



Lab Migration Report

on

To Study Residence Time Distribution Under Laminar Flow
Using Passive Scalar In CFD Simulations

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1. Governing Equations and Models

1.1 Problem Statements

To study Residence Time Distribution (RTD) for laminar flow using the passive scalar as tracer.

Objective: - To learn to use passive scalar to model and simulate tracer (non-reactive chemical species) in CFD simulations. Also to learn as to how to carry out RTD study for a given geometry under laminar flow condition. Then using passive scalar as tracer to study RTD for laminar flow in a straight cylinder tube. RTD study is inherently transient in nature so unsteady-state solver is to be used for this study. The study is generalized in nature and can be extended to other geometries as well.

1.2 Governing Equations

The continuity and momentum conservation equations are solved for the calculation of flow parameters like velocity and pressure. The conservation equations are expressed below:

Continuity Equation:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

Momentum Equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} (\nabla p) + \nu \nabla^2 \mathbf{u} \quad (2)$$

where ν is the kinematic viscosity, ρ is the density, \mathbf{u} is the velocity vector and p is the pressure.

A concentration transport equation is incorporated for the calculation of passive scalar concentration using modified solver.

Equation to model the transport of Passive Scalars (S1):

$$\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S = \nabla \cdot (\Gamma \nabla S) + S_c \quad (3)$$

Where S is the passive scalar, Γ is the diffusion coefficient and S_c is the source term of the passive scalar. The source term would be required to model chemical reaction related to S which would be 0 here. For more information regarding the source term, you can refer to this document [Theory](#).

Residence Time Distribution calculations for laminar flow – Residence time distribution is calculated based on time taken by different fluid elements from inlet to outlet in a given geometry. The flow needs to be fully developed from inlet onwards. For laminar flow, this will lead to parabolic velocity profile at the inlet itself. The residence time of any fluid element is given by $\tau = L/u$, where L is the length of the path and u is the velocity of the fluid element. Thus, the average residence time based on average velocity would be $\bar{\tau} = L/u_{avg}$. For laminar flow, $u_{avg} = u_{max}/2$, and the maximum velocity exists in the center of the flow. So, the central fluid element will take half the time compared to any fluid element will take on an average, i.e. $\theta = t/\bar{\tau} = 0.5$. Since the flow is in straight cylinder, so each fluid element across the inlet cross-section will reach the same relative position at outlet based on its inlet velocity without radial mixing. If tracer is

injected throughout the inlet cross-section, the first appearance of tracer will occur at $\theta = 0.5$, and then it will rise further to reach concentration same as inlet. Afterwards no variation in outlet tracer concentration is observed and hence the exercise of measuring RTD will be stopped. So, the study of RTD is inherently transient in nature.

After the first appearance, the tracer for plug flow, the velocity profile remains flat throughout from inlet to outlet, so there the first appearance occurs at same time as average residence time, i.e. $\theta = 1$. In reality, plug flow is approached using turbulent flows.

1.3 Geometry and Mesh.

The domain is a straight cylindrical tube with length of 0.5 m and diameter of the cross section as 0.01 m. The geometry is 3D. The geometry is long enough for the flow to fully develop. The scalar S1 will be injected at the inlet. The flow is already fully developed for laminar flow as parabolic velocity profile is taken at the inlet as boundary condition.

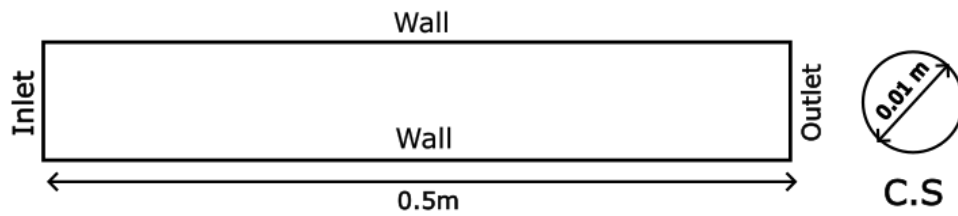


Fig 1: Schematic Diagram of Computational Domain

The meshing is done using blockMesh utility, openFOAM's built-in tool. The geometry is divided into 5 blocks and 18 vertices and the number of cells is 672000 for this case. The user is free to choose different types of meshing and numbers to get the similar results. For the detailed meshing process, one can go through the openFOAM spoken tutorial number 6. [spoken tutorial](#)

