

CFD Project

Mixing of liquids with different substance concentrations at 90° junctions

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Abstract

Liquid-liquid and liquid-gas mixing in ducts are of great importance for applications such as drug delivery, microfluidic devices, potable water distribution, etc. Many factors can affect this mixing phenomenon. Some of these factors are relative volume fluxes, entrance/exit lengths, surface tension and the relative properties of liquids.

In this project, mixing of two separate flows having the same fluids with different concentration of a substance is studied. It is assumed that the concentration of the substance does not affect the liquid properties. The flow is also assumed to be in the laminar region to avoid difficulties associated with turbulence, and an incompressible fluid assumption is also added since the liquid is flowing at very low Mach numbers.

A control volume-based staggered meshing is applied to the domain and the equations of mass, momentum and concentration are solved for velocities, pressure, and concentration. The solver is an explicit scheme for the time discretization and uses 2nd order approximations for derivatives on the boundary. Steady state solutions of velocities, pressure and concentration are compared for different inlet velocities, entrance lengths, and fluid properties to get a better understanding of the effect of each factor on the general flow and concentration fields. A fine mesh is also studied at different times to show the progress of the mixing in time.

The results show that relative velocity determines the area fraction of inlet that is taken by each flow which is visible in the concentration contours. Also, fluid with higher diffusive parameters result in a better mixing of the fluids and the “concentration boundary” between the two flows begin to vanish. The entrance length affects the pressure and velocity profiles but has negligible effect on the concentration profile.

Literature survey

T-junction flow with different fluids is addressed in a lot of microfluidic-based applications where different flow conditions are experimented-modeled. These results are highly affected by the surface tension which results in bubble generation and immiscible two-phase flow. For example, Steijn et al. [1] showed the velocity contour at different stages of bubble generation provided in fig 1.

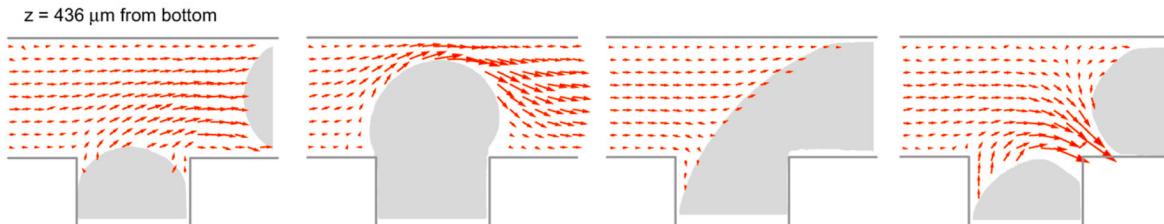


Fig 1

However, due to the dominance of surface tension forces in microscale, these cases will give a different solution to the flow field due to the droplet formation and may not be used as a reference in this project where we neglect those forces.

The other similar experiments that are similar to our problem are those that study turbulence mixing of water (or any other liquid) with different concentration of a substance. Conservation of mass and momentum equations along with a concentration equation govern this type of mixing problems. Sroka and Forney [2] theoretically and experimentally studied the mixing of a jet with pipeline liquid at turbulent flow regimes. Their results indicated that the mixing quality increases with increasing vertical flow (jet) momentum and distance from injection point. Fig 2 shows the concentration profile at distance x from the injection which is calculated by a similarity solution and verified later with an experimental setup.

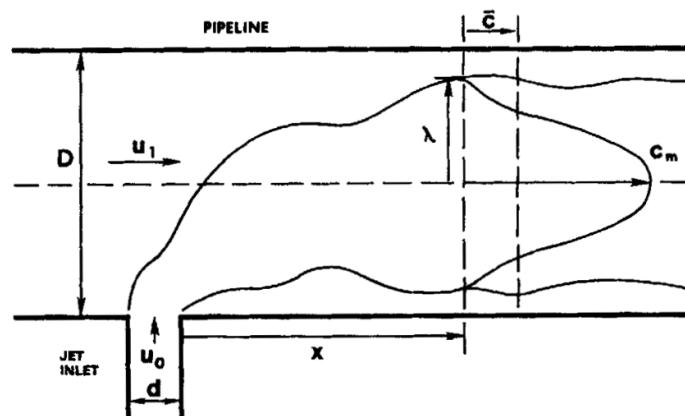


Fig 2

Wang et al. [3] used the ADINA software to simulate the flow at junctions with different angles for turbulent conditions. They used a 3D model along with finite element and finite volume formulations to solve incompressible Navier-Stokes equations. Giorges et al. [4] did a similar numerical study for single and multiple jet mixing. Walker et al. [5] also used a finite volume model to simulate mixing of two water flows with different ion concentrations in a horizontal pipe configuration.

Webber et al. [6] provided the velocity contours from Doppler velocimeter measurements in 3D channel flow. Fig 3 shows the surface x-velocity contour in which the backflow downstream the vertical inlet can easily be seen.

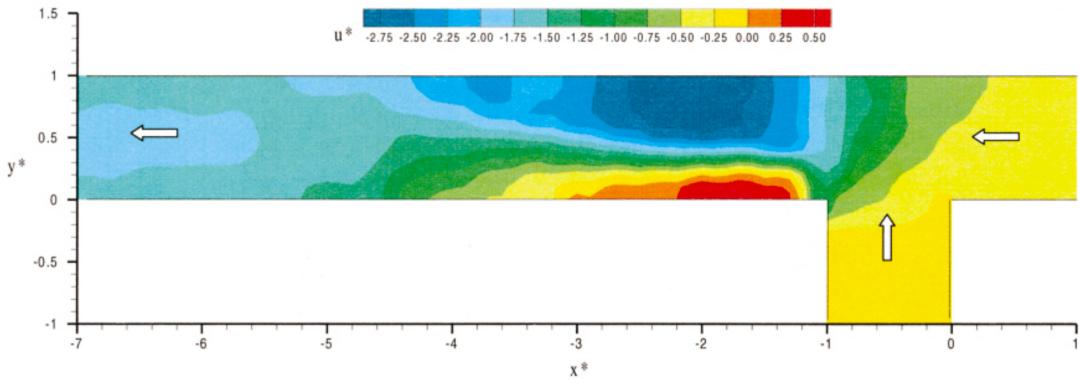


Fig 3

Although these experiments are done under turbulent flow conditions, the results can be used to get a general idea of the flow field close to the junction.

I was not able to find any papers on the exact condition of our problem, which is, laminar flow with different concentration of a substance and neglecting the surface tension. The closest papers to our problem are the ones mentioned above. These experiments are not directly used in the validation of results from the CFD simulation, since they all have different conditions such as turbulent flow. The results are assumed to be correct based on intuition.

Governing equations and physics of the problem

The governing equations include the mass and momentum conservations, which determine the velocities and pressure, and a coupled concentration equation, as it can be seen below:

$$\begin{aligned}
 \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0 && \text{continuity} \\
 \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= -\frac{1}{\rho} \frac{\partial P}{\partial x} + \vartheta \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) && \text{x-momentum} \\
 \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} &= -\frac{1}{\rho} \frac{\partial P}{\partial y} + \vartheta \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) && \text{y-momentum} \\
 \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} &= D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) && \text{concentration}
 \end{aligned}$$

In these equations, ρ is the density, ϑ is the kinematic viscosity, C is the concentration, and D is the mass diffusivity. The velocity field can be moved by convection, diffusion, and by pressure gradients. The concentration, however, is only affected by convection and diffusion. These effects are later studied in the results. As it can be seen, the concentration doesn't affect the velocities and pressure (since we assumed it has no effect on the properties of the liquid) but is affected by the velocity field through convection.

A no-slip condition is assumed at the walls, and v and u are assumed to be known at the inlets.

Geometry Discretization

The problem geometry consists of a simple T-junction, as shown in fig 4. These lengths are inputted by user and are flexible to build different geometries. This effect is studied in results.

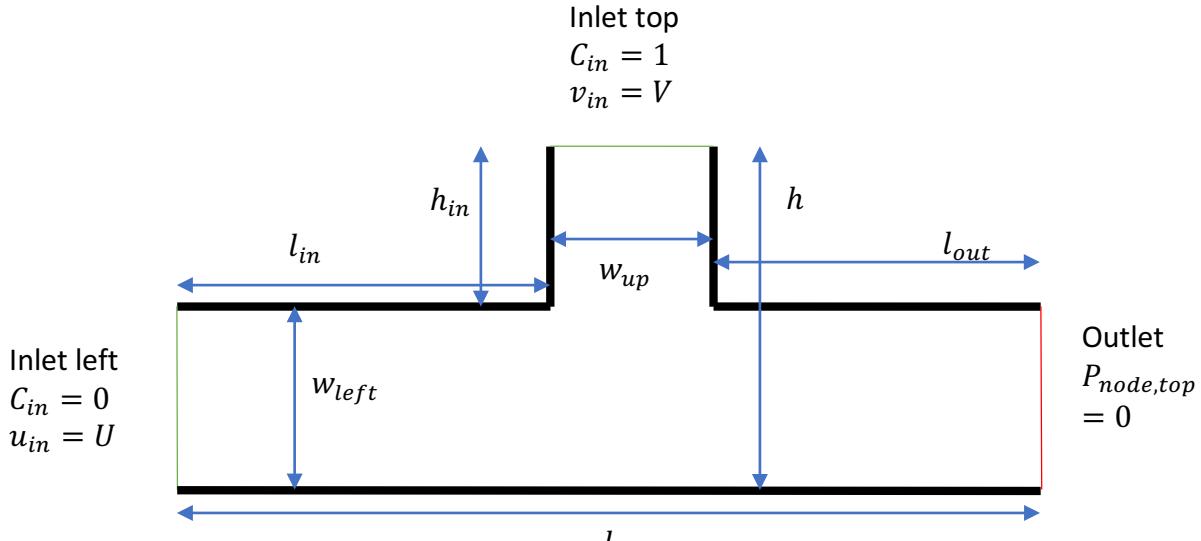
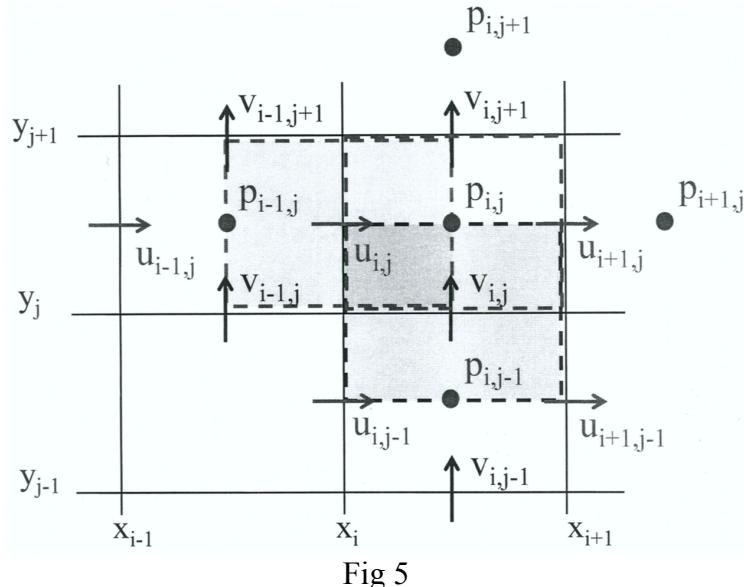


Fig 4

This geometry is then discretized by inputting the number of cells in each row and column. The code has the option of having different node spacing in x- and y-directions. However, in all the test cases they are set to the same value. A staggered mesh is used where concentration nodes have the same control volume as the pressure nodes. u-nodes and v-nodes are $\frac{dx}{2}$ and $\frac{dy}{2}$ behind the P-nodes respectively. The meshing is shown in fig 5.

For example, on the left boundary, the leftmost u-nodes are on the boundary but P- and v-nodes are $\frac{dx}{2}$ away from the boundary. All the other boundaries are similar. Appropriate expressions are used for the properties and derivatives on the boundary in calculating different terms of the PDEs.



The integral form of the equations is used for a control-volume-based approach. The Euler explicit scheme is used to achieve high speed and simplicity of calculations.

The error associated with the problem is dominant in the convective term. Since we are using a central difference approximation for the first derivative in the convective term, and the Euler explicit method for the time derivative approximation, the order of error of the finite difference formula would be $O(dt, dx^2)$.

Boundary and initial conditions

On the boundaries, appropriate conditions are set based on the type of boundary:

Walls: If the velocity node is on the wall, the value is set to zero based on the no slip-condition. If it's half-a-grid-length off the wall, a 2nd order assumption is assumed for the derivative at boundary using 3 points.

Inlets: Similar to walls, except that the known value is not zero and equal to a given number, e.g. inlet x-velocity in the left inlet.

Outlet: A $\partial/\partial x$ assumption is made, leading to setting to the boundary x-velocities equal to the value of the previous node, and setting the derivatives to zero for the convective and diffusive terms in y-momentum.

For the initial condition, the velocity and concentration at each of the entrance regions is set to the inlet value to get a faster solution for the steady state. However,

for the case of transient response, the initial condition is set to zero velocity and concentration everywhere in the domain to study the effects of concentration propagation.

Algorithm

At each time step, first the concentration is updated (since it doesn't affect the other fields). Then the velocities are updated from the momentum equation and boundary conditions are applied. The mass outlet is manually set to the sum of the mass inlet from the two sources by multiplying the boundary velocities by the appropriate factor. Then the pressure correction is calculated based on the divergence of the velocity field. Pressure is then corrected by setting one node to atmospheric pressure (the top node at outlet is selected in the code). Then from the pressure correction terms, the velocity corrections are calculated and velocities are corrected. The code is stopped when the change in all the fields after one second is less than an epsilon value ($\varepsilon_u = \varepsilon_v = 1e - 14$, $\varepsilon_p = 1e - 10$, $\varepsilon_c = 1e - 12$).

