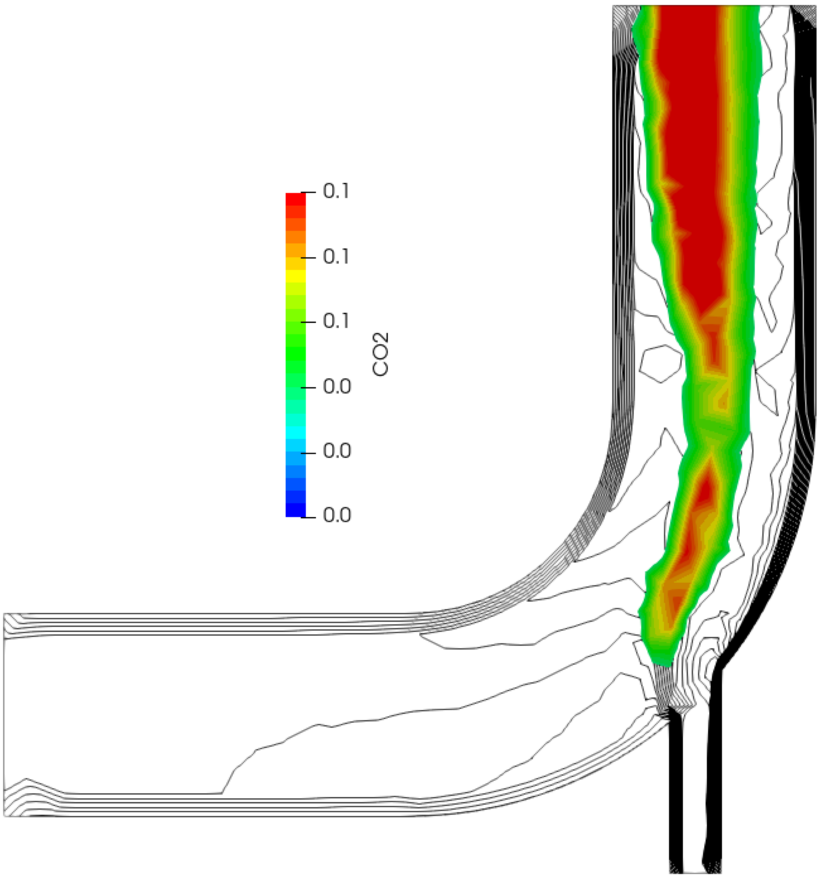
Tutorial Eleven

Reaction



Bahram Haddadi

ENGINEERING
FLUID
DYNAMICS

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Contributors:

- Bahram Haddadi
- Christian Jordan
- Michael Harasek
- Clemens Gößnitzer
- Sylvia Zibuschka
- Yitong Chen

Technische Universität Wien

Institute of Chemical, Environmental

& Bioscience Engineering

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Available from: www.fluiddynamics.at

Background

In computational fluid dynamics (CFD) and chemical reaction modeling, two commonly used approaches to simulate reactive flows are the Partially Stirred Reactor (PaSR) Model and the Eddy Dissipation Concept (EDC) Model. These models help in understanding and predicting how chemical reactions occur in different flow environments, such as combustion, industrial chemical processing, pollutant dispersion, and atmospheric chemistry.

1. Partially stirred reactor (PaSR) Model

Partially stirred rector (PaSR) model is used to model thermodynamic and chemical reactions numerically, for example, combustion. In the PaSR approach, a computational cell is split into two different zones: a reacting zone and a non-reacting zone. The reacting zone is modeled as a perfectly stirred reactor (PSR), and all reactants are assumed to be perfectly mixed with each other.

For the reactor, we are interested in three concentrations, 1) mean concentration of key component in the feed, c_{in}; 2) mixture concentration in the reacting zone, c; 3) concentration at the reactor exitc_{exit}.

In the reacting zone, reaction occurs for a duration of τ_c, so the concentration of mixture changes from c_{in} to c. In the non-reacting zone, the reacted mixture is getting mixed up with the non-reacted mixture for a duration of τ_{mix}, resulting in the final exit concentration, c_{exit}.

A key parameter to be calculated in this model would be the reaction rate, and it is clear that the reaction rate is proportional to the ratio of the chemical reaction time to the total conversion time in the reactor (i.e. sum of reacting and mixing time), κ_k:

$$\kappa_k = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

2. Eddy dissipation concept (EDC) Model

The Eddy Dissipation Concept (EDC) model looks at the interaction between reaction and turbulence, where the overall reaction rate is controlled by turbulent mixing. It is widely used for combustion modeling for a great variety of combustion environments with great success.

