



Lab Migration

Report

On

**Modelling and Simulation of two unmixed passive scalars as
diffusive reactive chemical species with second order
chemical reaction**

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1. Governing Equations and Models

1.1 Problem Statements

To model **passive scalars** as unmixed **reactive** chemical species **with** diffusion following **second order chemical reaction** and simulate the reaction in a laminar **flow reactor**.

Objective – The purpose is to understand how passive scalars can be used as reactive chemical species **without** diffusion under **flow** conditions. To do this we need a model for chemical reactions involving desired chemical species which is taken to be second order here. The chemical reaction term is incorporated as **source term** in the passive scalar transport equation. The effect of flow process (convection and diffusion both) and chemical reaction on resulting reaction due to mixing of chemical species from both upper and lower half along the flow is to be observed.

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 & S2):

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

Where S (in our case S1, S2 & S3) is the passive scalar, Γ is the diffusion coefficient and S_C is the source term of respective passive scalar. The source term would be required to model chemical reaction related to S1, S2 and S3.

Let the chemical reaction be $A + B \rightarrow C$ and assume the rate of reaction is of **second** order in a batch reactor, i.e.

$$-r_A = -\frac{dC_A}{dt} = kC_A C_B = -r_B = -\frac{dC_B}{dt} = r_C = \frac{dC_C}{dt} \quad (4)$$

C_{A0} , C_{B0} are the initial concentration of A and B, while the initial concentration of C would be zero.

Let S1, S2 and S3 represent the concentration of chemical species A, B and C respectively. As we can see, A and B are reactants and will be consumed in the reaction whereas C is product and thus will be produced during the reaction. So, the source term for S1 would be

$$S_{C1} = -r_A = -kC_A C_B \quad (5a)$$

for S2, it would be

$$S_{C2} = -r_B = -kC_A C_B \quad (5b)$$

and for S3, it would be

$$S_{C3} = r_C = kC_A C_B \quad (5c)$$

So the transport equation for C_A can be written as

$$\frac{\partial C_A}{\partial t} + \mathbf{u} \cdot \nabla C_A = \nabla(\Gamma \nabla C_A) + (-r_A) = \nabla(\Gamma \nabla C_A) - kC_A \quad (6)$$

The ideal laminar flow reactor in context of straight cylindrical tube means to have parabolic radial velocity profile from inlet to outlet with **no** radial mixing. The only way a particle can move radially would be through diffusion only. Both the reactants A and B are injected in separate halves of the cylinder thus ensuring unmixed condition. So, they must mix to cause chemical reaction. Since diffusion is the only driving force to cause mixing in the current case, theoretically, the chemical species should diffuse to opposite half of the cylinder depending on their respective diffusivities while moving along the flow in their respective halves. So, we should observe chemical reaction along the interface and the bulk of the halves along the flow. The purpose of this exercise is to observe the effect of diffusion on the chemical reaction.

For more information regarding the source term, you can refer to this document [Theory](#).

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 as shown in Fig. 1. The geometry is 3D. The geometry is long enough for the flow to fully develop. The chemical species S1 will be injected at upper half and S2 will be injected at lower half of the inlet.

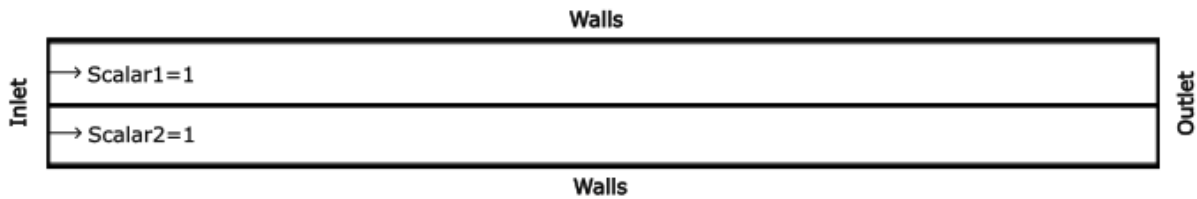


Fig 1: Schematic Diagram of Computational Domain

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. The user is free to choose different types of meshing and numbers to get similar results. For the detailed meshing process, one can go through the openFOAM spoken tutorial number 6. [spoken tutorial](#)

