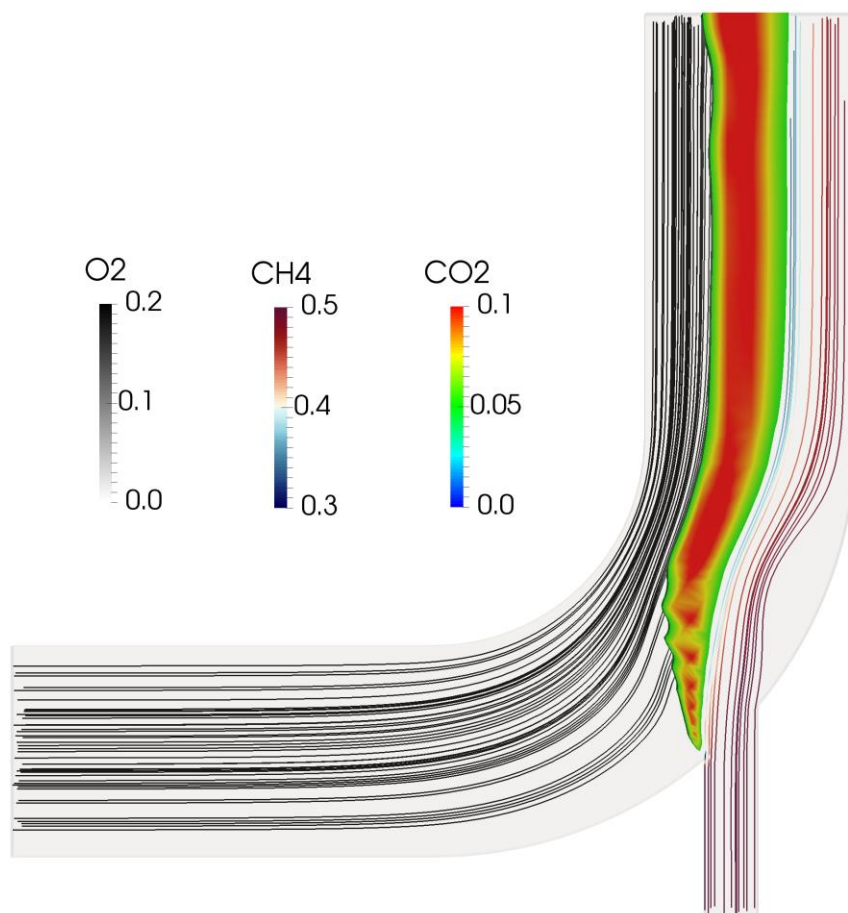


Tutorial Eleven

Reaction



6th edition, April 2023



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Background

There are two common approaches in modeling reactions:

1. Partially stirred reactor (PaSR) Model

Partially stirred reactor (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 exit c_{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 located 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.

reactingFoam – reactingElbow

Tutorial outline

Use the reactingFoam solver; simulate combustion of CH₄ and O₂ in a mixing elbow:

- Use the two times finer Hex mesh from Example One
- Domain initially filled with N₂
- velocity-inlet-5:
 - Velocity: 1 m/s
 - Mass fractions: 23 % O₂, 77 % N₂
 - Temperature: 800 K
- velocity-inlet-6:
 - Velocity: 3 m/s
 - Mass fractions: 50 % CH₄, 50 % N₂
 - Temperature: 293 K
- Operating pressure: 10⁵ 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/combustion/reactingFoam/laminar/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 CH₄ combusting with O₂ creating CO₂ and H₂O. N₂ is the non-reacting species. The boundary conditions and


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

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

N₂ is defines as `inertSpecie`. In reaction solvers in OpenFOAM® the inert specie is calculated explicitly using the mass balance equation (to satisfy mass conservation):

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

Involved species are listed in the `thermo.compressibleGas` file, which was included at the end of `physicalProperties` file. The species in this simulation are O₂, H₂O, CH₄, CO₂ and N₂. 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 `irreversibleArrhenius` 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             1.67212e-06;
    Ts             170.672;
  }
}
...
// * * * * *
* * * * *//

```

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      reactingFoam;

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
```

