

## **THERMODYNAMIC ALGORITHM FOR THE PREDICTION OF FLAME SPREAD RATE OVER SOLID FUELS: QUANTITATIVE EVALUATION OF VALIDITY**

A. I. Karpov, V. K. Bulgakov and A. A. Galat

Khabarovsk State University of Technology

**RUSSIA**

### **ABSTRACT**

An algorithm for the prediction of flame spread rate based on the principle of minimal entropy production is evaluated by the numerical investigation of the downward flame spread process. The main purpose of this study related to the selection of proper input data allowing a quantitative comparison of calculated results with experimental data to be made. The influence of fuel bed thickness and ambient oxygen mass fraction on the flame spread rate has been investigated and satisfactory agreement with measurements has been achieved.

**Keywords:** Flame spread, solid fuel, numerical modeling.

### **INTRODUCTION**

The general output of mathematical modeling of flame spread provides various parameters characterizing the process. One of them, the flame propagation velocity, may be considered as the most essential for fire safety, because it is a resulting factor describing the overall effect of the flame spread process. The present study focused on the flame spread modes, enabling the stationary regime under which the flame propagates at constant velocity to be assessed. Such a case is usually associated<sup>1-3</sup> with opposed-flow (downward) flame spread while the opposite one – flow-assisted (upward) flame spread, is an essentially unsteady process characterized by accelerating flame propagation.

A significant number of steady flame spread models have been developed<sup>3</sup>, from the pioneering work of de Ris<sup>4</sup> who assumed a series of simplifications allowing an analytical solution to be obtained, to the later comprehensive numerical models. Among later studies, mention should be made of the

studies of Di Blasi et al.<sup>5</sup> and of Bhattacharjee and Altenkirch<sup>6</sup>. This is because these investigations, having actually achieved equal levels of penetration into physical details of the process, show clearly the fundamental differences of general approaches to the prediction of steady flame spread rate. Model [5] uses the unsteady conservation equations, and has a clear mathematical basis, but needs substantial computer resources. In contrast, model [6] is based on the steady-state equations written in flame-fixed coordinates, which allows the number of independent variables to be reduced, but such an approach faces a difficulty in specifying the eigenvalue problem. The features of the eigenvalue closure problems have been discussed in previous papers<sup>7,8</sup>. This analysis results in a new approach for the prediction of flame spread rate and the formulation of a steady-state model has been proposed. Revealing the foundations of irreversible (non-equilibrium) thermodynamics, steady flame spread is considered as a stationary state of a thermodynamic system, which could be characterized by the minimal entropy production.

Previous investigations by the current authors have provided an adequate physical background of this 'thermodynamic' algorithm of flame spread rate prediction. These results appear to be in satisfactory agreement with the exact solution for one-dimensional premixed flame propagation<sup>9</sup> and are a reasonable description of the two-dimensional diffusive flame over solid combustible materials. Regarding the latter case, effects of fuel-bed thickness and ambient oxygen mass fraction<sup>8</sup> and opposed forced flow<sup>10</sup> have been estimated, however, in mostly qualitative terms. In view of the practical needs of fire safety applications, quantitative calibration of the model is highly important, which is a primary aim of the present paper.

## MODEL

The model of two-dimensional downward flame spread over a solid combustible is shown in Figure 1. The problem is formulated in the steady-state coordinate system fixed on the moving flame front. The governing equations for conservation of momentum, energy and mass in the gas phase are:

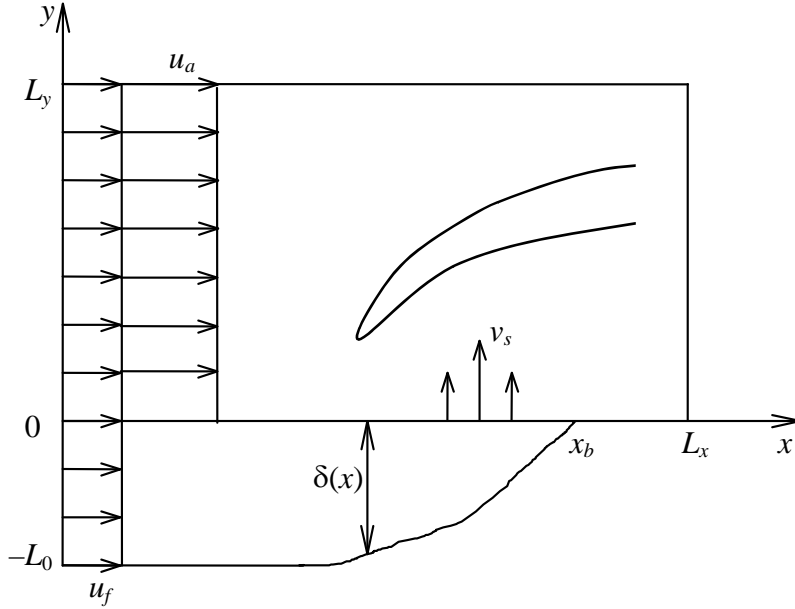
$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \frac{\partial}{\partial x} \frac{\text{Pr} \lambda}{C} \frac{\partial u}{\partial x} + \frac{\partial}{\partial y} \frac{\text{Pr} \lambda}{C} \frac{\partial u}{\partial y} - \frac{\partial p}{\partial x} + (\rho_a - \rho)g \quad (1)$$

$$\rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} = \frac{\partial}{\partial x} \frac{\text{Pr} \lambda}{C} \frac{\partial v}{\partial x} + \frac{\partial}{\partial y} \frac{\text{Pr} \lambda}{C} \frac{\partial v}{\partial y} - \frac{\partial p}{\partial y} \quad (2)$$

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \quad (3)$$

$$C \rho u \frac{\partial T}{\partial x} + C \rho v \frac{\partial T}{\partial y} = \frac{\partial}{\partial x} \lambda \frac{\partial T}{\partial x} + \frac{\partial}{\partial y} \lambda \frac{\partial T}{\partial y} + Q \rho W \quad (4)$$

$$\rho u \frac{\partial Y_O}{\partial x} + \rho v \frac{\partial Y_O}{\partial y} = \frac{\partial}{\partial x} \frac{Le \lambda}{C} \frac{\partial Y_O}{\partial x} + \frac{\partial}{\partial y} \frac{Le \lambda}{C} \frac{\partial Y_O}{\partial y} - v_O \rho W \quad (5)$$



**Figure 1:** Flame spread model.

$$\rho u \frac{\partial Y_F}{\partial x} + \rho v \frac{\partial Y_F}{\partial y} = \frac{\partial}{\partial x} \frac{Le\lambda}{C} \frac{\partial Y_F}{\partial x} + \frac{\partial}{\partial y} \frac{Le\lambda}{C} \frac{\partial Y_F}{\partial y} - v_F \rho W \quad (6)$$

$$\rho = p / RT \quad (7)$$

The balance of energy in the solid fuel is expressed as:

$$C_s \rho_s u_f \frac{\partial T_s}{\partial x} = \frac{\partial}{\partial x} \lambda_s \frac{\partial T_s}{\partial x} + \frac{\partial}{\partial y} \lambda_s \frac{\partial T_s}{\partial y} + Q_s \rho_s W_s \quad (8)$$

The gas-phase combustion reaction and solid fuel pyrolysis both are described by Arrhenius-type formulas:

$$W = k Y_O Y_F \exp(-E / R_0 T) \quad (9)$$

$$W_s = k_s \exp(-E_s / R_0 T_s) \quad (10)$$

Boundary conditions, correspondingly to the configuration shown in Figure 1, are:

$$y = 0 \quad (0 < x < x_b) : u = u_f \quad (11)$$

$$\rho v = \rho_s v_s \quad (12)$$

$$-\lambda \frac{\partial T}{\partial y} + \rho v C T = -\lambda_s \frac{\partial T_s}{\partial y} + \rho_s v_s C_s T_s \quad (13)$$

