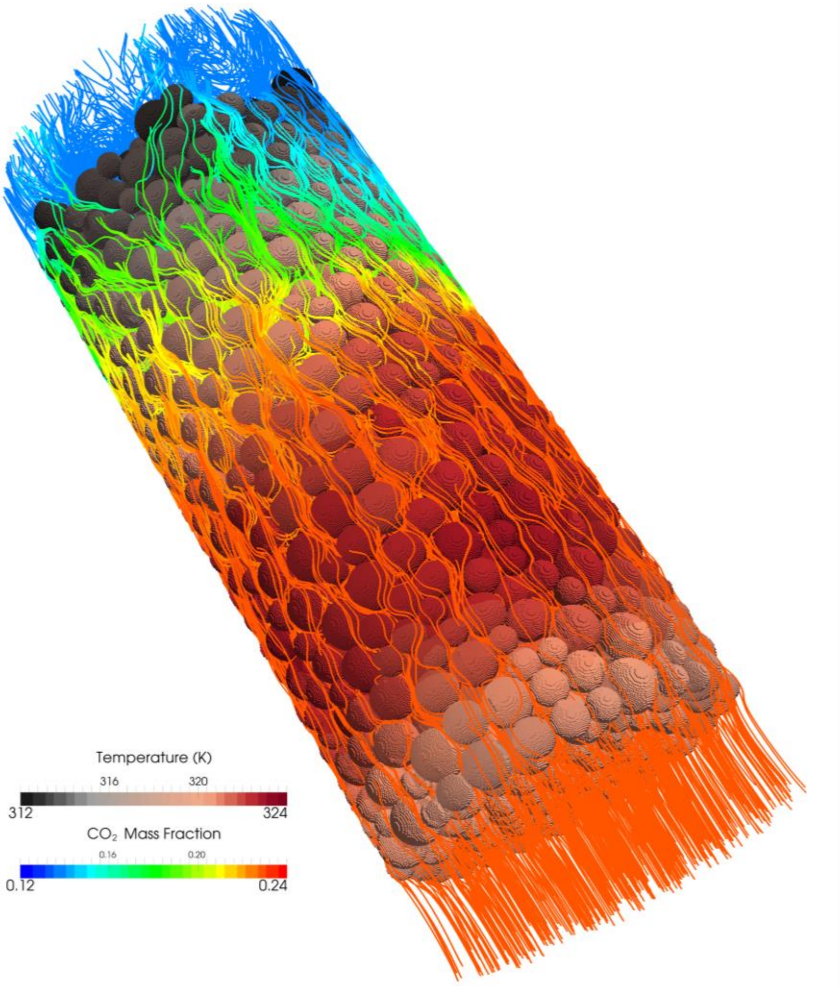
OpenFOAM® Basic Training

Tutorial Eleven



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Cover picture from:

- Bahram Haddadi, The image presented on the cover page has been prepared using the Vienna Scientific Cluster (VSC).

reactingFoam – reactingElbow

Simulation

Use the reactingFoam solver, simulate combustion of CH_4 and O_2 in a mixing elbow:

- Use the two times finer Hex mesh from Example One
- 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

Objective

- Understanding multi-species and reaction modeling in OpenFOAM®

Post processing

Evaluate your results in ParaView.

Step by step simulation

Copy tutorial

Copy the following tutorial to your working directory:

~/OpenFOAM/OpenFOAM-2.3.0/tutorials/combustion/reactingFoam

/ras/counterFlowFlame2D

Copy the GAMBIT mesh from example one (two times finer mesh) to the case main directory.

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 condition 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.

constant directory

In the thermophysicalProperties file the physical properties of the species can be set:

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

inertSpecie N2;

chemistryReader foamChemistryReader;

foamChemistryFile "$FOAM_CASE/constant/reactions";

