CHEMICAL MECHANISMS AND THE METHOD OF ONE-DIMENSIONAL TURBULENT FLAME

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An approximate but simple method for predicting kinetic parameters of empirical mechanisms modeling combustion reactions in a turbulent medium is suggested. With a single optimally selected fitting parameter the method satisfactorily approximates experimental functions, it also indicates that the kinetic parameters of empirical reaction mechanisms in laminar and turbulent flames can differ.

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Nonempirical detailed kinetic oxidation and combustion mechanisms (DKM) can comprise hundreds of species and thousands of elementary steps (see, e.g., [1]). These mechanisms are too cumbersome to be used at present in calculations of reacting turbulent flows in two-, and the more so, in three-dimensional approaches. This makes one invoke much simpler kinetic mechanisms of a semi-empirical or even purely empirical nature comprising only a small number of species and reaction steps.

The commonly recognized drawback of all empirical mechanisms, as distinct from DKM, is that they can be used only under particular conditions corresponding to those under which they have been developed. We reported previously [2] that the Arrhenius parameters of simplified empirical mechanisms derived from self-ignition experiments, e.g. from measured induction periods, model with a certain accuracy the induction periods themselves, but fail to describe propagation of a laminar flame. At the same time, one could reasonably hope that the Arrhenius parameters for the reaction rates derived from experimental data on propagation of laminar flames would suit also, to some extent, modeling of turbulent combustion. Applicability of these parameters to calculations of turbulent combustion must be checked directly. The best and only way to solve the two basic problems arising in this modeling — to elucidate how various empirical
mechanisms manifest themselves in turbulent flames and to establish whether the Arrhenius parameters of reaction rates chosen for these mechanisms adequately reproduce the chemical behavior of the system — is to use a well grounded and rigorous turbulent combustion model. However an excessively long computation time presents at present unsurmountable difficulties in performing such an analysis, therefore one has to look for simplified models.

To do this, we can use the method of a one-dimensional turbulent flame. Clearly, the idea of the method itself and the appropriate computation techniques provide quite a rough approximation to real turbulent combustion, however, if only a qualitative solution to the problem is sought for and the obtained results are considered as a zero approximation to a rigorous model of turbulent combustion, the application of the method has been repeatedly justified by its simplicity and accessibility. Here we employ a slightly modified model of a one-dimensional turbulent flame [3]. The set of equations for a one-dimensional flame is written in terms of average temperatures and concentrations, but, unlike the appropriate equations for a laminar flame, the set includes only a very simple empirical probability density function (PDF) for the reaction rate. This latter assumption allows us, although only approximately but fundamentally correctly, to use average values of temperature and concentrations.

First, we write the set of equations governing propagation of a one-dimensional laminar flame

\[ d[D_j \rho d(n_j/\rho)/dx]dx - \rho_j u_j d(n_j/\rho)/dx + \Sigma_j W_{ij} = 0, \]  

\[ d(dT/dx)/dx - \rho_j u_j c_p dT/dx + \Sigma_j h_j W_{ij} = 0 \]

(1)

(2)

where \( x \) is the coordinate along which the flame spreads, \( T \) is temperature, \( \lambda \) is the molecular heat conductivity, \( u_0 \) is the laminar burning velocity, \( \rho_0 \) and \( \rho \) are the initial and instantaneous gas density, \( n_j \) and \( D_j \) are the concentration and diffusion coefficient of the \( j \)-th component involved in the chemical reaction, \( c_p \) is the specific heat, and \( W_{ij} \) and \( h_j \) are the rate and heat of the \( i \)-th elementary reaction step involving the \( j \)-th component (\( W_{ij} = k \Pi_{j=1} n_j, k = AT\exp(-(E/R)T), AT^\prime \) is the preexponential factor, \( n \) is the temperature exponent, \( E \) is the activation energy, and \( R \) is the gas constant).