$$T = T_s \quad (14)$$

$$-\frac{Le\lambda}{C} \frac{\partial Y_O}{\partial y} + \rho v Y_O = 0 \quad (15)$$

$$-\frac{Le\lambda}{C} \frac{\partial Y_F}{\partial y} + \rho v Y_F = \rho_s v_s \quad (16)$$

$$y = 0 (x > x_b): \quad \rho v = 0, \quad \frac{\partial T}{\partial y} = 0, \quad \frac{\partial u}{\partial y} = 0 \quad (17)$$

$$x = 0: \quad u = u_f + u_a \quad (18)$$

$$v = 0, \quad T = T_a, \quad Y_F = 0, \quad Y_O = Y_{O,a} \quad (19)$$

$$y = L_y: \quad u = u_f + u_a, \quad \frac{\partial v}{\partial y} = 0, \quad T = T_a, \quad Y_F = 0, \quad Y_O = Y_{O,a} \quad (20)$$

$$x = L_x: \quad \frac{\partial u}{\partial x} = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \frac{\partial T}{\partial x} = 0, \quad \frac{\partial Y_F}{\partial x} = 0, \quad \frac{\partial Y_O}{\partial x} = 0 \quad (21)$$

$$y = -\delta(x): \quad \frac{\partial T_s}{\partial n} = 0 \quad (22)$$

The mathematical statements defined by Equations 1 to 8 provide eight equations for eight variables which are  $u, v, p, T, Y_O, Y_F, \rho, T_s$ . Besides these, conservation equations and boundary conditions contain three additional unknown parameters: linear pyrolysis rate  $v_s$ , burning surface profile  $\delta(x)$  and flame spread rate  $u_f$  which are the eigenvalues of the problem. Therefore, they should be determined through the other variables as a result of the problem's solution. The expressions for the first two of these parameters have been defined through the integration of the mass balance equation in the solid fuel, which results in the following<sup>8</sup>:

$$v_s = \int_{-\delta(x)}^0 W_s dy \quad (23)$$

$$\delta(x) = L_0 - \frac{1}{u_f} \int_0^x v_s dx \quad (24)$$

The algorithm for the prediction of flame spread rate is based on the principle of minimal entropy production. Among the possible solutions corresponding to every assigned value of flame spread rate  $u_f$ , the stationary one is that which provides the minimum of the following integral describing the summary entropy production within the solid fuel<sup>8,10</sup>:

$$P = \int_0^{x_b} \int_0^\delta (J_X X_X + J_Y X_Y + J_W X_W) dy dx \quad (25)$$

where thermodynamic fluxes and generalized forces due to the thermal conduction and chemical reaction are:

$$J_X = -\lambda_s \frac{\partial T_s}{\partial x}, \quad X_X = -\frac{1}{T_s^2} \frac{\partial T_s}{\partial x} \quad (26)$$

$$J_Y = -\lambda_s \frac{\partial T_s}{\partial y}, \quad X_Y = -\frac{1}{T_s^2} \frac{\partial T_s}{\partial y} \quad (27)$$

$$J_W = \rho_s W_s, \quad X_W = Q_s \left( \frac{1}{T_s} - \frac{1}{T_s^*} \right) - R \ln \xi \quad (28)$$

where  $T_s^*$  is the maximal temperature in the solid fuel and reaction's coordinate  $\xi$  of solid fuel's pyrolysis is described correspondingly to fuel bed thickness as:

$$\xi(x) = 1 - \delta(x) / L_0 \quad (29)$$

The numerical solution of the problem defined above is obtained by combined finite difference (for gas phase) – finite element (for solid fuel) procedure described in<sup>8</sup>.

