

AE471A Project Report

Modeling Pyrolysis and Combustion in Naturally Smoldering Cigarettes



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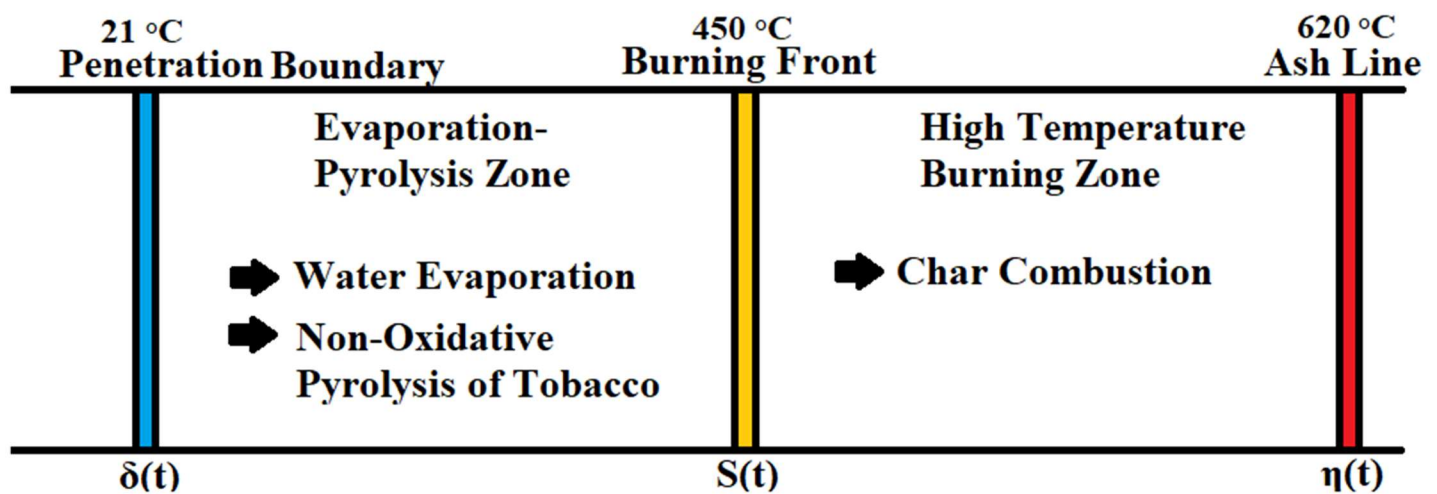
Motivation

Tobacco smoking, despite being harmful, continues to be the most common form of recreational drug use; practiced by millions around the world. It is the second leading cause of preventable deaths globally, accounting for more than 18% of deaths worldwide. With prevention difficult and widespread prevalence, it has become more critical than ever to understand the mechanisms involved in a burning cigarette and improve their construction to reduce associated risk factors.

A robust numerical simulation can supply us with data not obtainable through experiments, aid in analysis by providing the temperature and density profiles, and perform predictions when cigarette construction, initial densities, or dimensions are altered.

Introduction

This project aims to implement a 1D model of combustion processes during smoldering, the process of slow and flameless combustion that occurs when a cigarette is set alight. To set up the governing equations required for such a model, the cigarette is divided into two major reaction zones: (a) the **evaporation-pyrolysis zone** and (b) the **high-temperature burning zone**.



The boundaries of the two zones are defined at positions with a specific temperature. All three boundaries recede with time, and at steady state, their receding rate becomes constant. This rate is called the **Linear Burn Rate (LBR) or smoldering speed** and is an input to our model.

1. **Penetration Boundary** (at 294 K) – It is assumed that beyond this boundary, the temperature stays at the initial value of 294 K, and no heat is transferred through it.
2. **Burning Front** (at 723 K) – This boundary separates the pyrolysis and burning zones and marks the position where all the tobacco has been converted into volatile smoke and residual char.
3. **Ash Line** (at 893 K) – The right boundary of the burning zone, which marks the end of combustion. The side-stream smoke flows out of this boundary.

