Some challenges of numerical modeling and simulation of hydrogen kinetic combustion

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Introduction

• Currently approx. 14 mio gas appliances installed within the EU
• All residential and commercial gas appliances installed within the EU today designed for operation with natural gas
• Demand of renewable energy solutions is growing
• Hydrogen combustion in case of a gas condensing boiler:
  – Clean and efficient solution for heating and hot water generation
• EHI association: every natural gas fired boiler in domestic-scale (≤ 45kW) has to be hydrogen-ready from 2026
Key challenges of hydrogen combustion modelling

• **High reaction rate** leading to short chemical timescales
• **Detailed chemistry** increase the model's complexity
• **High diffusivity of hydrogen** due to its low molecular weight influences on buoyancy forces and mixing quality
• **Multiscale phenomena** from microscopic chemical reactions to macroscopic fluid dynamics
• **Turbulence-Combustion interactions** is crucial for accurately predicting flame behavior
• **Radiation heat transfer** due to high combustion temperature
• **Inlet Boundary conditions** are crucial for realistic hydrogen combustion modelling
Hydrogen premixed combustion problems

• Major problems of lean premixed hydrogen/air combustion:
  – Flashback to premixing duct
  – Ignition delay
  – Flame stabilisation
  – Non uniform mixture inlet boundary conditions

• The overall objective:
  “Avoid flashback to the premixing duct”
  – Premixing section is not designed for high temperature and pressure peaks
  – Can cause critical damage to the heating device

Source: Laboratory of Bekaert Combustion Technology B.V.
The impact of hydrogen mixing degree on FB

• Flashback (FB) phenomena in premixed or partially premixed combustion
  – FB in the core flow
  – FB due to combustion instabilities
  – Boundary layer FB
  – FB due to autoignition

• Major influence of mixing degree on combustion stability and FB

→ Objective: To evaluate the mixing degree, influencing mixture inlet BC of combustion chamber
Location of the investigated area

Combustion chamber

Perforated flat flame burner

Mixing stage

Interface to manifold - evaluated area

Source: Own illustration

Gas-Valve

$\text{H}_2$

Premixed

Ambient Air

Venturi

Source: Own illustration
Integrated mixing device

a) Front view

Hydrogen/Air mixture outlet

b) Top view

Air inlet

c) Side view

Hydrogen inlet
Modelling conditions

- Different angular velocities: 9500, 8000, 5000 rpm
- Total pressure increase estimated via similarity laws:

<table>
<thead>
<tr>
<th>Angular velocity [rpm]</th>
<th>$\dot{m}_{H_2+air}$ [g/s]</th>
<th>$\Delta p_{tot}$ [Pa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>9500</td>
<td>4.8074</td>
<td>703</td>
</tr>
<tr>
<td>8000</td>
<td>4.0483</td>
<td>499</td>
</tr>
<tr>
<td>5000</td>
<td>2.5302</td>
<td>194</td>
</tr>
</tbody>
</table>

- Inlet temperature $H_2 = 288$ K
- Inlet temperature Air = 323 K
- Constant excess air ($\lambda=1.3$)
Modelling of mixing efficiency

• Based on the idea of Weltens, a uniformity index for degree of premixing (UI\textsubscript{pre}) was derived

• Area averaged concentration

\[ \overline{c_{H_2}} = \frac{\sum_{i=1}^{N} c_{H_2,i} * A_i}{A_{out}} \]

• Local non-uniformity index

\[ \omega_{H_2,i} = \frac{\sqrt{(c_{H_2,i} - \overline{c_{H_2}})^2}}{\overline{c_{H_2}}} \]

• Non-uniformity index

\[ \overline{\omega} = \frac{\sum_{i=1}^{N} \omega_{H_2,i} * A_i}{A_{out}} \]

• Mixing efficiency

\[ UI_{pre} = 1 - \frac{\overline{\omega}}{2} \]
Modelling geometry

- Rot. domain
- Outlet
- Free-slip nozzle
- Volute
### Boundary conditions

<table>
<thead>
<tr>
<th>Boundary / Cell zone</th>
<th>Condition</th>
<th>Condition details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet air</td>
<td>Pressure inlet</td>
<td>Normal to boundary, $P = 0$ Pa, $T = 323$ K</td>
</tr>
<tr>
<td>Inlet $\text{H}_2$</td>
<td>Mass flow inlet</td>
<td>Normal to boundary, $T = 288$ K</td>
</tr>
<tr>
<td>Outlet</td>
<td>Pressure outlet</td>
<td>Gauge pressure, $P = 930$ Pa</td>
</tr>
<tr>
<td>Counter rotating wall</td>
<td>Rotational wall</td>
<td>No-slip, $n = x$ rpm (rel. to adjacent cell zone)</td>
</tr>
<tr>
<td>Nozzle wall</td>
<td>Stationary wall</td>
<td>slip</td>
</tr>
<tr>
<td>Volute + Impeller</td>
<td>Stationary wall</td>
<td>No-slip</td>
</tr>
<tr>
<td>Nozzle</td>
<td>Stationary domain</td>
<td>Air + $\text{H}_2$</td>
</tr>
<tr>
<td>Volute + Venturi</td>
<td>Stationary domain</td>
<td>Air + $\text{H}_2$</td>
</tr>
<tr>
<td>Impeller</td>
<td>Rotational domain</td>
<td>Air + $\text{H}_2$, $n = x$ rpm</td>
</tr>
</tbody>
</table>
## Solver settings (ANSYS Fluent)