## INPUT DATA

The assignment of proper input data for the mathematical model seems to be one of the most crucial factors providing the success and reliability of the simulation procedure. The mathematical formulation described above contains a number of empirical coefficients, which should be determined with a sufficient degree of accuracy. Thermophysical properties (conductivity, specific heat, diffusion coefficient, viscosity, density) of gas phase and solid fuel depends upon the composition of the gas mixture and the type of material. These parameters may be considered as knowns, as they can at least in principle be estimated through direct measurements. Almost the same arguments relate to the kinetic parameters (preexponential factor, activation energy, heat release) of the solid fuel's pyrolysis reaction (for example<sup>11</sup>). The most difficult task is the determination of kinetic parameters of the gas phase combustion reaction. Since the detailed kinetic scheme includes many steps, even for the combustion of simple gas mixtures, the gas phase combustion of polymeric materials is usually described by a one-step macrokinetic reaction with effective coefficients selected through comparison with experimental data. Flame spread rate is considered as a major criterion for such a comparison.

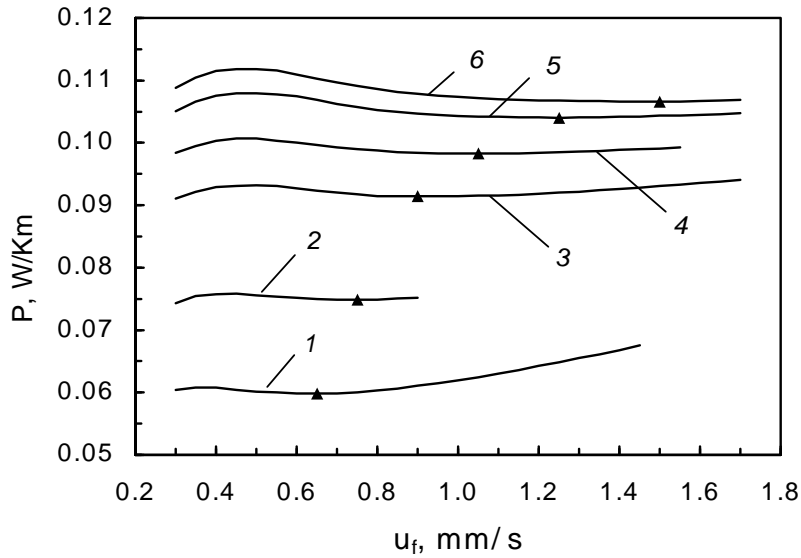
The prediction of the steady rate of downward flame spread over a thin sheet of paper has been carried out in this study. Following previous studies<sup>7,8,10</sup>, the gas phase and solid fuel properties proposed in<sup>12</sup> are used. These values are listed in Table 1. It may be noticed that a preexponential factor of the gas-phase reaction is not specified, because it is assigned as a free parameter for the calibration of the model.

Figure 2 presents the distribution of entropy production, defined by Equation 25, as a function of flame spread rate. Every curve, corresponding to a different value of preexponential factor, has a point of minimum, which is presumed to be the searched steady flame spread rate. These results show that flame spread rate increases as preexponential factor increases. The achieved overall dependence  $u_f(k)$ , shown in Figure 3, has a nearly linear character. The same feature has been found elsewhere<sup>12</sup>. The set of input data for the calculated results of Figures 2 and 3 correspond to the downward flame spread over a thin paper sheet ( $2L_0 = 0.19$  mm) in normal conditions – atmospheric pressure ( $P = 10^5$  Pa), ambient oxygen mass fraction of air ( $Y_{O,a} = 0.21$ ), absence of forced flow ( $u_a=0$ ). Comparing the data of Figure 3 with corresponding experimental results<sup>13-18</sup>, it may be found that the appropriate value of preexponential factor is  $k = (0.8 \text{ to } 1.0) \times 10^9$  1/s.

