



Lab Migration Report

on

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

Proposed By:

Prof. Dhiraj Garg

Solution By:

John Pinto

Manjil Sitoula

## Table of Contents

1. Governing Equations and Models .....	3
1.1 Problem Statements.....	3
1.2 Governing Equations.....	3
1.3 Geometry and Mesh. ....	4
1.4 Solver Setup .....	5
1.4.1 Fluid Properties .....	5
1.4.2 Case Setup.....	5
1.4.3 Initial and Boundary Conditions .....	9
2. Results and Discussions.....	10
3. Conclusion. ....	11

## List of Figures

Fig 1: Schematic Diagram of Computational Domain .....	4
Fig 2: Mesh Generation using BlockMesh .....	4
Fig 3 Tree diagram of the main folder .....	6
Fig 4 Detailed Tree diagram of the directories .....	6
Fig 5 Scalar Concentration along the tube at various time steps .....	10
Fig 6 Scalar concentration vs time at the Outlet.....	11

## List of Tables

Table 1-1 Boundary Conditions for U .....	9
Table 1-2 Boundary Conditions for p .....	9
Table 1-3 Boundary Conditions for scalar.....	10

# 1. Governing Equations and Models

## 1.1 Problem Statements

To study Residence Time Distribution (RTD) for plug 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 plug flow condition. Then using passive scalar as tracer to study RTD for plug flow in a straight cylinder tube. In ideal plug flow, the velocity profile in radial direction is flat and fully mixed. In reality, plug flow is approached using turbulent flow. 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  $\nu$  is the kinematic viscosity,  $\rho$  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):

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

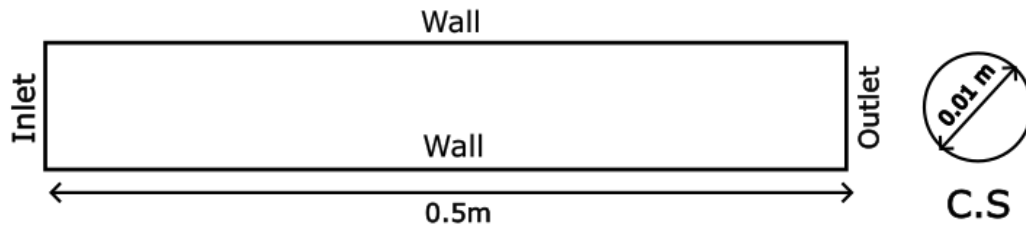
Where  $S$  is the passive scalar,  $\Gamma$  is the diffusion coefficient and  $S_c$  is the source term of the passive scalar. The source term would be required to model chemical reaction related to  $S$  which would be 0 here. For more information regarding the source term, you can refer to this document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

**Residence Time Distribution calculations for plug 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. In ideal plug flow, the radial velocity profile is flat with complete mixing in radial direction. In reality, plug flow is approached using turbulent flows. 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 plug flow,  $u_{avg} = u_{max}$ . So, all fluid elements will

take same to reach outlet, i.e.  $\theta = t/\bar{\tau} = 1$ . If tracer is injected throughout the inlet cross-section, the first appearance of tracer will occur at  $\theta = 1$ , and that too at 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.

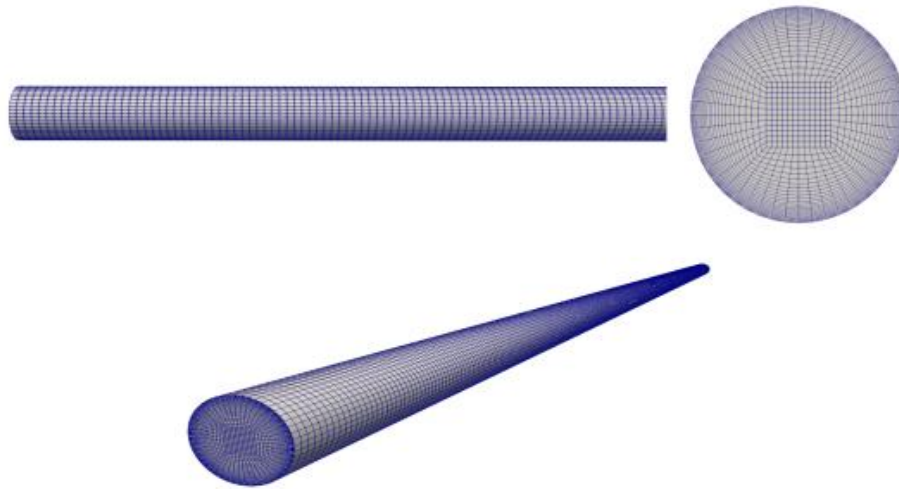
### 1.3 Geometry and Mesh.