The reactions that occur in the Pyrolysis Zone include the evaporation of water in the tobacco and the non-oxidative pyrolysis of virgin tobacco, which lead to the formation of residual char and volatile smoke. In the Burning Zone, the density change is characterized by char combustion and the formation of ash.

Methodology

Two numerical Python codes have been written for this project. Both utilize a different mathematical model for smoldering but attempt to solve for the same parameters.

1. **Muramatsu's Approach:** A set of governing partial differential equations were written to express the heat and mass transfer phenomena in the Pyrolysis Zone. These set of 6 simultaneous PDEs were solved with the Runge-Kutta-Gill Method to obtain temperature and density distributions in the Pyrolysis Zone.
2. **Chen's Approach:** In this model, temperatures in the pyrolysis and combustion zones were assumed to have a given functional form that satisfied the boundary conditions. These temperature profiles were integrated across both zones to match the overall mass and energy balance constraints. This model goes further in its analysis than Muramatsu's approach as it outputs temperatures and densities in both zones; however, some prior knowledge about the temperature profile is required.

So, with these two methods, we can build a clearer picture of how parameters vary inside a naturally smoldering cigarette. Moreover, predictions can be performed regarding the effect of input parameters such as the radius and packing density of cigarettes, smoldering speed, and air mass flow rate on the cigarette's smoldering features.

Governing Equations in Muramatsu's Approach

When writing the governing equations, it is helpful to be in the frame of reference of the moving boundaries. Since the linear burn rate becomes constant at steady state, we can solve for temperatures and compound densities with respect to a spatial axis rather than time. So, we input $x = z + ut$ in our heat and mass balances, with dx/dt being the linear burn rate, u . The position of the burning front is taken as **origin**.

For Muramatsu's Approach, a set of six simultaneous ordinary and partial differential equations were used to describe the pyrolysis and evaporation processes.

- A. The reaction rate of virgin tobacco pyrolysis follows the n^{th} order Arrhenius equation and is the sum of the reaction rates of four major compounds involved in the pyrolysis.

$$\frac{d\rho_v}{dx} = \frac{1}{u} \sum_{i=1}^4 -Z_i e^{\left(-\frac{E_i}{RT}\right)} \left(\frac{\rho_{vi}}{\rho_{vi0}}\right)^{n_i} \rho_{vi0}$$

- B. The char formation reaction describes the conversion of tobacco into char. The char formation ratio is taken to be 0.34 for our purposes.

$$\frac{d\rho_c}{dx} = -\frac{\rho_f}{\rho_{v0}} \frac{d\rho_v}{dx}, \text{ where } \frac{\rho_f}{\rho_{v0}} \text{ is the char formation ratio.}$$

- C. The evaporation of water and subsequent water loss due to diffusion is described by the following two partial differential equations, one for water density and the other for the vapor pressure.

$$\frac{d\rho_w}{dx} = -\frac{Z_w}{u} e^{\left(-\frac{8430}{T}\right)} \left(\frac{\rho_w}{\rho_{v0}} - w_{eq}\right)^{1.81}, \text{ where } w_{eq} \text{ is a function of } P_w.$$

$$\frac{dP_w}{dx} = \frac{P_w}{T} \frac{dT}{dx} - \frac{\frac{P_w}{T} \left(\frac{d^2 T}{dx^2} \right) + \frac{0.03}{r d\phi_w} (P_w - P_{w0} \frac{T}{T_0}) + \frac{uRT}{\phi_w m D_x} \frac{d\rho_w}{dx}}{\frac{u}{D_x} + \frac{0.25}{T} \frac{dT}{dx}}$$

D. Finally, the equation for temperature gradient is determined by performing a heat balance within the Pyrolysis Zone. Heat transfer via thermal conduction, heat loss due to convection and radiation through the outer surface, and thermal energy used in the reaction are considered in the heat balance.

