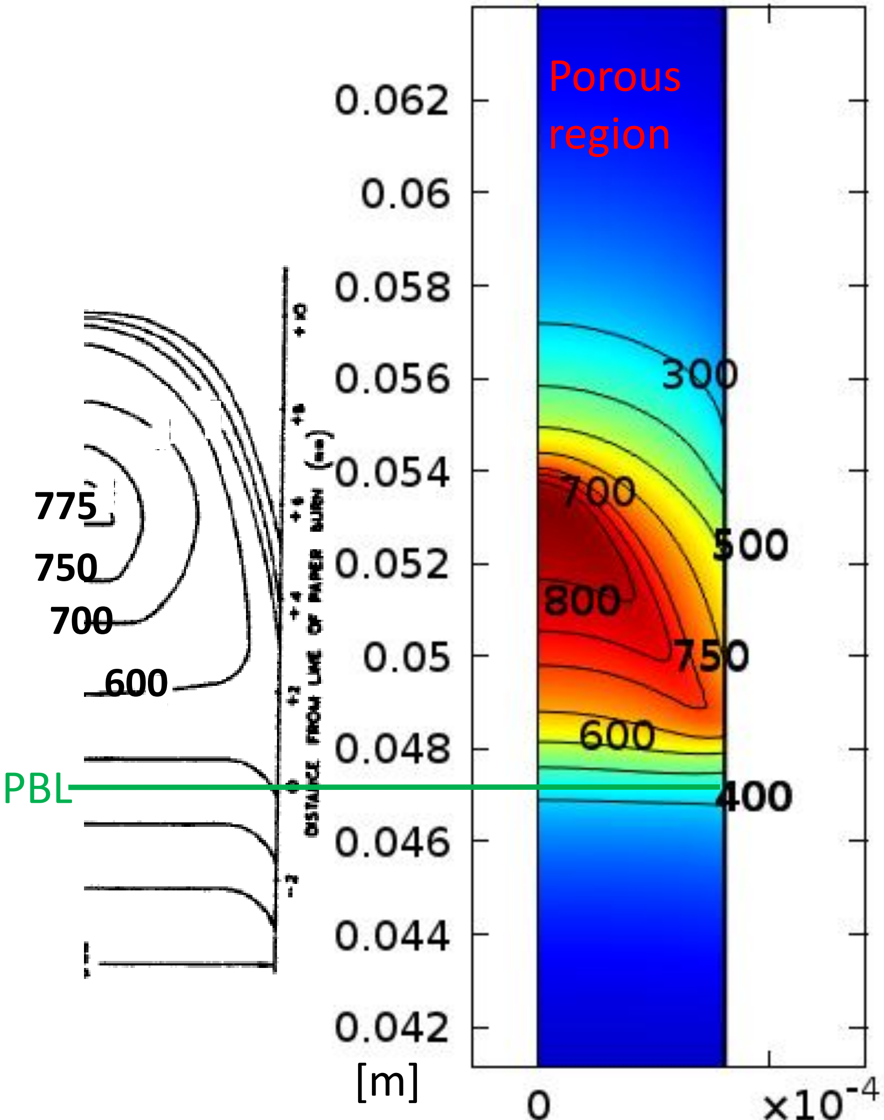


Char and Volatile-Precursor Density Profiles



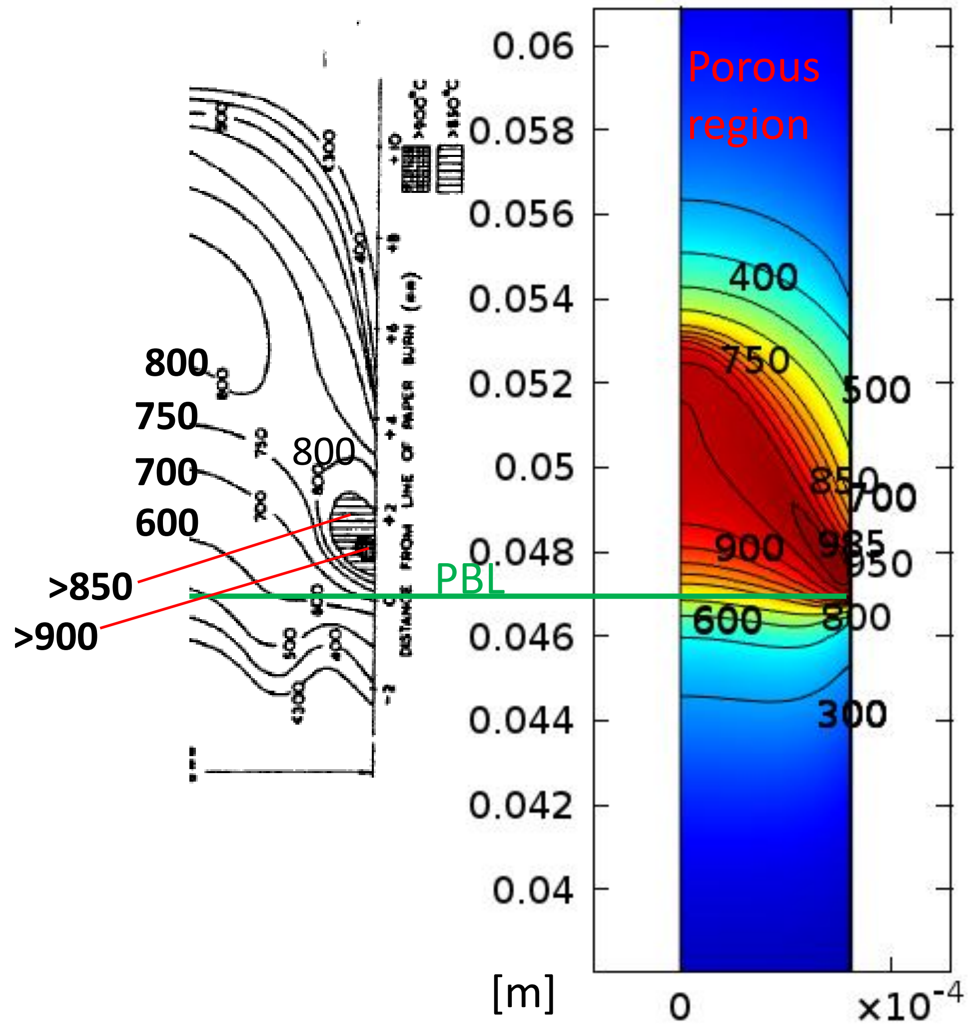
Experimental and Simulated Solid Temperatures (˚C)