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 3 dimensional and the simulation is carried out in 3d with flat velocity at the inlet. The geometry is long enough for the flow to fully develop.



*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. The number of cells is 672000. 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 Reynolds number is expressed as:

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

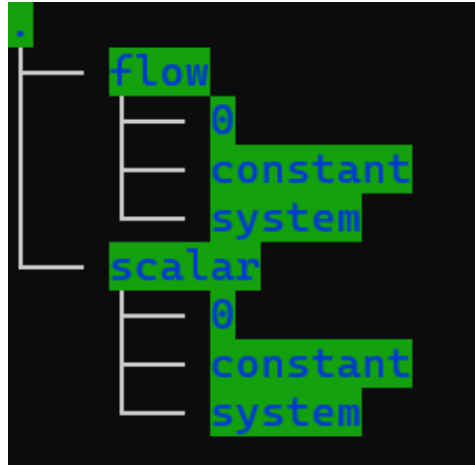
Where  $U_{avg}$  is the average velocity,  $D$  is the diameter of the tube and  $\nu$  is the kinematic viscosity. For the above input flow parameters, the Reynolds number of the flow is 1165 which is in the laminar regime (<2100). So, a laminar model is used for the simulation.

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

For this case, to simulate plug flow, the radial velocity profile during the flow from inlet to outlet must remain flat. To achieve this type of velocity profile, a flat velocity profile needs to be imposed at inlet as boundary condition. To prevent any change in the velocity profile during flow, the boundary condition at walls will be “Slip” and the velocity will be same as average velocity at inlet. This will simulate the plug flow condition throughout the flow through cylindrical tube. The user can use actual turbulent flow condition also for obtaining actual RTD values.

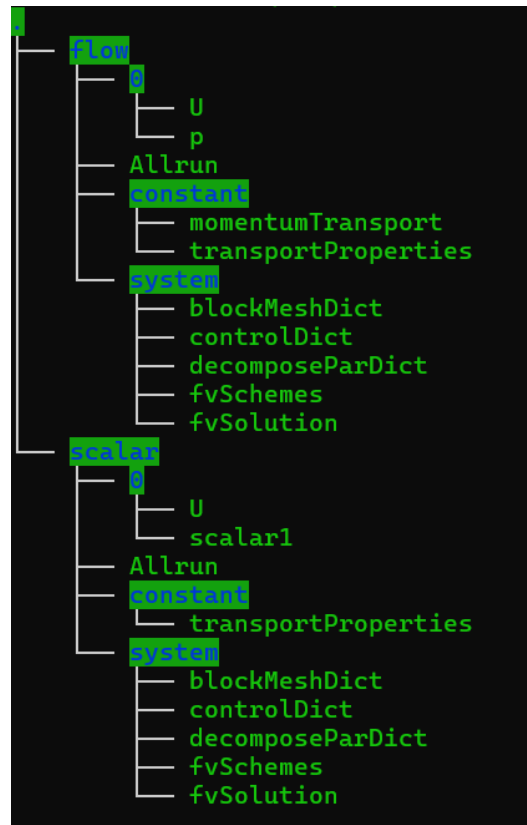
### 1.4.2 Case Setup

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 and the scalar folder has the necessary files to simulate the scalar. The velocity field solved using flow folder is used by the scalar to move along the tube and trace the path of the flow. Since, newScalarTransportFoam, doesnot solve for velocity, we need to simulate for the flow field and provide as a path for the scalar. 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\_Uniform/flow**

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

The Allrun file consists of 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. At last, reconstructPar command is used to reconstruct a single domain from the processor sub-domains.

### **Scalar Case setup:**

#### **Solver modification and compilation**

To simulate the 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\_Uniform/scalar**

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

The Allrun file consists of 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 diffusivity and kS1 is the kinetic rate coefficient. For this case, both are set to zero since there is no diffusion and chemical reaction.

### 1.4.3 Initial and Boundary Conditions

The initial and boundary conditions for the flow and scalar simulation 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 through which scalar moves. The flow field conditions for the scalar simulation are provided by the flow simulation and a new solver is implemented to simulate the concentration of passive scalar. For the flow simulation, simple Foam, a steady state solver is used whereas newScalarTransportFoam, an incompressible transient solver is used for the scalar.

