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ON THE MODELING OF LAMINAR-TURBULENT TRANSITION IN FIRE APPLICATION: EFFECT OF INTERACTION BETWEENCHEMICAL REACTION AND TURBULENCE

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ABSTRACT

A model for the prediction of the chemical reaction rate in a gas flowing over a burning surface has been developed. Special emphasis was given to describing the characteristics of the process under transition conditions from laminar to turbulent regimes. The application to flow-assisted flame spread over solid fuel is considered.

Keywords: Turbulent combustion, flow-assisted flame spread, modeling.

BACKGROUND

A self-sustained combustion reaction is the very essence of the flame spread process (Figure 1). Hence, the reasonable prediction of a flame's heat release rate provides a basis for proper modeling of the general effect of fire phenomenon. The combustion process is affected by a number of factors surrounding flame propagation. Some of the most important factors involve features of the fluid flow. Substantial qualitative (obviously, quantitative too) change of flow properties occurs during the transition from laminar to turbulent flow regimes. Correspondingly, the features of chemical reactions in the gas phase are also affected.

When examining the spread of fires over the surface of solid fuels, the two generally distinguished modes of flame spread (e.g. [1,2]) are considered: opposed-flow and flow-assisted. The first of these is usually associated with laminar flow while the latter case depends upon the specific condition of the process – either laminar or turbulent regimes may prevail. Usually, flame spread in a concurrent flow that takes place in different space orientations due to the buoyancy force: from upward, which mostly relates to accelerating propagation of strongly turbulent flame, to horizontal, under which a gradual laminar-turbulent transition is expected.

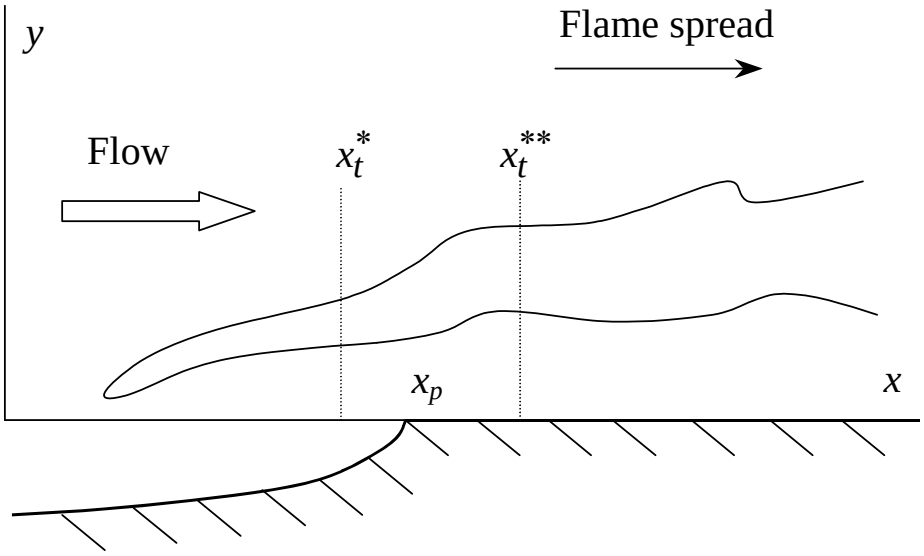

Figure 1: Flame spread model.

Apparently, intermediate cases may appear for every possible flame spread mode, especially if non-stationary processes such an ignition and extinction are considered. Approaches to flame spread modeling usually postulate the flow mode in advance – laminar or turbulent. However, the visible turbulent character of the flow over combustible materials does not necessarily mean that flame spread itself is controlled by turbulence.

Consider the flame spread configuration shown in Figure 1. The value of flame propagation velocity is determined by the characteristics of heat and mass transfer near the 'pyrolysis' point x_p, where solid fuel starts to vaporise. Another characteristic point of the process (x_t) relates to transition of flow structure from laminar to turbulent, which can be caused both by flame or wall induced turbulence. The mutual location of these points determines which mechanism is more important for flame propagation: laminar (x_t^*), turbulent (x_t^{**}) or both of them ($x_t \approx x_p$).