At the end of every step, the Reynolds number and CFL numbers are checked to make sure the flow is laminar and the solution is stable. Criteria set in the code is for the CFL (both v and u) and sigma (both for ϑ and D) values to be less than 0.1 and for the Reynolds number (both u and v) to be less than 1000. Note that for stability σ and CFL need to be less than 1; Reynolds number needs to be less than 2300 for laminar flow. The maximum Reynolds and CFL numbers are mentioned at the steady state condition for each case. These numbers are computed from the following equations:

$$CFL_u = dt / \min(|dx/u|) \quad (\text{variable, checked at every time step})$$

$$\sigma_D = dt / \min(dx^2/D, dy^2/D) \quad (\text{constant, checked at t=0 only})$$

$$Re_u = \max(|u|) * w_{left} / \vartheta \quad (\text{variable, checked at every time step})$$

(total Re can be as large as $\sqrt{Re_u^2 + Re_v^2}$)
(still lower than 2300)

Results

1. Transient behavior

In order to study the transient behavior of the flow, a fine mesh is used. The initial condition is such that the fluid is stationary with zero concentration everywhere in the domain. The inlets pump fluid with different concentration at time 0. The properties of this case are in the tables below:

Geometry	
l_{in} (m)	0.2
h_{in} (m)	0.2
l_{out} (m)	0.6
w_{left} (m)	0.2
w_{up} (m)	0.2
l (m)	1.0
h (m)	0.4

Fluid properties	
ρ (kg/m ³)	1000
ϑ (m ² /s)	9e-4
D (m ² /s)	2e-4

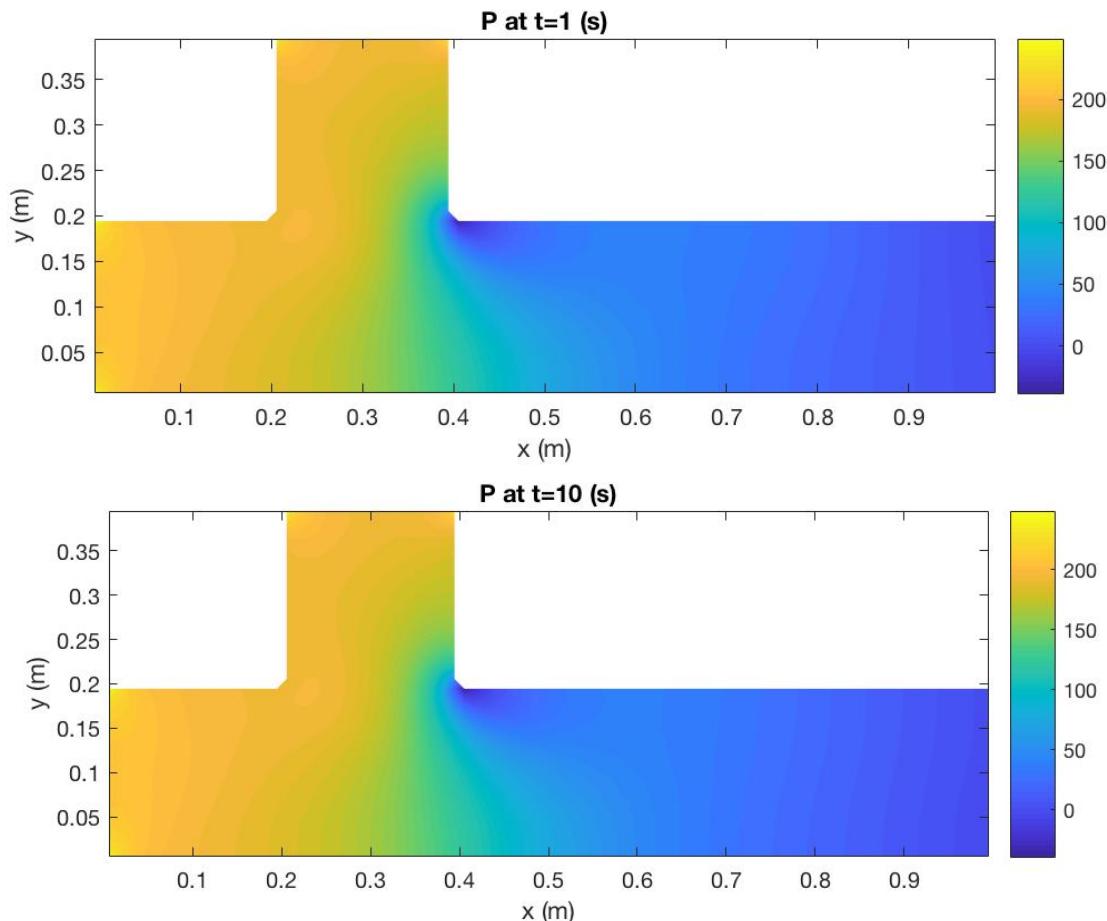
Discretization	
dx (m)	0.01111
dy (m)	0.01111
dt (s)	2e-4
cells in a row	90
cells in a column	36

Inlets	
$u_{in,left}$ (m/s)	0.2
$v_{in,left}$ (m/s)	0
$C_{in,left}$	0
$u_{in,up}$ (m/s)	0
$v_{in,up}$ (m/s)	-0.2
$C_{in,up}$	1

The contours of different properties at different times are given in fig 6-20. (The junction edges are sharp but in MATLAB's contours they look like smooth entrances)

In this case the maximum Reynolds number at the steady state is 133 and the maximum CFL number is 0.0107. σ is on the order of 0.001. These numbers show that the flow is laminar and the time step is small enough for the solution to be stable.

Pressure plots



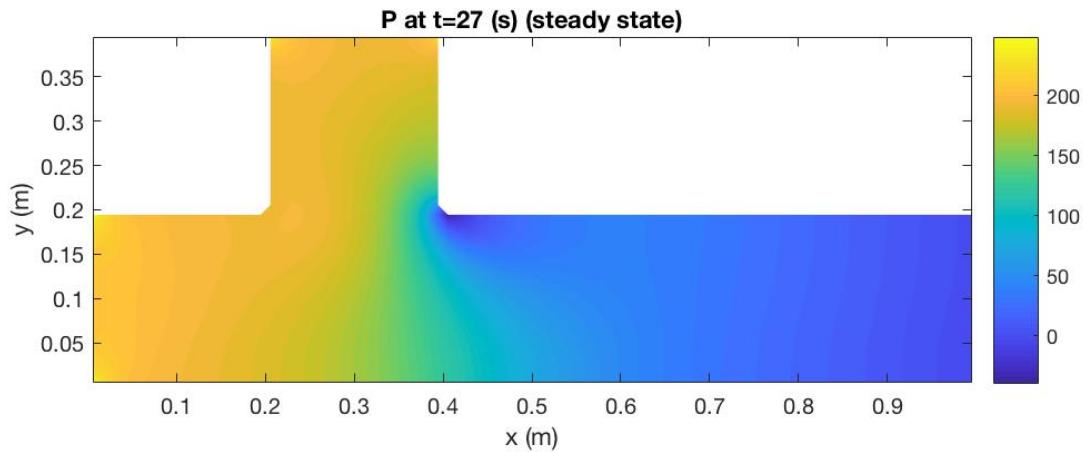
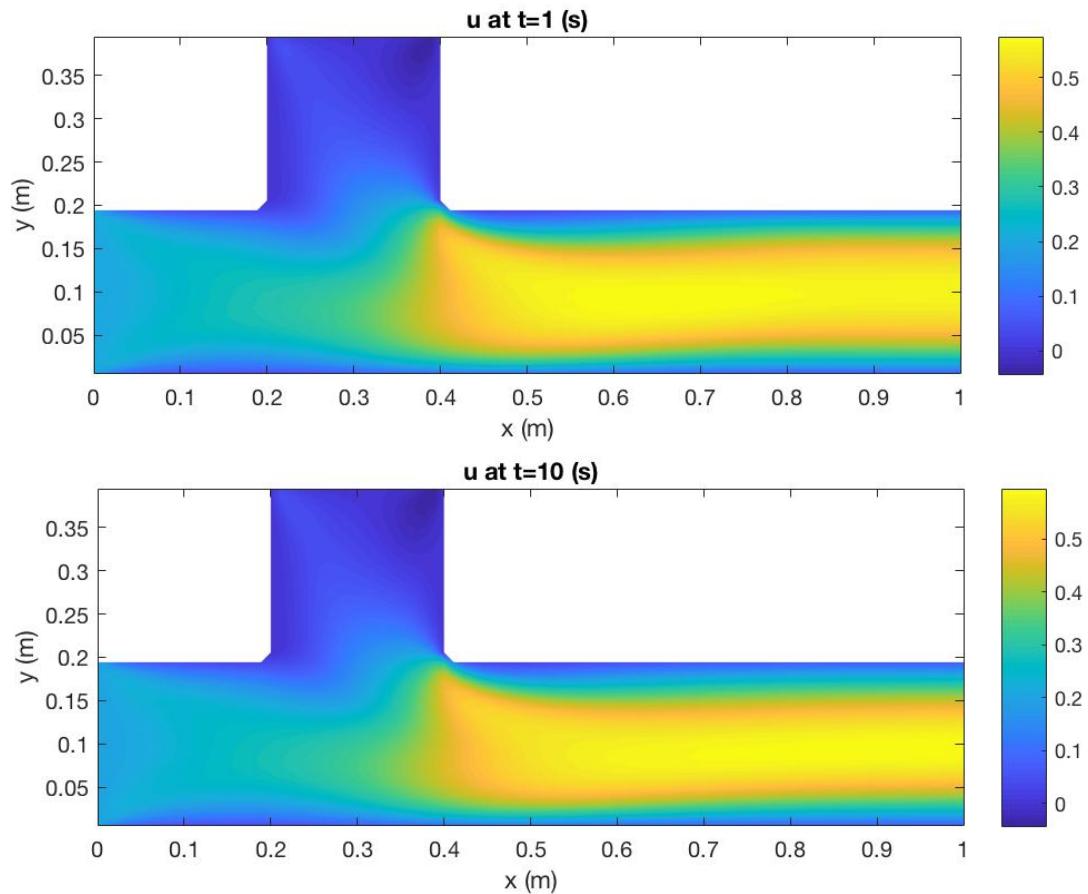


Fig 6

u-velocity plots



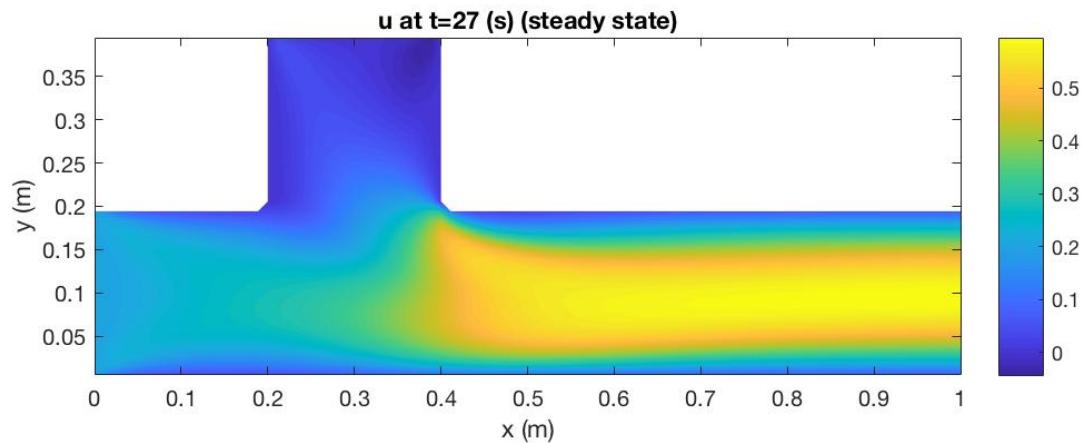
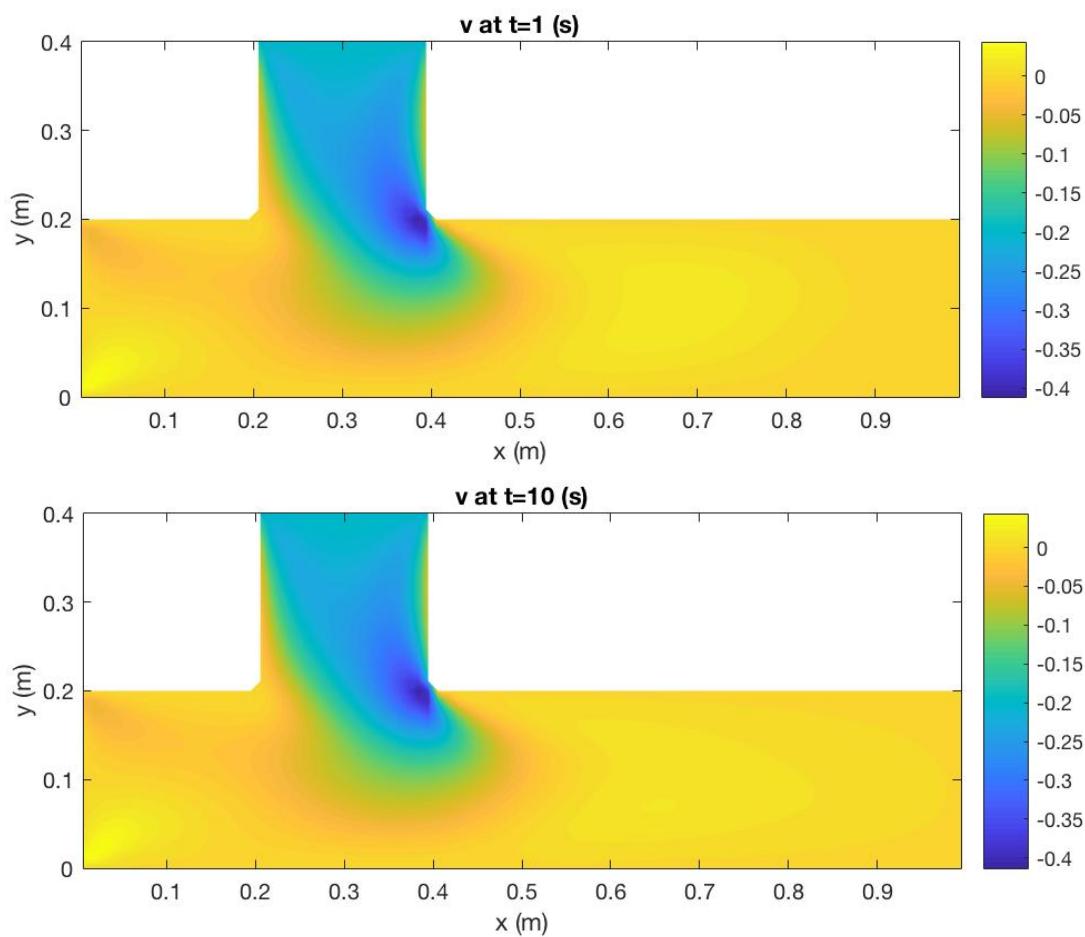


