P2.2 NON-LOCAL CHEMISTRY IMPLEMENTATION IN HIGRAD/FIRETEC

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1. ABSTRACT

In order to study the interactions between the important processes within a wildland fire, Los Alamos National Laboratory and the USDA Forest Service are continuing to develop the HIGRAD/FIRETEC wildfire behavior model. HIGRAD/FIRETEC is a coupled atmosphere/wildfire behavior model and is based on conservation of mass, momentum, species and energy. HIGRAD/FIRETEC is a three-dimensional transport model that uses a compressible-gas formulation to couple its physics based wildfire model with the motions of the local atmosphere. Currently, all of the chemistry and heat production occurs within the same computational cell as the burning wood and a fraction of the heat produced is returned to the wood to sustain combustion. In some situations, this is very realistic; however, in other situations, this treatment is not as realistic since it is possible for volatilized hydrocarbons to travel tens of meters before they combust. We are investigating the trade offs involved in a local burning scheme by separating the pyrolysis from the combustion of the various pyrolysis products. The initial products of pyrolysis (an endothermic process) in our scheme are char, a generic hydrocarbon mixture, and inert gas. We are allowing the overall gas/char ratio to vary with temperature and fuel type (e.g. grass or wood). In a separate step the hydrocarbon mixture is allowed to mix with oxygen and combust with the only product being an inert gas. The hydrocarbon combustion is exothermic and a fraction of the heat produced is returned to the wood to sustain combustion. Char is tracked explicitly and allowed to combust in a slower exothermic step. Here we report on preliminary investigations into this simple non-local chemistry scheme.

2. INTRODUCTION

Current wildfire model vary in origin from purely empirical formulations, (Andrews (1986); Finney (1998)) to physics-based algorithms (Dupey and Larini (2000); Porterie *et al.* (2000); Grishin (2001A) and (2001B)) to combinations of the two (Clark *et al.* (1996); Coen and Clark (2000)). These models of differing complexity and origin are appropriate for different applications. FIRETEC (Linn (1997)) is a coupled atmospheric transport/wildfire behavior model being developed at Los Alamos National Laboratory, and is based on the principals of conservation of mass, momentum, and energy as well as representations of some of the physical processes that drive wildfires. The physically based nature of FIRETEC could make it a useful learning tool and allow it to be used to examine some of the more complex wildfire behaviors. FIRETEC is combined with the hydrodynamics model, HIGRAD (Reisner *et al.* (2000), Reisner *et al.* (2003)), in order to simulate three-dimensional wildfires moving over a terrain-following grid and to couple FIRETEC with the motions of the local atmosphere. Some examples of the physical phenomena being studied with FIRETEC are the effects of transient wind conditions, nonhomogeneous terrain, nonuniform fuel beds with patchy distributions and different vertical fuel structures.

The chemistry currently employed in FIRETEC is relatively simple and some basic improvements can easily be envisioned. The ‘wish list’ for improved chemistry within FIRETEC includes: a three component wood model (cellulose, hemicellulose, and lignin), Arrhenius form kinetics, an improved probability distribution function for temperature (Gaussian is currently employed), a char formation/oxidation scheme, a

soot formation/transport scheme, and gas phase oxidation of pyrolysis products. We feel that the most important step is to separate the pyrolysis of wood (an endothermic process) from the gas phase combustion of pyrolysis products. This should be important when the distance that reactive gases travel before combusting is larger than the typical dimension of the resolved volume. We are currently running with resolved volumes on the order of 1 m^3 near the ground. The improved chemistry should allow us to simulate a more realistic behavior of fuel and flames. With this improved representation we hope to characterize, understand, and simulate transitions to extreme fire behaviors such as blow-ups and crowning under realistically complex meteorological and topographical conditions. Here we describe some initial attempts to incorporate some of these improvements into FIRETEC.