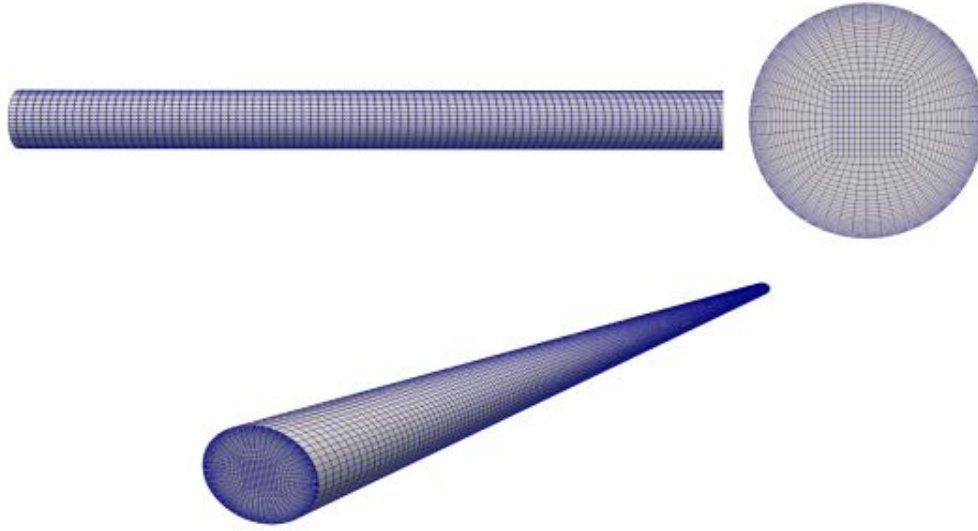


Fig 2: Mesh Generation using BlockMesh

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 are taken for calculations. The kinematic viscosity of water at room temperature (300 K) is $8.58 \times 10^{-7} \text{ m}^2/\text{s}$ and the average velocity of the flow is 0.1 m/s , which is half the maximum velocity. 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.(Re) | 1165 |
| Scalar Diffusivity constant (DS) | $10^{-7} \text{ m}^2/\text{s}$, $2 \times 10^{-7} \text{ m}^2/\text{s}$ & $3 \times 10^{-7} \text{ m}^2/\text{s}$ |
| Scalar Kinetic rate coefficient (kS) | 1 s^{-1} |

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:

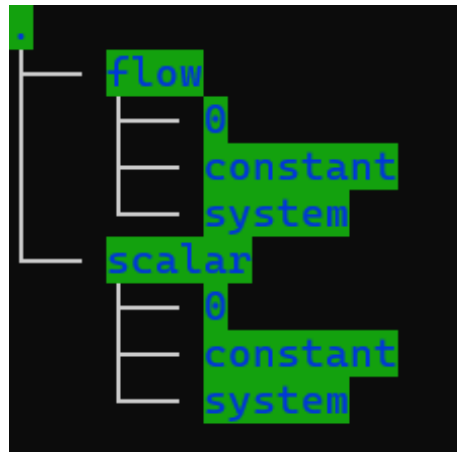


Fig 3 Tree diagram of the main folder

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, **newScalarTransportFoam2S**, does not solve for velocity, we need to simulate for the flow field and provide as a path for the scalar. The scalar folder is used in simulating the scalar change depicting the chemical reaction. The folders can be further expanded along this tree:

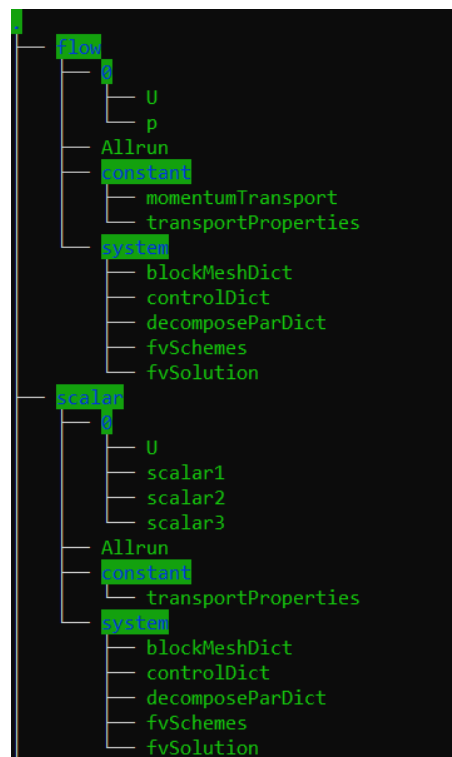


Fig 4 Detailed Tree diagram of the directories

The 0 directory of scalar folder consists of initial and boundary conditions for scalar1, scalar2 and scalar3. Scalar1 and Scalar2 is used to model the chemical species which after reaction are converted to another species, modeled by scalar3.

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 HalfBore_D_New/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 newScalarTransportFoam2S. 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 newScalarTransportFoam2S
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 2HalfBore_D_Source/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 newScalarTransportFoam2S -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] 1e-7;
DS2            [0 2 -1 0 0 0 0] 1e-7;
DS3            [0 2 -1 0 0 0 0] 1e-7;
kS             [0 0 -1 0 0 0 0] 1;

```

```

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

DS1            [0 2 -1 0 0 0 0] 2e-7;
DS2            [0 2 -1 0 0 0 0] 2e-7;
DS3            [0 2 -1 0 0 0 0] 2e-7;
kS             [0 0 -1 0 0 0 0] 1;

```

```

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

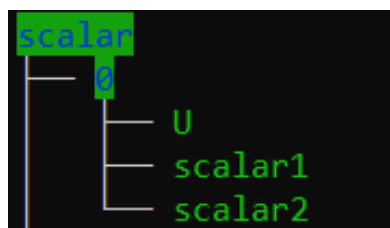
DS1            [0 2 -1 0 0 0 0] 3e-7;
DS2            [0 2 -1 0 0 0 0] 3e-7;
DS3            [0 2 -1 0 0 0 0] 3e-7;
kS             [0 0 -1 0 0 0 0] 1;

```

Here, DS1, DS2 and DS3 are the diffusivities of Scalar1, Scalar2 and Scalar3 respectively and kS is the kinetic rate coefficient. Here, three different cases with different diffusivity values are taken. There is diffusion of all scalars, and all are assumed to have equal value for the same case. The user can choose different values for each of them and observe the difference in the new results. Since, it models chemical reactions, the kinetic rate coefficient is set to 1. The user can change its value also and observe the differences in the results.

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 newScalarTransportFoam2S, an incompressible transient solver is used for the scalar. The initial and boundary conditions are provided in the 0 directory which contains U, Scalar1, Scalar2 and Scalar3 dictionary.



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.

```
inlet
{
    type            codedFixedValue;
    value           uniform (0 0 0);

    name parabolicVelocity;
    code
    #{
        const vectorField& Cf = patch().Cf();

        vectorField& field = *this;
        const scalar R = 0.005;
        const scalar c = 0;
        const scalar Umax = 0.2;

        forAll(Cf, faceI)
        {
            const scalar x = Cf[faceI][0];
            const scalar y = Cf[faceI][1];

            field[faceI] = vector(0,0,Umax*(1-((pow((y-c)/R,2)))+(pow((x-c)/R,2)))));
        }
    #};
}
```

The velocity at the inlet is computed using the coded boundary condition.

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 (Scalar1, Scalar2 & Scalar3)

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. Firstly, the scalar1 and scalar2 are injected at the upper half and lower half of the inlet cross section respectively with concentration of 1. Then, Scalar1 and Scalar2 using their non-zero values in a given mesh, would react to produce Scalar3.

1.4.3.2.2 Boundary conditions

The flow field is used from the flow simulation and the boundary conditions for the scalar1, scalar2 and scalar3 is tabulated below:

Table 1-3 Boundary Conditions for Scalar1

| Patch | Condition |
|--------|-----------------|
| Inlet | codedFixedValue |
| Outlet | zeroGradient |
| Walls | zeroGradient |

codedFixedValue for Scalar1:

```
inlet
{
    type            codedFixedValue;
    value           uniform 1;

    name halfBore;
    code
    #{
        const vectorField& Cf = patch().Cf();

        scalarField& field = *this;

        forAll(Cf, faceI)
        {
            const scalar r = Cf[faceI][1];
            if (r>=0)
            {
                field[faceI] = 1;
            }

            else
            {
                field[faceI] = 0;
            }
        }
    };
}
```

Here, r takes the y coordinates of the inlet face and if r is greater than zero i.e. the upper half, it assigns the value of scalar field at inlet to 1, otherwise 0.

codedFixedValue for Scalar2:

```

inlet
{
    type          codedFixedValue;
    value         uniform 1;

    name halfBore1;
    code
    #{
        const vectorField& Cf = patch().Cf();

        scalarField& field = *this;

        forAll(Cf, faceI)
        {
            const scalar r = Cf[faceI][1];
            if (r>=0)
            {
                field[faceI] = 0;
            }

            else
            {
                field[faceI] = 1;
            }
        }
    #};
}

```

Here, r takes the y coordinates of the inlet face and if r is less than zero i.e. the lower half, it assigns the value of scalar field at inlet to 1, otherwise 0.

Boundary condition for Scalar2:

Table 1-4 Boundary Conditions for Scalar2

| Patch | Condition |
|--------|-----------------|
| Inlet | codedFixedValue |
| Outlet | zeroGradient |
| Walls | zeroGradient |

The boundary condition at the inlet is set to codedFixedValue for both scalar1 and scalar2 which after reaction converts to scalar3 modeled in newScalarTransportFoam2S solver with necessary formulations.

Boundary condition for Scalar3:

Scalar3 is set to zero at the inlet and zeroGradient at the outlet and walls.

```

FoamFile
{
    format      ascii;
    class       volScalarField;
    object       scalar3;
}

dimensions      [0 0 0 0 0 0 0];

internalField   uniform 0;

boundaryField
{
    inlet
    {
        type      fixedValue;
        value      uniform 0;
    }

    outlet
    {
        type      zeroGradient;
    }

    wall
    {
        type      zeroGradient;
    }
}

```

1.4.3.2.3 Source term

The scalar S1 and S2 are consumed during reaction which is modeled by newScalarTransportFoam2S solver through source term.

```

while (simple.correctNonOrthogonal())
{
    fvScalarMatrix scalar1Eqn
    (
        fvm::ddt(scalar1)
        + fvm::div(phi, scalar1)
        - fvm::laplacian(DS1, scalar1)
        ==
        -kS*scalar1*scalar2
    );

    fvScalarMatrix scalar2Eqn
    (
        fvm::ddt(scalar2)
        + fvm::div(phi, scalar2)
        - fvm::laplacian(DS2, scalar2)
        ==
        -kS*scalar1*scalar2
    );