End of 58 [s] Smolder



PBL = paper burn line location at start of 3rd Puff

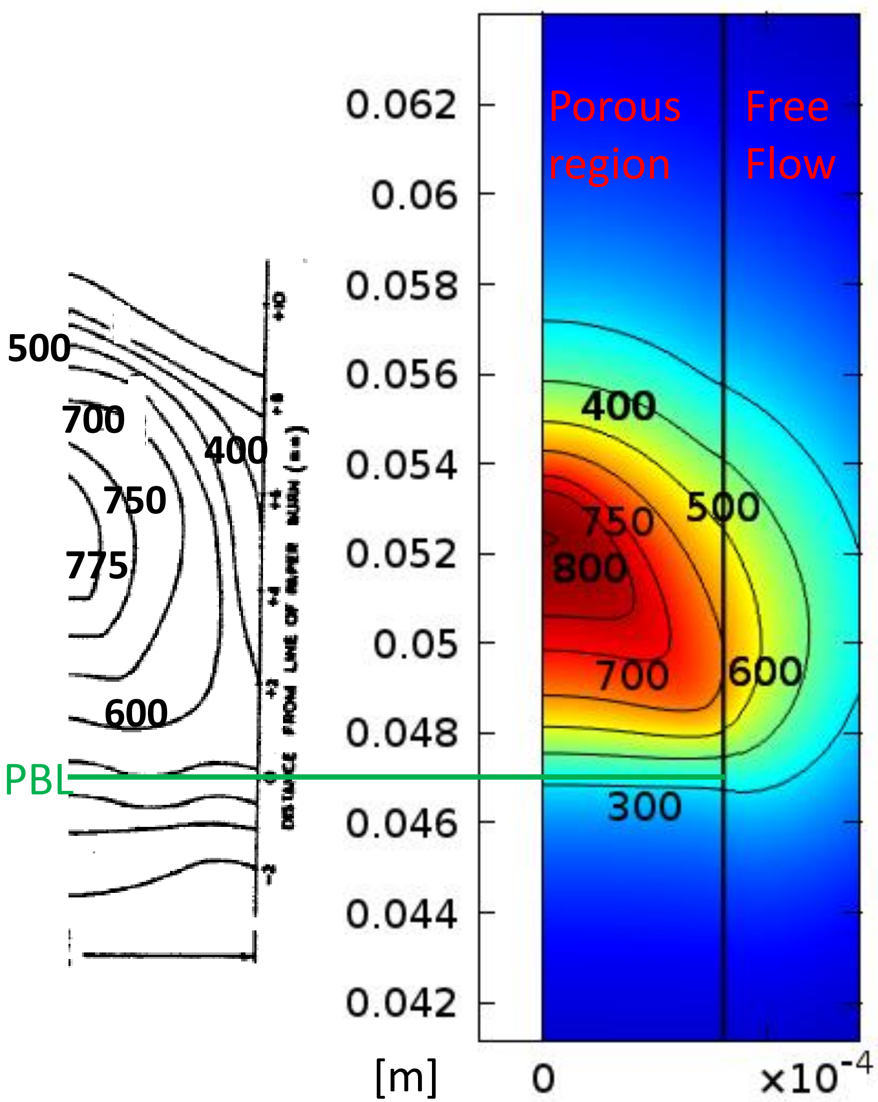