Fig 7

v-velocity plots



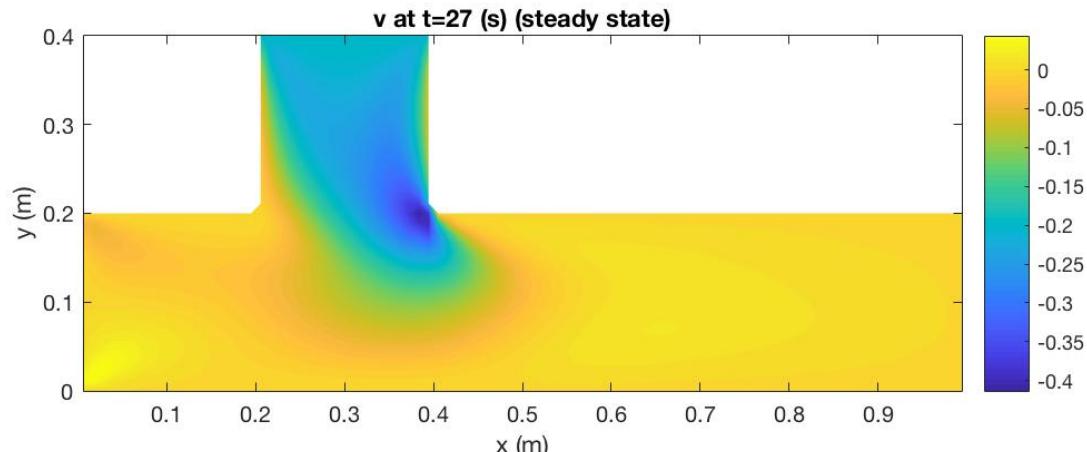


Fig 8

Velocity quiver at steady state

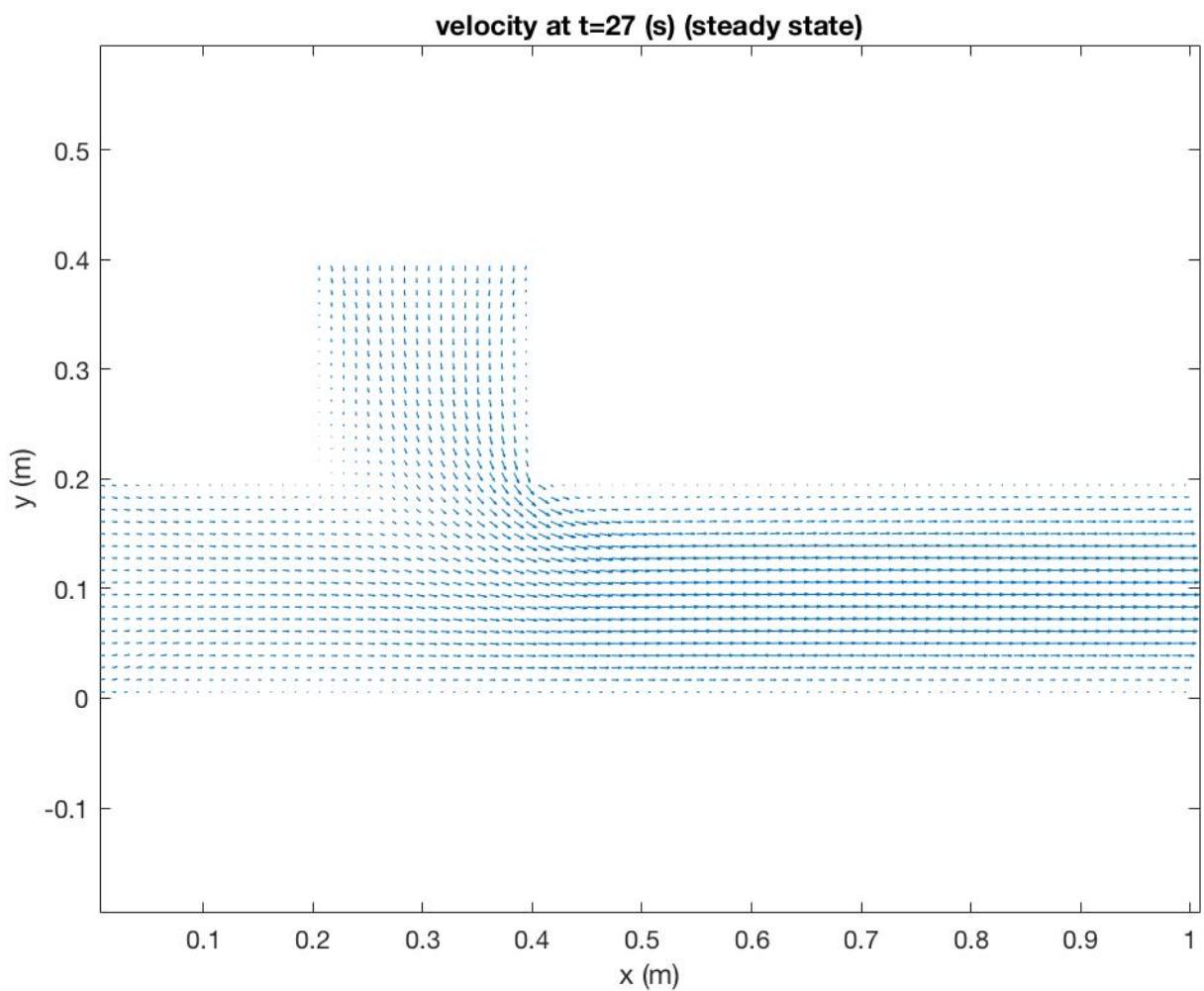
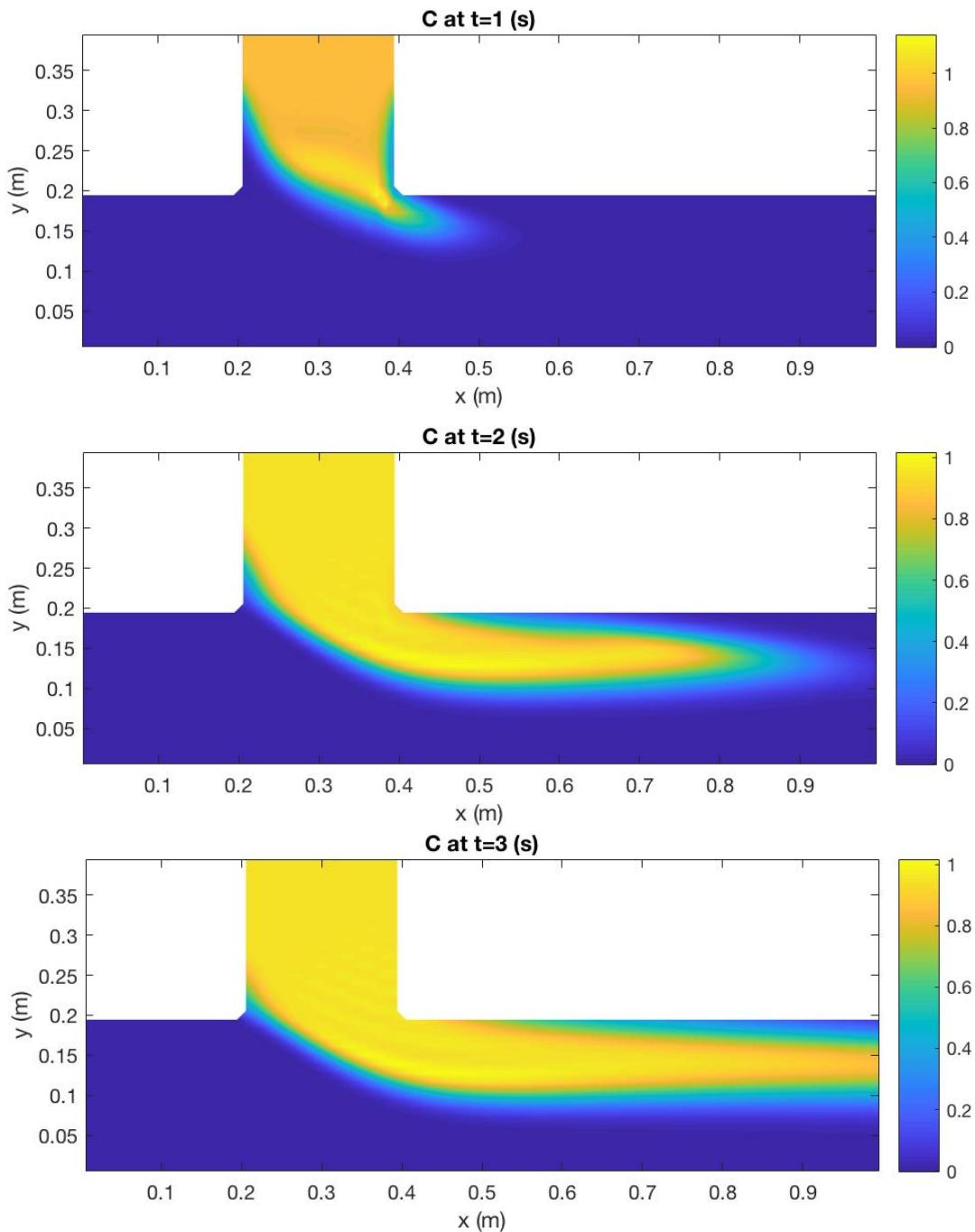


Fig 9

Concentration plots



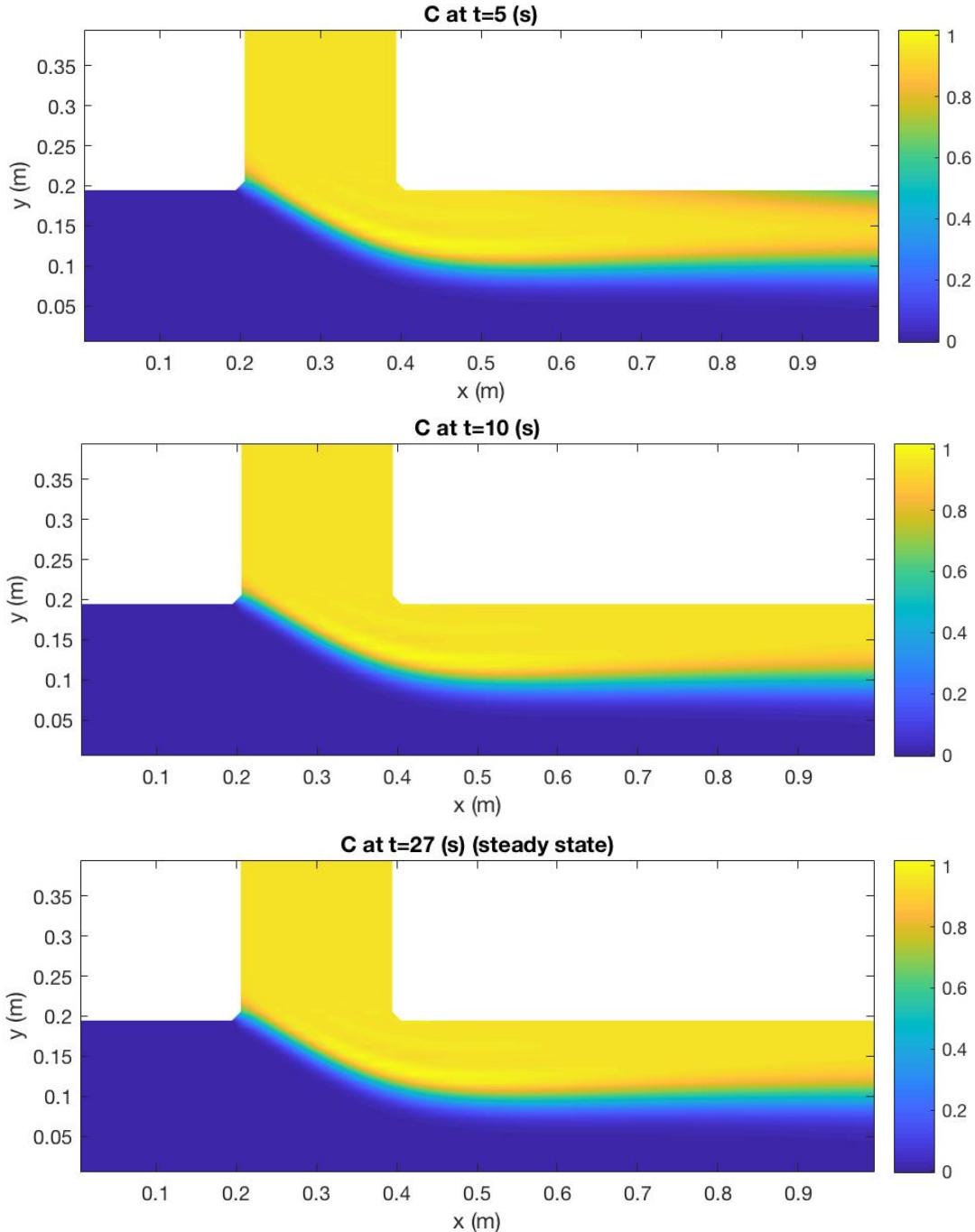


Fig 10

As it can be seen from the plots, the pressure and velocity fields reach the steady state very quickly (around 2 seconds) since the propagation in these fields is due to the pressure waves and conservation of mass in each cell (continuity). This results in the information to be transferred without the need for actual mass transfer. However, for the concentration field to propagate, mass must be transferred from

one cell to the other due to convection or diffusion, this results in a more required time to reach steady state.