    fvScalarMatrix scalar3Eqn
    (
        fvm::ddt(scalar3)
        + fvm::div(phi, scalar3)
        - fvm::laplacian(DS3, scalar3)
        ==
        kS*scalar1*scalar2
    );
}

```

1.4.3.3 Steady State Study of Scalar

The scalar steady case is to see the steady state of the simulation. If one is interested in the final results or when the solution doesnot change with time and don't want to trace the scalar with time, once can navigate to this folder `cd 2HalfBore_D_Source /scalar_steady` and type `./Allrun` and press enter. This only provides the steady state solution and observe the final state of the scalar.

2. Results and Discussions

The scalar1 is injected from the upper cross section and scalar2 at the lower cross section of the inlet of the inlet each with the concentration 1. Since there is diffusivity of the scalar, the scalars will diffuse to other half and in the process, the chemical reaction will take place from interface towards bulk. The extent of chemical reaction will depend on the extent of diffusion taking place which will depend on the value of diffusion coefficient of individual reacting scalars.

The scalar concentration along the tube is shown below at steady state in Fig 5. The scalar1 and scalar2 react to form scalar3 as the flow proceeds. Since the diffusion seems to be low, the chemical reaction is majorly limited to the interface of the two halves. If the diffusion could be increased or the velocity of the flow could be reduced, the diffusion process will cause more radial mixing. This interplay of velocity (convection) and diffusion on mixing is given by Peclet number, $Pe_a = \frac{uL}{D}$, where u is velocity in axial direction, L is the length and D is the diffusion coefficient.