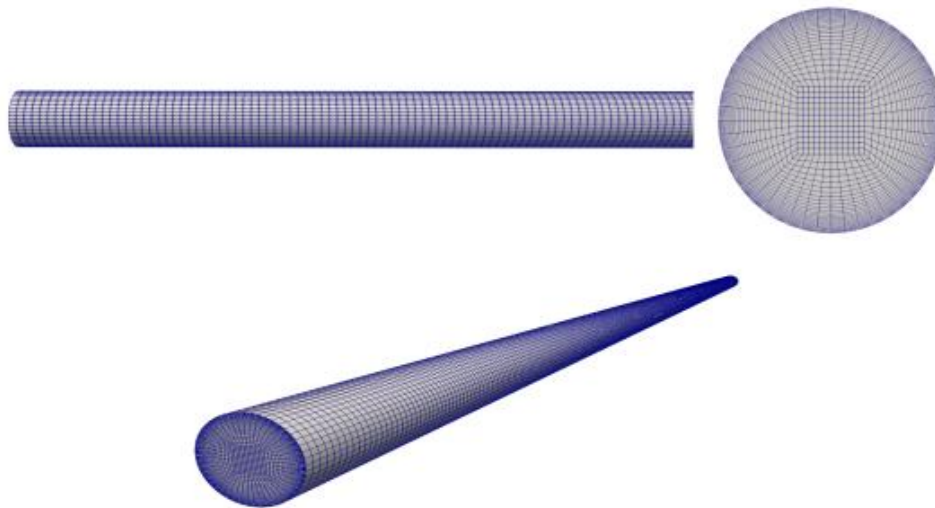


Fig 2: Mesh Generation using BlockMesh

1.4 Solver Setup

1.4.1 Fluid Properties

Water at room temperature is used as the fluid and the thermo physical properties of water at 300K are taken for calculations. The kinematic viscosity of water at room temperature is $8.58 \times 10^{-7} \text{ m}^2/\text{s}$. The average velocity of the flow is 0.1 m/s , which is half the maximum velocity as per given parabolic velocity profile. The Reynolds number is expressed as:

$$Re = \frac{U_{avg} * D}{\nu}$$

Where U_{avg} is the average velocity, D is the diameter of the tube and ν is the kinematic viscosity. For the above input flow parameters, the Reynolds number of the flow is 1165 which is in the laminar regime (<2100). So, a laminar model is used for the simulation.

Flow Parameters	Value
Max. Velocity (U_{max})	0.2 m/s
Average Velocity (U_{avg})	0.1 m/s
Density (ρ)	1000 kg/m ³
kinematic viscosity (ν)	$8.58 \times 10^{-7} \text{ m}^2/\text{s}$
Reynolds No.	1165
Scalar Diffusivity constant (DS1)	0 m ² /s
Scalar Kinetic rate coefficient(kS1)	0 s ⁻¹
S_c	kS1*S1
Residence Time	5 sec.