The boundary conditions at \( x = 0 \) and \( x = l \) (beginning and end of the reaction zone) read

\[ [T - (\lambda/\rho_j u_j c_p dT/dx)]_{x=0} = T_0, \]

\[ [n_j - (\rho D_j/u_0 \rho_0) dn_j/dx]_{x=0} = n_{j0}. \]

(3)
It turns out that a similar approach can be used in calculating turbulent flames, if one writes averaged differential equations (the bar over a function stands for average quantities) and introduces probability density functions

\[ P(T, \tilde{T}) \] for the temperature:

\[
d[D_T \bar{\rho} d(\bar{n}/\rho)]/dx + \rho \bar{\mu}_T d(\bar{n}/\rho)]/dx + \sum_{j} \int_{T_0}^{T_1} W_{j} P(T, \tilde{T}) dT = 0, \tag{4}\]

\[
d(\lambda_T d\tilde{T}/dx) + \rho \bar{\mu}_T c_p d\tilde{T}/dx + \sum_{j} \int_{T_0}^{T_1} h_{j} W_{j} P(T, \tilde{T}) dT = 0, \tag{5}\]

where \( \lambda_T \) and \( D_T \) are the phenomenological coefficients of turbulent heat transfer and diffusion. The boundary conditions are similar to the laminar case, \( T_i \) pertains to point \( x = L \).

In conformity to the well-known theoretical laws of heat and mass transfer in a turbulent medium, we approximately assumed that

\[
D_T = u L, \quad \lambda_T = D_T c_p, \]

where \( u \) and \( L \) are the root mean square fluctuation velocity and turbulence scale, respectively, the effect of combustion on the above transport coefficients was disregarded.

By definition, temperature PDF is the probability of temperature \( T \) from the \( T_0 - T_i \) interval to arise in the medium whose average temperature equals \( \tilde{T} \)

\[
\int_{T_0}^{T_1} P(T, \tilde{T}) dT = 1. \tag{6}\]

It can be shown that the overall reaction rate in Eq.(1) and the total heat release rate in Eq.(2) can be written in some equivalent form, where the sum of the rates of elementary steps and the sum of products of the elementary-step rates by the reaction heats are replaced by the rates of changes in the species concentration and by the sum of products of the rates of changes in the concentrations of species participating in the chemical
process by the heats of species decomposition into atoms $Q_j$ (quantity available in the thermodynamic database [4]) or by enthalpies of formation, i.e. $\Sigma W_b = W_f$ and $\Sigma h_j W_j = \Sigma Q_j W_f$. Similar replacements can be made in Eqs. (4) and (5).

Then we introduced another simplification which is crucial for the method suggested, namely, the rate of variations in the concentration of species $j$ as a function of the temperature $W_j(T)$ in a turbulent flame was identified with its analog in a laminar flame; to this end, calculations of a turbulent flame were preceded by calculations of the appropriate laminar flame and the resulting $W_j(T)$ values were stored in the memory. Thus, in the final run, we solved the following set of equations for a one-dimensional turbulent flame:

$$
\frac{d\left[D_p (\bar{\nu}/p)(dx)\right]}{dx} - \rho_0 \mu_d (\bar{\nu}/p)(dx) + \int_{T_0}^{T_1} W_j(T) P(T,T)dT = 0,
$$

(7)

$$
\frac{d(\lambda_\tau dT)}{dx} - \rho_0 \mu_\tau \lambda_\tau dT + \sum_{j} \int_{T_0}^{T_1} Q_j W_j(T) P(T,T)dT = 0.
$$

(8)

On the strength of the adopted assumption, Eqs. (7) and (8) become independent.

Generally, the PDF can be taken from experiment or from direct numerical calculation. In this work we used a model tub-shaped PDF qualitatively consistent with the experimental fact that in turbulent flames, one normally observes either the initial or final temperature, whereas the probability of recording intermediate temperatures is fairly low [5-7]. The model PDF was constructed as follows. First, for each average temperature we evaluated $P(T, \bar{T})$ at points with the initial temperature $T = T_0$ and final temperature $T = T_1$ by formulas: $P(T, \bar{T}) = \frac{T_1 - \bar{T}}{T_1 - T_0}$ and $P(T, \bar{T}) = \frac{T - T_0}{T_1 - T_0}$. It can easily be verified that these PDF values at the extreme points of the temperature scale with $P(T, \bar{T}) = 0$ at any intermediate temperature are equivalent to an assumption of an infinitely thin flame front, the average temperature in this case is a result of simple mixing of the unburnt mixture and combustion products. However at intermediate temperatures $T_0 < T <
\( T_1 \), we ascribed to \( P(T, \tilde{T}) \) a fixed value the same at all the values of the arguments, except \( \tilde{T} = T_0 \) and \( \tilde{T} = T_1 \), where \( P(T, \tilde{T}) \) was set at zero. This corresponds to a finite flame thickness. Then the PDF was constructed in compliance with Eq.(6).

