SAFe and Efficient hydrocarbon oxidation processes by KINetics and
Explosion eXpertise and development of computational process engineering
tools

Project No. EVG1-CT-2002-00072

Work-package 3

Contractual deliverable No. 15

Validation of laminar burning velocity model

A.A. Konnov, J. De Ruyck

Vrije Universiteit Brussel

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Introduction

Present report is prepared at the VUB within the Task 3.1 “Modeling of laminar burning velocity”. The Task 3.1 includes two parts: development of the model and software for calculation of laminar burning velocity and also validation of the laminar burning velocity model. These two parts are to be presented as contractual deliverables No. 14 and 15 on months 14 and 34 respectively.

Deliverable No. 14 “Model and software for calculation of laminar burning velocity” presented the report on the development of the model and software for calculation of laminar burning velocity and demonstrated the ability of the combustion chemical kinetic model and of the existing software package Chemkin to predict laminar burning velocities in the mixtures of simple hydrocarbons with oxygen and inert gases. At this stage, a satisfactory qualitative agreement between model predictions and available literature data was demonstrated. In the Deliverable No. 14 the software package Chemkin was described. Required information for the flame modeling was outlined. Typical cases of the calculation of laminar burning velocity were discussed. Adiabatic flame modeling and flame modeling with heat losses were presented. Typical problems related to the accuracy of the solution, its convergence, boundary conditions, etc. were also discussed.

Validation of the laminar burning velocity model was thought in the project planning as an important step for prediction of the temperature and pressure dependence of the laminar burning velocities. These calculations, in turn, will be used in the model of turbulent flame propagation which is under development within the Work Package 3.

As it is stated in the “Detailed project plan”, the main variables that should be considered in the flame modeling are: kind of mixture, the initial pressure and the temperature. A significant number of experiments has been performed at the VUB to determine flame burning velocities at atmospheric pressure and room temperature within the Task 4.2.6. Major part of these results are outlined in the present deliverable and compared with the modeling. In addition available results from the literature for high pressures are also presented and modeled.

Some results of the mechanism validation have been already published in scientific journals or presented at symposia. To avoid unnecessary duplication these papers / presentations are not copied in the present report but outlined shortly citing major accomplishments.

Modeling approach

A detailed C/H/N/O reaction mechanism for the combustion of small hydrocarbons is used for the modeling [1]. The current version of the mechanism (Release 0.5) consists of 1200 reactions among 127 species. This mechanism has been validated with experimental data available for oxidation, ignition, and flame structure of hydrogen, carbon monoxide, formaldehyde, methanol, methane, ethane, propane, and some of their mixtures. This
mechanism was used as a starting point for the development of the C1 - C3 combustion mechanism in the Safekinex project.

The SAFEKINEX C1-C3 mechanism developed within WP 4 and reported in the deliverable No. 34 was not used in the present modeling for several reasons:

1. The C1-C3 mechanism is too big for the flame modeling: it consists of about 2700 reactions between about 400 species. The 1-D modeling with this mechanism could only be performed on modern super-computers.
2. The current version of the C/H/N/O mechanism (Release 0.5) [1] has been used in many cases by the authors and in other Universities; good performance for many fuels was generally found.
3. Although the Safekinex C1-C3 mechanism includes many reactions important at lower temperatures, as compared to the Konnov mechanism (Release 0.5) [1], these reactions are generally considered as non-important for flame propagation.

The CHEMKIN - II collection of codes [2 - 4], including transport properties [5] from Sandia National Laboratories, were used. Multi-component diffusion and thermal diffusion options were taken into account. Adaptive mesh parameters were GRAD = 0.1 and CURV = 0.5.

## Laminar flames at atmospheric pressure

In the following the results of experiments performed at the VUB to determine flame burning velocities at atmospheric pressure and room temperature within the Task 4.2.6 are presented and compared with the modeling.