3. FUEL MODEL

3.1 Local Fuel Model

The set of chemical reactions occurring in a wildfire is extremely complex and has many intermediate transient species. In the fuel model currently employed by FIRETEC (Linn (2002)) the set of chemical reactions was simplified to a single solid-gas reaction that is presented in equation 1.

$$N_{wood}(wood) + N_{O_2}(oxygen) \rightarrow (products) + (heat) \quad (1)$$

The stoichiometric coefficients, N_{wood} and N_{O2}, describe the net amount of wood and oxygen consumed through pyrolysis and all of the intermediate reactions when a unit mass of 'inert' products is formed. The reaction rate, F_{wood}, is described by equation 2.

$$F_{wood} = \rho_{wood} \rho_{O_2} \nu \quad (2)$$

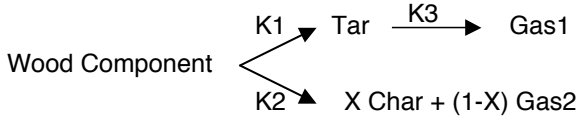
Where ρ_{wood} and ρ_{O2} are the local densities of wood and oxygen respectively, ν is the turbulent diffusion coefficient, which is calculated based on the local turbulent kinetic energy and vegetation geometry, and Γ is a function of: the stoichiometry assumed in equation (1), the local densities of the reactants, and a probability distribution function for the temperature (which is employed to give an 'ignited volume fraction', i.e. the fraction of wood in a resolved volume that is actively burning).

The philosophy behind this particular model is that the rate of pyrolysis is ultimately related to the heat flux to the solid wood, which is tied to the nearby gaseous reactions that are limited by the amount of oxygen. We assume that the rates of the exothermic reactions are limited by the rate at which reactants can be brought together (mixing limited), this is justified since the dominant exothermic reactions all involve oxidation by O_2, which is by far the limiting reagent in the case of actively burning wood. Thus, the heat fluxes to the solids, and so the rate of pyrolysis will ultimately be limited by the mixing process. A simple function is used to represent the fraction of heat released from the gas phase that is deposited directly back to the solid, this function is assumed to be in direct proportion to the amount of wood that has burned. This is meant to represent the fact that the primary nature of burning at a given location changes over time from flaming combustion, with much of the heat escaping with the gases, to smoldering combustion where catalysis and insulation by char and ash cause a larger proportion of the heat to be recaptured by the solid.

3.2 Nonlocal Fuel Model.

A first step towards adding detailed chemistry to FIRETEC is to separate the pyrolysis from the gas phase combustion in a semi-global kinetics scheme. In general semi-global kinetics are defined as those comprising more than one explicit reaction step, wherein the steps themselves are not necessarily elementary. Criteria for a useful semi-global kinetics scheme in this case are that it must reproduce the correct magnitudes of the temperature dependence (global intrinsic activation energy) and concentration dependence (global intrinsic reaction order) during steady state combustion across the various temperature ranges of interest. We would like to take into account the formation of

char, tar, and gas (both combustible and inert) from the act of pyrolysis. It would also be useful to be able to account for different types of fuels by having separate schemes for cellulose, hemicellulose, and lignin. These three loosely defined types are the major components of all wildfire fuels. The scheme employed here is a modified form of a scheme taken from the literature (see for example Miller and Bellan (1997), and Di Blasi (1998) and references therein) where tar formation competes with char formation.



The rates are determined from Arrhenius form kinetics (characterized by a rate constant A_j and an activation energy E_j) combined with a probability distribution function for temperature, which will be discussed later. The reaction parameters depend on the wood component (cellulose, hemicellulose, and lignin) being combusted. This allows different types of wildfire fuels to produce more or less char and tar when burned under identical conditions. Fractions of these components in different types of wildfire fuels are available in the literature. Currently we assume that all tar formed immediately is converted to our generic Gas mixture. This is to avoid having to transport two types of reactive gases as well as to avoid having to model the semi-volatile nature of tar. Values employed for X are 0.35, 0.60, and 0.75 in the case of cellulose, hemicellulose, and lignin respectively. The values employed for A_j and E_j are compiled in table 1.

Table 1.

