Numerical Simulation of Forward and Static Smoldering Combustion

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Introduction: Understanding the formation and transport of toxins in cigarette smoke can be aided by numerical simulation. Smoldering combustion in a cigarette is comprised of many physical, chemical and morphological processes, all of which must be included in the model.

- Simulation domain encompasses tobacco rod, filter, paper and surrounding air
- Pyrolysis zone exist ahead of oxidation zone
- Transient problem due to alternation between static and forced smoldering (puffing)
- Most air enters at paper burn line
- Fundamentally a 2-D (or 3-D) problem
- Local thermal equilibrium between gas and solid does not always hold
- System of equations is highly nonlinear and possesses a range of time and length scales

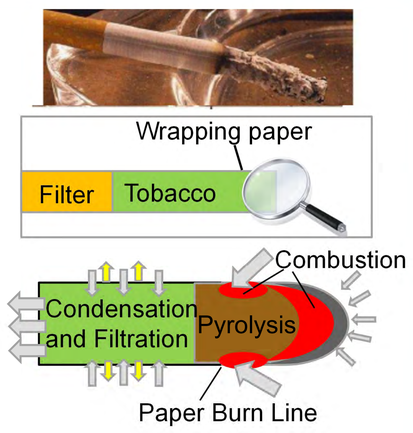


Fig 1. Schematic of burning cigarette showing convective and diffusive fluxes.

Computational Methods: A 2-D axisymmetric domain is employed, with conservation equations supplemented by expressions defining transport, thermodynamic and kinetic properties of the gas and the porous solid.

Conservation Equations

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

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

For free flow region: $\phi=1,\ Q=0\ and\ \kappa\to\infty$

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

Gas Species: $$\phi\rho\left(\frac{\partial w_j}{\partial t}+\mathbf{u}\circ\nabla w_j\right)=-\nabla\circ\mathbf{J}_j+\sum_k\nu_{j,k}\Re_k-w_jQ$$ Maxwell-Stefan model for diffusion

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

Physics Interfaces Employed in Each Region

- **Reaction Engineering** synced with:
- **Free and Porous Media Flow**: Regions 1,2,3,4
- **Transport of Concentrated Species**: Regions 1,2,3,4
- **Heat Transfer in Fluids**: Regions 1,2,3,4
- **Heat Transfer in Solids**: Regions 2,3,4
- **Domain ODEs**: Region 2 (four tobacco components, two char components, etc.)
- **Domain ODE**: Region 4 (for paper permeability)

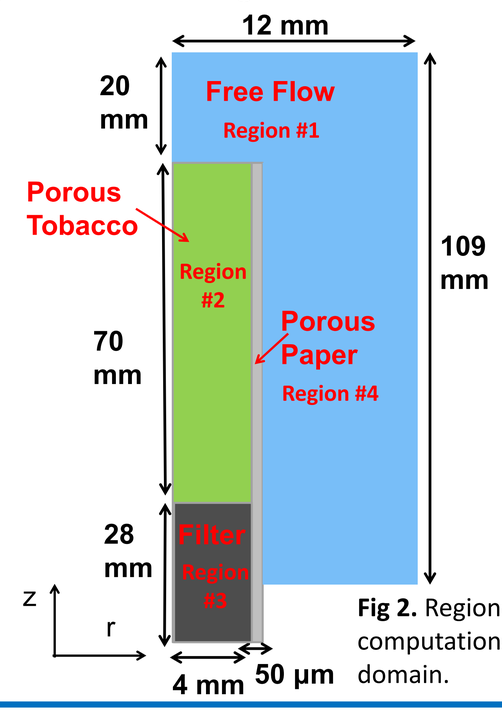
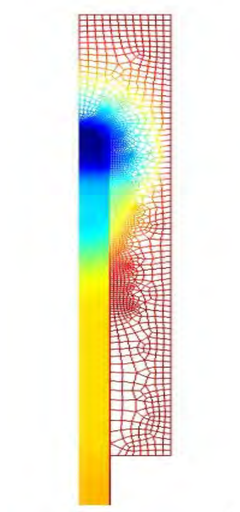


Fig 2. Regions of computational domain.