1.4.2 Case Setup

The case files for the current session are available in this [link](#). Download and extract these files into your run directory. A general overview of the setup is explained below:

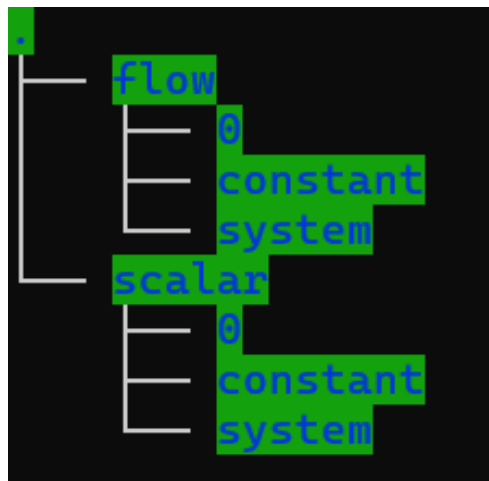


Fig 3: Tree diagram of the main folder

The main folder consists of flow and scalar folder as in Fig 3. The flow folder consists of files to solve the flow field. The scalar folder has the necessary files to simulate the scalar. Since, newScalarTransportFoam, does not solve for velocity, we need to first simulate the flow field. So, initially, the steady state velocity field is solved using flow folder. This flow field is then used by the scalar to move along the flow through local velocity. This is explained more in section 1.6. The folders can be further expanded along this tree:

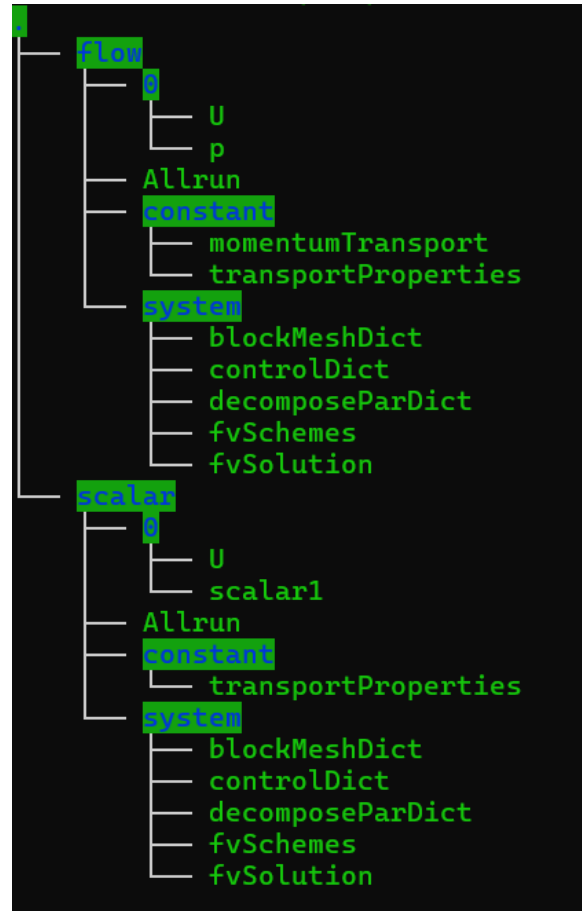


Fig 4: Detailed Tree diagram of the directories

Flow case setup:

The initial and boundary conditions for velocity and pressure are provided in the U and p files of 0 directory. You can see the boundary conditions by accessing these files. The boundary conditions are further explained in the next section.

- The kinematic viscosity of fluid is provided in **constant/transportProperties**.

```

transportModel  Newtonian;

nu              [0 2 -1 0 0 0 0] 8.58E-07;

```

- Similarly, in momentumTransport dictionary, type of model for the simulation is provided. In our case, we have used the laminar model.

```
FoamFile
{
    format      ascii;
    class       dictionary;
    location    "constant";
    object      momentumTransport;
}

simulationType laminar;
```

- The blockMeshDict consists of mesh information and the controlDict dictionary consists of case controls like timing, write information etc.
- System/decomposeParDict dictionary is used for parallel computing.