Finite-rate combustion reaction under laminar flow is associated with an Arrhenius-type formula describing the chemical kinetics:

$$W = k_g Y_F^{n_F} Y_O^{n_O} \exp\left(-E / R_0 T\right) \tag{1}$$

Reaction rates controlled by turbulent mixing in a fully developed turbulent flow is described by an eddy-break-up model[3,4]:

$$W = C_A \frac{\varepsilon}{k} \min\left[Y_F, \frac{Y_O}{\nu}, \frac{Y_P}{C_B(1+\nu)} \right] \tag{2}$$

Thus, the reaction mechanisms defined by Equations 1 and 2 are completely different. A possible combination of them[5] employs a simple comparison between values obtained from Equations 1 and 2 among which the smaller one is chosen to be the actual reaction rate. Such an approach, assuming abrupt changes in characteristics of the process, cannot provide an adequate description if both

mechanisms are significant. Then, the eddy-break-up model is a rather simplified approach to the description of turbulent combustion[6].

The analysis presented below outlines a model making it possible to predict a chemical reaction rate without *a priori* assignment of a flow structure.

MODEL

The mathematical formulation of the flame spread model shown in Figure 1 has been drawn up with some simplifications which are not too crucial to the analysis. Firstly, a boundary layer approach is used assuming that gas-phase convection in the direction of flame propagation is the dominant (actually, the sole) mechanism of flame spread. Secondly, stationary equations are considered, which assumes the flow is 'frozen'. The governing equations describing the turbulent reacting flow are as follows:

$$\bar{\rho}\bar{u}\frac{\partial \bar{u}}{\partial x}+\bar{\rho}\bar{v}\frac{\partial \bar{u}}{\partial y}=\frac{\partial}{\partial y}\left[\mu_m\frac{\partial \bar{u}}{\partial y}-\overline{u'(\rho v)'}\right]-\frac{\partial \bar{p}}{\partial x} \tag{3}$$

$$\bar{\rho}\bar{u}\frac{\partial \bar{T}}{\partial x}+\bar{\rho}\bar{v}\frac{\partial \bar{T}}{\partial y}=\frac{\partial}{\partial y}\left[\frac{\lambda_m}{C}\frac{\partial \bar{T}}{\partial y}-\overline{T'(\rho v)'}\right]+\frac{Q}{C}\bar{\rho}\bar{W} \tag{4}$$

$$\bar{\rho}\bar{u}\frac{\partial \overline{Y_F}}{\partial x}+\bar{\rho}\bar{v}\frac{\partial \overline{Y_F}}{\partial y}=\frac{\partial}{\partial y}\left[\frac{Le\lambda_m}{C}\frac{\partial \overline{Y_F}}{\partial y}-\overline{Y_F'(\rho v)'}\right]-\nu_F\bar{\rho}\bar{W} \tag{5}$$

$$\bar{\rho}\bar{u}\frac{\partial \overline{Y_O}}{\partial x}+\bar{\rho}\bar{v}\frac{\partial \overline{Y_O}}{\partial y}=\frac{\partial}{\partial y}\left[\frac{Le\lambda_m}{C}\frac{\partial \overline{Y_O}}{\partial y}-\overline{Y_O'(\rho v)'}\right]-\nu_O\bar{\rho}\bar{W} \tag{6}$$

$$\frac{\partial \bar{\rho}\bar{u}}{\partial x}+\frac{\partial \bar{\rho}\bar{v}}{\partial y}=0 \tag{7}$$

$$\bar{p}=R\left(\bar{\rho}\bar{T}+\overline{\rho'T'}\right) \tag{8}$$

To complete the statement defined by Equations 3 to 8, boundary conditions on y and initial conditions on x have to be specified. They are omitted here implying their conventional form depends upon the model for the solid fuel gasification process and the structure of inlet ambient flow.

Since dynamical turbulence is not affected by chemical reaction, the Reynolds stress in momentum Equation (3) is described simply as for non-reacting flow:

$$-\overline{u'(\rho v)'}=\mu_t\frac{\partial \bar{u}}{\partial y} \tag{9}$$

where the generally employed expression for turbulent viscosity is used in the form

$$\mu_t=C_\mu\bar{\rho}k^2/\varepsilon \tag{10}$$

To achieve the values of kinetic energy of turbulence and energy dissipation rate, a turbulence model must be introduced such as a the well-known $k-\varepsilon$ model[7] or one of its possible modifications.