For radial Peclet number, $Pe_R = \frac{uR}{D} = Pe_a \left(\frac{R}{L}\right)$. Since radial velocity is zero in our case, axial velocity will do with aspect ratio $\left(\frac{R}{L}\right)$. For diffusion to be significant compared to convection, $Pe \ll 100$.

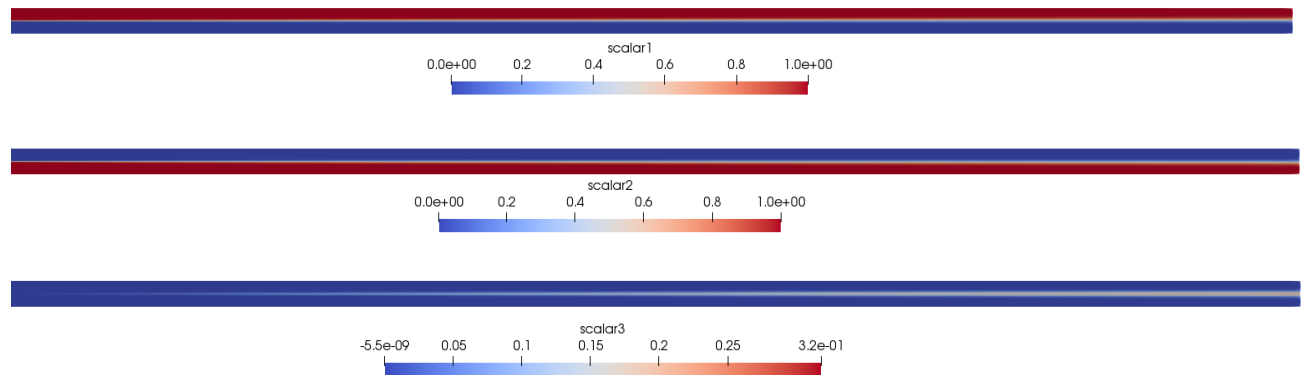


Fig 5 Scalar Concentration along the tube at diffusivity value of $1e-7$.

The scalar concentration at the cross section of the tube at outlet is shown in **Error! Reference source not found.**. Since there is diffusion, the scalar1 and scalar2 crosses the centre. Scalar3 is formed only at the interface of scalar1 and scalar2 where reaction takes place. Due to diffusion, the scalars are being spread over the half line and scalar3 is formed at the interface which also diffuses itself.

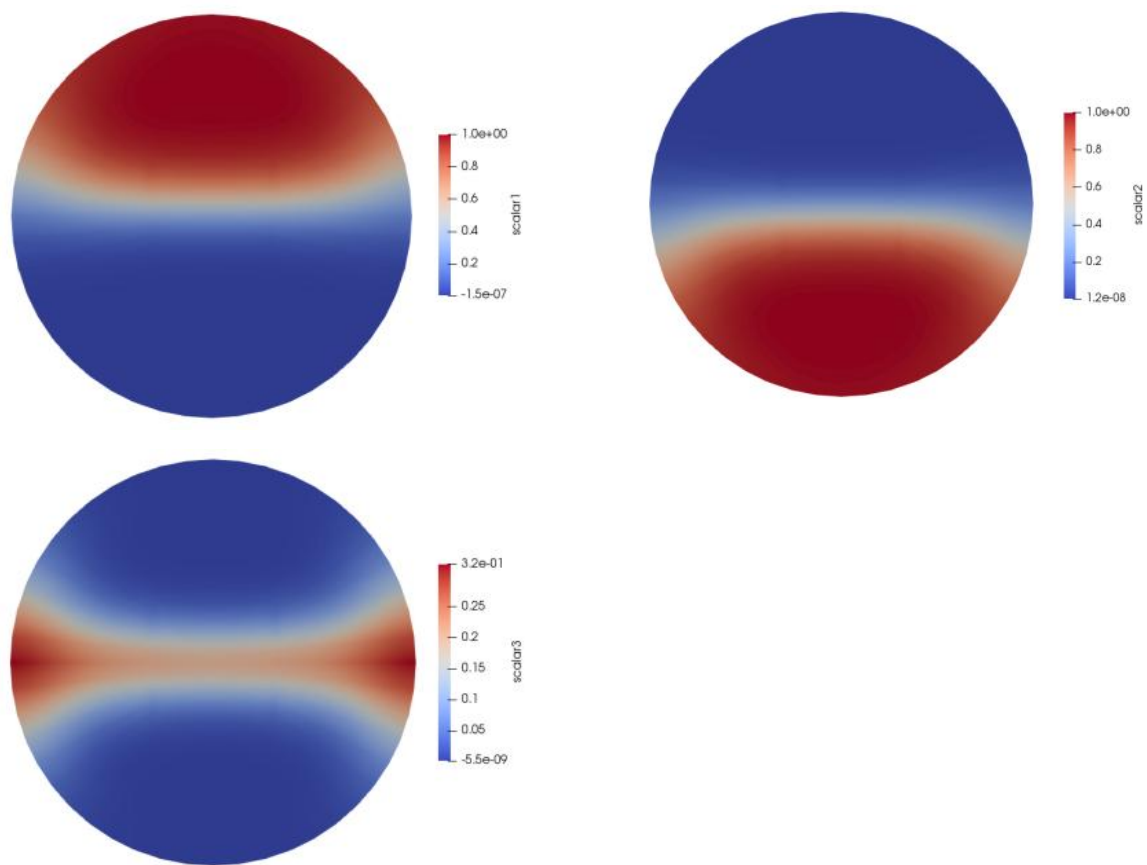


Fig 6 Scalar concentration at outlet after steady State at diffusivity value of $1e-7$.

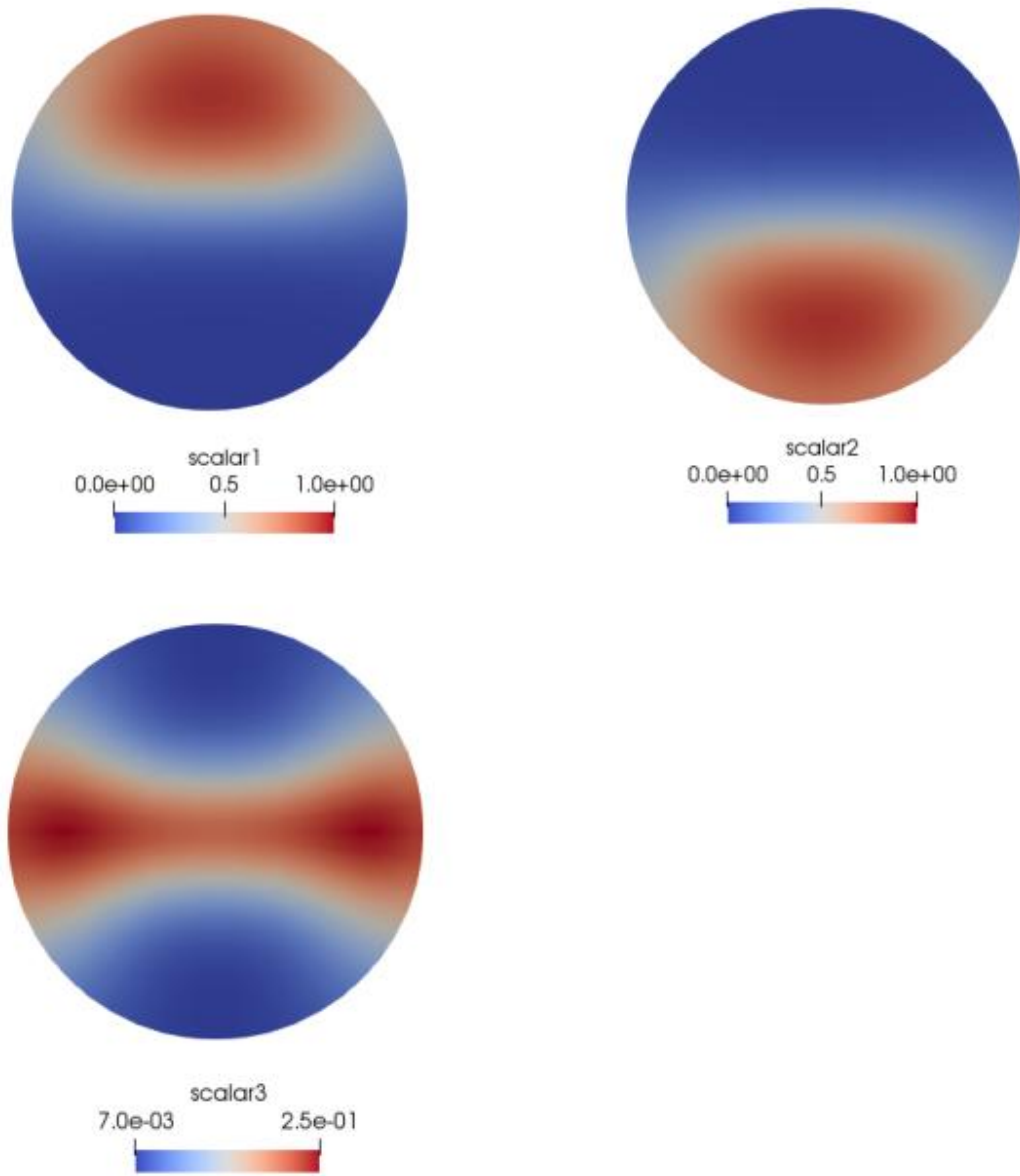


Fig 7 Scalar concentration at outlet after steady State at diffusivity value of $3e-7$.

After the flow reaches steady state, the area averaged concentration of scalar3 is calculated at various sections of the tube (0.125 m, 0.25 m, 0.375 m) and cup average concentration is calculated at the outlet.

The area average concentration can be calculated as:

$$S_{avg} = \frac{\int S. dA}{A_{cross-section}}$$

The cup average concentration can be calculated as:

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

Where u is the velocity and S is the scalar concentration at area dA.