From the velocity plots and quiver, the effect of no slip walls is observable, which leads to higher velocities in the center of the channel. Also the effect of the perpendicular flows can be seen in the v-velocity to be pushed to the left, and the u-velocity to be pushed down, due to the other flow hitting them.

It can be seen in concentration plots from 1-5 seconds that the concentration at the center is being propagated more quickly as the velocities are higher at the center of the channel (observable in quiver and u-velocity plots), resulting in more convective propagation which is the dominant term in concentration propagation in this case.

In the pressure plots, it can be observed that pressure increases as we move upstream, also at the junction (right corner) there is a decrease in pressure due to the increased velocity at that point from the mixing. This pressure, if is low enough, can cause a back flow at that point which is usually observed at higher velocities and turbulent flows.

Eventually, at steady state, about half of the channel is taken by each flow due to the same mass fluxes from the inlets. Since the mass diffusion is low, the flows are not mixed well. The effect of mass diffusion is studied in next parts.

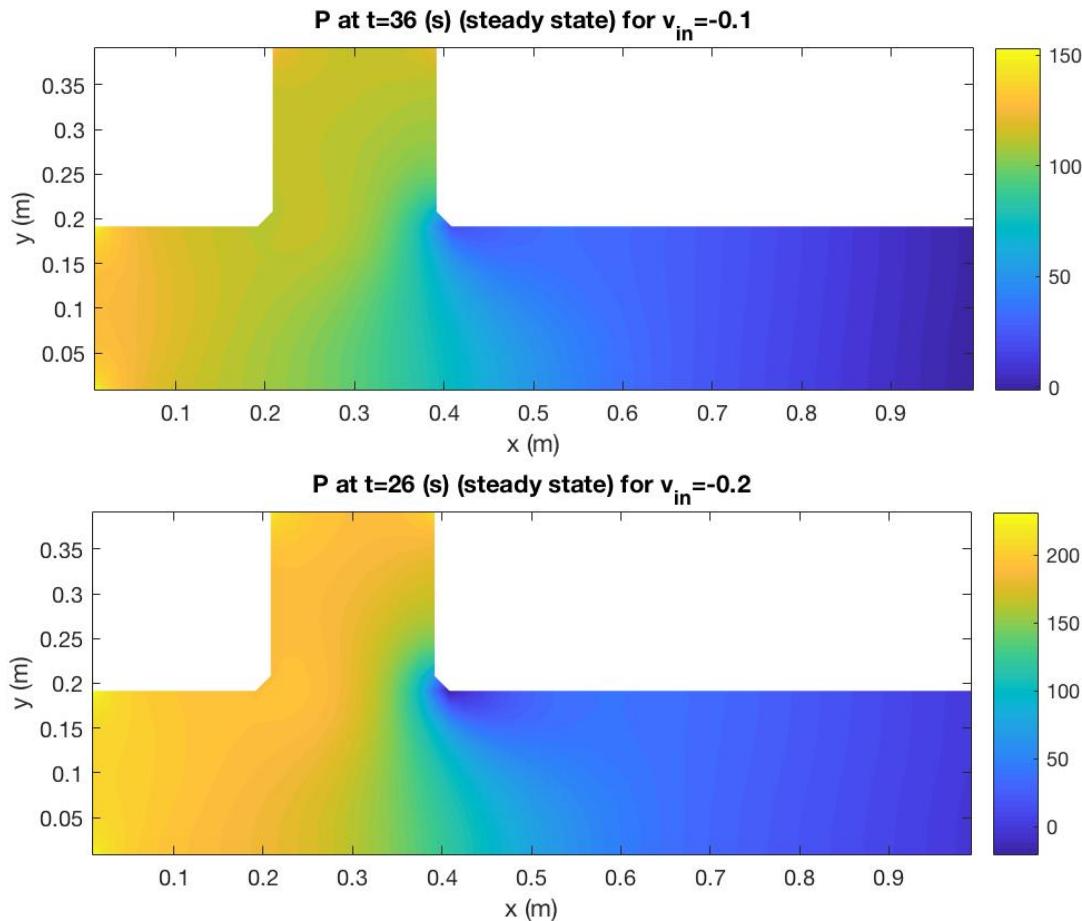
In the next sections, a coarser mesh is used to achieve a lower computation time. $Dx=dy=0.016667$ and dt for each case is selected such that the solution would be stable. All the other parameters are kept the same except when mentioned. The steady state CFL and Reynolds numbers are given for each case.

*note that the quiver data everywhere is plotted assuming that u and v are known on the P-nodes. They are actually $\frac{dx}{2}$ and $\frac{dy}{2}$ off from the P-nodes.

2. Effect of relative mass flux

In this section, the v-velocity from the upper inlet is changed to study the effect of the relative mass flux on different fields. The maximum steady state Reynolds numbers are, in order, 99, 132, 198 and 283. The maximum CFL numbers are 0.013, 0.014, 0.021 and 0.015.

Pressure plots



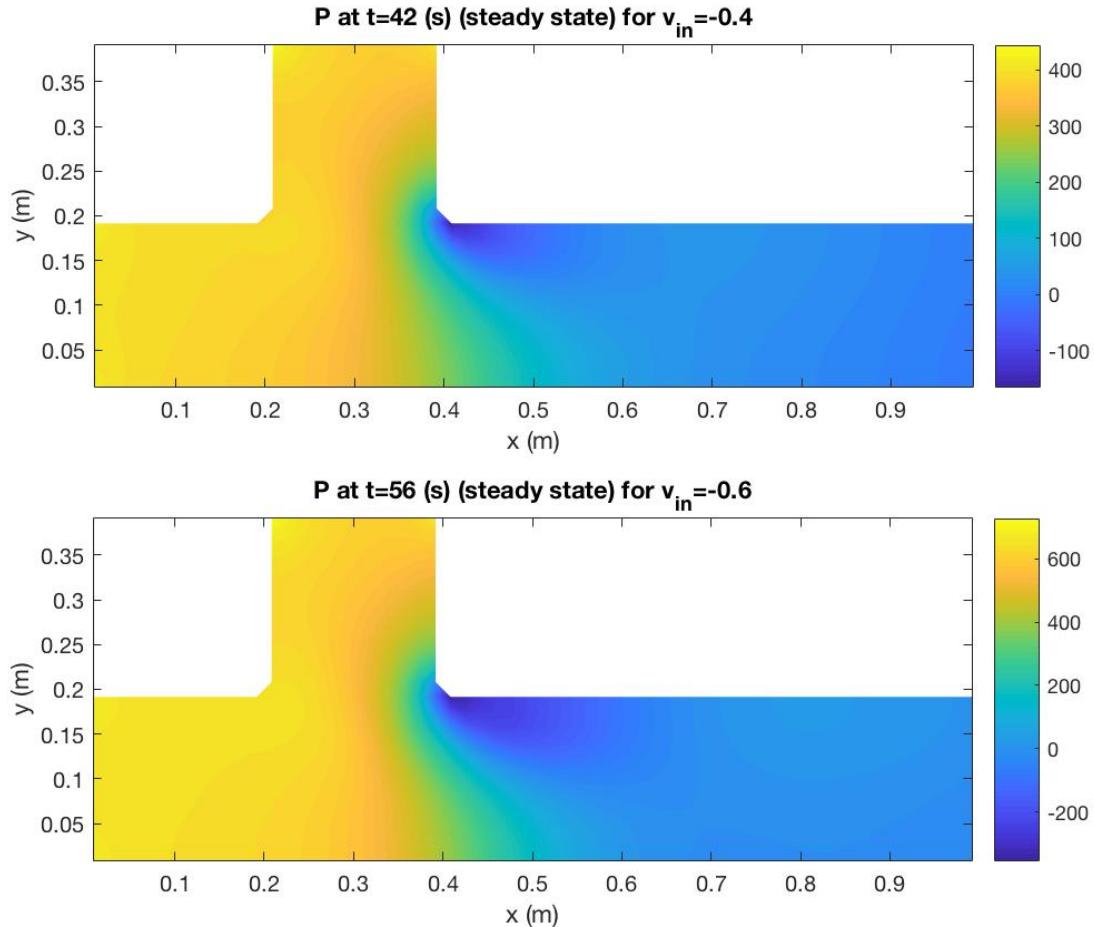
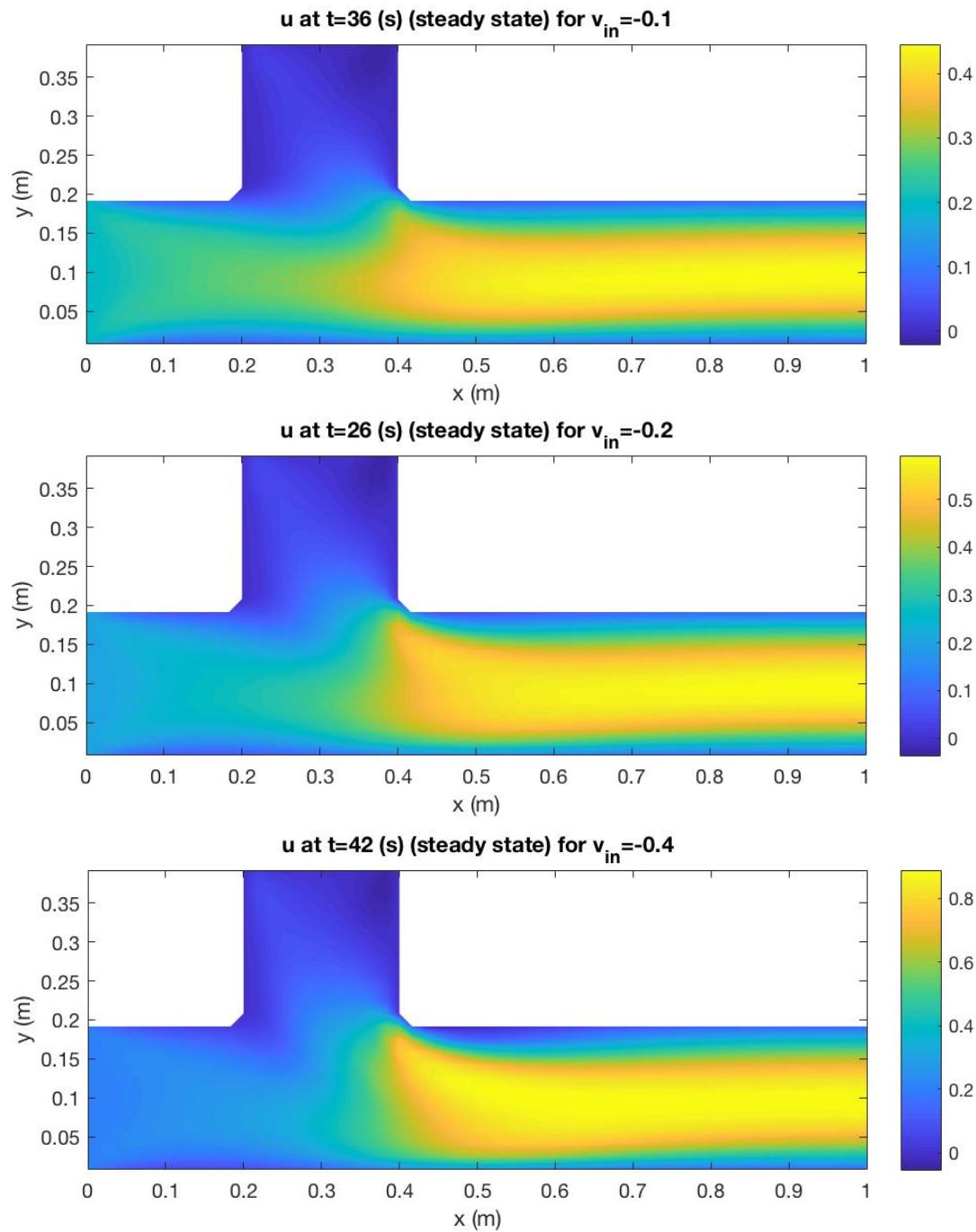


Fig 11

We can observe that increasing the influx from the upper channel would lead to a higher pressure drop along the channel because of the higher velocities. Also, the pressure drop at the junction (right edge) would increase as the influx increases, which is due to the higher velocity gradient at that point.