Numerical Implementation

Mesh of 8341 elements is sufficiently refined



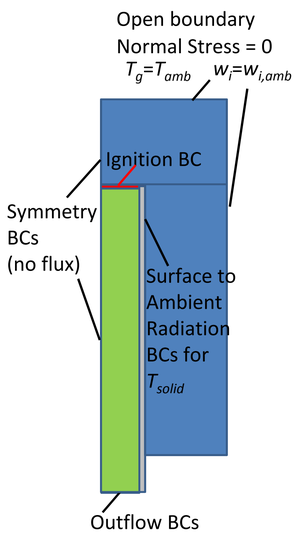


Figure 3. (a) Mesh and (b) Boundary conditions.

Initial and Boundary Conditions

- Atmospheric ICs with zero velocity
- Puffing/smoldering transition via application of 17.5 cc flow rate at outlet for 2 [s] every 60 [s]

Mesh and Elements Details:

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

Solver Settings:

- Time dependent BDF solver
- Newton's Method at each time step
- Direct MUMPS linear solver

Results: The agreement between simulation and experiment[1,2] is qualitatively and quantitatively reasonable.

Solid and Gas Temperatures

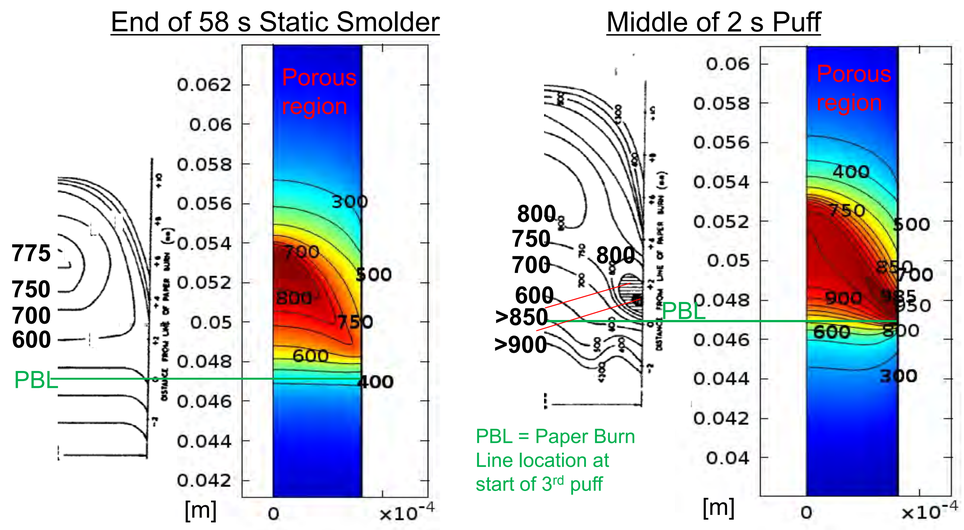


Fig 4. Experimental and Simulated Solid Temperatures (˚C) at two times.