The steps for the simulation are provided below:

1. First, you need to navigate to the flow folder in your run directory.

```
cd $FOAM_RUN
```

```
cd RTD_Parabolic/flow
```

2. The Allrun file consists of necessary commands to run the simulation. Type **./Allrun** and press enter.

The Allrun file consists of the following commands:

```
blockMesh
decomposePar
mpirun -np 6 simpleFoam -parallel
reconstructPar
```

The blockMesh command is used to generate the mesh. Command decomposePar decomposes the domain into subdomains and assigns the number of processors to these subdomains based on the method like simple, scotch etc. In this case, 6 processors are used in parallel and simpleFoam solver is used. The user is free to choose different numbers of core based on availability and requirement. Finally, reconstructPar command is used to reconstruct a single domain from the processor sub-domains.

Scalar case setup:

Solver modification and compilation

To simulate the passive scalar, we have modified the scalarTransportFoam solver and named it newScalarTransportFoam. To make executables for this solver, we will need to compile it first. To do that follow the steps given below:

1. Open your terminal and navigate to the run directory.
cd \$FOAM_RUN
2. Navigate to the solver folder by typing the following command.
cd newScalarTransportFoam
3. Compile the solver by typing the following command and press enter.
wclean
wmake

After this the following steps are required.

1. First, you need to navigate to the flow folder.

cd RTD_Parabolic/scalar

2. The Allrun file consists of necessary commands to run the simulation. Type **./Allrun** and press enter.

The Allrun file consists of the following commands:

```
blockMesh
decomposePar
mpirun -np 6 newScalarTransportFoam -parallel
reconstructPar
```

These commands are explained in the previous section.

Transport Properties:

```
FoamFile
{
    format      ascii;
    class        dictionary;
    location     "constant";
    object       transportProperties;
}

DS1              [0 2 -1 0 0 0 0] 0;
kS1              [0 0 -1 0 0 0 0] 0;
```

Here, DS1 is the diffusion coefficient and kS1 is the kinetic rate coefficient. For this case, both are set to zero since there is no diffusion and chemical reaction of the tracer.

1.4.3 Initial and Boundary Conditions

The initial and boundary conditions for the flow and scalar simulations are used separately. The scalar term represents the concentration of the passive scalar in the simulation. At first, the flow is simulated as steady state to obtain a velocity field throughout the cylindrical tube. This flow field

is then used for the scalar simulation and a new solver is implemented to simulate the concentration of passive scalar. A steady state solver simpleFoam is used for the flow simulation, whereas an incompressible transient solver newScalarTransportFoam, is used for the scalar transport.

1.4.3.1 Flow Field

The initial conditions are set to zero and the necessary boundary conditions for the flow are tabulated below:

Table 1-1 Boundary Conditions for U

Patch	Condition
Inlet	codedFixedValue
Outlet	zeroGradient
Walls	noslip

Table 1-2 Boundary Conditions for p

Patch	Condition
Inlet	zeroGradient
Outlet	fixedValue(uniform 0)
Walls	zeroGradient

Since, the velocity at the inlet is parabolic and the cylinder is 3D, velocity at various locations (x, y) is calculated using a code which can be accessed in U file of 0 folder. A steady state simulation is done to calculate the steady state velocity profile in the tube. This is then used as an input to the scalar which is carried out as transient simulation.

1.4.3.2 Scalar

1.4.3.2.1 Initial Conditions

The steady state velocity profile obtained from the flow simulation is used as a local flow field for the scalar to trace the path of flow. The U file of last time step from the flow simulation is kept in the 0 directory of the scalar.

1.4.3.2.2 Boundary conditions

The flow field is used from the flow simulation and the boundary conditions for the scalar is tabulated below:

Table 1-3 Boundary Conditions for scalar

Patch	Condition
Inlet	fixedValue (uniform 1)
Outlet	zeroGradient
Walls	zeroGradient

2. Results and Discussions

Post processing of simulation data is done in paraView. The cup average (or volumetric flow average) concentration of passive scalar is calculated at the outlet. It is plotted with time to observe the change in concentration of tracer at the outlet. The cup average concentration can be calculated as:

$$S_{avg} = \frac{\int u \cdot S \cdot dA}{\int u \cdot dA} = \frac{\int u \cdot S \cdot dA}{U_{avg} * A_{outlet}}$$

where u is the velocity and S is the scalar concentration at various meshes of the outlet. The results at different times are shown in Fig 5.