u-velocity plots



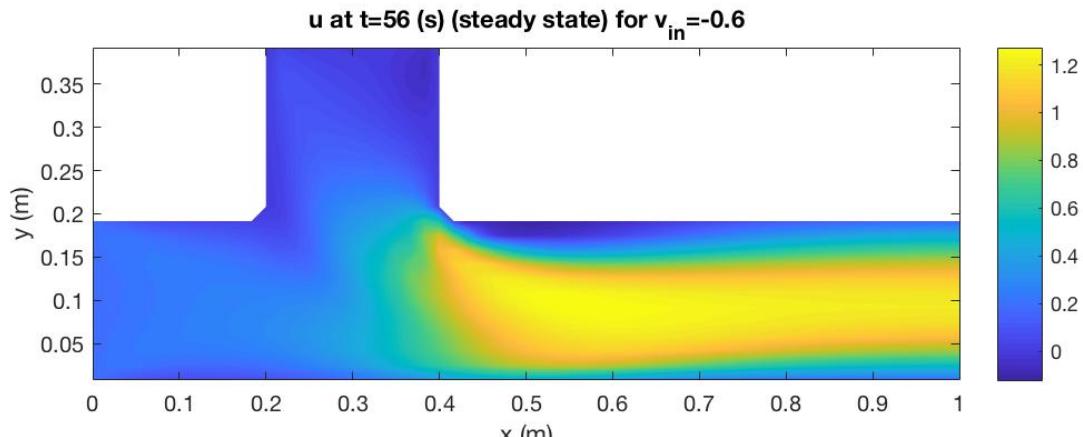
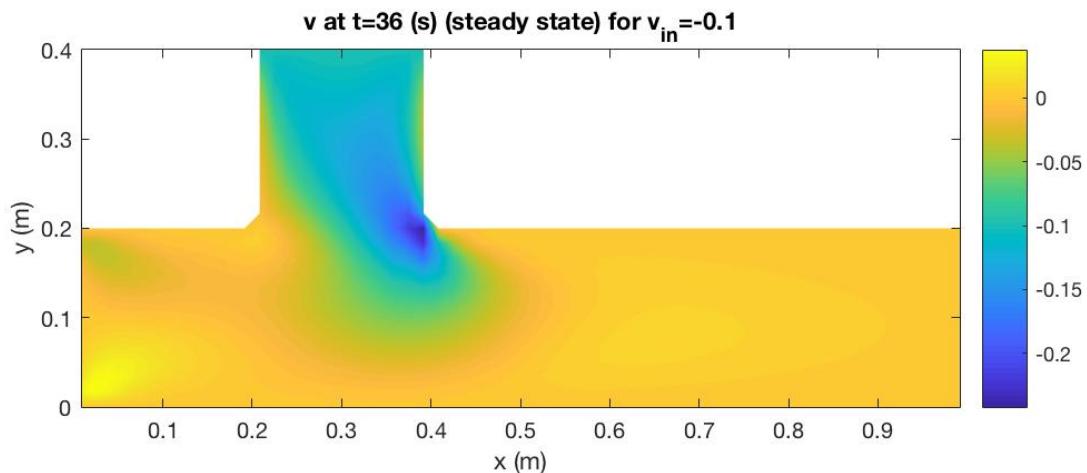


Fig 12

Increasing the influx would lead to higher velocities at the outlet channel (more mass flux). The profile is also pushed to the bottom wall due to the effect of coming v -velocity from the vertical channel.

v-velocity



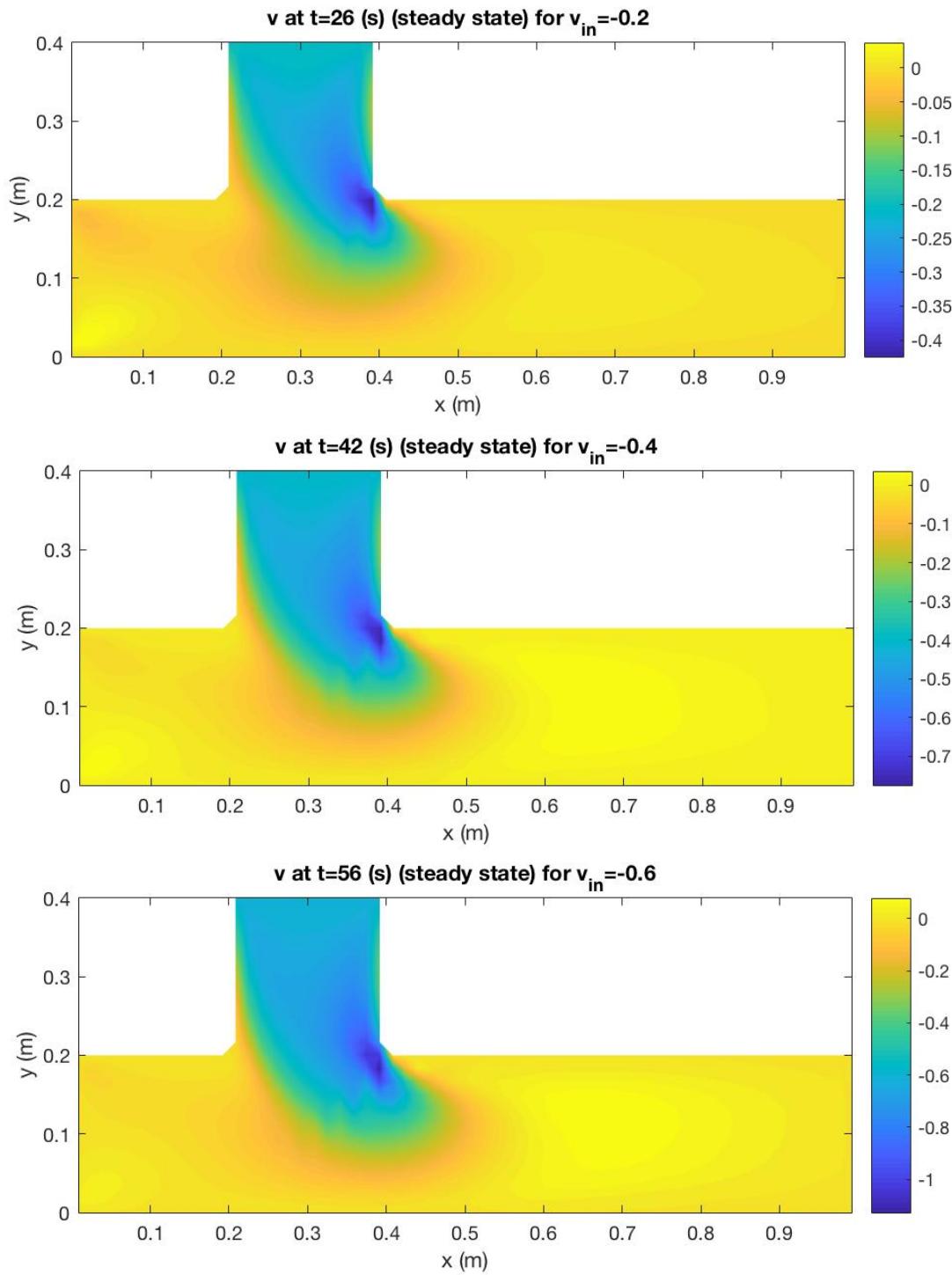
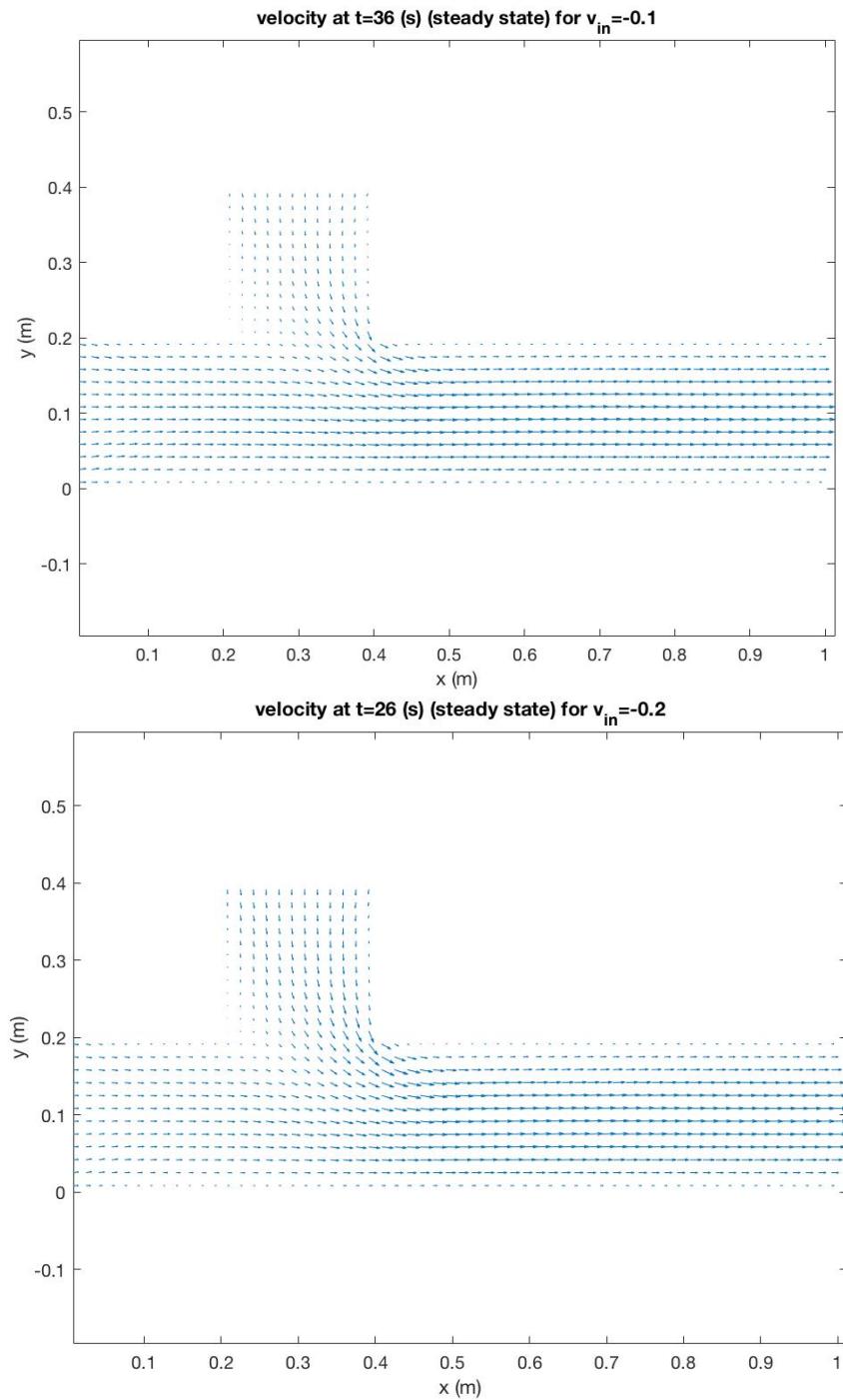


Fig 13

The v -velocities look very similar, the only difference is that the values would be higher everywhere at higher influxes.

Velocity quivers



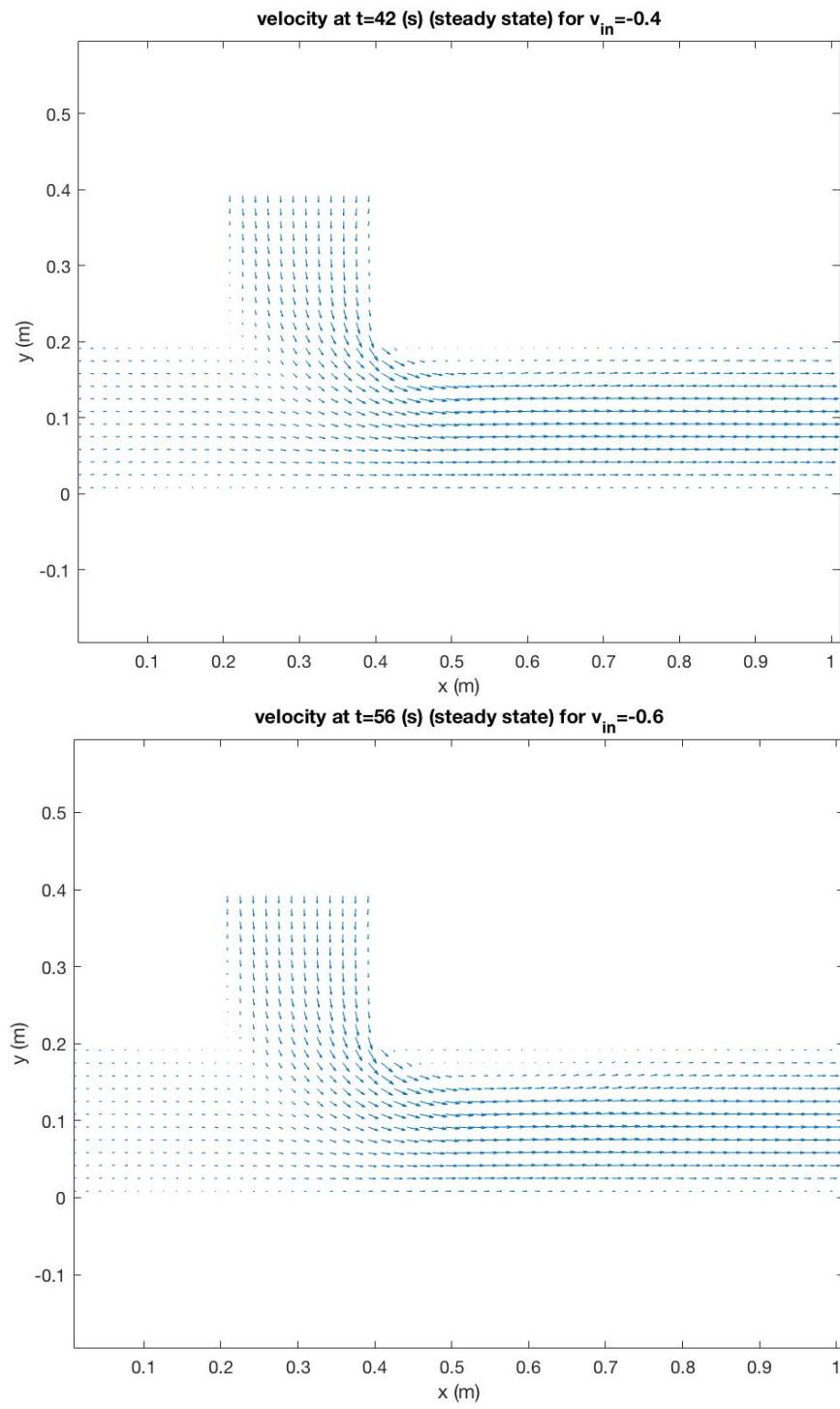
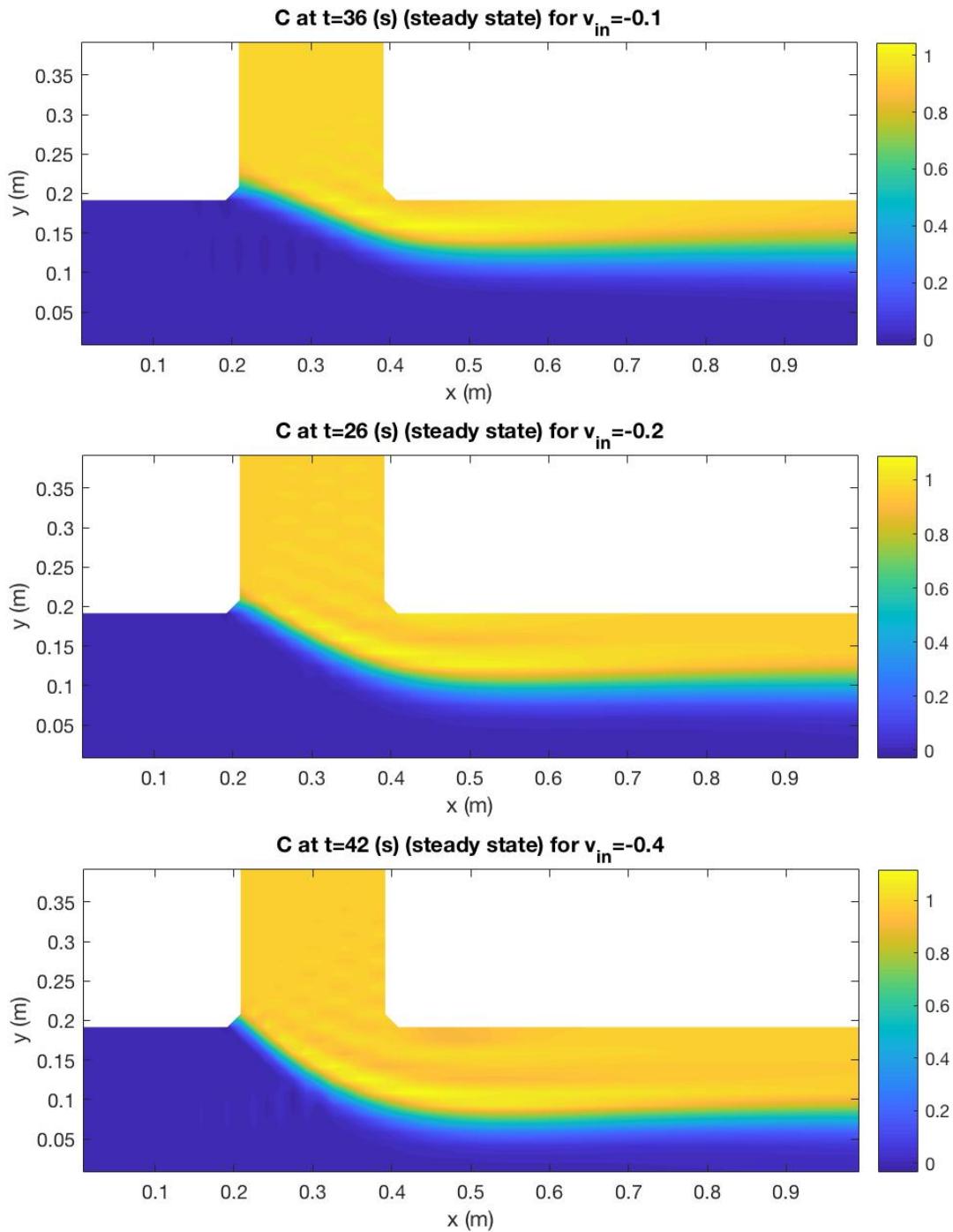