$$\frac{dy}{dx} = \frac{y}{K_e} \left\{ u(\rho_v C_{pv} + \rho_c C_{pc} + \rho_w C_{pw}) - \frac{dK_e}{dx} \right\} + \frac{2}{rK_e} \{ h(T - T_\infty) + \sigma \epsilon_s (T^4 - T_\infty^4) \} +$$

$$\frac{u}{K_e} \left\{ (T - T_\infty) \left(C_{pv} \frac{d\rho_v}{dx} + C_{pc} \frac{d\rho_c}{dx} + C_{pw} \frac{d\rho_w}{dx} \right) - Q_p \frac{d\rho_v}{dx} - Q_w \frac{d\rho_w}{dx} \right\}$$

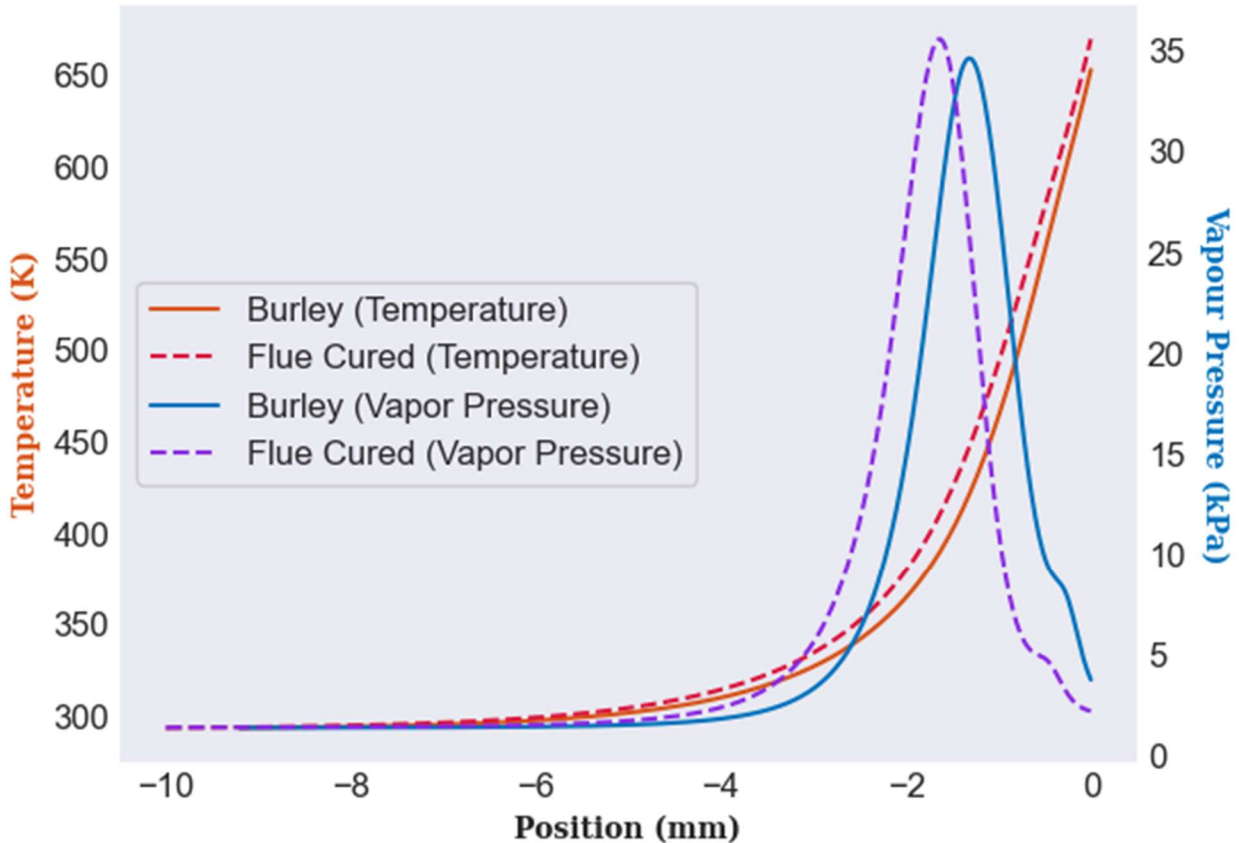
An additional ODE needs to be solved to obtain the temperature from its gradient,

