Tutorial Ten Residence Time Distribution



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Compatibility:

- OpenFOAM[®] 5.0
- OpenFOAM[®] v1712

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Background

In this tutorial we will carry out Residence Time Distribution (RTD) analysis of fluid flow through a T-junction pipe.

1. Residence Time Distribution (RTD)

Residence time distribution is a probability distribution function that provides information about the amount of time a tracer element spends within a process unit, such as a reactor or a column. RTD analysis is important because in almost all real-life processes, the mixing is not ideal and chemical engineers will need RTD to analyze the real mixing characteristics inside for example, a continuously stirred reactor. They can also use RTD analysis and to obtain information about the flow pattern, back mixing and bypassing behavior of a process unit.

2. Tracer Analysis



Tracer analysis and RTD distribution of an ideal process

Sometimes a radioactive tracer is usually used to determine RTD of a process unit. Based on the above diagram, first the tracer is injected into the inlet, and then the exit tracer concentration, C(t), is measured at regular time intervals. This allows the exit age distribution, E(t), to be calculated.

$$E(t) = \frac{C_T(t)}{\int_0^\infty C_T(t) dt} = \frac{Tracer \ concentration \ at \ time \ t}{Total \ tracer \ concentration}$$

It is clear from the above equation that the fraction of tracer molecules exiting the reactor that have spent a time between t and t + dt in the process unit is E(t)dt. Since all tracer elements will leave the unit at some point, RTD satisfies the following relationship:

$$\int_0^\infty E(t)\,dt=1$$



simpleFoam & scalarTransportFoam - TJunction

Simulation

Use the simpleFoam and scalarTransportFoam to simulate the flow through a square cross section T pipe and calculate RTD (Residence Time Distribution) for both inlets using a step function injection:

- Inlet and outlet cross sections: $1 \times 1 \text{ m}^2$
- Gas in the system: air at ambient conditions
- Operating pressure: 10⁵ Pa
- Inlet 1: 0.1 m/s
- Inlet 2: 0.2 m/s

Objectives

- Understanding RTD calculation using OpenFOAM[®]
- Using multiple solver for a simulation

Data processing

Plot the step response function and the RTD curve.



1. Pre-processing

1.1. Copy tutorial

Copy the following tutorial to your working directory as a base case:

\$FOAM TUTORIALS/incompressible/simpleFoam/pitzDaily

1.2. 0 directory

Update p, U, nut, nuTilda, k and epsilon files with the new boundary conditions, e.g. U:

```
// * * * * * * * * * *
                                            * *
                                                                                * * * * * * * * //
dimensions
               [0 1 -1 0 0 0 0];
internalField uniform (0 0 0);
boundaryField
{
    inlet one
    {
                     fixedValue;
uniform (0.1 0 0)
        type
        value
    1
    inlet two
    {
        type
                       fixedValue;
                       uniform (-0.2 0 0)
       value
    }
   outlet
    {
                       zeroGradient;
        type
    }
    walls
    {
                       fixedValue;
        type
        value
                       uniform (0 0 0)
    }
                                                                      * * * * * * * * * * * * * //
    * * * * *
                                                *
```

1.3. constant directory

Check turbulenceProperties file for the turbulence model (kEpsilon).

```
// * * * * * * * *
                  * * *
                                           +
                                              * * *
                                                       * * *
                                                            * * * * * * * * * * * * * * * //
simulationType RAS
RAS
{
      RASModel
                     kEpsilon;
       turbulence
                      on;
       printCoeffs
                      on;
                                   * * * * * * * * * * * * *
                                                                    * * * * * * * * * * * //
11
```

1.4. system directory

(

Edit the blockMeshDict to create an appropriate geometry.