Fig 14

The quivers clearly show how the fluid moves which is very similar for all the cases. The only difference is the effect of pressure drop at the junction edge which leads to a higher distance of the high-speed fluid from the edge in higher influxes.

Concentration plots



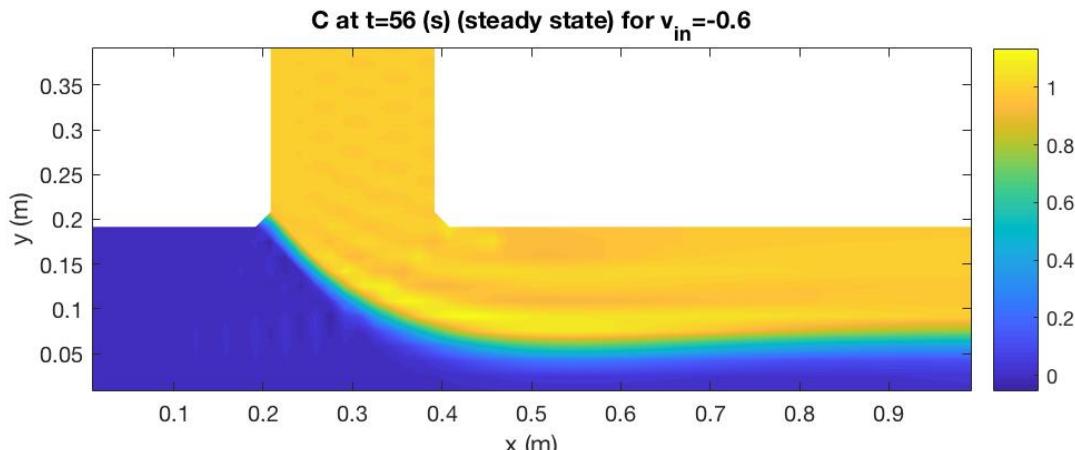


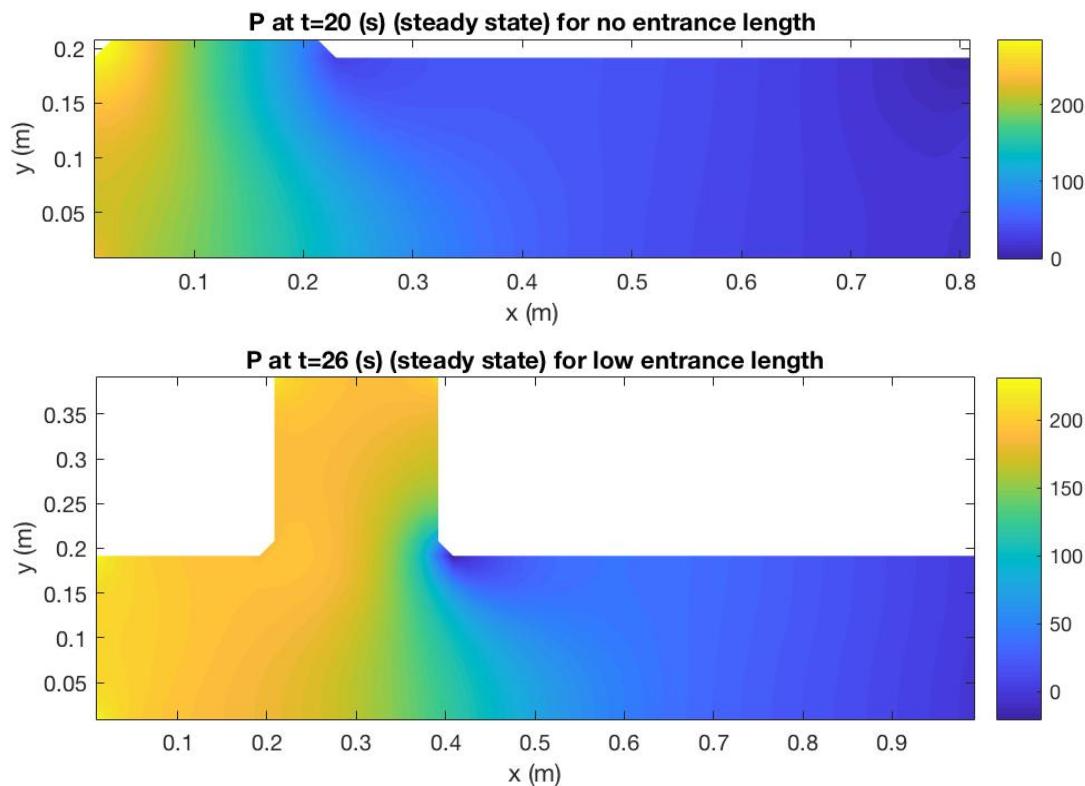
Fig 15

Since the mass diffusivity is low, the concentration doesn't dissipate well and flows move separately on top of each other. Higher influx leads to more of the outlet channel being taken by the upper flow. In lower influxes, the effect of diffusion is more observable as the convective term decreases, so the concentration dissipates more along the width of the channel.

3. Effect of entrance length

In this section, the entrance length of both inlets is changed and 3 cases are compared, one with almost no entrance region (one cell), other with a low entrance length, and the last one with a higher entrance length to let the flows become fully-developed before mixing. The maximum Reynolds number for the steady states are 136, 132 and 132 respectively. The CFL numbers are 0.014, 0.014 and 0.017.

Pressure plots



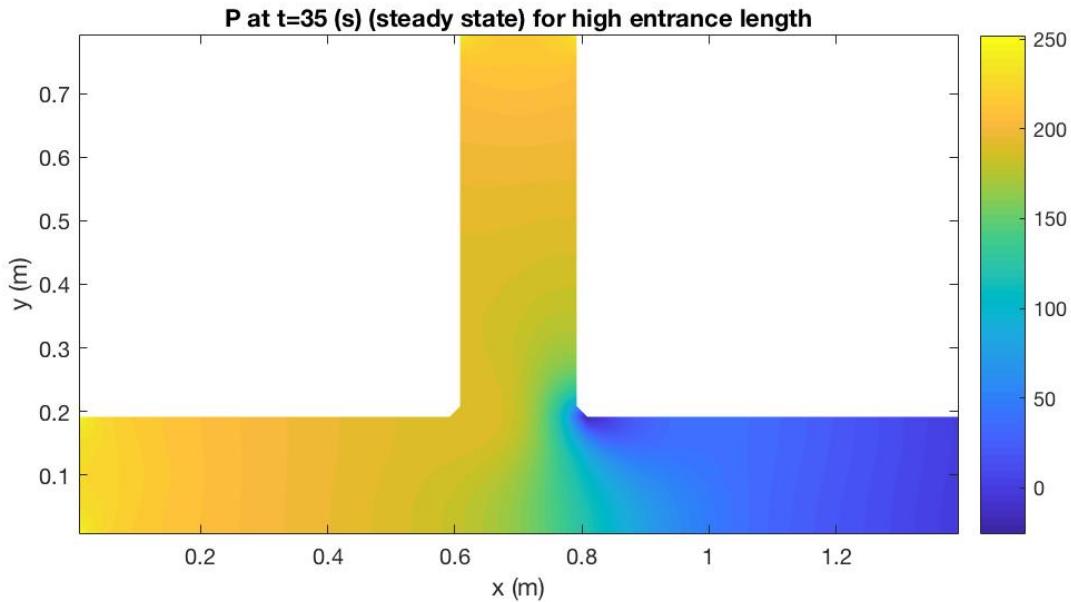
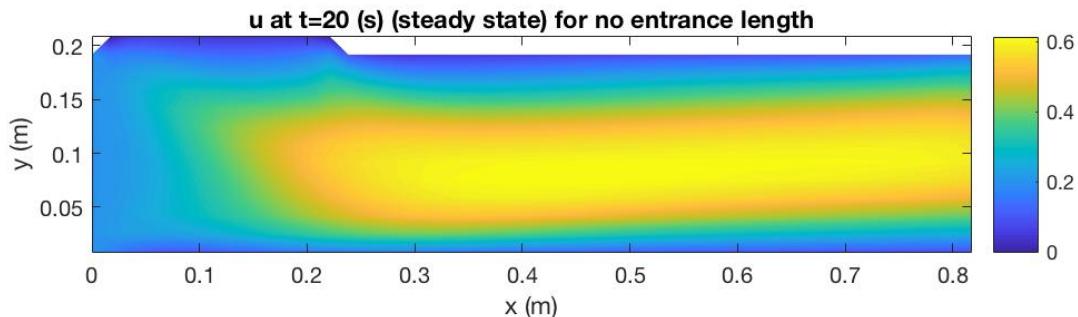


Fig 16

From the plots, we can conclude that a higher entrance length and allowing the flow to become fully-developed would lead to a lower pressure drop in the outlet channel (by comparing pressures at the left edge of the junction). This is because mixing is done in a more “laminar” condition when flow is fully developed and the pressure losses would be less due to the lower velocity gradients.