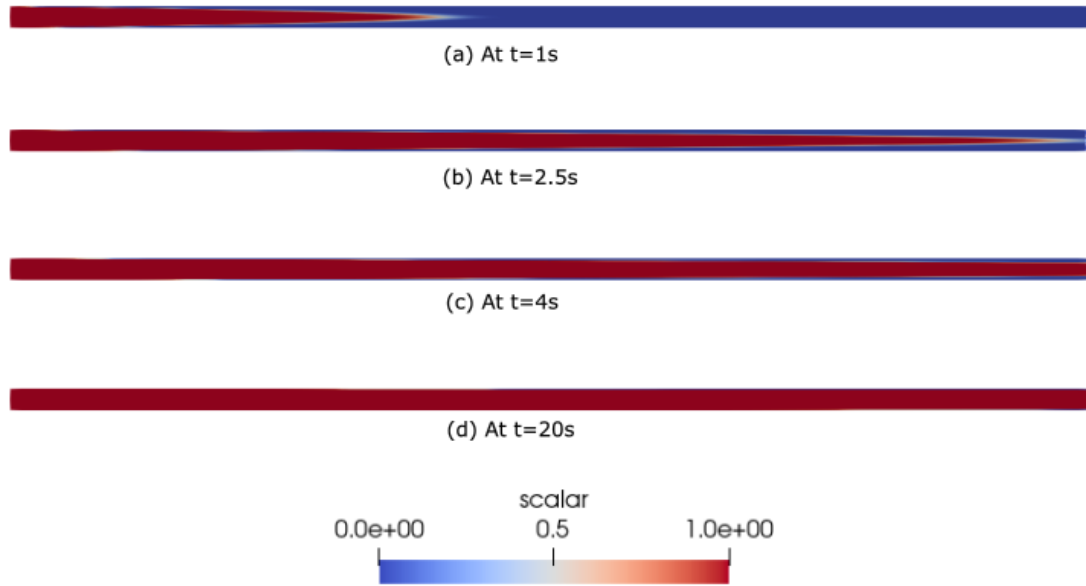


Fig 5: Scalar Concentration along the tube at various time steps

The first appearance of tracer at the outlet is observed to occur at half the residence time (5 sec.) as shown in Fig 6. This agrees with the theory as the center velocity is maximum and twice the average velocity. At around three times the residence time, the scalar reaches the inlet concentration asymptotically. The scalar concentration within a volume does not change with time once the steady state situation is approached after three residence times. The concentration of tracer is uniform throughout the cylinder since there is no chemical reaction.

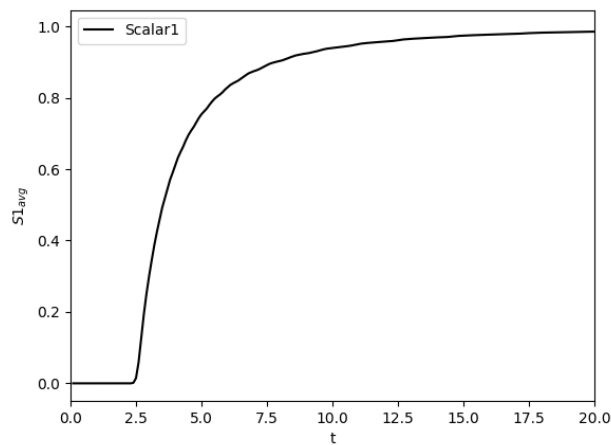


Fig 6: Scalar concentration vs time at the Outlet

3. Conclusion

The use of passive scalar for modelling and simulation of tracer (non-reacting chemical species) to predict and estimate RTD is shown successfully. The tracer needs to be both non-diffusive and non-reactive and the flow should be fully developed at inlet for correct RTD calculations.