Middle of a 2[s] Puff



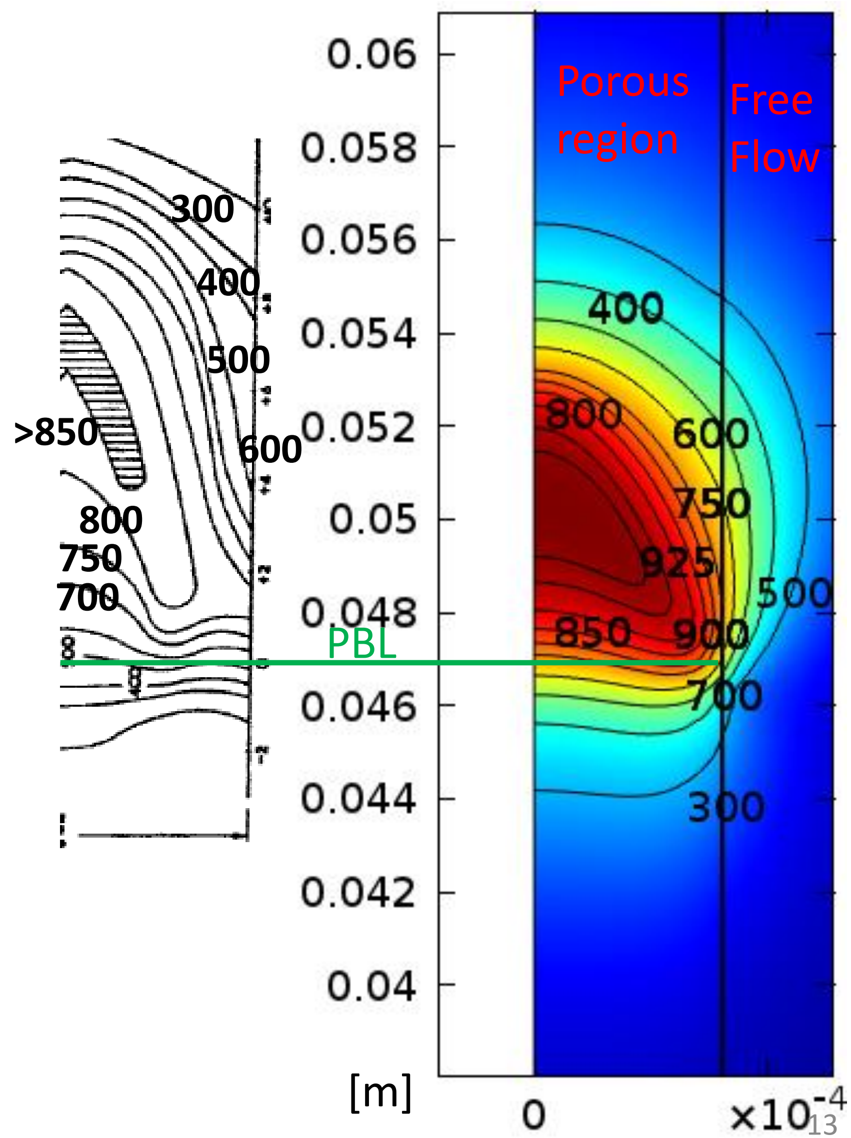
Baker, R R, *High Temp. Science*, 7 (1975) 236-247

