Numerical Simulation of Hydrogen Gas Turbines using Flamelet Generated Manifolds technique on Open FOAM

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Overall objective of the H$_2$-IGCC project is

• To provide and demonstrate technical solutions for reliable gas turbines (GTs) in the next generation of Integrated Gasification Combined Cycle (IGCC) plants.
• The goal is to enable combustion of undiluted hydrogen-rich syngas with low NOx emissions and also allowing for high fuel flexibility.

• The H$_2$-IGCC project brings together 24 partners from industry and academia with the common goal to increase gas turbine efficiency and fuel flexibility without affecting the reliability and availability in a pre-combustion IGCC-CCS plant configuration.

For more informations: http://www.h2-igcc.eu
Aim of SP1 is to develop safe and low emission combustion technology for undiluted, hydrogen-rich syngas.

In order to achieve this, problems resulting from the differences in combustion properties of hydrogen and natural gas need to be addressed and solved.

Partners involved, together with TU/e in the SP1, are:

- Siemens AG
- EDF
- E.ON
- Ansaldo Energia
- PSI
- Cardiff University
- DLR
- NUI
- University of Genoa
- Enel
TU/e work for SP1

• Developing of RANS and LES model based on Flamelet Generated Manifolds technique with a special focus on preferential diffusion effects

• Heat loss at non adiabatic walls has to be accounted

• The code and table generation will be done with the use of TU/e CHEM1D code

• Numerical Simulation is done with the open source toolbox OpenFOAM

• Validation test case, in accordance with Siemens AG, will be DLR jet flames.
The addition of Hydrogen in the fuel mixture is important in order to evaluate the knowledge about the effects of biomass and coal gasification. Last, but not least, the reducing of thermal NOx formation has to be taken into account.

- Hydrogen is highly diffusive and affects chemical process and stability of flames.

- Hydrogen Lewis Number, which is the ratio between thermal and species diffusion, is very low, meaning that there is a preferential diffusion effect which becomes important when hydrogen is added and causes the so-called thermo-diffusive instabilities.

- The large diffusion of hydrogen causes an increase of fuel consumption and a local increase of burning velocity in these regions.
• Reasons of using a *reduced numerical method*: detailed reaction mechanism is extremely time consuming, due to:

  • PDE for each chemical component
  • Non-linear coupling of equations by hundreds of chemical reactions
  • Stiffness of system because of a broad range of time scales.

• FGM is the solution to this with very good *accuracy*, respect to detailed chemistry, but with reduction in CPU time (2 orders of magnitude)

2D methane-air Bunsen flame

from: Jeroen A. van Oijen
The idea is to solve a multidimensional flame considering it as a set of many 1D flames called **flamelets**

Conservation equations for a premixed flame are adapted in terms of the **Controlling Variables** $Y_i$

A **manifold** is built in the way that mixture composition is described by a small number of controlling variables.

**Flamelet equations** are obtained considering the conservation equations for a premixed flame in a system along the coordinate $s$ perpendicular to the flame:

\[
\frac{\partial}{\partial s} \left( \rho s L_i Y_i - \frac{\lambda}{Le_i c_p} \frac{\partial Y_i}{\partial s} \right) - \omega = P_i
\]
Flamelet Generated Manifolds (III)

• From this equation the source term (st) is unclosed but can be obtained from the manifold.

• Specialized 1D flame code (CHEM1D) will be used.

• Pre-processing: manifold is computed and variables needed to solve conservation equations (ρ, Y, st, ...) are stored in a database.

• With the use of FGM it is possible to predict minor species.

• CFD code solves flow field equations and equations for controlling variables (i.e. Y and h).
In order to start, an extra equation for $C$ is set with source term defined as an analytical function dependent on $C$. The constant in the source term expression affects the power of it and can determine whether the flame in the domain can blow out or have a flashback.

Velocity field is given with parabolic profile inside a very simple and easy 2D flame in a box mesh ($U_{\text{max}} = 1 \text{m/s}$). A transient laminar incompressible solver has been used for the test case. $C$ has been initialized to 1 in all the domain, except the inlet ($C_{\text{inlet}}=0$).

\[
\dot{C} = [C \cdot (1 - C)]^2 \cdot \text{constant}
\]
Open FOAM implementation

- Use of **icoFoam** which is a transient, laminar and incompressible in order to evaluate the 1D flamelet and modification of the solver in **fanzysource**
- Velocity field with parabolic profile ($U_{\text{max}} = 1 \text{ m/s}$) using **groovyBC**
- Addition of scalar transport equation for $C$, declaration of volScalarField and other parameters in createFields.H

```cpp
volScalarField AF = fanzy*pow(((1-C)*C),2); //where AF is the source term

solve
{
    fvm::ddt(C)
    +fvm::div(phi, C)
    -fvm::laplacian(nu, C) == AF
};

dimensionedScalar fanzy
{
    transportProperties.lookup("fanzy")
};

Info<< "Reading field C\n" << endl;
volScalarField C
{
    I0object
    {
        "C",
        runTime.timeName(),
        mesh,
        I0object::MUST_READ,
        I0object::AUTO_WRITE
    },
    mesh
};

solve(UEqn == -fvc::grad(p));

// --- PISO loop
for (int corr=0; corr<nCorr; corr++)
{
    include "Ceqn.H"
    volScalarField rUA = 1.0/UEqn.A();
}
```
Flame in a box results

Time (seconds) = 0.005

Time (seconds) = 0.01

Time (seconds) = 0.02

Time (seconds) = 0.03
• Once the transport equation and source term are working, it is possible to consider the progress variable with the values given from a table (1D manifold).

• For each value of C, which goes from 0 (unburnt) to 1 (burnt) there is a specific value for the source term.

• Interpolation is necessary, considering the discrete values available in the table

• After the method is working for a laminar case, it will be possible to include the compressibility and turbulence for a 3D mesh.

• Preferential Diffusion for H₂ effects will be added after Methane simulations are validated.

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Thank you for your attention