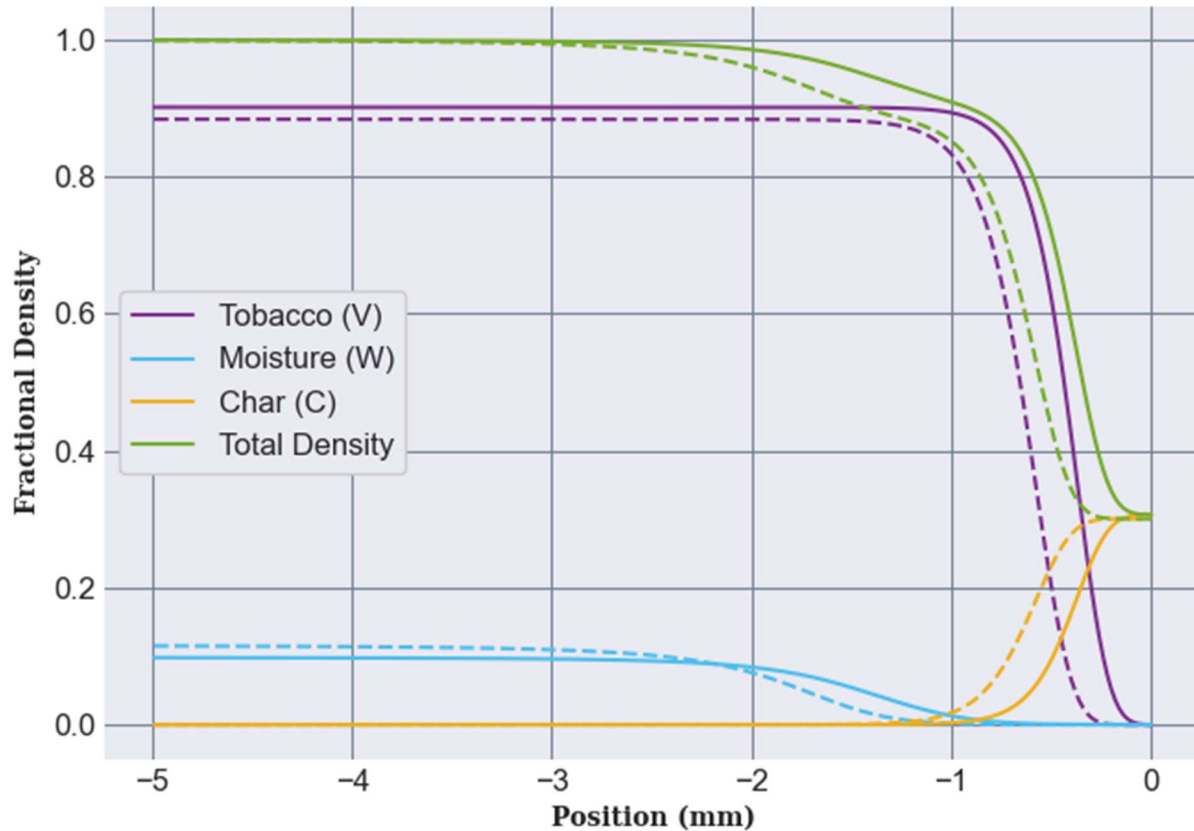
$$\frac{dT}{dx} = y$$

Results from Muramatsu's Approach

The above-mentioned simultaneous equations were solved with the Runge-Kutta Gill method, and the temperature and density profiles for two kinds of tobacco commonly used in cigarettes were obtained:

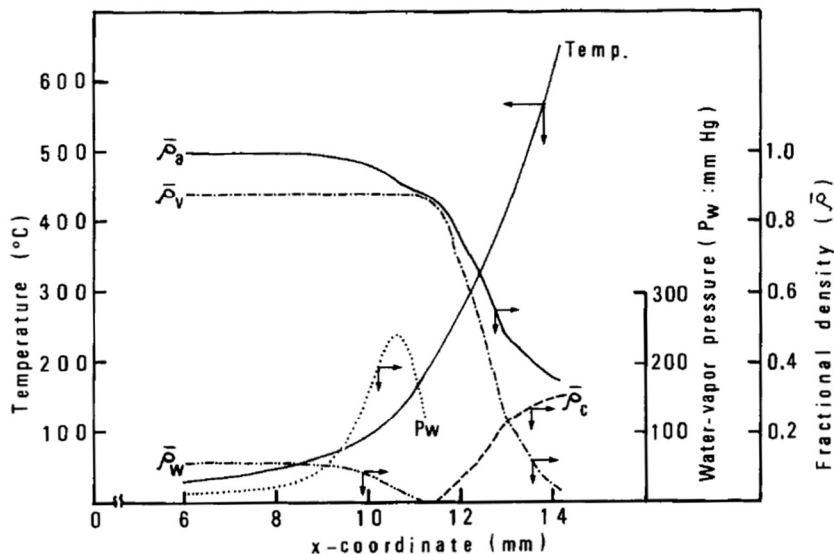
(1) **Burley** (Solid line) and (2) **Flue Cured** (Dashed line).



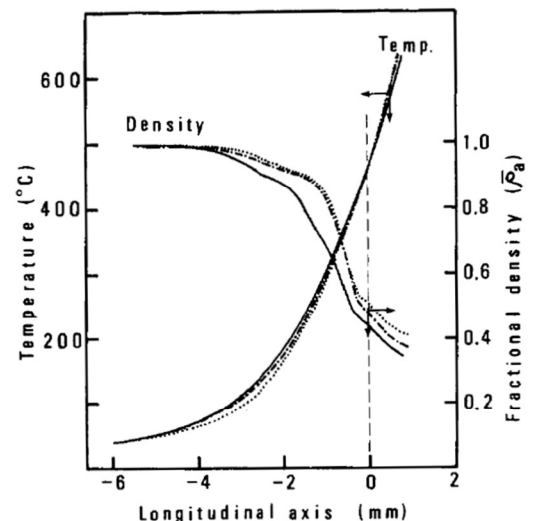


From the above plots, we can make the following observations:

1. We clearly observe the decrease in total density when water evaporation starts at around 340 K. This is consistent with an increase in vapor pressure and a decrease in water density in that region.
2. From 450 K, a sharp decrease in total density is observed corresponding to the onset of tobacco pyrolysis into residual char—the char density increasing as a result.
3. The evaporation of water takes place prior to the pyrolysis of tobacco in distinct regions.
4. The temperature and density profiles are similar in both kinds of tobacco; however, we can observe that the reactions occur earlier spatially in the flue-cured tobacco cigarettes.



Theoretical profiles of temperature, density, and water-vapor pressure in evaporation-pyrolysis zone of a cigarette containing flue-cured tobacco.



Comparison of theoretical temperature and density profiles for cigarettes containing different types of tobacco: —, flue cured (F); ····, burley (B); -·-·-·, Matsukawa (M_2).

All these observations are consistent with theoretical models and experiments conducted by Muramatsu (1979). Shown above are relevant results from the paper under consideration.

Governing Equations in Chen's Approach

In the model given by Chen (2002), the **integral method** is utilized to solve the partial differential equations. This method involves substituting an assumed temperature profile (a cubic function) into the heat and mass balances. The boundary conditions and set of obtained equations can be used to calculate the unknowns in the temperature function.

➤ In the Pyrolysis Zone, the following temperature profile was assumed,

$$T = T_{\delta} + (T_s - T_{\delta}) \left(\frac{x + L_p}{L_p} \right)^3, \text{ where } L_p \text{ is the length of the Pyrolysis Zone.}$$

Once we substitute the temperature profile in the heat balance equation, we get a quadratic equation in L_p that can be solved.

$$u = \frac{3k_{eff}}{\rho c_p L_p} - \frac{h'(T_s - T_a)}{2r\rho c_p (T_s - T_{\delta})} L_p, \text{ where } u \text{ is the known Linear Burn Rate.}$$

The tobacco pyrolysis and char formation equations are the same as the ones used in Muramatsu's approach. However, the water density is modeled such that the vapor pressure is not required.

$$\frac{d\rho_w}{dx} = -\frac{Z_w}{u} e^{\left(-\frac{E_w}{RT}\right)} \left(\frac{\rho_w}{\rho_{v0}}\right)^{n_w} \rho_{v0}$$