u-velocity plots



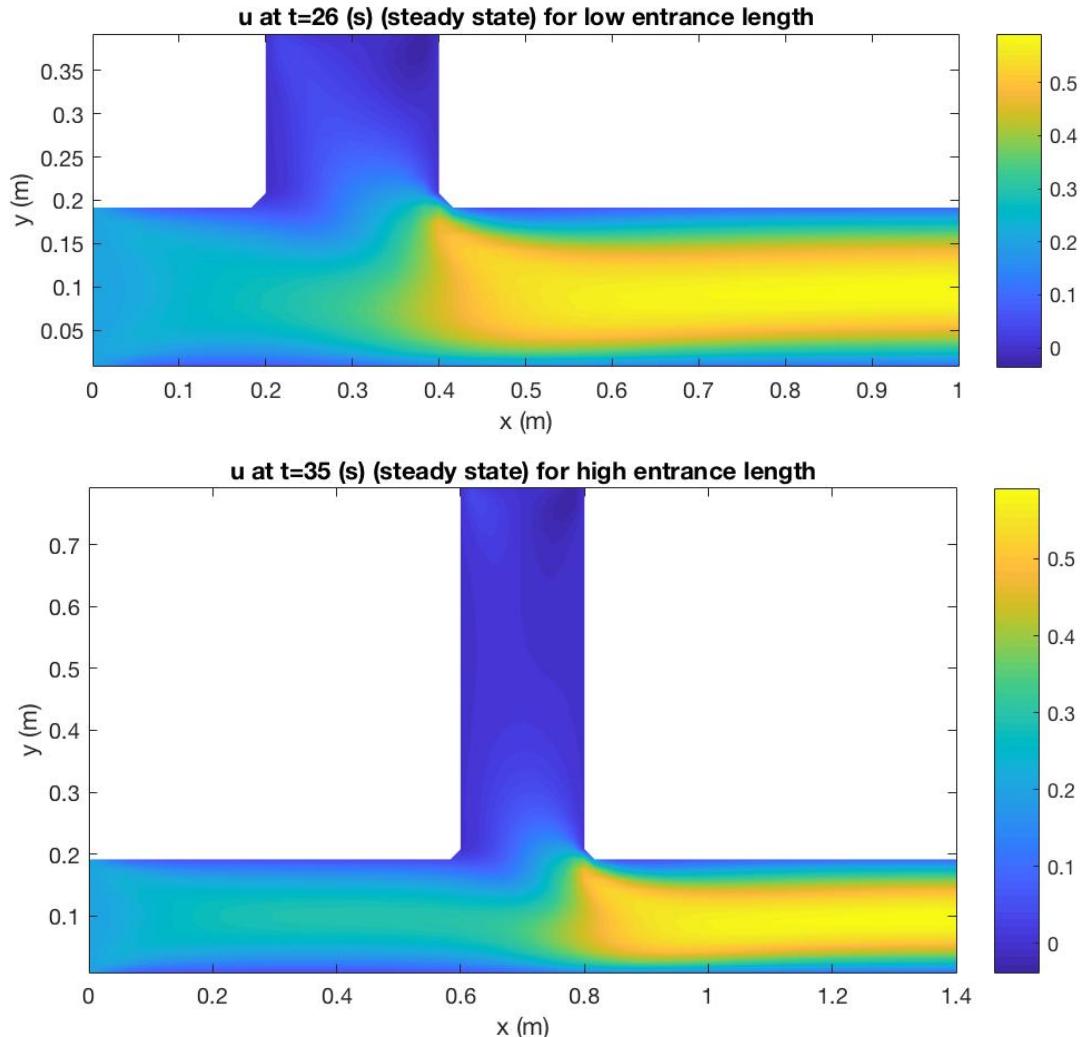


Fig 17

From the u -velocity plots, we can observe that when the flows mix at a uniform profile (not developed) they don't affect each other that much (since the highest velocities at the center are not achieved). This results in the flows to divert less. So we can see that the left flow is not pushed down as much as the fully developed case and this leads to the other flow to start getting momentum in the x -direction at around the middle of the junction, where in the other case it would be at the right edge.

v-velocity plots

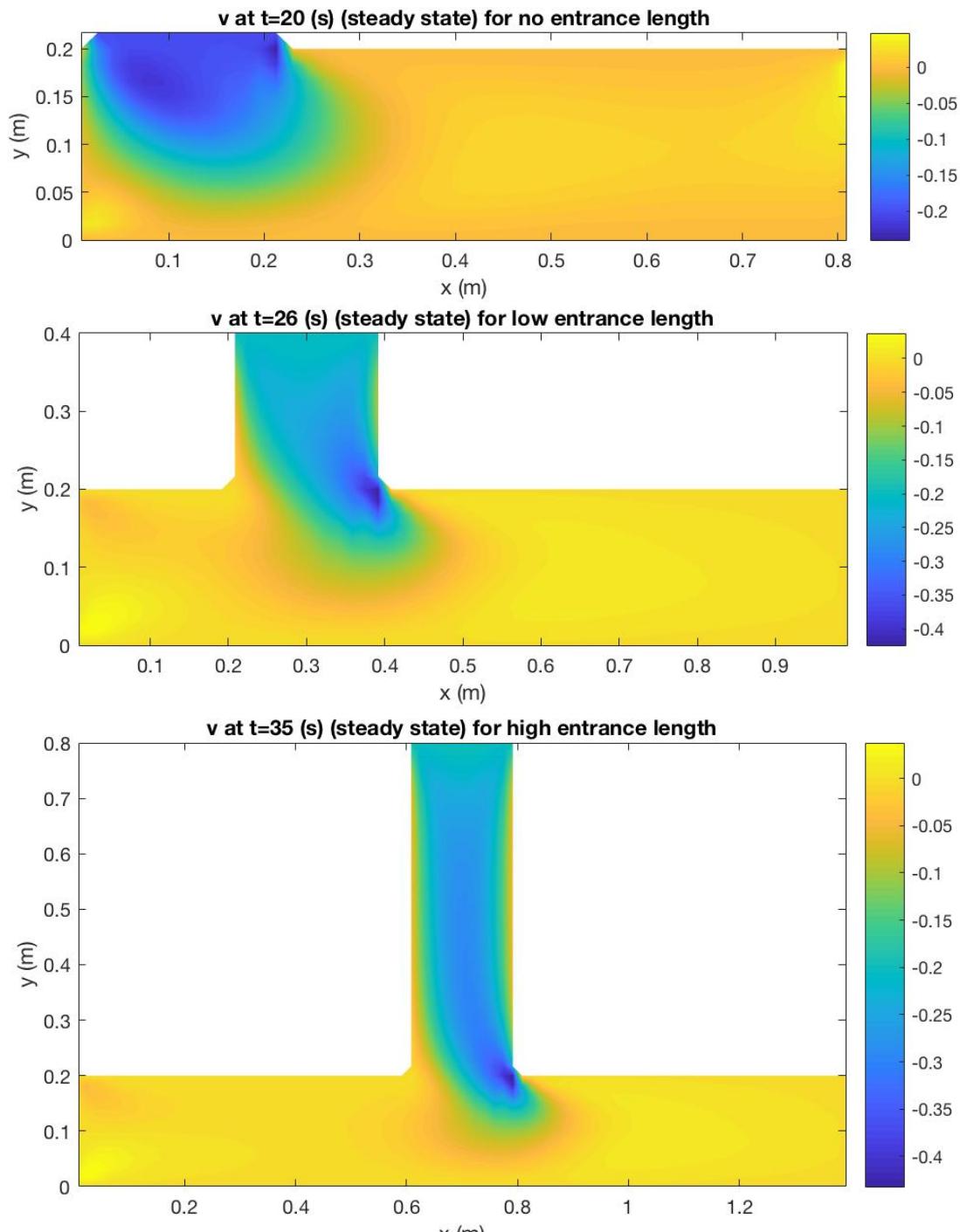
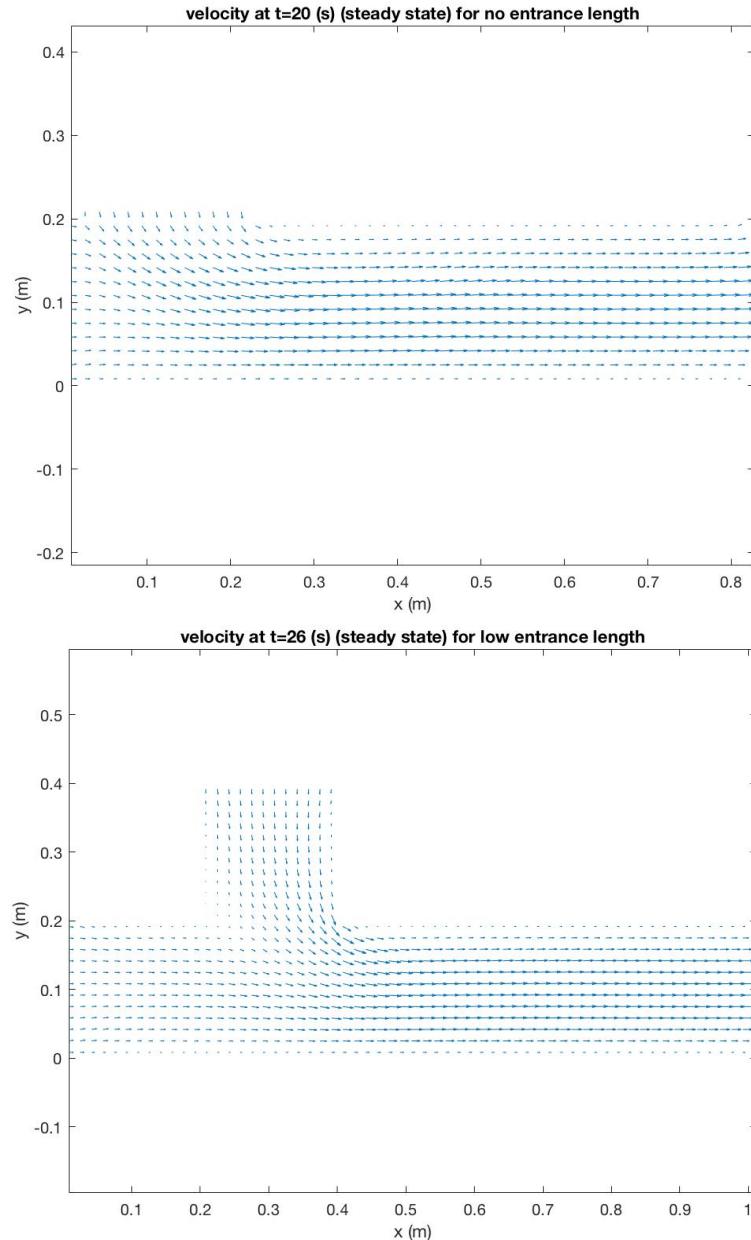


Fig 18

Results are similar to what discussed for the u-velocity. When the flows are not developed, the upper flow is not pushed to the right that much. This leads to the points in the middle of the junction to gain velocity in the y-direction.

Velocity quivers



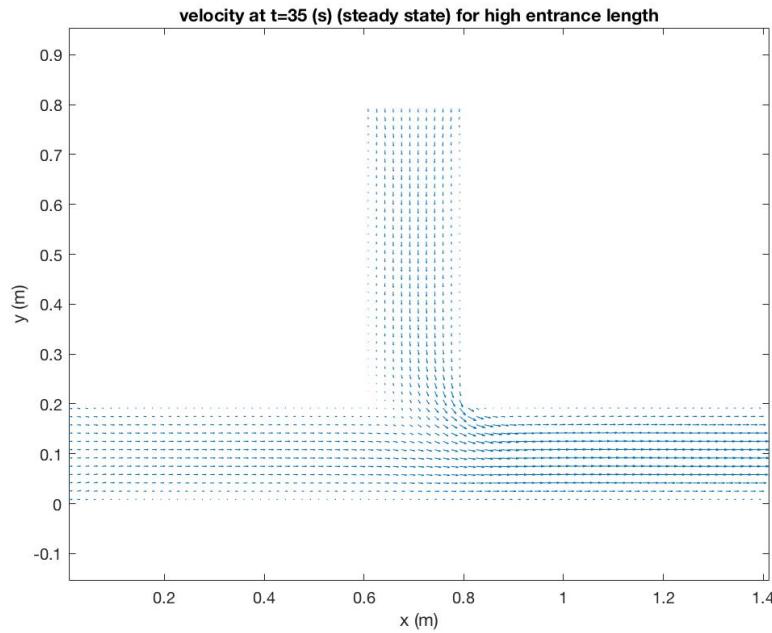
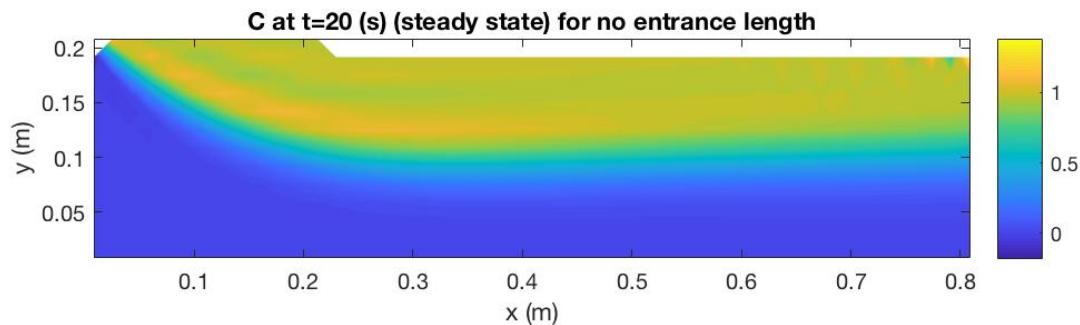


Fig 19

The discussion for velocities can also be observed in the quivers. Fully developed mixing would push the flows away from the center of the junction and causes a high velocity at the right edge of the junction.