Experimental and Simulated Gas Temperatures (˚C)

End of 58 [s] Smolder



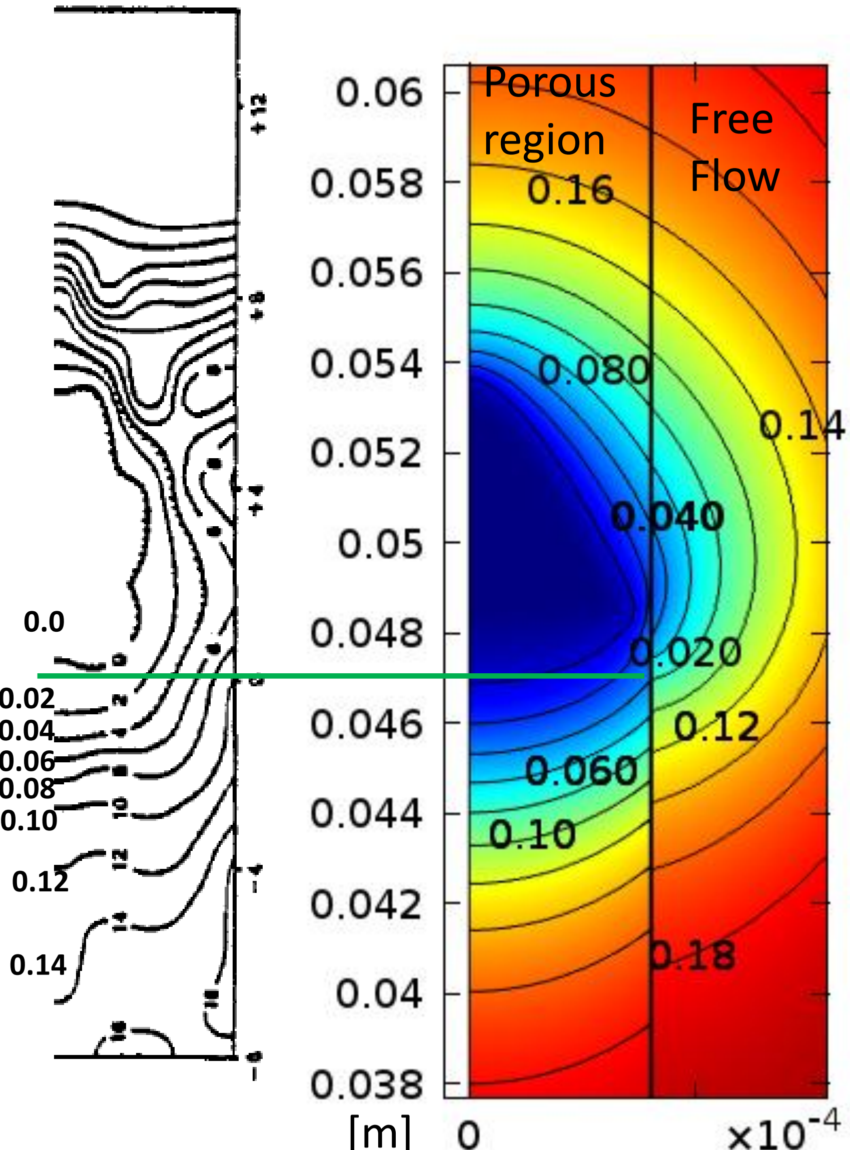
Middle of a 2[s] Puff



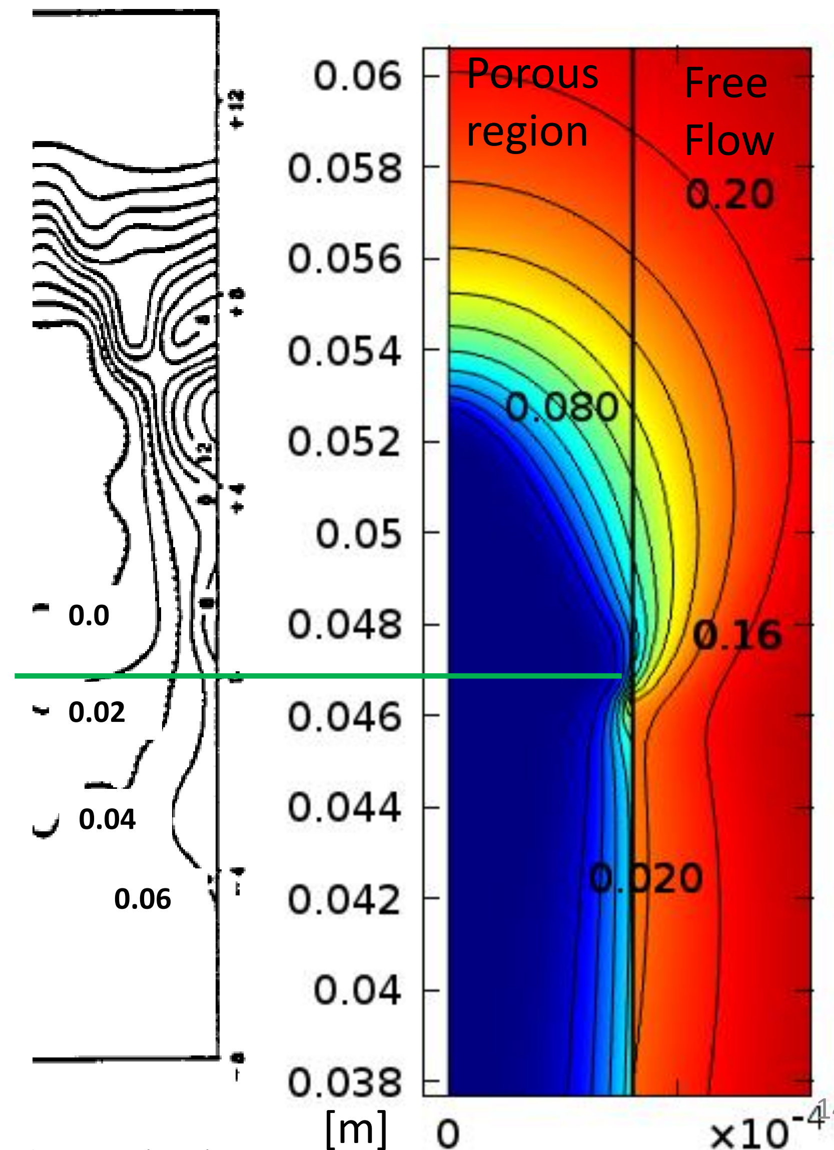
Baker, R R, *High Temp. Science*, 7 (1975) 236-247

Experimental and Simulated Oxygen Mass Fraction

End of 58 [s] Smolder



Middle of a 2[s] Puff



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Conclusions and Directions for Further Work

- Simulation for full puffing/smoldering cycle on entire domain has been constructed in 2-D
- Model agrees reasonably well with experimental data
- Discrepancies may be due to unknown sub-model parameters, questionable applicability of sub-models or REV assumption
- Future work could attempt to resolve smaller scales, since separation of scales is questionable

Acknowledgments

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Cold Flow, Velocity Magnitude