Unlike the momentum Equation 3, turbulent heat and mass transfer are different in non-reaction flow due to the combustion reaction described by last terms of Equations 4 to 6. The previous analysis (summarized in paper[8] available in English) of a solid propellant premixed flame has shown that chemical reaction significantly dampens the turbulent fluctuations in the flame zone. There is a local-isotropic approach that has been derived by keeping only the generation and dissipation terms in the transport equation for turbulent heat flux $-\overline{T'(\rho v)'}$. Hence, the partial differential equation is reduced to algebraic formula:

$$-\overline{T'(\rho v)'} = \frac{\mu_t}{\mathrm{Pr}_t}\frac{\varphi}{(1-\delta_T)}\frac{\partial \overline{T}}{\partial y} \tag{11}$$

where:

$$\varphi = 1-\exp\left(-B\frac{\varepsilon}{k\overline{W}}\right) \tag{12}$$

$$\delta_T = \frac{1}{C_T}\frac{k\varphi}{\varepsilon}\frac{Q}{C}\frac{\partial \overline{W}}{\partial \overline{T}} \tag{13}$$

Equation 11 differs from commonly used expressions for non-reacting flow by the factor $\varphi/(1-\delta_T)$, which describe the influence of chemical reaction on turbulent heat transfer. Then, a feedback effect of turbulent fluctuations on reaction rate is considered.

Strong non-linearity of the dependence of the reaction rate upon the temperature and mass fractions expressed by Equation 1 gives $\overline{W(Y_F, Y_O, T)} \neq W(\overline{Y_F}, \overline{Y_O}, \overline{T})$. Expanding this function into a power series and averaging the resulting expression yields:

$$\overline{W(Y_F, Y_O, T)} = W(\overline{Y_F}, \overline{Y_O}, \overline{T}) + 0.5W_{Y_FY_F}\overline{(Y_F')^2} + 0.5W_{Y_OY_O}\overline{(Y_O')^2} + 0.5W_{TT}\overline{(T')^2} +$$
$$+ W_{Y_FY_O}\overline{(Y_F'Y_O')} + W_{Y_FT}\overline{(Y_F'T')} + W_{Y_OT}\overline{(Y_O'T')} \tag{14}$$
$$\text{where} \qquad W_{AB} = \frac{\partial^2 W}{\partial A \partial B}.$$

Thus, some expressions are needed to determine the correlations of turbulent fluctuations appearing in Equation 14. A comprehensive way to do that leads to the full transport equation, which, for the example for temperature fluctuation, has the following form[8]:

$$\overline{\rho u}\frac{\partial \overline{(T')^2}}{\partial x} + \overline{\rho v}\frac{\partial \overline{(T')^2}}{\partial y} = \frac{\partial}{\partial y}\left[\frac{\lambda_m}{C}\frac{\partial \overline{(T')^2}}{\partial y} - \overline{(T')^2(\rho v)'}\right] +$$
$$+ 2\overline{T'(\rho v)'}\frac{\partial \overline{T}}{\partial y} - 2\beta_T\frac{\overline{\rho}\varepsilon}{k\varphi}(1-\delta_T)\overline{(T')^2} \tag{15}$$

where turbulent transfer term is expressed similar to Equation 11:

$$-\overline{(T')^2(\rho v)'} = \alpha_T \frac{\mu_t}{\mathrm{Pr}_t} \frac{\varphi}{(1-\delta_T)} \frac{\partial \overline{(T')^2}}{\partial y} \tag{16}$$

In fact, such an approach significantly complicates the problem, since six (compared with four in the basic statement, Equations 3 to 6) additional partial differential equations have to be solved. Using the local-isotropic assumption[8], only source terms are kept in Equation 15 and algebraic formulas result for averaged temperature fluctuations:

$$\overline{(T')^2} = C_1 \frac{k}{\varepsilon} \frac{\varphi}{(1-\delta_T)} \overline{T'(\rho v)'} \frac{\partial \overline{T}}{\partial y} \tag{17}$$