It is assumed in the model that most reaction takes place within fine turbulence structures, which are modeled as perfectly-mixed reactors. We need to know the reaction mass fraction and the mass transfer rate between the fine structures and its surrounding fluid.

The mass fraction occupied by the fine structures, γ^*, is expressed as:

$$\gamma^* = \left\{\frac{u^*}{u'}\right\}^2$$

Where u^* is the mass average fine structure velocity. The fine structures are in regions with nearly constant turbulent kinetic energy given by u'^2.

The mass transfer rate between fine structure and surrounding fluid per unit of fluid and per unit of time is modeled as:

$$\dot{m} = 2 \cdot \frac{u^*}{L^*} \cdot \gamma^*$$

where L^* is the characteristic length of the fine structure.

multicomponentFluid – reactingElbow

Tutorial outline

Use the multicomponentFluid solver; simulate combustion of CH_4 and O_2 in a mixing elbow:

- Use the two times finer Hex mesh from Example One
- Domain initially filled with N_2
- velocity-inlet-5:
  - Velocity: 1 m/s
  - Mass fractions: 23 % O_2, 77 % N_2
  - Temperature: 800 K
- velocity-inlet-6:
  - Velocity: 3 m/s
  - Mass fractions: 50 % CH_4, 50 % N_2
  - Temperature: 293 K
- Operating pressure: 10^5 Pa
- Operating temperature: 298 K
- Isolated walls

Objectives

- Understanding multi-species and reaction modeling in OpenFOAM®

Data processing

Evaluate your results in ParaView.

1. Pre-processing

1.1. Copying tutorial

Copy the following tutorial to your working directory:

`$FOAM_TUTORIALS/multicomponentFluid/counterFlowFlame2D`

Copy the GAMBIT® mesh from Tutorial One (two times finer mesh) to the case main directory.

1.2. 0 directory

Update all the files in 0 directory with new boundary conditions, e.g. U:

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * * *//

dimensions      [0 1 -1 0 0 0 0];

internalField   uniform (0 0 0);

boundaryField
{
    wall-4
    {
        type            fixedValue;
        value           uniform (0 0 0);
    }

    velocity-inlet-5
    {
        type            fixedValue;
        value           uniform (1 0 0);
    }

    velocity-inlet-6
    {
        type            fixedValue;
        value           uniform (0 3 0);
    }

    pressure-outlet-7
    {
        type            zeroGradient;
    }

    wall-8
    {
        type            fixedValue;
        value           uniform (0 0 0);
    }

    frontAndBackPlanes
    {
        type            empty;
    }
}

// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * * *//
```

The reaction taking place in this simulation CH_4 combusting with O_2 creating CO_2 and H_2O. N_2 is the non-reacting species. The boundary conditions and initial value of all species should be defined in the 0 directory. These values are mass fractions (between 0 and 1) and dimension less, e.g. CH$_4$:

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

dimensions      [0 0 0 0 0 0 0];

internalField   uniform 0.0;

boundaryField
{
    wall-4
    {
        type            zeroGradient;
    }

    velocity-inlet-5
    {
        type            fixedValue;
        value           uniform 0; //no CH4 at this inlet
    }

    velocity-inlet-6
    {
        type            fixedValue;
        value           uniform 0.5; //50% CH4 mass fraction at this inlet
    }

    pressure-outlet-7
    {
        type            zeroGradient;
    }

    wall-8
    {
        type            zeroGradient;
    }

    frontAndBackPlanes
    {
        type            empty;
    }
}

// ************************************************************************* //
```

Note: If the file for a species does not exist in the 0 directory, the values from Ydefault will be used for that species.

Note: For the `pressure-outlet-7` set the species boundary conditions to `zeroGradient`.