The scalar3 concentration is plotted along the tube at various cross sections in Fig 8. The scalar3 concentration along the tube length is plotted for two different values of diffusivity referred by Scalar3_1D, Scalar3_2D and Scalar3_3D (1×10^{-7} , 2×10^{-7} and 3×10^{-7}). When the diffusivity value is higher, the slope of the graph is higher than that of low diffusivity value. This occurs as a result of more mixing of scalar1 and scalar2 due to diffusion as the flow proceeds along the tube and higher formation of scalar3 at the interface. When compared with the previous case with no diffusion, the graph with no diffusion seems to be constant relative to that with diffusion.

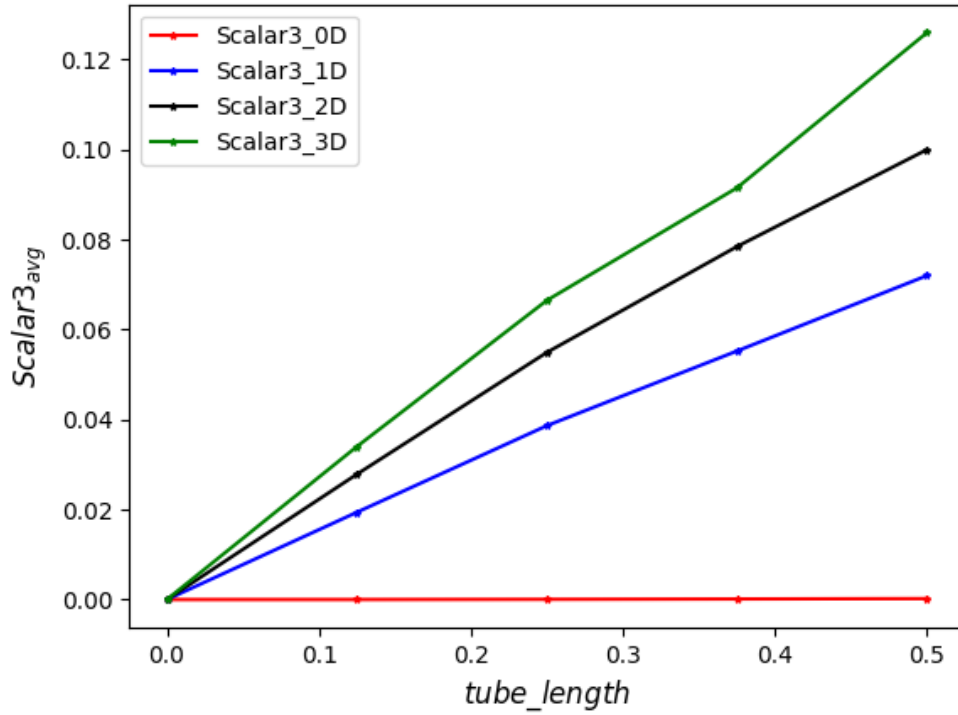
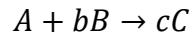


Fig 8 Scalar3 Concentration along various sections of the tube

The user can change the value of kinetic rate coefficient and individual diffusion coefficients of all the scalars and observe the effect on chemical reaction and thus, the concentration profile of each scalar across the cross section along the flow. The user can also implement a higher order reaction rate. The example is given below. Let the kinetic scheme be



Where b and c are stoichiometric coefficient of B and C respectively. The initial concentration of A, B and C are C_{A0} , C_{B0} and C_{C0} . The rate

$$-r_A = -\frac{dC_A}{dt} = kC_A^n C_B^m = -\frac{r_B}{b} = \frac{r_C}{c} \quad (7)$$

where $n + m$ is the order of the reaction and can have any value from 0 onwards. The user can obtain an analytical solution corresponding to this and compare the results obtained by the simulation under plug flow or batch reactor condition.