(0 4 0) // 0 (0 3 0) // 1 (3 3 0) // 2 (3 0 0) // 3 (3 0 0) // 3 (4 0 0) // 4 (4 3 0) // 5 (7 3 0) // 6 (7 4 0) // 7 (7 4 0) // 8 (3 4 0) // 9 (0 4 1) // 10 (0 3 1) // 10 (0 3 1) // 11 (3 3 1) // 12 (3 0 1) // 13 (4 0 1) // 14 (4 3 1) // 15 (7 3 1) // 16 (7 4 1) // 17 (4 4 1) // 18 (3 4 1) // 19); blocks (hex (0 1 2 9 10 11 12 19) (10 30 10) simpleGrading (1 1 1) hex (9 2 5 8 19 12 15 18) (10 10 10) simpleGrading (1 1 1) hex (8 5 6 7 18 15 16 17) (10 30 10) simpleGrading (1 1 1) hex (2 3 4 5 12 13 14 15) (30 10 10) simpleGrading (1 1 1)); edges (); patches (patch inlet_one ((0 10 11 1)) patch inlet_two ((7 6 16 17)) patch outlet ((4 3 13 14)) wall walls ((0 1 2 9) (2 5 8 9) (5678) (2 3 4 5) (10 19 12 11) (19 18 15 12) (18 17 16 15) (15 14 13 12) (0 9 19 10) (9 8 18 19) (8 7 17 18) (2 1 11 12) (3 2 12 13) (5 4 14 15) (6 5 15 16))); mergePatchPairs (); * * * * * * * * * * * // 11



2. Running simulation

>blockMesh



>simpleFoam

Wait for simulation to converge. After convergency check the results to be sure the solution is converged.

>foamToVTK

The simulation results are as follows (results are on the cut plane in the middle):



Simulation results after convergence (65 iterations)

3. RTD calculation

3.1. Copy tutorial

Copy following tutorial to your working directory:

\$FOAM_TUTORIALS/basic/scalarTransportFoam/pitzDaily

3.2. 0 directory

Delete the U file and replace it with the calculated velocity field from the first part of the tutorial (use the latest time step velocity field from previous part of simulation to calculate RTD for this geometry). There is no need to modify or change it. The solver will use this field to calculate the scalar transportation.



Update T (T will be used as an inert scalar in this simulation) file boundary conditions to match new simulation boundaries, to calculate RTD of the inlet_one set the internalField value to 0, T value for inlet one to 1.0 and T value for inlet two to 0.

3.3. system directory

Replace the blockMeshDict file with the one from the first part of tutorial.

In the controlDict file change the endTime from 0.1 to 120 (approximately two times ideal resistance time) and also deltaT from 0.0001 to 0.1 (Courant number approximately 0.4).

4. Running Simulation

```
>blockMesh
>scalarTransportFoam
>foamToVTK
```

5. Post-processing



Contour plots scalar T at 120 s for inlet 1

5.1. Calculating RTD

To calculate RTD the average T value at the outlets should be calculated first. The "integrate variables function" of ParaView can be used for this purpose.

>foamToVTK

Load the outlet VTK file into paraview using following path:

File > Open > VTK > outlet > outlet_..vtk > OK > Apply

Select T from variables menu, and then integrate the variables on the outlet:

Filters > Data Analysis > Integrate Variables > Apply

The values given in the opened window are integrated values in this specific time step. By changing the time step values for different time steps are displayed. As mentioned before, the average value of the property is needed. Therefore, these values should be divided by outlet area to get average values $(1m \times 1m)$.

The same procedure should be followed for calculating RTD of inlet_two, except T value for inlet_one should be 0 and for inlet_two it should be 1.0.





Average value of T on the outlet for two inlets versus time

The average value of T for each outlet approaches a certain constant value, which is the ratio of that scalar mass inlet to the whole mass inlet. For plotting data over time "Plot Selection Over Time" option in ParaView can be used, in the opened SpreadSheetView window (IntegrateVariables) select the set of data which you want to plot over time and then:

Filters > Data Analysis > Plot Selection Over Time > Apply

Next, to obtain the RTD plots, simply calculate the gradient of change in average value of T on the outlet from time 0 to 120s, export the data to Excel, and plot the results.



RTD of two inlets