#### 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	FixedValue (uniform 0.1)
Outlet	zeroGradient
Walls	slip

*Table 1-2 Boundary Conditions for p*

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

A steady state simulation is done to calculate the steady velocity profile in the tube which is 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

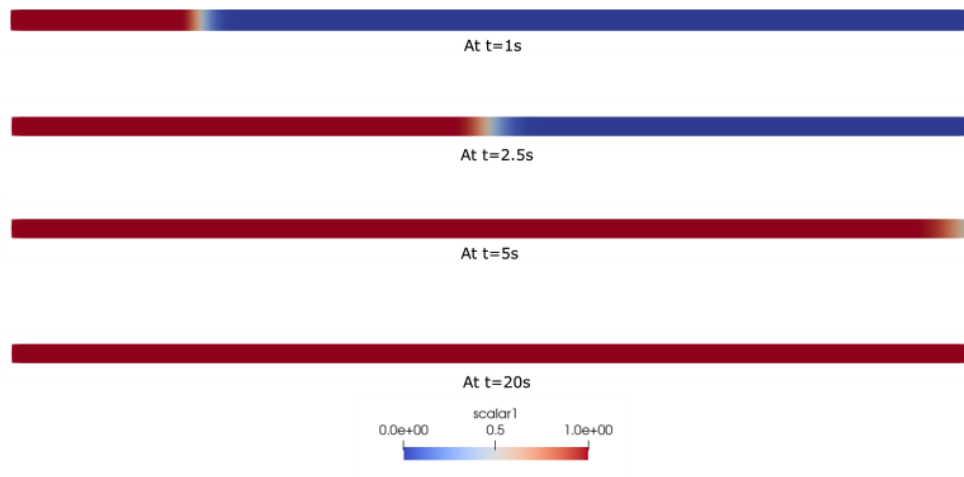
## 2. Results and Discussions

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 is calculated as:

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

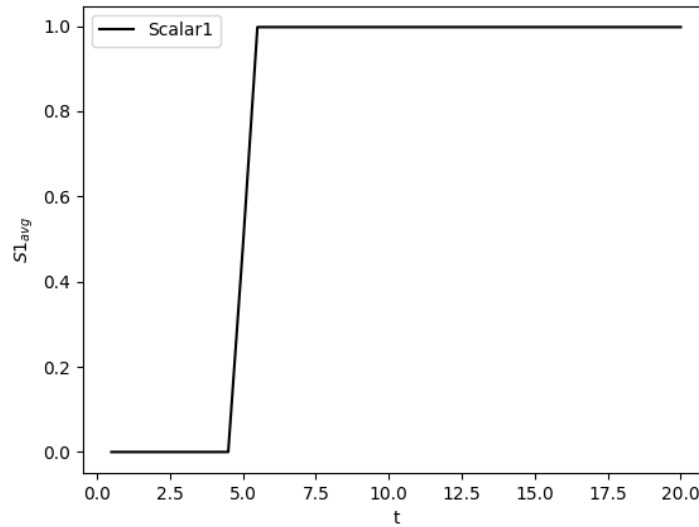
where  $u$  is the velocity and  $S$  is the scalar concentration at various meshes of the outlet. The results at different times are shown in Fig 5.

The residence time (length of the tube/average cross-sectional velocity at inlet) is 5 seconds. The first appearance of tracer at the outlet occurs at same as the residence time. This is because the maximum velocity is same as average velocity and velocity is uniform everywhere cross-sectionally throughout the flow. Thus, the residence time of any point on the cross-section remains same from inlet to outlet.



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

The scalar is injected at the inlet with the concentration 1 and is gradually moving along the tube with time. At time equals the residence time, the scalar reaches the outlet and the concentration increases sharply to the level of the inlet concentration like a unit step function as can be seen in Fig 6. Due to limitation of meshing size resolution at the outlet in flow direction, the scalar reaches the outlet slightly lesser than the residence time.



*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 of plug flow is shown successfully. The tracer needs to be both non-diffusive and non-reactive. The flow should be fully developed with flat velocity profile throughout flow for correct RTD calculations. The same was incorporated through uniform velocity boundary condition at inlet and slip velocity boundary condition at walls in this case. In real situation, the plug flow can be approximated through turbulent flow.