➤ For the case of the burning zone, we again assume that temperature has a cubic profile. However, there are several unknowns in this profile, even after making it satisfy the boundary conditions.

$$T = T_s + (T_{max} - T_s) \left(\frac{3x}{2\gamma L_c} - \frac{1}{2} \left(\frac{x}{\gamma L_c} \right)^3 \right)$$

- T_{max} , the maximum temperature in the combustion zone, is calculated from an empirical relation dependent on the radius of the cigarette and the mass flow rate of air.
- γ is the relative position of maximum temperature in the burning zone and is given by a cubic equation derived from the temperature profile, $\frac{T_{\eta} - T_s}{T_{max} - T_s} = \frac{1}{2\gamma} \left(3 - \frac{1}{\gamma^2} \right)$. This cubic was converted to a **depressed cubic** and solved analytically via the cubic formula.
- Finally, the length of the burning zone, L_c , was calculated by equating the heat transferred from the burning zone to the pyrolysis zone by performing a heat balance at the burning front.

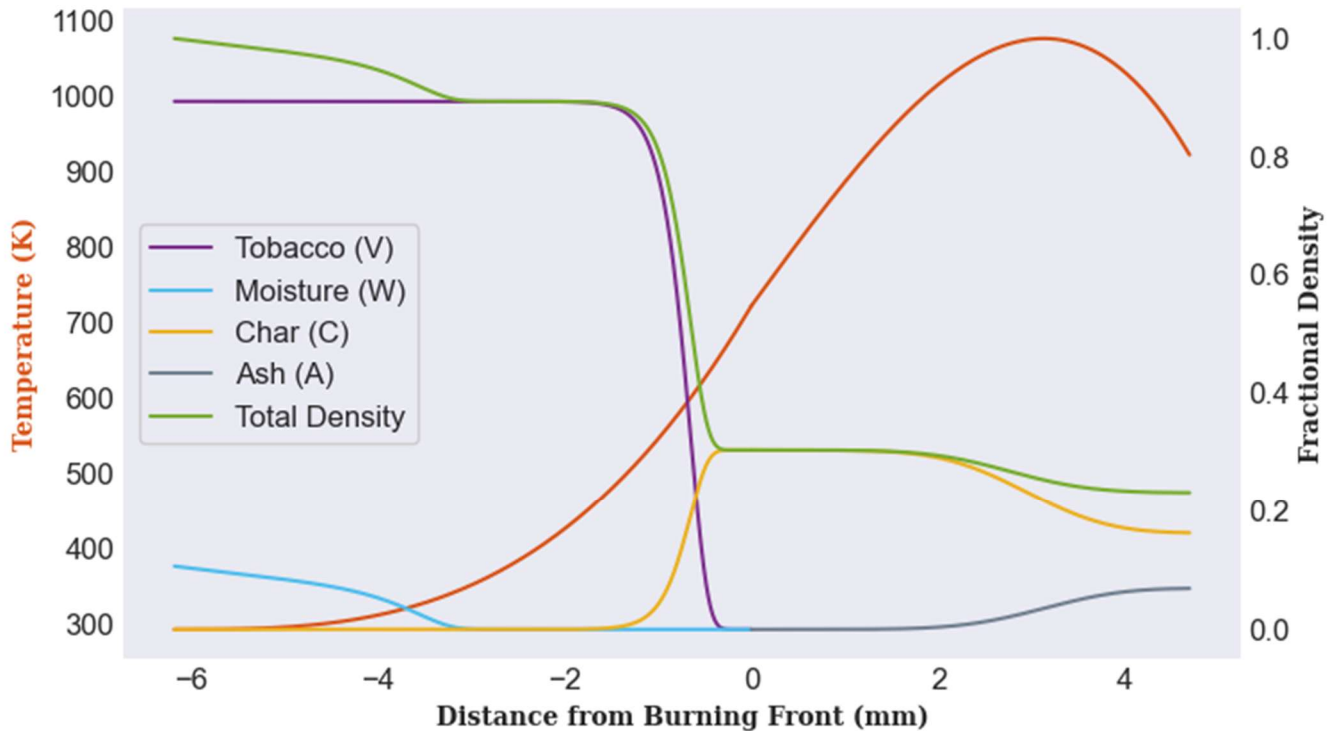
The reactions in the burning zone are characterized by the combustion of char and the formation of ash. A first-order Arrhenius reaction is used to model the reaction rate of char. An ash formation ratio of 0.38 is used.