When solving Eqs.(7) and (8) by iterations, the reaction zone length \( l \) was so chosen that the temperature \( T_1 \), calculated in the laminar flame be preserved in the turbulent flame.

As seen, the above model of a one-dimensional turbulent flame is very simplified and approximate. However we believe it would be pertinent to use this model to qualitatively explore possible manifestations of various simplified chemical mechanisms in modeling turbulent combustion and to test the Arrhenius parameters of the reaction mechanisms. For this purpose, we developed a code which allowed us, within the adopted assumptions, to calculate a one-dimensional turbulent flame. Owing to the simplified assumptions, the computation time for a one-dimensional turbulent flame was shorter than the computation time for the appropriate laminar flame. Since the turbulent flame model and the computation procedure call for further modification, the results discussed below (although are compared with experiment) should be considered as tentative.

Three kinetic mechanisms of hydrogen combustion were chosen for calculations.

(a) A detailed mechanism comprising, according to [8], eight species \( \text{H}_2, \text{O}_2, \text{OH}, \text{H}, \text{O}, \text{H}_2\text{O}, \text{HO}_2, \) and \( \text{H}_2\text{O}_2 \) and 42 reaction steps and designated by 8/42.

(b) An empirical mechanism comprising 4 species (\( \text{H}_2, \text{O}_2, \text{H}_2, \) and \( \text{R} \)) and three reaction steps (4/3) [2]. For brevity, in the latter mechanism, dissociation was taken into account by introducing two mutually reverse reactions involving a new species — radical \( \text{R} \). These reactions are similar to the well-studied dissociation of water molecules, \( \text{H}_2\text{O} + \text{M} = \text{H} + \text{OH} + \text{M} \), but with an empirical replacement of \( \text{H} \) atoms and hydroxyl radicals OH by a single radical: \( \text{H}_2\text{O} + \text{M} = \text{R} + \text{R} + \text{M} \), where \( \text{R} \) stands for species of the type of \( \text{H} \) and \( \text{OH} \).

(c) An empirical mechanism comprising two species (\( \text{H}_2 \) and \( \text{H}_2\text{O} \)) and one reaction (2/1). Generally, this applies only to mixtures lean in hydrogen where variations of the oxygen concentration and dissociation can be neglected.

The above-mentioned mechanisms are summarized in Table 1.