The other correlations of Equation 14 could be achieved by the same way:

$$\overline{(Y_F')^2} = C_1 \frac{k}{\varepsilon} \frac{\varphi}{(1+\delta_{Y_F})} \overline{Y_F'(\rho v)'} \frac{\partial \overline{Y_F}}{\partial y} \tag{18}$$

$$\overline{(Y_O')^2} = C_1 \frac{k}{\varepsilon} \frac{\varphi}{(1+\delta_{Y_O})} \overline{Y_O'(\rho v)'} \frac{\partial \overline{Y_O}}{\partial y} \tag{19}$$

$$\overline{Y_F' Y_O'} = C_2 \frac{k}{\varepsilon} \frac{\varphi}{(1+0.5\delta_{Y_F}+0.5\delta_{Y_O})} \left(\overline{Y_F'(\rho v)'} \frac{\partial \overline{Y_F}}{\partial y} + \overline{Y_O'(\rho v)'} \frac{\partial \overline{Y_O}}{\partial y} \right) \tag{20}$$

$$\overline{Y_F' T'} = C_2 \frac{k}{\varepsilon} \frac{\varphi}{(1+0.5\delta_{Y_F}-0.5\delta_T)} \left(\overline{Y_F'(\rho v)'} \frac{\partial \overline{Y_F}}{\partial y} + \overline{T'(\rho v)'} \frac{\partial \overline{T}}{\partial y} \right) \tag{21}$$

$$\overline{Y_O' T'} = C_2 \frac{k}{\varepsilon} \frac{\varphi}{(1+0.5\delta_{Y_O}-0.5\delta_T)} \left(\overline{Y_O'(\rho v)'} \frac{\partial \overline{Y_O}}{\partial y} + \overline{T'(\rho v)'} \frac{\partial \overline{T}}{\partial y} \right) \tag{22}$$

where

$$\delta_{Y_F} = \frac{1}{C_T} \frac{k\varphi}{\varepsilon} \nu_F \frac{\partial \overline{W}}{\partial \overline{Y_F}} \tag{23}$$

$$\delta_{Y_O} = \frac{1}{C_T} \frac{k\varphi}{\varepsilon} \nu_O \frac{\partial \overline{W}}{\partial \overline{Y_O}} \tag{24}$$

The turbulent diffusive flux is expressed in a similar way to Equation 11 for heat flux:

$$-\overline{Y_F'(\rho v)'} = \frac{Le_t \mu_t}{\mathrm{Pr}_t} \frac{\varphi}{(1+\delta_{Y_F})} \frac{\partial \overline{Y_F}}{\partial y} \tag{25}$$

$$-\overline{Y_O'(\rho v)'} = \frac{Le_t \mu_t}{\mathrm{Pr}_t} \frac{\varphi}{(1+\delta_{Y_O})} \frac{\partial \overline{Y_O}}{\partial y} \tag{26}$$

NOMENCLATURE

B	constant in Equation 12
C	Specific heat
C_1, C_2	Constants in Equations 17 to 22
C_A, C_B	Constants in Equation 2
C_T	Constant in Equations 13, 23 to 24
C_μ	Constant in Equation 10
E	Activation energy
k	Kinetic energy of turbulence
k_g	Preexponential factor
Le	Lewis number
n	Reaction's order
Pr	Prandtl number
p	Pressure
Q	Effective heat of reaction
R	Specific gas constant
R_0	Universal gas constant
T	Temperature
u , v	Velocity components
W	Chemical reaction's rate
x	Coordinate along the fuel's surface
Y	Mass fraction
y	Coordinate normal to the fuel's surface

Greek symbols

α_T	Constant in Equation 16
β_T	Constant in Equation 15
ε	Dissipation rate of turbulence energy
λ	Thermal conductivity
μ	Viscosity

ν	Stoichoimetric coefficient
ρ	Density

Superscripts

$(\bar{...})$	Reynolds averaged variable
$(...)'$	Fluctuation

Subscripts

F	Fuel
O	Oxidizer
m	Molecular
P	Product
P	Pyrolysis
T	Turbulent

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