$$\frac{d\rho_c}{dx} = \frac{-Z_c}{u} e^{\left(-\frac{E_c}{RT}\right)} \rho_c \text{ and } \frac{d\rho_{ash}}{dx} = -0.38 \frac{d\rho_c}{dx}$$

Results from Chen's Approach

Using the Runge-Kutta Gill method, we can separately calculate the density profiles in both zones and stitch them together in one plot. In the code, since both the water and char density reaction rates depend on tobacco density, the mesh **must be doubly fine** for tobacco. This is because the availability of values of independent variables at every half-step is a prerequisite for iterating with the RK Gill method.

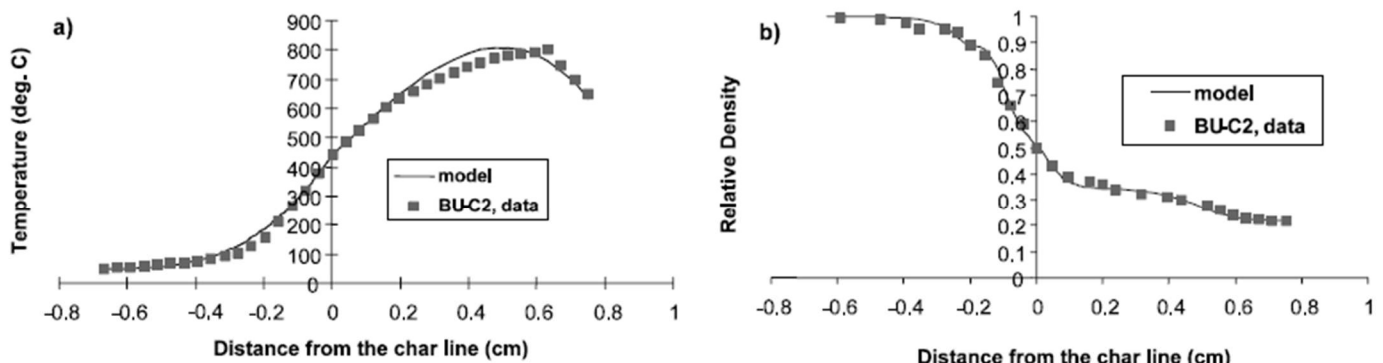
In the pyrolysis zone, a mesh size of 10000 for water and char densities and 20000 for tobacco was required for convergence and 300 and 600 respectively for ash and char in the burning zone.



For **Burley tobacco**, some relevant parameters that were obtained as part of the calculation are:

- Pyrolysis Zone Length, $L_p = 6.17$ mm
- Burning Zone Length, $L_c = 4.69$ mm
- Maximum Temperature, $T_{max} = 1077$ K at relative position, $\gamma = x/L_c = 0.667$.

The solutions are consistent with the profiles obtained by Chen (2002).



Temperature (a) and density (b) profiles of smoldering BU-C2 cigarette

The pyrolysis zone profiles also agree well with those obtained from Muramatsu's approach, with a point of difference being the length of the pyrolysis zone. The length obtained here is much shorter than from the previous method (10 mm).

Closing Remarks

The motivations behind the project were two-fold, understanding a real-world combustion problem in detail and applying numerical techniques to solve such a problem. Smoldering combustion was a perfect candidate for such an endeavor – not so complicated that modeling takes too much time but also elaborate enough to include both heat and mass transfer and reactive mechanisms.

Although the process of understanding, writing, and debugging was arduous (sometimes mind-numbingly so), I am happy to have been able to achieve what I set out to do. I want to thank my advisor, Prof. Ashoke De, for introducing me to such an interesting topic and his course on combustion, AE663A, without which understanding the literature would have been impossible.

References

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