1.3. constant directory

In the *physicalProperties* file the physical properties of the species can be set:

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * * *//
thermoType
{
    type            hePsiThermo;
    mixture         coefficientWilkeMultiComponentMixture;
    transport       sutherland;
    thermo          janaf;
    energy          sensibleEnthalpy;
    equationOfState perfectGas;
    specie          specie;
}
```

```
defaultSpecie N2;

#include "thermo.compressibleGas"
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * *//
```

The mixture type is set to a multi-component mixture for calculating the mixture properties and the heat capacities are calculated using “janaf polynomials”.

N_2 is defines as `defaultSpecie`. In reaction solvers in OpenFOAM® the default specie is calculated explicitly using the mass balance equation (to satisfy mass conservation):

$$\mathit{mass\ fraction\ of\ inert\ specie} = 1 - \sum \mathit{mass\ fraction\ of all\ other\ species}$$

Involved species are listed in the *thermo.compressibleGas* file, which was included at the end of *physicalProperties* file. The species in this simulation are O_2, H_2O, CH_4, CO_2 and N_2. They are defined in the `species` sub-dictionary:

```
species
(
    O2
    H2O
    CH4
    CO2
    N2
);
```

The reactions are addressed in the *reactions* file:

```
reactions
{
    methaneReaction
    {
        type     irreversibleArrhenius;
        reaction "CH4 + 2O2 = CO2 + 2H2O";
        A        5.2e16;
        beta     0;
        Ta       14906;
    }
}
```

in the `reactions` sub-dictionary. The reaction of methane combustion is defined and it is of `type` irreversible Arrhenius reaction, `irreversibleArrhenius`.

In the Tutorial Two it was explained that the coefficients for calculating gas mixture properties are defined in the `mixture` sub-dictionary because it was a homogeneous mixture. However, in this example the mixture is not homogenous so coefficients for calculating properties of each species are needed separately to calculate mixture properties based on each cell composition. The coefficients of each species are defined in the *thermo.compressibleGas* file from the constant directory. For example, the `O2` coefficients for each model are shown below:

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * *//

O2
{
    specie
    {
        molWeight       31.9988;
    }
    thermodynamics
    {
        Tlow            200;
        Thigh           5000;
        Tcommon         1000;
        highCpCoeffs    ( 3.69758 0.00061352 -1.25884e-07 1.77528e-11 -
                          1.13644e-15 -1233.93 3.18917 );
        lowCpCoeffs     ( 3.21294 0.00112749 -5.75615e-07 1.31388e-09 -
                          8.76855e-13 -1005.25 6.03474 );
    }
    transport
    {
        As              1.753e-06;
        Ts              139;
    }
}
…

// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * */
```

In the `thermodynamics` sub-dictionary, the janaf polynomial model coefficients for calculating the heat capacity can be found and in `transport` the sutherland model coefficients for viscosity are stored.

1.4. system directory

By setting the `adjustTimeStep` to `yes` in the *controlDict*, the solver automatically ignores `deltaT`, and calculates the `deltaT` based on the maximum Courant number `maxCo` defined for it. Change the `endTime` to `120` (approximately one time the volumetric residence time based on velocity-inlet-5) and `writeInterval` to `10`, to write every 10 s to case directory.

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * */

application     foamRun;

solver          multicomponentFluid

startFrom       startTime;

startTime       0;

stopAt          endTime;

endTime         120;

deltaT          1e-6;

writeControl    adjustableRunTime;

writeInterval   10;

purgeWrite      0;

writeFormat     ascii;

writePrecision  6;

writeCompression off;

timeFormat      general;

timePrecision   6;
```

```
runTimeModifiable true;

adjustTimeStep  yes;

maxCo           0.4;

// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* * * * * *//
```

2. Running simulation