First we calculated laminar flames using all the three mechanisms with Arrhenius parameters in the empirical mechanisms chosen to obtain the best fit to experimental burning velocities.
<table>
<thead>
<tr>
<th>Reaction</th>
<th>$h$, kcal/mol</th>
<th>Direct</th>
<th></th>
<th></th>
<th>Reverse</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$h$, kcal/mol</td>
<td>$A$, mol, l, s</td>
<td>$n$</td>
<td>$E$, kcal/mol</td>
<td>$A$, mol, l, s</td>
<td>$n$</td>
<td>$E$, kcal/mol</td>
</tr>
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<td>OH + H₂ = H + H₂O</td>
<td>15</td>
<td>2.2 + 0.5</td>
<td>1.5</td>
<td>3.5</td>
<td>1.0 + 06</td>
<td>1.5</td>
<td>18.6</td>
</tr>
<tr>
<td>OH + O = H + O₂</td>
<td>16</td>
<td>2.8 + 12</td>
<td>-0.8</td>
<td>-0.1</td>
<td>1.9 + 11</td>
<td>0.0</td>
<td>16.4</td>
</tr>
<tr>
<td>OH + H = O + H₂</td>
<td>2</td>
<td>6.9 + 09</td>
<td>0.0</td>
<td>7.0</td>
<td>1.5 + 10</td>
<td>0.0</td>
<td>8.9</td>
</tr>
<tr>
<td>OH + OH = O + H₂O</td>
<td>17</td>
<td>6.0 + 05</td>
<td>1.3</td>
<td>0.0</td>
<td>6.3 + 06</td>
<td>1.3</td>
<td>17.0</td>
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<td>H + H + M = H₂ + M</td>
<td>103</td>
<td>2.0 + 10</td>
<td>-0.3</td>
<td>0.0</td>
<td>1.0 + 17</td>
<td>-1.3</td>
<td>104.8</td>
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<tr>
<td>O + O + M = O₂ + M</td>
<td>118</td>
<td>3.6 + 09</td>
<td>-0.6</td>
<td>0.0</td>
<td>1.6 + 17</td>
<td>-1.6</td>
<td>120.0</td>
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<tr>
<td>OH + H = H₂O</td>
<td>118</td>
<td>6.8 + 10</td>
<td>0.1</td>
<td>0.0</td>
<td>1.6 + 15</td>
<td>-0.9</td>
<td>120.0</td>
</tr>
<tr>
<td>O + H + M = OH + M</td>
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<td>4.7 + 09</td>
<td>0.0</td>
<td>0.0</td>
<td>1.1 + 13</td>
<td>0.0</td>
<td>104.0</td>
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<tr>
<td>H + HO₂ = H₂ + O₂</td>
<td>56</td>
<td>6.0 + 09</td>
<td>0.0</td>
<td>0.0</td>
<td>1.1 + 09</td>
<td>0.0</td>
<td>56.0</td>
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<td>H + O₂ = HO₂</td>
<td>47</td>
<td>1.2 + 09</td>
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<td>1.6 + 12</td>
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<td>48.8</td>
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<td>H + HO₂ = OH + OH</td>
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<td>1.6 + 09</td>
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<td>37.6</td>
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<tr>
<td>O + HO₂ = O₂ + OH</td>
<td>54</td>
<td>6.0 + 10</td>
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<td>9.4 + 10</td>
<td>0.0</td>
<td>54.0</td>
</tr>
<tr>
<td>OH + HO₂ = O₂ + H₂O</td>
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<td>6.0 + 09</td>
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<td>1.0 + 11</td>
<td>0.0</td>
<td>71.2</td>
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<tr>
<td>H + HO₂ = H₂O + O</td>
<td>54</td>
<td>6.0 + 08</td>
<td>0.0</td>
<td>0.0</td>
<td>5.3 + 08</td>
<td>0.0</td>
<td>54.4</td>
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<tr>
<td>OH + H₂O₂ = HO₂ + H₂O</td>
<td>31</td>
<td>1.8 + 09</td>
<td>0.0</td>
<td>0.3</td>
<td>1.9 + 09</td>
<td>0.0</td>
<td>31.2</td>
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<td>Reaction</td>
<td>Rate Coefficient</td>
<td>Preexponential</td>
<td>Activation Energy</td>
<td>Preexponential</td>
<td>Activation Energy</td>
<td>Preexponential</td>
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<tr>
<td>H + H₂O₂ = H₂O + OH</td>
<td>66</td>
<td>7.1 + 09</td>
<td>0.0</td>
<td>4.2</td>
<td>6.4 + 08</td>
<td>0.0</td>
<td>72.6</td>
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<tr>
<td>OH + OH = H₂O₂</td>
<td>50</td>
<td>3.4 + 07</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0 + 16</td>
<td>0.0</td>
<td>50.0</td>
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<tr>
<td>O + H₂O₂ = O₂ + H₂O</td>
<td>85</td>
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<td>6.4</td>
<td>4.8 + 10</td>
<td>0.0</td>
<td>91.4</td>
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<td>H + H₂O₂ = H₂ + HO₂</td>
<td>16</td>
<td>7.0 + 09</td>
<td>0.0</td>
<td>4.2</td>
<td>1.6 + 09</td>
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<td>20.0</td>
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<td>HO₂ + HO₂ = H₂O₂ + O₂</td>
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<td>41.8</td>
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<td>O + H₂O₂ = HO₂ + OH</td>
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<td>6.4</td>
<td>2.9 + 09</td>
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<td>20.4</td>
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<thead>
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<th>Preexponential</th>
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<td>H₂ + H₂ + O₂ = H₂O + H₂O</td>
<td>114</td>
<td>7.0 + 13</td>
<td>0.0</td>
<td>21.0</td>
<td>-</td>
<td>-</td>
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<tr>
<td>H₂O + M = R + R + M</td>
<td>-109</td>
<td>8.8 + 22</td>
<td>0.0</td>
<td>120.0</td>
<td>3.0 + 13</td>
<td>0.0</td>
<td>0.0</td>
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<th>Equation</th>
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<tr>
<td>H₂ = H₂O</td>
<td>57</td>
<td>2.3 + 6</td>
<td>0.0</td>
<td>22.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
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</table>
FIGURE 1. Calculated profile of the reduced temperature in a turbulent flame over the burning zone for a hydrogen-air mixture: $[\text{H}_2]_0 = 17.5\%$, $T_0 = 293$ K, $P = 1$ atm, $T_m = 1638$ K. Calculations are carried out by DKM at $P_f(T,T)$ $= 10^{-5}$, $L = 0.75$ cm.