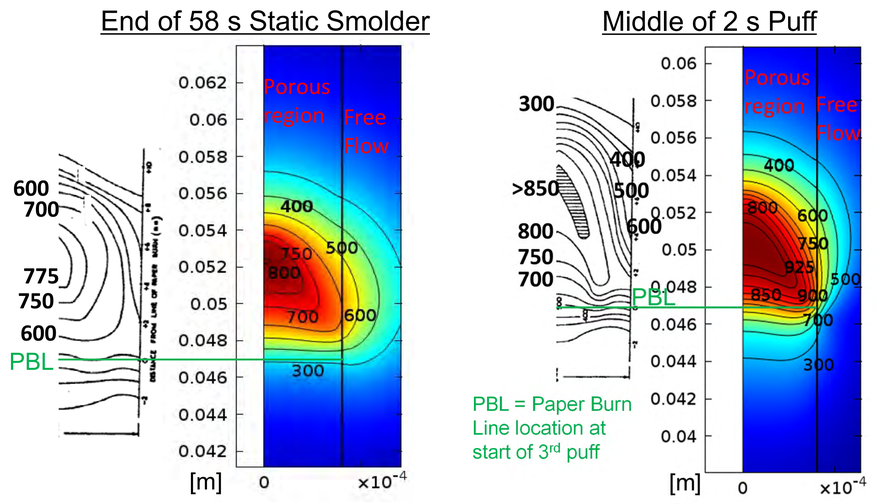
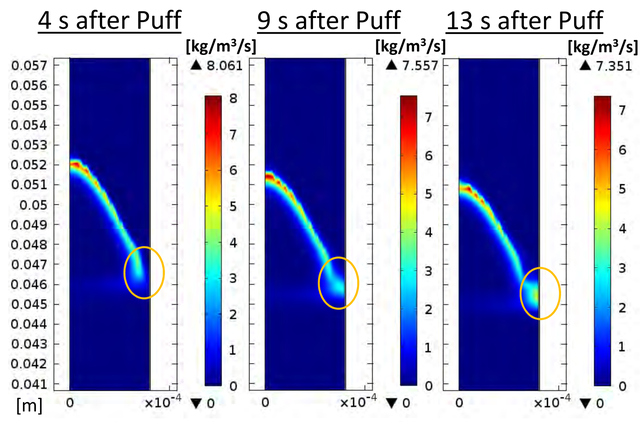


Fig 5. Experimental and Simulated Gas Temperatures (˚C) at two times.

- Solid temperatures are highest along axis during the static smolder and highest along periphery, just in front of the burn line, during forward smoldering
- Maximum gas and solid temperatures are within 50-75 (˚C) of experimental data[1]
- Deviations between experiments and simulations mostly due to shape of char coal

Char Oxidation Rate



- Char oxidation along periphery pauses for ~10 s after puff, **similar to experimental observation**[1] that paper burn line does not advance for ~15 s after puff!
- "Pause" is due to build-up of products at expense of O_2 as puff ends and lasts until diffusion can replenish O_2 concentrations

Fig 6. Char oxidation rate profiles during static smolder period.

Oxygen Mass Fraction

- O_2 depletion zone during static smolder is roughly 6 mm in length for both the simulations and experiments[2]
- During forward smoldering, predicted O_2-starved region extends further downstream than experiment…
- Assumption of a *homogeneous porous medium* is questionable

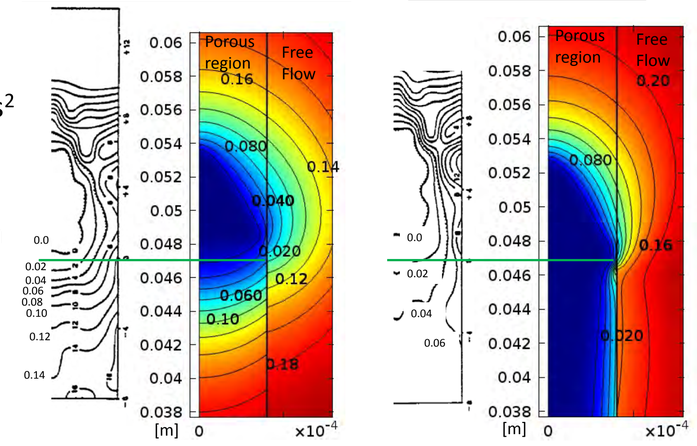


Fig 7. Experimental and Simulated Oxygen mass fractions.

Conclusions: A simulation of a static and forward smoking cycle in and around a burning cigarette has been validated. Ongoing work is focused on incorporating more detailed pyrolysis models. Future work may attempt to resolve smaller scales, since scale separation is weak.

References:
1. Baker, R R, *High Temp. Science,* 7 (1975) 236-247
2. Baker, R R, *Beitr. Tabakforsch*, 11, (1981), 1-17

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