	A_j [1/s]	E_j [kj/mol]	Source
K_{1c}	3.3×10^{14}	196.5	Di Blasi and Russo (1994)*
K_{2c}	1.3×10^{10}	150.5	Di Blasi and Russo (1994)*
K_{1h}	8.8×10^{15}	202.4	Di Blasi and Russo (1994)*
K_{2h}	2.6×10^{11}	145.7	Di Blasi and Russo (1994)*
K_{1l}	1.5×10^{9}	143.8	Koufopanos *et al.* (1989)*
K_{2l}	7.7×10^{6}	111.4	Koufopanos *et al.* (1989)*

The subscripts c, h, and l represent cellulose, hemicellulose, and lignin respectively
* these values were modified somewhat by Miller and Bellan (1997)

We observe from table 1 that in general the char producing pathway has a lower value for both Aj and Ej. Thus char will form in abundance from relatively low temperature combustion, but at higher temperatures tar and gas formation will dominate. It can also be gleaned that fuels with a high fraction of lignin will produce the most char. Data on the heat of reaction for each step in the kinetic scheme is limited and so a single value is used for each step independent of the component combusting.

Table 2

Property	Value	Source
Δh_1	255 kJ/kg	Koufopanos *et al.* (1991)
Δh_2	-20 kJ/kg	Koufopanos *et al.* (1991)
Δh_3	-42 kJ/kg	Curtis and Miller (1988)

We observe from table 2 that tar formation is relatively strongly endothermic, and char formation only weakly exothermic. Thus the energy that supports fire propagation must come primarily from the combustion of reactive gasses released by pyrolysis. Char combustion is also exothermic (Δh = -7030 kJ/kg) and so will also help to support continued pyrolysis. It is handled here by employing the Arrhenius form kinetics described in C Di Blasi (1999) in conjunction with a probability distribution function for temperature. The only product of Char combustion is currently assumed to be inert gas. It is important to track Char explicitly because it affects the heat transfer properties of the solid fuel, it is also important for modeling smoldering fires.

The gas phase products of pyrolysis are a mixture of reactive and inert gasses. We are currently assuming that Gas1 and Gas2 in the kinetic scheme are equivalent. However we are considering a scheme whereby the heat of reaction of the transported reactive gasses would change based on its relative proportion of Gas1 and Gas2 within each resolved volume.

Experimental data (Hajaligol (1982), Nunn (1985(a) and 1985(b)), Grishin (1997)) shows that the gas produced during pyrolysis is roughly 68% reactive (mostly CO but also containing CH_4, H_2, CH_3CHO, CH_3OH, C_2H_4 and traces of longer chain hydrocarbons) and 32% inert (CO_2 and H_2O), these data were used to compute an approximate heat of combustion for the reactive portion of the gas (8800 kJ/kg) as well as the stoichiometric coefficients of the combustion. That is, the mass of reactive gas and oxygen that react to produce a unit mass of inert products.

$$N_{reactive gas}(\text{reactive gas}) + N_{O2}(\text{oxygen}) \rightarrow (\text{inert gas}) + (\text{heat}) \quad (3)$$

The reactive gas is then reacted with oxygen following a scheme proposed for FIRETEC by Linn (1997).

$$F_{wood} = \frac{\rho_{reactivegas}\rho_{O2}\Delta}{2\left(N_{O2}\rho_{reactivegas} + N_{reactivegas}\rho_{O2}\right)} \quad (4)$$

Where the symbols have the same meaning as described for equation 1. There are some differences in the numerical constants used in the formulation of Δ and ρ. The new term in the denominator results from a simple description of the correlations between the density of the reactive gas and that of oxygen within a resolved volume. The only product of the combustion of the reactive gas is an inert gas. Once again this is a huge oversimplification of the complex chemistry occurring in gas phase combustion. It is simply meant as one step beyond the combustion chemistry currently employed by FIRETEC.

4. PROBABILITY DISTRIBUTION FUNCTION FOR TEMPERATURE.

In the FIRETEC model our resolved volume is on the order of 1 m^3 as mentioned above. Even within this volume there can be a wide range of temperatures. The temperature at any point is not a quantity we are able to determine, yet the local temperatures are the temperatures that determine ignition and burn intensity at that point. We use a probability distribution function (PDF) for temperature to estimate the fraction within a resolved volume that is at a given temperature. This approach is based on the assumption that there is some universality and characterizability to the temperature distributions in a region.