Table 1. Summary of the burning velocity + species profiles studied at the VUB at atmospheric pressure and 298 K.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Oxidiser</th>
<th>O₂/(O₂+Inert)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>O₂+N₂</td>
<td>0.209, 0.16, 0.17, 0.18</td>
</tr>
<tr>
<td>CH₄</td>
<td>O₂+CO₂</td>
<td>0.26, 0.29, 0.3155, 0.35</td>
</tr>
<tr>
<td>CH₄</td>
<td>O₂+Ar</td>
<td>0.17, 0.16, 0.15</td>
</tr>
<tr>
<td>CO(45%)+H₂(5%)+CO₂</td>
<td>air</td>
<td></td>
</tr>
<tr>
<td>CO(50%)+H₂(50%)</td>
<td>O₂+N₂</td>
<td>0.09, 0.08, 0.07</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>O₂+N₂</td>
<td>0.209, 0.18, 0.17, 0.16, 0.15</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>O₂+Ar</td>
<td>0.16, 0.15, 0.14</td>
</tr>
<tr>
<td>C₂H₄</td>
<td>O₂+CO₂</td>
<td>0.26, 0.29, 0.3155, 0.35</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>O₂+N₂</td>
<td>0.18, 0.17, 0.16, 0.15, 0.14</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>O₂+CO₂</td>
<td>0.23 0.209, 0.18</td>
</tr>
<tr>
<td>CH₄ (65-100%)+H₂(0-35)</td>
<td>O₂+N₂</td>
<td>0.209, 0.19, 0.18, 0.17, 0.16</td>
</tr>
</tbody>
</table>
**H2 flames**

**Related publications**


Modeling range covers flame burning velocities in hydrogen - oxygen - inert mixtures from 0.35 up to 4 atm; hydrogen flame structure at 1 and 10 atm.

![Graph](image)

Fig. 1. (from HERMANNS et al., submitted) Laminar burning velocities of H2-O2-N2 mixtures at atmospheric pressure. The presented results are at O2/(O2 + N2) = 0.077 with different equivalence ratios. The measurements and modeling were performed with a gas-flow temperature of 298 K and ambient pressure. O: heat Flux measurements; ◘: measurements by Egolfopoulos and Law; line: calculations with the present mechanism.
H2/CO flames

Related publications


Hydrogen (50\%) + carbon monoxide (50\%) + oxygen + nitrogen flames at \( P = 1 \), \( T_{in} = 298 \) K. Oxygen contents \( D = \frac{O_2}{(O_2 + N_2)} \) in the artificial air was 7\%; 8\%; 9 \%. Lean to rich.

Fig. 2. Adiabatic burning velocities in flames of \( \text{H}_2 + \text{CO} + \text{CO}_2 \) and air. Two series of symbols represent day-to-day repeatability of measurements; solid line: modeling.
CH4 flames

Related publications


Table 2. Adiabatic burning velocities in cm/s for CH₄ - O₂ - N₂ flames with different dilution ratio O₂/(O₂+N₂).