foamChemistryThermoFile "$FOAM_CASE/constant/thermo.compressibleGas";
// ************************************************************************* //
```

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

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

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

The species and the reactions are addressed using `foamChemistryFile`. In this simulation reactions and species are read from reactions file in the constant directory:

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

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

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. In the `reactions` sub-dictionary, reactions are specified. The reaction of methane combustion is defined and it is of `type` irreversible Arrhenius reaction, `irreversibleArrheniusReaction`.

In the Example Two it was explained the coefficients for calculating gas mixture properties are defined in the `mixture` sub-dictionary because it was a homogeneous mixture. But 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 `foamChemistryThermoFile`, which reads the file thermo.compressibleGas from the constant directory, e.g. for `O2` coefficients for each model is mentioned bellow:

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

O2
{
    specie
    {
        nMoles          1;
        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.

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 `writeTimeInterval` 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;

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

Running simulation

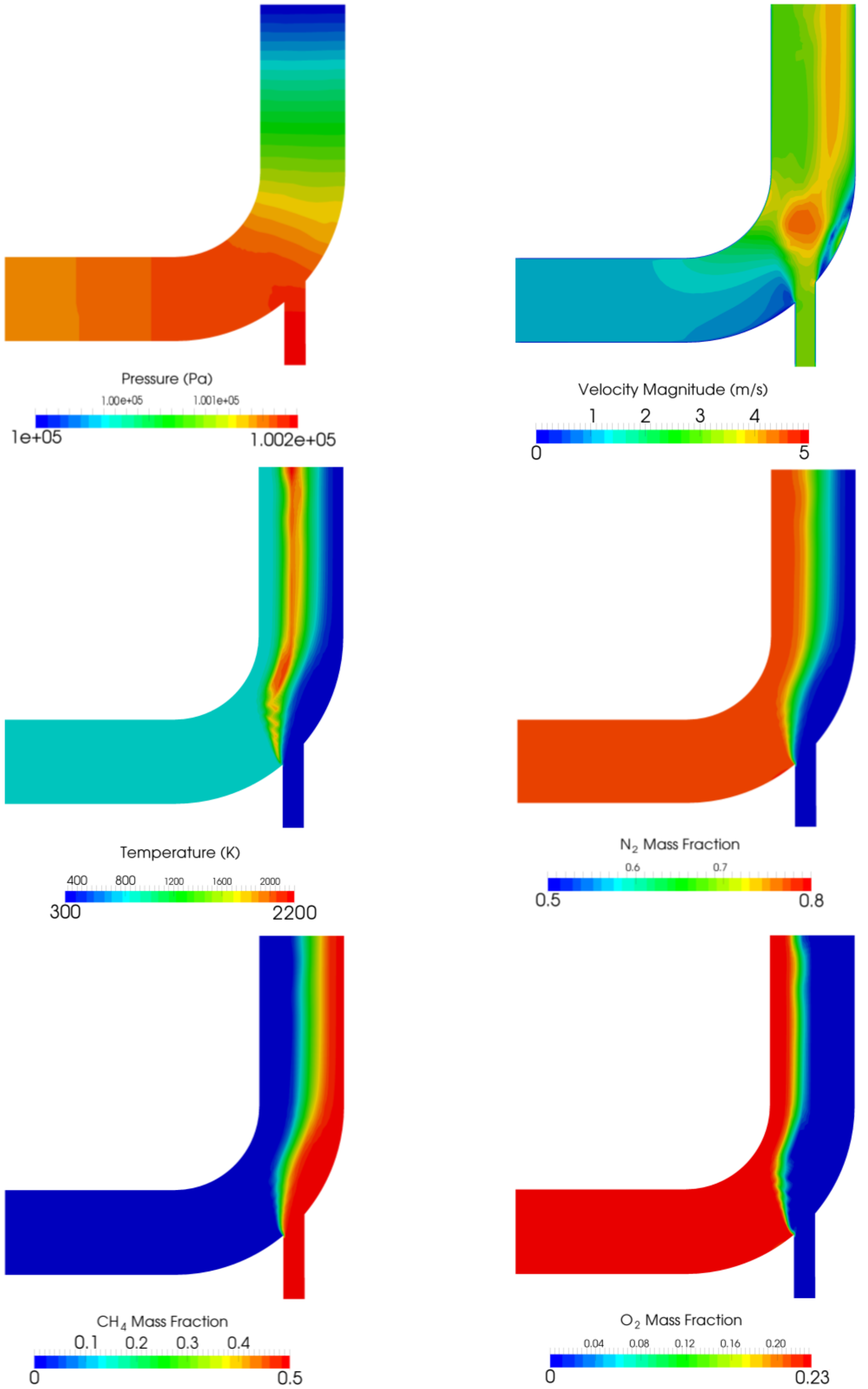
```
>fluentMeshToFoam fineHex.msh
```

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
```

The simulation results are as follows:



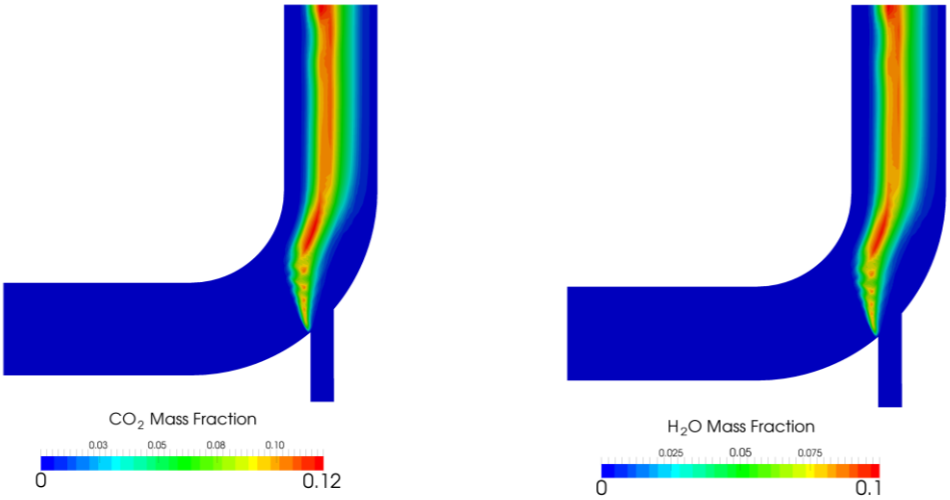


Figure 11.1 Simulation results after 120 s