Improving FGM: multiple chemical time scales

Citation for published version (APA):

Document status and date:
Published: 06/10/2016

Document Version:
Other version

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher’s website.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.

Link to publication

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the “Taverne” license above, please follow below link for the End User Agreement:
www.tue.nl/taverne

Take down policy
If you believe that this document breaches copyright please contact us at:
openaccess@tue.nl
providing details and we will investigate your claim.
Improving FGM: multiple chemical time scales
Applied to predict the fate of NO and CO in Nozzle Guide Vanes

Introduction
- Flamelet Generated Manifolds (FGM) reduced chemistry model yields accurate representation of the conversion of the fuel into the major products.
- Usually, FGM accounts only for one chemically reactive time scale, described by the reaction progress variable.
- In this work: improvement of the general accuracy of the FGM by allowing for additional degrees of freedom.
- Inclusion of additional chemical processes with different characteristic times scales.

Method
- Extending FGM following the ideas of ILDM.
- Perform a time scale analysis of chemical source term locally in each grid point of the FGM.
- Assumption: chemistry evolution quickly varies in the directions of the fast reaction groups.
- FGM is extended locally by the directions of the slow chemistry.

FGM generation
- Premixed free propagating stoichiometric methane/air flames, GRI 3.0, Le = 1.
- Enthalpy and pressure are additional FGM dimensions.
- FGM N_r = 1, total of 3 dimensions (\( \Psi, T, \ldots \)) = \( f(p, h, \Psi_0) \)
- FGM N_r = 2, total of 4 dimensions (\( \Psi, T, \ldots \)) = \( f(p, h, \Psi_0, \Psi_1) \)
- Tabulated on a curvilinear grid, table retrieval done by linear interpolation.

Results
- Comparing FGM with \( N_r = 2 \) to the standard FGM (\( N_r = 1 \)).
- Detailed chemistry (DC) as reference.
- CO and NO mass fractions for NGV, residence time \( r = 0.1 \) ms.
- CO and NO mass fractions for a nozzle geometry with an increased residence time of \( r = 10 \).

Test case
- Combustor: CO and NO are formed.
- Focus of this work: Stators / turbine. What is the fate of CO and NO freeze?

FGM generation
- Typical directions of \( \Psi_0 \) and \( \Psi_1 \)

<table>
<thead>
<tr>
<th>( i )</th>
<th>( \lambda_i )</th>
<th>( H_2 )</th>
<th>( O_2 )</th>
<th>( H_2O )</th>
<th>( CO )</th>
<th>( CO_2 )</th>
<th>( NO )</th>
<th>( N_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1.06 ( \times ) 10^7</td>
<td>0.065</td>
<td>-0.279</td>
<td>-0.099</td>
<td>-0.030</td>
<td>0.135</td>
<td>0.135</td>
<td>0.830</td>
</tr>
<tr>
<td>2</td>
<td>-1.25 ( \times ) 10^7</td>
<td>0.175</td>
<td>-0.361</td>
<td>-0.021</td>
<td>-0.045</td>
<td>0.011</td>
<td>0.011</td>
<td>0.000</td>
</tr>
</tbody>
</table>

2 slowest time scales
- Effect on the other species is included
- The chemistry of CO and NO is coupled

Obtained FGM is parametrized by multiple chemically reactive control variables:

\[ \Psi_i = \sum_j Y_i \Psi_{ij} \quad \frac{\partial \Psi_i}{\partial t} + F \cdot (\nabla \Psi_i) = P \left( \frac{1}{M_i} \nabla \cdot \Psi_{ij} \right) = u_{ij} \quad i = 1, \ldots, N_r \]

- \( N_r \) — number of reactive dimensions
- \( \Psi_{ij} \) — primary reactive control variable (reaction progress variable)
- \( \Psi_{ij} \) — secondary reactive control variable (extra chemical degrees of freedom)

Test case
- Nozzle Guide Vanes (NGV).
- Flow through a decreasing area duct.
- Enthalpy is converted into kinetic energy.
- High velocities, Mach number range given by: \( 0.1 < M < 0.98 \).
- Residence time in the order of: \( r = 0.1 \) ms.

\[ \Psi_{ij} = \sum_k Y_i \Psi_{ij} \quad \frac{\partial \Psi_i}{\partial t} + F \cdot (\nabla \Psi_i) = P \left( \frac{1}{M_i} \nabla \cdot \Psi_{ij} \right) = u_{ij} \quad i = 1, \ldots, N_r \]

Conclusions
- FGM can be extended with additional chemically reactive dimensions.
- The new developed model captures the fate of CO and NO under conditions of Nozzle Guide Vanes, characterized by fast time scales of the thermodynamic processes (expansion and cooling).

\[ \Psi_{ij} = \sum_k Y_i \Psi_{ij} \quad \frac{\partial \Psi_i}{\partial t} + F \cdot (\nabla \Psi_i) = P \left( \frac{1}{M_i} \nabla \cdot \Psi_{ij} \right) = u_{ij} \quad i = 1, \ldots, N_r \]

\[ \Psi_{ij} = \sum_k Y_i \Psi_{ij} \quad \frac{\partial \Psi_i}{\partial t} + F \cdot (\nabla \Psi_i) = P \left( \frac{1}{M_i} \nabla \cdot \Psi_{ij} \right) = u_{ij} \quad i = 1, \ldots, N_r \]

\[ \Psi_{ij} = \sum_k Y_i \Psi_{ij} \quad \frac{\partial \Psi_i}{\partial t} + F \cdot (\nabla \Psi_i) = P \left( \frac{1}{M_i} \nabla \cdot \Psi_{ij} \right) = u_{ij} \quad i = 1, \ldots, N_r \]