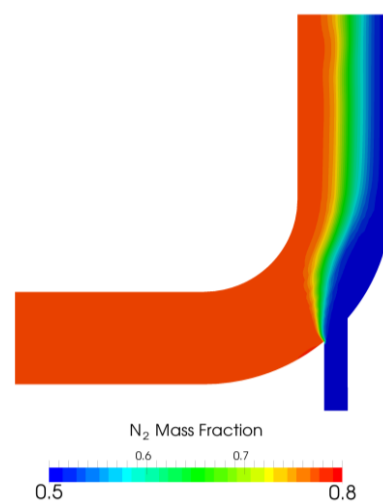
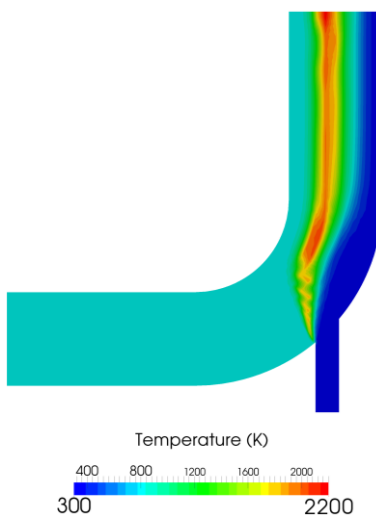
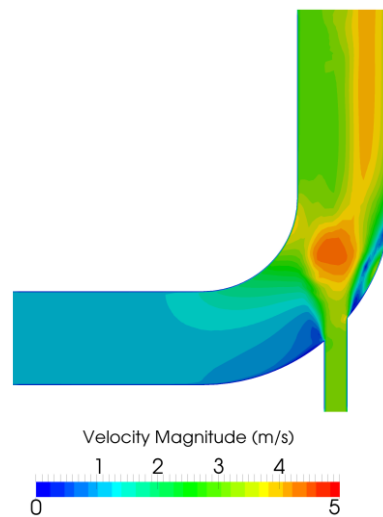
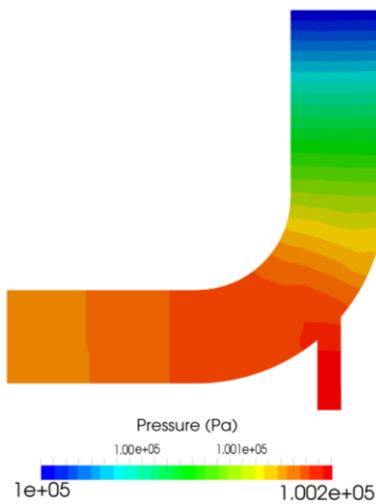
After converting the mesh, check the boundary file in the constant/polyMesh directory and change the `type` and `inGroups` of boundary `frontAndBackPlanes` from `wall` to `empty` (it is a 2D simulation).

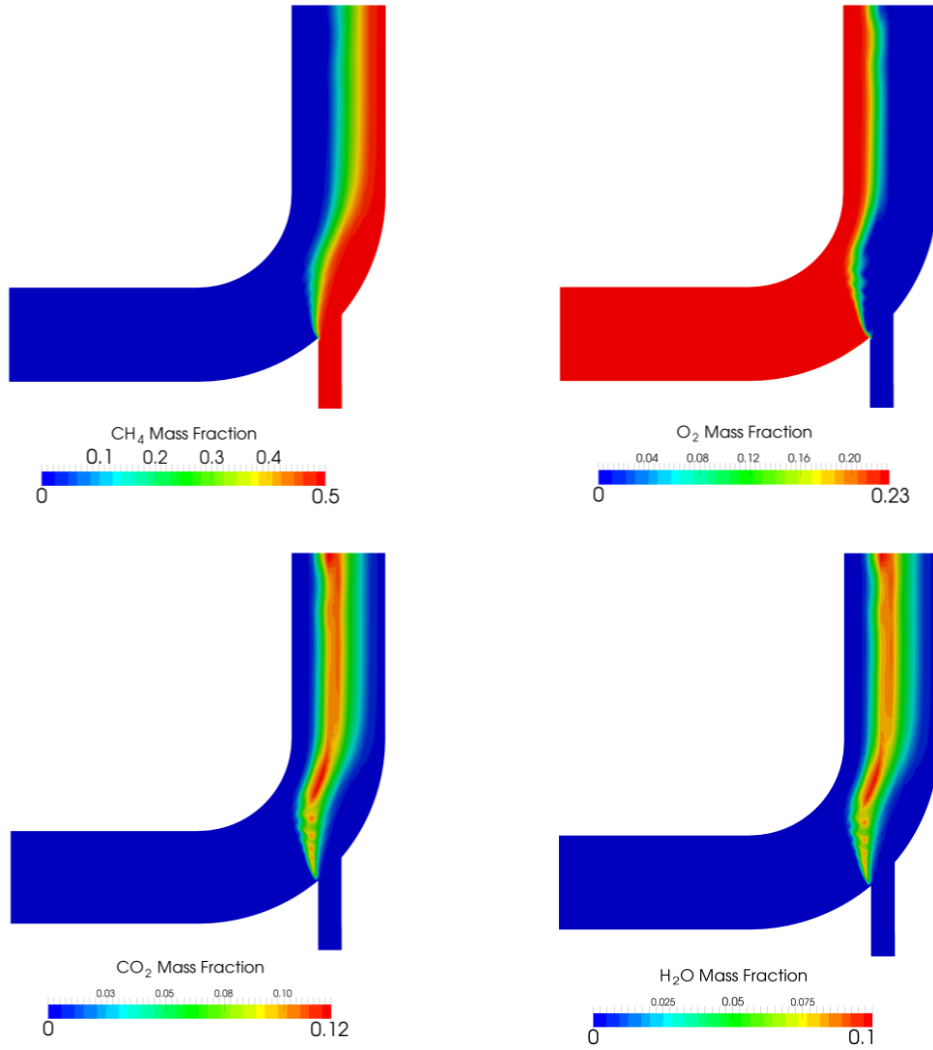
```
>reactingFoam
```

```
>foamToVTK
```

3. Post-processing

The simulation results at 120 s are as follows:





Simulation results after 120 s

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