NUMERICAL SIMULATION OF TURBULENT COMBUSTION PROCESSES USING A FRONT TRACKING TECHNIQUE

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Comparison of Flamelet and PDF Models with Detailed Experimental Data for Turbulent Combustion
CONTENTS

• model of turbulent combustion
• application to a rapid compression device
• comparison with experimental data
• evaluation of model parameters
MODEL OF TURBULENT COMBUSTION

- Based on front tracking methods
  - Development in time of an interface due to a flow field and due to self-advancement
  - Similar to G-equation approach, but without solving a transport equation

- Methods are applied to the turbulent combustion zone
  - The interaction of a complex chemistry with a turbulent flow field is transformed into the **kinematic** problem of the evolution of the combustion zone
  - Thickness must be considered
CALCULATION OF FLOW FIELD

Poisson equation

\[
\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = -\frac{1}{\rho} \frac{d\rho}{dt} = S_{ij}
\]

with source terms

\[
S_{ij} = \frac{f_{ij}^n - f_{ij}^{n-1}}{\Delta t} \rho_u^n - \rho_b^n - \frac{f_{ij}^{n-1}}{\Delta t} \rho_b^n - \rho_b^{n-1} - \frac{1 - f_{ij}^n}{\Delta t} \rho_u^n - \rho_u^{n-1}
\]

reaction compression burnt compression unburnt

POSITION OF SOURCES
ASSUMPTIONS
FOR THERMODYNAMIC CALCULATION

- Combustion chamber contains only burnt and unburnt fluid (infinitely thin laminar flame zone)
- crevices contain only unburnt gas at ambient temperature
- volume of crevices is constant
- uniform pressure in the whole system
- the ideal gas law holds in each zone
- chemical equilibrium in the burnt gas
- uniform temperatures in each zone
- heat transfer only to the walls
EQUATIONS
FOR THERMODYNAMIC CALCULATION

\[ V_t = V_u + V_b + V_c \]

\[ m_t = m_u + m_b + m_c \]

\[ m_u c_{p_u} dT_u = dQ_u + V_u dp - dm_c (h_c - h_u) \]

\[ m_b c_{p_b} dT_b = dQ_b + V_b dp + dm_b (h_u - h_b) \]

\[ p = \frac{m_u R_u T_u + m_b R_b T_b + m_c R_u T_w}{V_t} \]
TURBULENT BURNING VELOCITY I

laminar flame area
\[ A_l = \bar{A} + A' \]

mean area
\[ \bar{A} \sim l^2 \]
excess area
\[ A' \sim lL \]

increase due to turbulence
\[ dA_1' \sim u'ldt \]
decrease due to burning of pockets
\[ dA_2' \sim s_l Ldt \]
TURBULENT BURNING VELOCITY II

ordinary differential equation

\[ \frac{da'}{A} = \frac{dA'}{A} = \frac{dA_1 - dA_2}{A} = c_1 \frac{u'}{T} dt - c_2 a' \frac{s_i}{T} dt \]

Solution of ode

\[ a' = \frac{c_1 u'}{c_2 s_i} (1 - e^{-2c_2 \frac{s_i}{T} t}) \]

With continuity across the combustion zone (Damköhler’s assumption)

\[ \rho_u s_i A_t = \rho_u s_b \bar{A} \]

Substitution:

\[ k_1 = c_1 / c_2; k_2 = 2c_2 \]

\[ s_b = s_i [1 + k_1 (\frac{u'}{s_i}) (1 - e^{-k_2 \frac{s_i}{T} t})] \]

Comparison with formula from literature:

\[ \frac{s_b}{s_i} = 1 + c \left( \frac{u'}{s_i} \right)^N \]

leads to:

\[ \frac{s_b}{s_i} = 1 + k_1 \left( \frac{u'}{s_i} \right)^N (1 - e^{-k_2 \frac{s_i}{T} t}) \]
FLAME ZONE THICKNESS

\[
\frac{A'}{A} \sim \frac{l^2}{lL}
\]

\[L = k_3 l a' = k_3 l \frac{A'}{A}\]

\[A_l = \tilde{A}_{s_l}^{s_b}\]
ENTRAINMENT MODEL

- unburnt gas enters the combustion zone as set of volume elements
- volume elements burn with laminar burning velocity
- volume fraction which actually burns depends on shape of volume element

<table>
<thead>
<tr>
<th>typ</th>
<th>volume</th>
<th>change of volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>flat</td>
<td>$V = l \times A$</td>
<td>$\dot{V} = -s_l \times A$</td>
</tr>
<tr>
<td>cylindrical</td>
<td>$V = \pi l^2 H$</td>
<td>$\dot{V} = -2\pi H s_l (r_0 - s_l \hat{t})$</td>
</tr>
<tr>
<td>spherical</td>
<td>$V = 4/3 \pi l^3$</td>
<td>$\dot{V} = -4\pi s_l (r_0 - s_l \hat{t})^2$</td>
</tr>
<tr>
<td>general</td>
<td>$V = k \times l^n$</td>
<td>$\dot{V} = -kn (r_0 - s_l \hat{t})^{n-1} s_l$</td>
</tr>
</tbody>
</table>

in the calculations a cylindrical shape is assumed
ENTRAINMENT MODEL II

- volume elements are transported with the flow field
- in the implementation the sources are transported instead of the volume elements
APPLICATION TO THE RAPID COMPRESSION DEVICE