<table>
<thead>
<tr>
<th>Solver settings</th>
<th>RANS (FRM)</th>
<th>URANS (TRS)</th>
<th>Hybrid RANS/LES (TRS)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Analysis typ</strong></td>
<td>Stationary/ Frozen Rotor</td>
<td>Transient/ Mesh moving</td>
<td>Transient/ Mesh moving</td>
</tr>
<tr>
<td><strong>Turbulence model</strong></td>
<td>SST k-ω</td>
<td>SST k-ω</td>
<td>DDES / SST k-ω</td>
</tr>
<tr>
<td><strong>Pressure-Velocity Coupling</strong></td>
<td>Coupled solver</td>
<td>Coupled solver</td>
<td>Coupled solver</td>
</tr>
<tr>
<td><strong>Pressure Scheme</strong></td>
<td>Second Order</td>
<td>Second Order</td>
<td>Second Order</td>
</tr>
<tr>
<td><strong>Advection Scheme</strong></td>
<td>Second Order Upwind</td>
<td>Second Order Upwind</td>
<td>Second Order Upwind</td>
</tr>
<tr>
<td><strong>Turbulence numerics</strong></td>
<td>Second Order Upwind</td>
<td>Second Order Upwind</td>
<td>Second Order Upwind</td>
</tr>
<tr>
<td><strong>Species</strong></td>
<td>Second Order Upwind</td>
<td>Second Order Upwind</td>
<td>Second Order Upwind</td>
</tr>
<tr>
<td><strong>Physical time-step</strong></td>
<td>Automatic</td>
<td>2.8707e-5 s for 9500 rpm</td>
<td>2.8707e-5 s for 9500 rpm</td>
</tr>
<tr>
<td><strong>Steps of iteration</strong></td>
<td>1000</td>
<td>40/TS</td>
<td>40/TS</td>
</tr>
<tr>
<td><strong>Residual target</strong></td>
<td>Res &lt; $10^{-3}$</td>
<td>Res &lt; $10^{-3}$</td>
<td>Res &lt; $10^{-3}$</td>
</tr>
<tr>
<td><strong>Residual target energy</strong></td>
<td>Res &lt; $10^{-6}$</td>
<td>Res &lt; $10^{-6}$</td>
<td>Res &lt; $10^{-6}$</td>
</tr>
</tbody>
</table>
Results – mixing efficiency
Velocity magnitude

- RANS
- URANS
- RANS/LES
Results – local $\lambda$ as a function of rpm (RANS/LES)
Local variation of excess air
Some findings of mixing simulation part

- Well mixed hydrogen and air is of crucial importance for stabil premixed combustion
  - Small range of $\lambda$ deviation may have strong impact on flame stability
  - Greater level of turbulence leads to smaller local $\lambda$ deviation
- Lower rotor rpm produces better mixing, 5000 rpm has been set for experimental setup
- To assure optimal mixing of air and hydrogen, the mixing devices should be properly designed (i.e., integrated venturi nozzle with fan housing)
- CFD simulations of mixing part help to determine the non-uniform inlet boundary conditions (IBC) of the combustion chamber
Combustion experimental setup

- Burner hood
- Perforated burner plate
- Burner gasket
- Mixing stage
- Mixing output = non-uniform IBC
- Heat exchanger / combustion chamber
- $d_{B2D}$
- $d_{CO}$
- Burner hood/distributor
- Heat exchanger
- Distributor
- Combustion chamber
- Restrictor
- Inlet
Perforated burner

Characteristic properties:
- Aluminum material
- 5x6 open clusters
- 5 holes per cluster
- Hole diameter $\sim 1$ mm

Previous findings:
- Massive thermoacoustic phenomena (TA) independent from Lambda and heat load
- TA results in flashback due to flow oscillation
- Maximum heat load: $Q_c = 14.0$ kW ($\lambda = 1.42 \rightarrow \bar{v}_{out,hole} = 15.1 \text{ m/s}$)

Detail A: CFD computational domain
CFD computational domain

- Detailed chemistry and radiation simulation:
  - 1st approach:
    - 3D simulation
    - Steady simulation
    - 1/8 slice of burner cluster
  - 2nd approach:
    - 2D simulation
    - Steady simulation
    - 5 holes of cluster

Computational effort vs. complex modelling of inlet conditions

Detail A
Limitations of numerical simulation

- **Detailed chemistry and radiation simulation:**
  - Hybrid RANS-LES (SST k-ω turbulence model)
  - Detailed chemistry using validated ANSYS Fluent Chemkin mechanism for hydrogen/air combustion
  - Turbulence-Chemistry Interaction Model: Eddy-Dissipation Concept
  - Conjugated heat transfer with solid boundary conditions: measurement data
  - Fully-premixed hydrogen/air mixture
  - $\lambda = 1.3$
  - App. 35% of heat input

- **Further objective:**
  - Modelling of burner stabilized premixed hydrogen/air combustion in case of a gas condensing boiler
  - Define requirements for the mesh to illustrate combustion stabilities correct
  - Evaluate influence of radiation models on the combustion
  - **Investigation of flame stability/ interaction of two or more single flames** by the variation of inlet conditions
Numerical results: Temperature

3D modelling of detailed chemistry and radiation simulation:

Fluid zone

Solid zone
Numerical results: water and OH radicals

Concentration $C_{\text{H}_2\text{O}}$

Concentration $C_{\text{OH}}$
Conclusions

• Well mixed hydrogen and air is of crucial importance for stabil premixed combustion in case of flat flame burner
• Hydrogen flame instability often leads to the FB
• CFD simulations of mixing part help to determine the non uniform inlet boundary conditions of the combustion chamber
• Simplified numerical models are useful for basic simulations of premixed hydrogen combustion in smaller limited computational domain
• Numerical modeling requires detailed combustion chemistry and interaction with turbulence
• Some decision factors ($dv/dt, T \ldots$) should be identified for FB detection
• Thermoacoustics represents additional issue of premixed hydrogen combustion depending on burner and combustion chamber type