Figure 1 shows the calculated temperature profile in a turbulent flame spreading through a lean hydrogen-air mixture under conditions of experiments in [9]. Calculations were carried out with a fixed PDF (hereinafter indicated are non-normalized PDF values) and a turbulence scale $L = 0.75$ cm (the scale was measured in [9] at about 1 cm). The thickness of the appropriate laminar flame of about 0.05 cm is much less than that of the turbulent flame which amounts to about 18 cm. The latter flame thickness should be treated as an overall width of the reaction zone extending between the extreme positions of the flame front within which the average temperature $\bar{T}$ rises from its initial value to the final one. Because of the adopted assumptions, this quantity is steady, whereas in experiments it is not the case.

Figure 2 illustrates experimental values of the turbulent burning velocity [9] and the calculated curves for mechanisms 8/42 (curve 2), 4/3 (curve 1), and 2/1 (the same curve 1). As seen, at a zero fluctuation velocity corresponding to a laminar flame, the calculated and measured burning velocities are identical. Further on, as the fluctuation velocity rises, the turbulent burning velocities $u_T$ for DKM and empirical mechanisms start diverging, although for mechanisms 4/3 and 2/1 they remain identical. It is evident that the curve calculated by DKM approximates fairly well the experimental data. At the maximum fluctuation velocity value, the deviation of calculations by the empirical mechanisms from experimental data on $u_T$
FIGURE 2. Turbulent burning velocity versus the fluctuation velocity for a hydrogen-air mixture: $[\text{H}_2]_0 = 17.5\%$, $T_0 = 293$ K, $P = 1$ atm. Dots are experimental data [9] and lines are calculated with $P_{T,T} = 10^{-4}$, $L = 0.75$ cm; (1) kinetic mechanisms 4/3 and 2/1, (2) DKM 8/42, (3) 2/1 at $W_{f,4H_2}(2/1) = W_{f,4H_2}(8/42)$.

FIGURE 3. Calculated laminar (1) and turbulent (2) burning velocities as a function of the preexponential factor $A_1$ in the expression for the rate of the first reaction of mechanism 4/3 for a hydrogen-air mixture (the experimental values of the laminar ($u_l$) and turbulent ($u_r$) burning velocities [9] are plotted on the y-axis; $[\text{H}_2]_0 = 17.5\%$, $T_0 = 293$ K, $P = 1$ atm, the fluctuation velocity $u = 900$ cm/s, $P_{T,T} = 10^{-4}$, $L = 0.75$ cm.

attains a factor of two. We have found that selecting a proper PDF, namely, $P(T,\tilde{T})$ values identical for all $T$ and $\tilde{T}$, one can make the $u_r$ values calculated by the empirical mechanisms much closer to the experimental data and even bring them together. There is another opportunity to improve
the fit of the empirical mechanisms to the experimental data, not invoking variation of $P(T, \tilde{T})$, this is optimization of the Arrhenius parameters of these mechanisms.