<table>
<thead>
<tr>
<th></th>
<th>Dilution ratio O₂/(O₂+N₂)</th>
</tr>
</thead>
<tbody>
<tr>
<td>φ</td>
<td>air</td>
</tr>
<tr>
<td>0.7</td>
<td>16.42</td>
</tr>
<tr>
<td>0.75</td>
<td>20.79</td>
</tr>
<tr>
<td>0.8</td>
<td>25.11</td>
</tr>
<tr>
<td>0.85</td>
<td>28.75</td>
</tr>
<tr>
<td>0.9</td>
<td>32.35</td>
</tr>
<tr>
<td>0.95</td>
<td>35.04</td>
</tr>
<tr>
<td>1</td>
<td>37.24</td>
</tr>
<tr>
<td>1.02</td>
<td></td>
</tr>
<tr>
<td>1.05</td>
<td>38.50</td>
</tr>
<tr>
<td>1.1</td>
<td>38.76</td>
</tr>
<tr>
<td>1.15</td>
<td>37.98</td>
</tr>
<tr>
<td>1.2</td>
<td>35.78</td>
</tr>
<tr>
<td>1.25</td>
<td>32.47</td>
</tr>
<tr>
<td>1.3</td>
<td>27.59</td>
</tr>
<tr>
<td>1.35</td>
<td>22.52</td>
</tr>
<tr>
<td>1.4</td>
<td>16.99</td>
</tr>
<tr>
<td>1.5</td>
<td>10.19</td>
</tr>
</tbody>
</table>
Fig. 3. Adiabatic burning velocity in methane – air mixtures. Diamonds: present measurements in CH₄ - air mixtures; crosses: present measurements in CH₄ - O₂ - N₂ mixtures; squares: Vagelopoulos et al. (1994); open triangles: Vagelopoulos and Egolfopoulos (1998); circles: van Maaren et al. (1994b); stars: Hassan et al. (1998); solid triangles: Gu et al. (2000); solid line: modeling.
Fig. 4. Adiabatic burning velocities for CH₄ - O₂ - N₂ flames with different dilution ratio. Crosses: 18 % of O₂ in air; circles: 17 %; squares: 16 %. Solid lines: modeling.
Fig. 5. Adiabatic burning velocities for CH₄ – O₂ – N₂ flames with different dilution ratio up to pure CH₄ – O₂ flames. Crosses: measurements of Jahn (1934) cited by B. Lewis, G. von Elbe (1987). Solid line: modeling.

G. Jahn, (1934) Der Zundvorgang in Gasgemischen, Oldenbourg, Berlin.

CH4/H2 flames

Related publications


$\alpha$ is defined as the mole fraction of hydrogen in the methane-hydrogen mixture: $\alpha = \frac{H_2}{(CH_4+H_2)}$

![Diagram](image_url)

Fig. 6. Adiabatic burning velocities in $(CH_4+H_2)+O_2+N_2$ flames with different dilution ratio (D) at standard temperature and pressure; $\alpha=0.05$. Symbols: experiment, lines: modeling. Crosses: D=0.209; diamonds: D=0.19; squares: D=0.18; circles: D=0.17; triangles: D=0.16.
Fig. 7. Adiabatic burning velocities in (CH₄+H₂)+O₂+N₂ flames with different dilution ratio (D) at standard temperature and pressure; α=0.15. Symbols: experiment, lines: modeling. Crosses: D=0.209; diamonds: D=0.19; squares: D=0.18; circles: D=0.17; triangles: D=0.16.
Fig. 8. Adiabatic burning velocities in (CH$_4$+H$_2$)+O$_2$+N$_2$ flames with different dilution ratio (D) at standard temperature and pressure; $\alpha=0.25$. Symbols: experiment, lines: modeling. Crosses: D=0.209; diamonds: D=0.19; squares: D=0.18; circles: D=0.17; triangles: D=0.16.
Fig. 9. Adiabatic burning velocities in (CH₄+H₂)+O₂+N₂ flames with different dilution ratio (D) at standard temperature and pressure; $\alpha=0.35$. Symbols: experiment, lines: modeling. Crosses: D=0.209; diamonds: D=0.19; squares: D=0.18; circles: D=0.17; triangles: D=0.16.
C2H6 flames

Related publications


Table 3. Adiabatic burning velocity (cm/s) in C2H6 - O2 - N2 (Ar) flames with different dilution ratio O2/(O2+Inert) as a function of equivalence ratio $\phi$.