**Table 1:** Gas phase and solid fuel properties<sup>12</sup>.

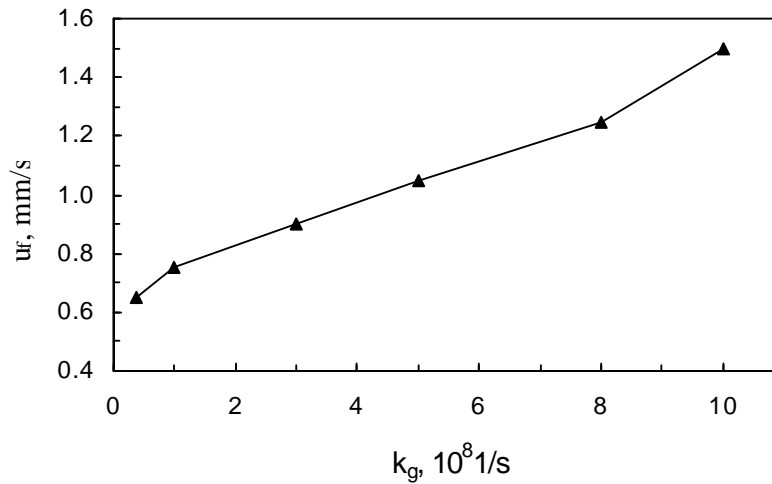
Symbol	Gas	Solid	Unit
$C$	1005.6	1257	J/(kg K)
$\lambda$	0.0254	0,1257	W/(m K)
$\rho$	1.0	650	kg/m <sup>3</sup>
$p$	$10^5$	–	Pa
$R$	333	–	J/(kg K)
$Q$	$1.68 \times 10^7$	$-7.54 \times 10^5$	J/kg
$k$	*)	$10^{10}$	1/s
$E$	62850	125700	J/mole
$v_F$	1.0	–	
$v_O$	1.185	–	
$T_a$	300	300	K
$Pr$	1.0	–	
$Le$	1.0	–	

\*) Should be defined through the calculations.



**Figure 2:** Dependence of entropy production versus flame spread rate distribution upon the preexponential factor of chemical reaction's rate in gas phase.

Curves: 1 –  $k = 3.7 \times 10^7$  1/s, 2 –  $k = 1 \times 10^8$  1/s, 3 –  $k = 3 \times 10^8$  1/s,  
 4 –  $k = 5 \times 10^8$  1/s, 5 –  $k = 8 \times 10^8$  1/s, 6 –  $k = 1 \times 10^9$  1/s;  
 ▲ – point of minimum.

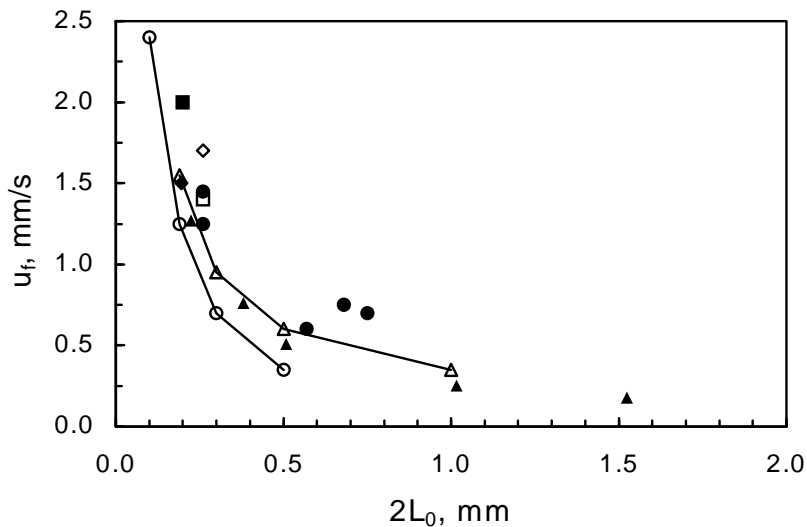


**Figure 3:** Overall dependence of the flame spread rate upon the preexponential factor of chemical reaction's rate in the gas phase.

## RESULTS AND DISCUSSION

Figure 4 presents the measured values of downward flame spread rate over paper sheets in the normal conditions defined above, under the different fuel-bed thicknesses available from known experimental investigations. Despite the obvious general effect of decreasing of flame spread rate as fuel-bed thickness increases, these data are somewhat scattered due to differences in sample properties (actual type of material, density, moisture content). Comparison of calculated results with experimental data shown in Figure 4 leads to the conclusion that a more appropriate value of the preexponential factor of gas-phase combustion reaction is  $k = 1 \times 10^9$  1/s.