Curves 1 and 2 in Fig.3 illustrate the dependence of laminar ($u_\lambda$) and turbulent ($u_T$) burning velocities on the preexponential factor $A_1$ of the 4/3 mechanism. As is seen, to predict the experimental $u_\lambda$ value, preexponential factor $A_1$ should be set at $3.5 \times 10^{14}$ $\text{m}^2\text{mol}^{-1}\text{s}^{-1}$, whereas to fit the experimental value of $u_T$ it should be equal to $5.4 \times 10^{14}$ $\text{m}^2\text{mol}^{-1}\text{s}^{-1}$. This discrepancy is not surprising, because in a turbulent flow, the reaction zone is affected not only by large-scale turbulent fluctuations wrinkling the flame front surface but by small-scale fluctuations, enhancing transport within the flame front, as well. Due to this the flame front spreads normally to its surface in a turbulent flow at a velocity that differs from the laminar burning velocity $u_\lambda$. The apparent full consistency between the experimental $u_T$ values and calculations with DKM (Fig.2) is a result of an appropriate choice of the optimal effective $P(T, \tilde{T})$ value. Indeed, here, as has often been done in rigorous models of turbulent combustion, we disregard the effect of small-scale fluctuations.

Then we found out whether the rates of changes in the hydrogen concentration $W_{f-H_2}$ (8/42) calculated with DKM could be transferred without modifying them to the simplest empirical mechanism 2/1, that is, whether we can assume that $W_{f-H_2}(2/1) = W_{f-H_2}(8/42)$. The results of this calculation are displayed in Fig.2 (curve 3). It is seen that the latter curve lies above the curves calculated by the other mechanisms.

The above-discussed method and calculations by it relate numerically the burning velocity to the chemical combustion mechanism in a turbulent flow. The solution furnish also the burning zone width. Nonetheless, we can mention some peculiarities inferred from the calculations. Figure 4 shows the calculated thickness of a turbulent flame against the fluctuation velocity for DKM. The flame thickness is a linear function of $\tilde{\mu}$ and attains the above-mentioned value of $\sim 18$ cm at $\tilde{\mu} = 900$ cm/s. It is difficult to say how well this result is consistent with experimental observations. Unlike the turbulent burning velocity, the reaction zone thickness is essentially unsteady, and virtually no experimental data on this parameter is available in the literature. As commonly recognized, in closed combustion chambers
in which a mixture is ignited at the center, the reaction zone thickness increases as the flame spreads, and when the leading flame front arrives at the wall, some inhomogeneities are still observed at the ignition site. These inhomogeneities are attributed to the continuing reaction. Calculations with the empirical mechanisms yield much wider flame zones than do DKM calculations, under identical conditions and at strictly equal burning velocities, the width is different for mechanisms 4/3 and 2/1 (Fig. 2).

Interestingly, calculations by mechanism 2/1 at $W_{f=H_2}(2/1) = W_{f=H_2}(8/42)$ not only the flame speeds are similar but the reaction zone width does not differ very much either from that calculated by DKM.

![Graph](image)

**FIGURE 4.** The width of a turbulent flame zone versus the fluctuation velocity for a hydrogen-air mixture: $[\text{H}_2]_0 = 17.5\%$, $T_s = 293$ K, $P = 1$ atm. Calculations by DKM at $P_f(T,T) = 10^{-4}$, $L = 0.75$ cm.

It should be found out whether the procedure used to derive the empirical mechanism 2/1 (calculation of the kinetic parameters based on DKM calculations of a laminar flame) is of a general nature, in order to extend it to two-dimensional calculations with more complex chemical reactions. This would allow application of DKM in more rigorous turbulent flame models, which has been so far impossible.

To sum up, we note that, presumably, if other models of turbulent combustion are used to elucidate how empirical mechanisms manifest themselves and how adequate are the Arrhenius parameters of the reaction rates assessed in a laminar flow, the results could differ from those discussed above. Hence we can draw a tentative conclusion that only direct numerical integration of non-simplified equations governing turbulent burning with DKM are capable of providing data consistent with experiment, the use of empirical mechanisms and approximate models of turbulence necessitates their validation.
CONCLUSIONS

1. An approximate, but quite simple, method for tentative assessment of the kinetic parameters of empirical mechanisms modeling combustion reactions in a turbulent flow is suggested.

2. The method offers a satisfactory approximation of an experimental $u_f(\bar{u})$ function and requires an optimal selection of only one parameter, $P_1(T, \bar{T})$.

3. The suggested method points to a possible discrepancy between the kinetic parameters of the empirical mechanisms in laminar and turbulent flames.

REFERENCES