- combustion chamber
- window
- turbulence generator
- piston
- driver section
- TDC stop

- turbulence generation
- BDC

- turbulence decay and compression
- $\Delta t$
- start of piston

- combustion and expansion
- TDC
INPUT DATA FROM EXPERIMENT

- piston position $H(t)$
- initial conditions $p_0, T_0$
- turbulence intensity at ignition $u'$
- compression ratio $\epsilon$

PARAMETER

- fuel: $C_3H_8$, $C_2H_2$
- equivalence ratio : 6.0 to 10
- turbulence intensity $u'$: 0.0 m/s to 2.0 m/s
INFLUENCE OF EXPERIMENTAL UNCERTAINTY

\[ C_3H_8, \lambda = 1, w' = 1.2m/s \]
INFLUENCE OF TURBULENCE INTENSITY

\[ C_3H_8, \lambda = 1 \]

\[ C_2H_2, \lambda = 1.34 \]
INFLUENCE OF COMPRESSION RATIO

\[ C_8H_8, \lambda = 1, u' = 0 \text{m/s} \]
DEVELOPMENT OF TURBULENT BURNING VELOCITY

$C_3H_8, \lambda$

$C_2H_2, \lambda = 1.8, u' = 1.04 m/s$
$C_5H_8$, $\lambda = 1.0$, $u' = 0.0\, \text{m/s}$, frame rate $0.6\, \text{ms}$
$C_3H_8$, $\lambda = 1.0$, $u' = 0.08m/s$, frame rate 0.6 ms
$C_3H_8$, $\lambda = 1.0$, $u' = 0.23 m/s$, frame rate 0.6 ms
$C_5H_8$, $\lambda = 1.0$, $u' = 0.74 m/s$, frame rate 0.6 ms
$C_9H_8$, $\lambda = 1.0$, $u' = 1.61\ m/s$, frame rate 0.6 ms
$C_2H_2, \lambda = 1.34, u' = 0.0 m/s, \text{ frame rate } 0.2 \text{ ms}$
$C_2H_2$, $\lambda = 1.34$, $u' = 0.08m/s$, frame rate 0.2 ms
\( C_2H_2, \lambda = 1.34, \ u' = 0.23 \text{m/s}, \ \text{frame rate} \ 0.2 \text{ms} \)
$C_2H_2, \lambda = 1.34, u' = 0.74 m/s$, frame rate 0.2 ms
$C_2H_2$, $\lambda = 1.34$, $u^' = 1.61m/s$, frame rate 0.2 ms
COMBUSTION ZONE THICKNESS

$C_3H_8, \lambda$

$C_2H_2, \lambda = 1.34$
SPATIAL DISTRIBUTION OF REACTION RATE

\[ C_3H_8, \lambda = 1.0, u' = 0.74 \text{m/s} \]
STATISTICAL PARAMETERS OF SOURCE STRENGTH DISTRIBUTION
STATISTICAL PARAMETERS OF SOURCE STRENGTH DISTRIBUTION

$t = 1$ ms

$t = 5$ ms

$t = 2$ ms

$t = 6$ ms

$t = 3$ ms

$t = 7$ ms

$t = 4$ ms

$t = 8$ ms
STATISTICAL PARAMETERS OF SOURCE STRENGTH DISTRIBUTION

- combustion zone thickness
- centre of gravity of profiles
  \[ M = K_1 \]
- varianz
  \[ V = \sqrt{K_2} \]
- skewness
  \[ S = \frac{K_3}{V^3} \]
- flatness
  \[ E = \frac{K_4}{V^4} \]
- integral
  \[ I = \sum dx_i s_i \]

\[ K_1 = \frac{\sum s_i x_i}{\sum s_i} \]
\[ K_2 = \frac{\sum s_i (x_i - K_1)^2}{\sum s_i} \]
\[ K_3 = \frac{\sum s_i (x_i - K_1)^3}{\sum s_i} \]
\[ K_4 = \frac{\sum s_i (x_i - K_1)^4}{\sum s_i} - 3K_2^2 \]
STATISTICAL PARAMETERS OF SOURCE STRENGTH DISTRIBUTION
EVALUATION OF MODEL PARAMETERS

results of 70 simulations: $C_3H_8$, $\lambda = 1$
EVALUATION OF MODEL PARAMETERS

results of 32 simulations: $C_2H_2, \lambda = 1.34$
CONCLUSIONS

• combustion model with the following features
  – no turbulence model
  – no detailed chemistry
  – **kinematic** problem of flame propagation
    is solved
  – spatial distribution of energy release
    in the combustion zone is modeled

• experimental results can be reproduced
  – thermodynamic or global properties
  – shape, position, thickness and development in time
    of the combustion zone
  – influence of various parameters

• coefficients of turbulent burning velocity are indepen-
dent of turbulence intensity