The effect of ambient oxygen mass fraction on downward flame spread rate is shown in Figure 5. Input data of these calculations correspond to measurements<sup>19</sup>:  $p = 0.68 \times 10^5$  Pa (10 PSIA),  $2L_0 = 0.19$  mm.



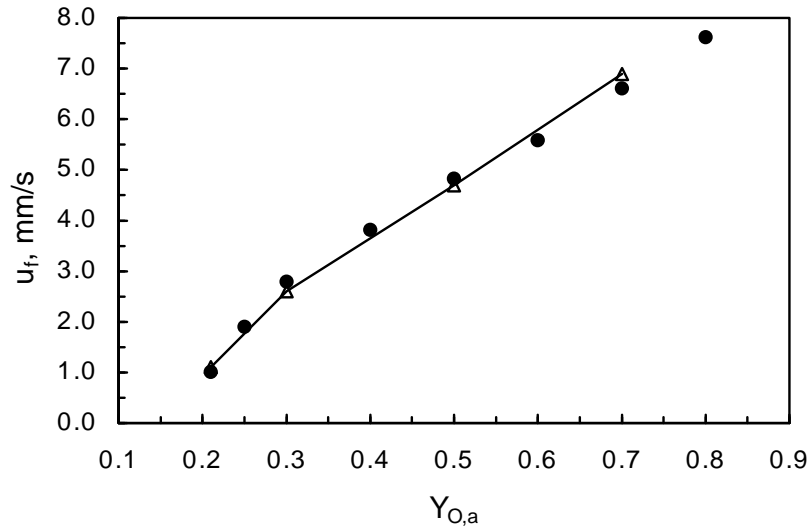
**Figure 4:** Dependence of flame spread rate upon the fuel-bed thickness.

Experiments: □ – [13], ▲ – [14], ■ – [15], ◆ – [16], ◇ – [17], ● – [18].

Calculations: ○ –  $k = 8 \times 10^8$  1/s, ▲ –  $k = 1 \times 10^9$  1/s.

Finally, results of numerical investigations presented in this paper show a satisfactory quantitative agreement with the experiments both for the effect of fuel-bed thickness and ambient oxygen mass fraction on the flame spread rate. Surely, much expanded studies are necessary to confirm the suitability of the proposed thermodynamic algorithm for flame spread rate's prediction.





**Figure 5:** Dependence of flame spread rate upon the ambient oxygen mass fraction.  
● – experiment<sup>19</sup>,  $\Delta$  – calculation,  $k = 1 \times 10^9$  1/s.

## NOMENCLATURE

$C$ :	Specific heat
$E$ :	Activation energy
$g$ :	Gravity acceleration
$J$ :	Thermodynamic flux
$k$ :	Preexponential factor
$L_0$ :	Half-thickness of fuel bed
$Le$ :	Lewis number
$n$ :	Coordinate normal to the solid fuel's surface
$P$ :	Entropy production
$Pr$ :	Prandtl number
$p$ :	Pressure

$Q$ :	Effective heat of reaction
$R$ :	Specific gas constant
$R_0$ :	Universal gas constant
$T$ :	Temperature
$u, v$ :	Velocity components
$u_f$ :	Steady flame spread rate
$v_s$ :	Linear pyrolysis rate
$W$ :	Chemical reaction's rate
$X$ :	Generalized force
$x$ :	Coordinate along the fuel's surface
$x_b$ :	Burnout position
$Y$ :	Mass fraction
$y$ :	Coordinate normal to the fuel's surface

#### **Greek symbols**

$\delta(x)$ :	Thickness of solid fuel bed
$\lambda$ :	Thermal conductivity
$\nu$ :	Stoichiometric coefficient
$\xi$ :	Reaction's coordinate
$\rho$ :	Density

#### **Subscripts**

$a$ :	Ambient
$F$ :	Fuel
$O$ :	Oxidizer
$s$ :	Solid phase
$W$ :	Chemical reaction
$X, Y$ :	Thermal conduction in $x$ and $y$ - directions

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