Another important aspect of CFD is that it is based on the law of conservation of mass and not moles. Moles are conserved only when there is no reaction. On the other hand, all chemical reaction rate equations are based on moles instead of mass as the units of concentration terms are in mol/vol and reaction rate is defined as mol/vol/time. The units of kinetic rate coefficient k can

be obtained accordingly. So, the rate equation, thus kinetic rate coefficient and concentration terms have to be made dimensionless in terms of moles. This is achieved by following method:

Applying following transformation in eqn. (7),

$$C'_A = \frac{C_A}{C_{A0}}, C'_B = \frac{C_B}{C_{B0}}, C'_C = \frac{C_C}{C_{A0}} \quad (8)$$

This will make initial concentration of A and B as 1 at inlet, while that of C be 0 which is the case here also.

$$\text{we have } -r'_A = -\frac{dC'_A}{dt} = k \cdot C_{A0}^{n-1} C_A'^n C_{B0}^m C_B'^m = k' C_A'^n C_B'^m \quad (9)$$

$$\text{Where } k' = k \cdot C_{A0}^{n-1} C_{B0}^m \quad (10)$$

Similarly for B (from eqn. (7))

$$-r'_B = -\frac{dC'_B}{dt} = b \cdot k \cdot C_{A0}^{n-1} C_A'^n C_{B0}^m C_B'^m \left(\frac{C_{A0}}{C_{B0}} \right) = b \cdot s \cdot k' C_A'^n C_B'^m \quad (11)$$

Where b is stoichiometric coefficient of B and $s = \left(\frac{C_{A0}}{C_{B0}} \right)$. This will work for all values of n making units of k as s^{-1} . This transformation will also achieve the purpose of normalization thus reducing the numerical errors also.

For $n = 1, m = 1, s = 1, b = 1$, this equation for current case can be found out.