The current fuel model employed in FIRETEC defines a function $\Delta(\overline{T})$, based on the mean temperature that describes the percentage of the reactants in a region that are above a 'critical temperature' and therefore able to react if they are properly mixed. Currently the PDF in use is a roughly symmetric, roughly bell-shaped, curve. It is assumed that the same PDF applies to both the gas and solid phases within a resolved volume. The shape of the PDF does not change with mean temperature. The temperature of combustion doesn't matter as the assumption is that the rate of reaction is mixing limited anyway.

In the new nonlocal fuel model, the temperature of pyrolysis is important because it determines the relative amount of the three-fuel component that combust and the relative amount of gas and Char produced. The assumption of pyrolysis being mixing limited is also somewhat questionable in this context since pyrolysis can occur in the absence of oxygen. The heat flux can be reasonably assumed to be mixing limited since the exothermic reactions involve reaction with oxygen, but those reactions will now be handled separately in the non-local scheme. Therefore, we are currently not using the 'fraction ignited' function for pyrolysis but are using a PDF for temperature directly. We have no specific data to support the use or rejection of any specific form for the PDF, this being the case we chose a well-studied function – the lognormal distribution. A lognormal PDF has the property of increased width as temperature increases, this seems intuitively right to us. It is very similar to the PDF currently used in the simple model to produce $\Delta(\overline{T})$. However, the lognormal PDF times the Ahrrenius rate equation is not fully integratable, thus we have employed the tactic of calculating the value of the PDF and rate equation offline,

then fitting their product to an equation of the form:

$$\text{Rate} = A_j e^{\left(\frac{-C_1}{T} + \frac{-C_2}{T^2} + \frac{-C_3}{T^3}\right)} \qquad (5)$$

which captures most of the variance; above 98% over the relevant temperature range. This fitting was done for each fuel component and the resulting equation can be used as part of the rate expression during computational runs.

In the case of the gas phase reaction we are still employing the same function for $\Box(\overline{T})$ as in the simple fuel model. As part of the derivation of $\Box(\overline{T})$ for the simple fuel model it is assumed that all the available fuel elements are thermally thin, so we expect the temperature distribution of the solid pockets to be similar to that of the gas because there is a rapid heat exchange between the two phases.

5. SIMULATIONS

At the present time we do not have any relevant simulations to present and are sorting through the varous issues related to specific numerical constants to be used as well as the specific form for the PDF. One of the numerical constants we are having problems with is associated with the current scheme for radiative heat transfer, which is calculated based on a two-field thermal radiation approximation, adapted from Stephens (1984). The primary emitter of radiation in a wildfire is soot, which is currently not being tracked explicitly. Thus the depletion of oxygen is used as a proxy for soot production, and that is combined with a T^4 dependence on temperature as for blackbody radiation. A constant, Crad, combines all other factors that are involved in going from these terms to the emissivity of the air. Some of these other factors have been changed due to our explicit inclusion of basic nonlocal combustion. Crad is a very important factor in keeping the nonlocal processes involved in wildfire combustion from 'blowing up', a careful balance must be achieved. The lognormal PDF for temperature needs both a mean and a deviation to be computed and different values for the deviation are still being tested. Initial simulations suggest that the size of the deviation may have to be implemented as a function of the strength of turbulence at small and medium spatial scales. It may in fact turn out that the lognormal PDF is not the best one for modeling a wildfire, we are currently searching for any experimental data that might give us a clue as to the proper shape of the PDF for temperature in a fire. The PDF need not be continuous due to the way in which we are currently fitting the product of the Ahrrenius expression and the PDF to a function offline.

6. CONCLUSIONS

We have described here a scheme for improving the representation of chemistry involved in wildfires in FIRETEC. With this improved representation we hope to characterize, understand and simulate transitions to extreme fire behaviors such as blow-ups and crowning under realistically complex meteorological and topographical conditions. Initial attempts have been made to incorporate some of these improvements into FIRETEC. There is still a good deal of calibration to be done, especially in the area of a probability distribution for temperature. At some point it will also be important to determine if and when the benefit of including these effects are worth their associated computational cost.

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