```
>fluentMeshToFoam fineHex.msh
```

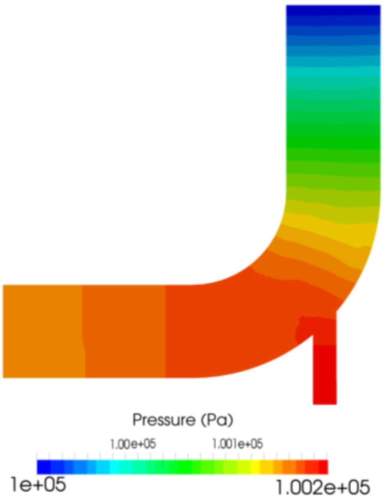
After converting the mesh, check the boundary file in the constant/polyMesh directory and change the `type` and `inGroups` of boundary `frontAndBackPlanes` from `wall` to `empty` (it is a 2D simulation).

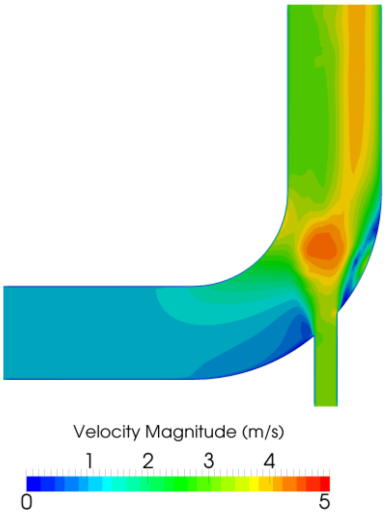
```
>foamRun -solver multicomponentFluid
```

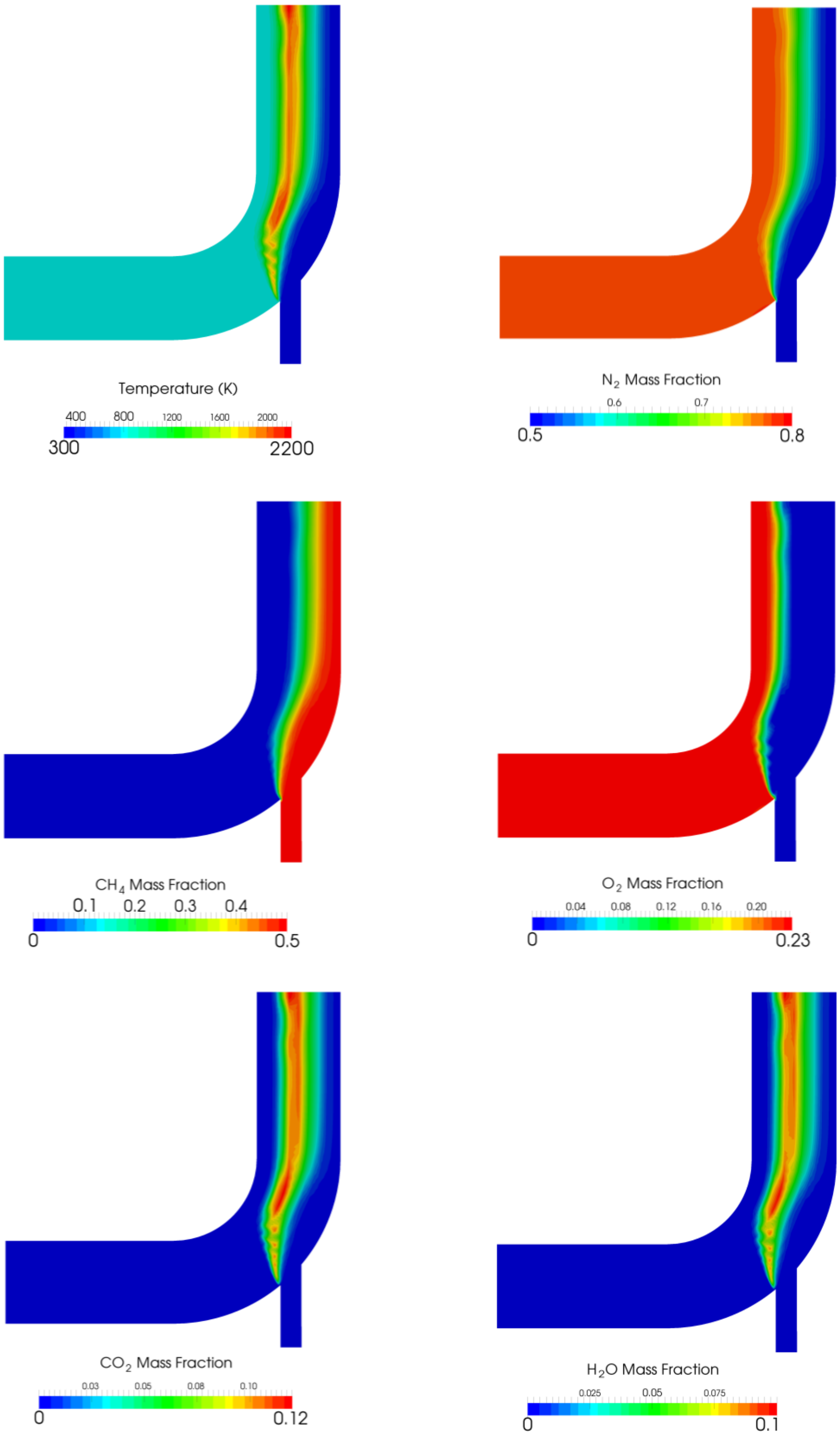
```
>foamToVTK
```

3. Post-processing

The simulation results at 120 s are as follows:







Simulation results after 120 s