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>Ratio O2/(O2+N2)</th>
<th>Ratio O2/(O2+Ar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6</td>
<td>0.209  0.209</td>
<td>0.18  0.17</td>
</tr>
<tr>
<td>0.65</td>
<td>14.23  14.87</td>
<td></td>
</tr>
<tr>
<td>0.7</td>
<td>22.42  22.32</td>
<td>13.56</td>
</tr>
<tr>
<td>0.75</td>
<td>16.31  13.88</td>
<td>24.81  21.95</td>
</tr>
<tr>
<td>0.8</td>
<td>30.2   30.37</td>
<td>19.11  16.23</td>
</tr>
<tr>
<td>0.85</td>
<td>33.95  21.7</td>
<td>18.86  15.21</td>
</tr>
<tr>
<td>0.9</td>
<td>36.6   36.78</td>
<td>24.51  20.55</td>
</tr>
<tr>
<td>0.95</td>
<td>39.25  26.53</td>
<td>22.32  18.56</td>
</tr>
<tr>
<td>1</td>
<td>40.74  28.25</td>
<td>23.85  19.77</td>
</tr>
<tr>
<td>1.05</td>
<td>41.8   29.43</td>
<td>24.65  20.6</td>
</tr>
<tr>
<td>1.1</td>
<td>42.04  29.71</td>
<td>24.98  20.9</td>
</tr>
<tr>
<td>1.15</td>
<td>41.56  29.43</td>
<td>24.61  20.4</td>
</tr>
<tr>
<td>1.2</td>
<td>40.15  28.31</td>
<td>23.19  19.08</td>
</tr>
<tr>
<td>1.25</td>
<td>37.92  25.94</td>
<td>21.12  17</td>
</tr>
<tr>
<td>1.3</td>
<td>35.28  31.07</td>
<td>23.05  18.22</td>
</tr>
<tr>
<td>1.35</td>
<td>31.07  19.84</td>
<td>15.19</td>
</tr>
<tr>
<td>1.4</td>
<td>26.9   26.54</td>
<td>16.19</td>
</tr>
<tr>
<td>1.45</td>
<td>22.74  18.68</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>18.8   18.68</td>
<td>20.73  16.97</td>
</tr>
<tr>
<td>1.55</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.6</td>
<td></td>
<td>16.8</td>
</tr>
</tbody>
</table>
Fig. 10 Adiabatic burning velocities in C₂H₆ - O₂ - N₂ (Ar) flames with different dilution ratio. Solid squares: O₂/(O₂+Ar) = 16 %; solid circles: O₂/(O₂+Ar) = 15 %; open squares: 18 % of O₂ in air; crosses: 17 % of O₂ in air; diamonds: 16 % of O₂ in air; open circles: 15 % of O₂ in air. Solid lines: modeling.
C2H4 flames

Fig. 11. Adiabatic burning velocities in C$_2$H$_4$ - O$_2$ - N$_2$ flames with 18% of O$_2$ in air. Points: measurements of Egolfopoulos et al. (1990). Solid line: modeling.
C2H2 flames

Fig. 12. Adiabatic burning velocities in C2H2 - O2 - N2 flames with 13% of O2 in air. Points: measurements of Egolfopoulos et al. (1990). Solid line: modeling.
C3H8 flames

Related publications


Fig. 13. Adiabatic burning velocities of C3H8 – air flames. Solid line: modeling.
Laminar flames at high pressures and variable temperatures

Fig. 14. Adiabatic burning velocities of stoichiometric CH4 – air flames as a function of pressure. Solid line: modeling at 328 K, dashed line: at 300 K.
Burning velocities at elevated temperatures and pressures were extensively studied [6 - 17], however most of these publications were devoted to methane combustion. Selected results are shown in Fig. 14 above and compared with the modelling. Although the model correctly reproduces temperature and pressure dependences, its agreement with the measurements deteriorates at higher pressures.

Concluding remarks

1. The model and software presented in this and in the previous Report No. 14 were validated and found in good agreement with adiabatic burning velocities for the following fuels: H2, H2/CO, CH4, CH4/H2, C2H4, C2H6 and C3H8 at atmospheric pressure and room temperature. The effects of inerts, N2, CO2 and Ar, and their amount are also accurately reproduced.

2. In the whole range of fuels, equivalence ratios, and inert concentrations at atmospheric pressure the accuracy of the model predictions is usually within 2 cm/s (or 5-10%) when compared with available measurements. At higher pressure the deviation of the model predictions from the experiments may reach 20-30 %.

3. For the model of turbulent flame propagation, which is under development within the Work Package 3, it is therefore recommended to use, whenever possible, experimental burning velocities at higher pressures.

4. On the other hand, the modeling could be useful for the fuels and their mixtures when experimental data are not available. The accuracy of this modeling hardly could be better than 30 %.

References