Concentration plots



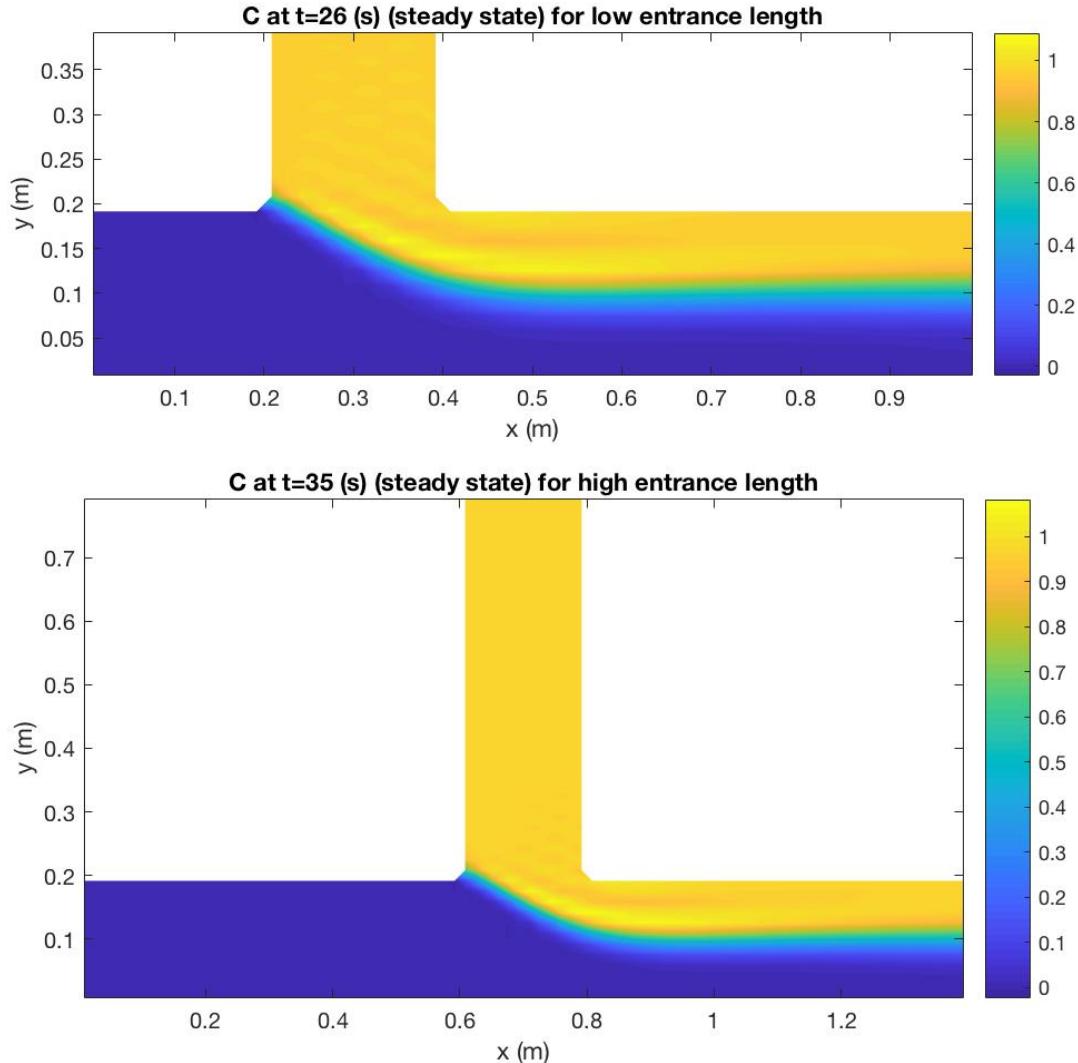


Fig 20

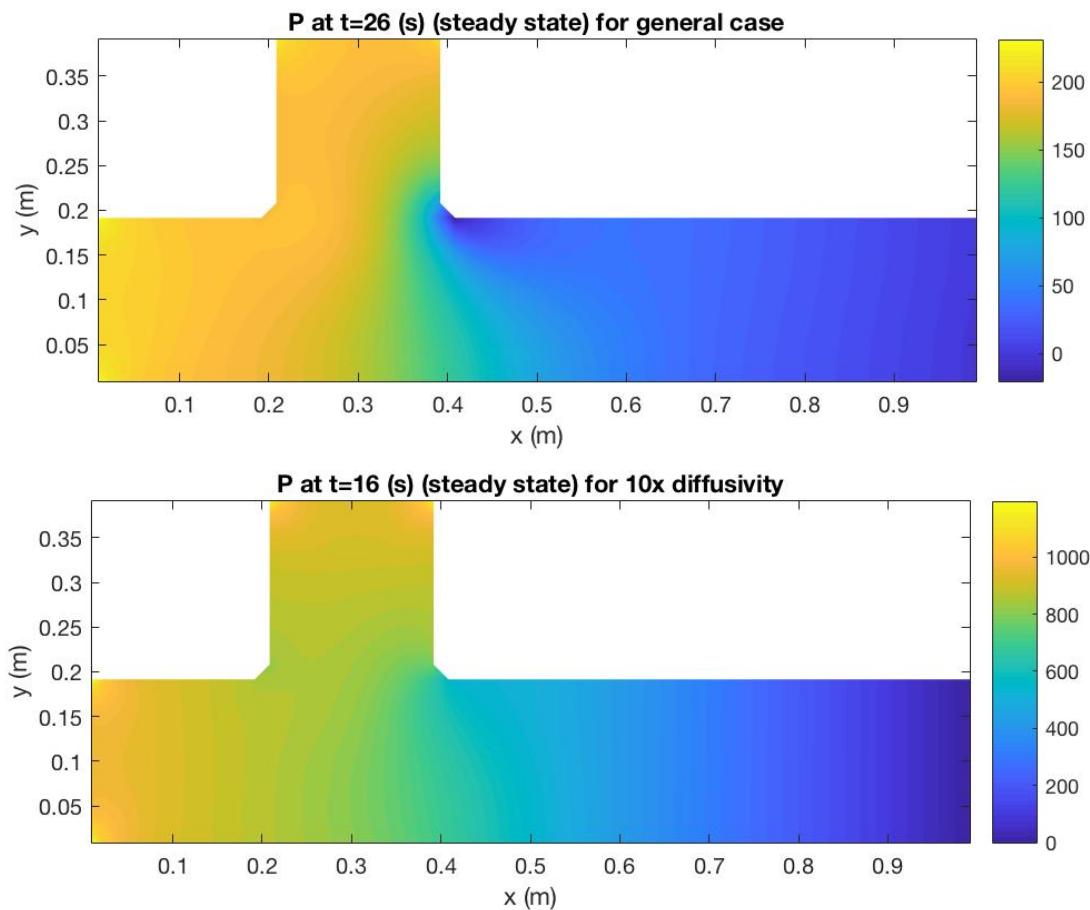
The concentration plots are not affected much by the entrance lengths as the flows would still move on top of each other. There's a slightly better mixing with not-developed mixing as the upper flow is moved closer to the upper wall. This effect, however, is negligible.

4. Effect of diffusive terms (ϑ and D)

In this section, the effect of diffusive terms in momentum and concentration equation is studied. This is done by comparing the general case against 5 and 10 times higher diffusive terms. This section doesn't concern a practical study since the values would be unrealistic (especially the mass diffusivities), but it illustrates the effect of diffusive terms in the plots perfectly.

For the cases, the Maximum Reynolds numbers at the steady state are 132, 13 and 1 respectively. Maximum CFL numbers are 0.014, 0.014 and 0.0014.

Pressure plots



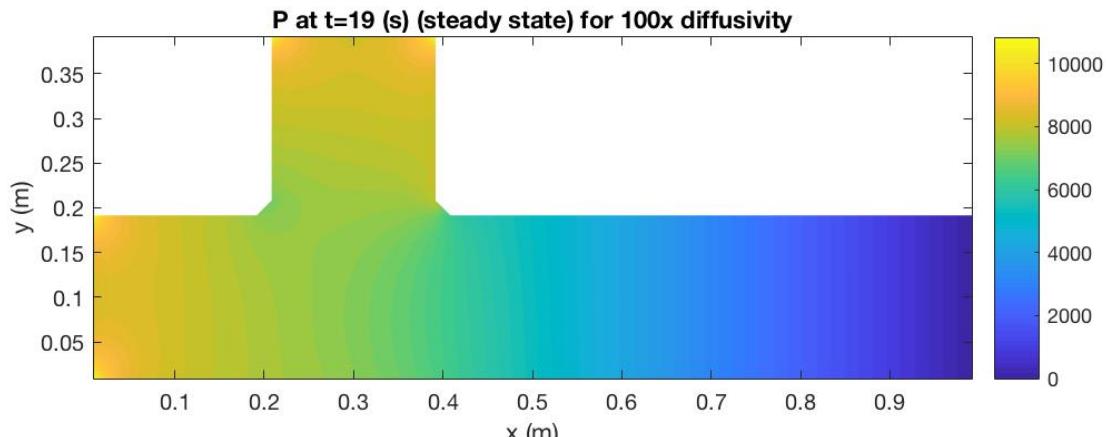
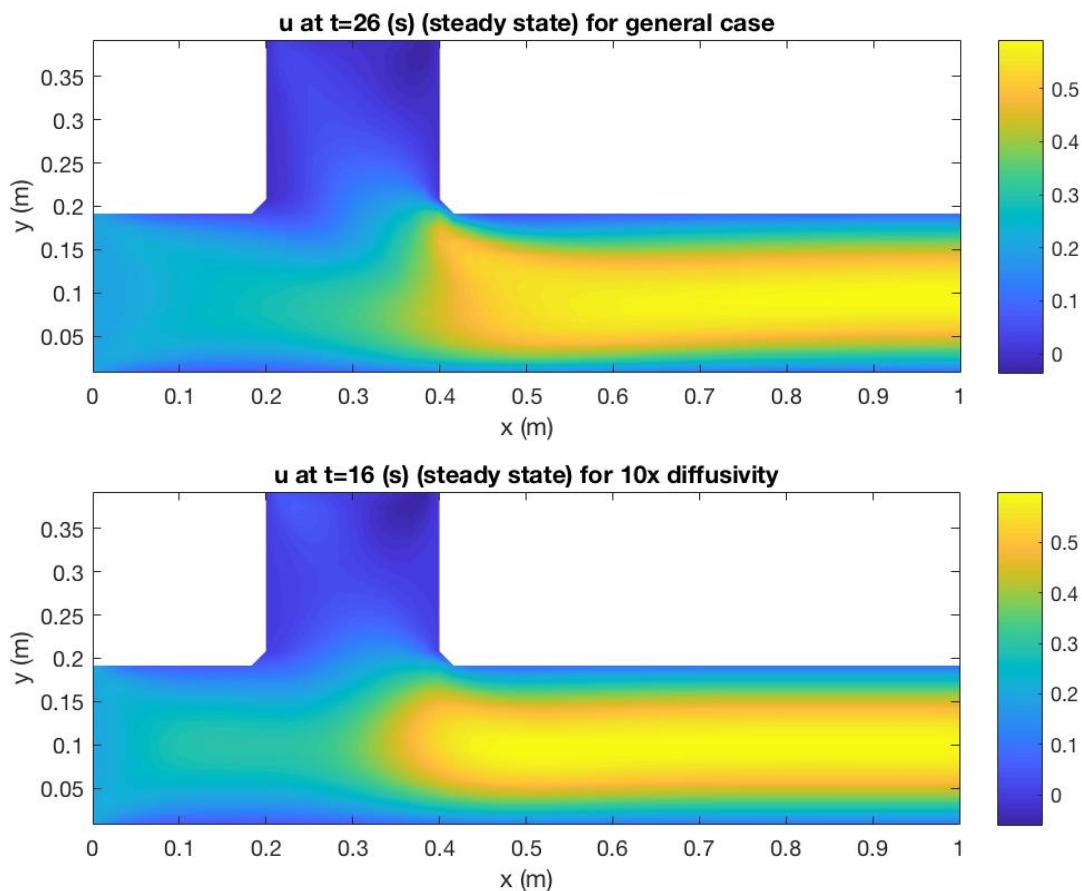


Fig 21

As it can be seen from the plots, higher viscosity would lead to an increase in the pressure drop in all sections of the channel by orders of magnitude. This is because of the high shear forces in the viscous liquid.

u-velocity profiles



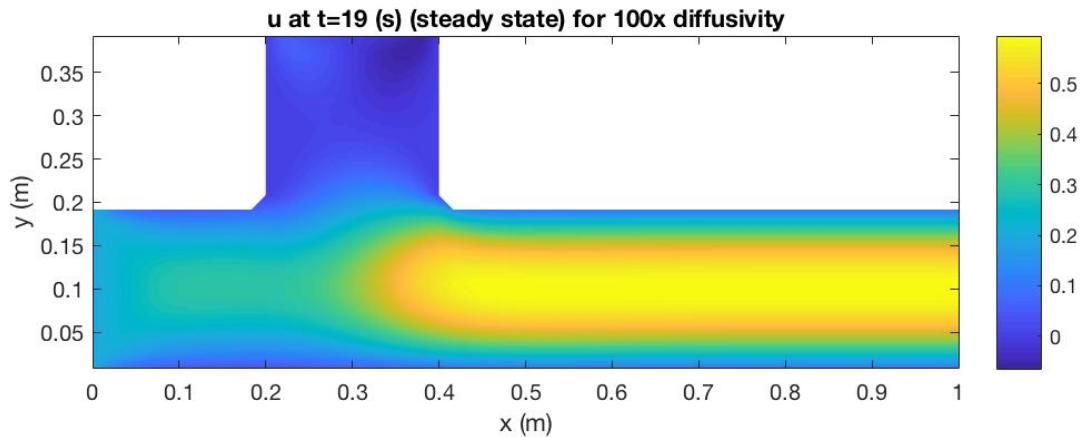
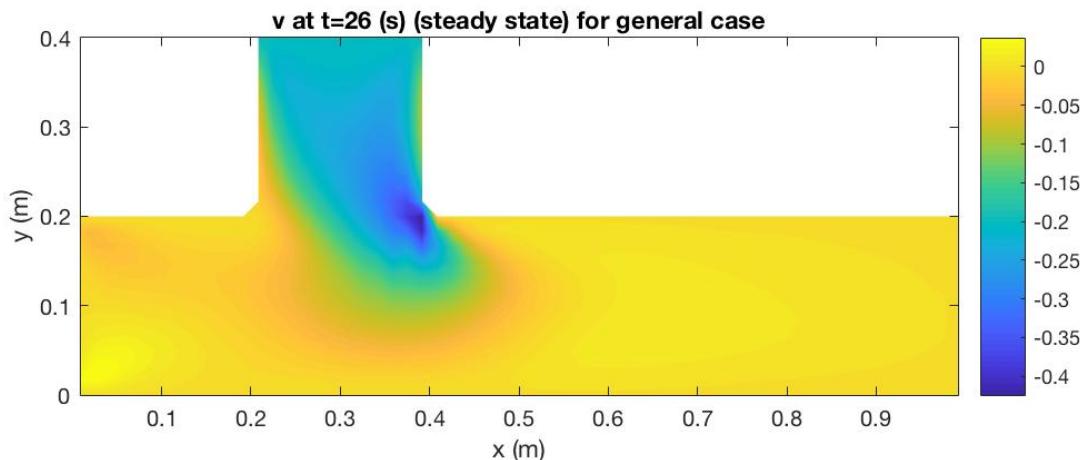


Fig 22

As we can see, the higher viscosity doesn't affect the profile at the outlet channel, but since the flows are more laminar, the effect of mixing is less and the left flow is not affected by the other one as much as it would for higher Reynolds numbers.

v-velocity plots



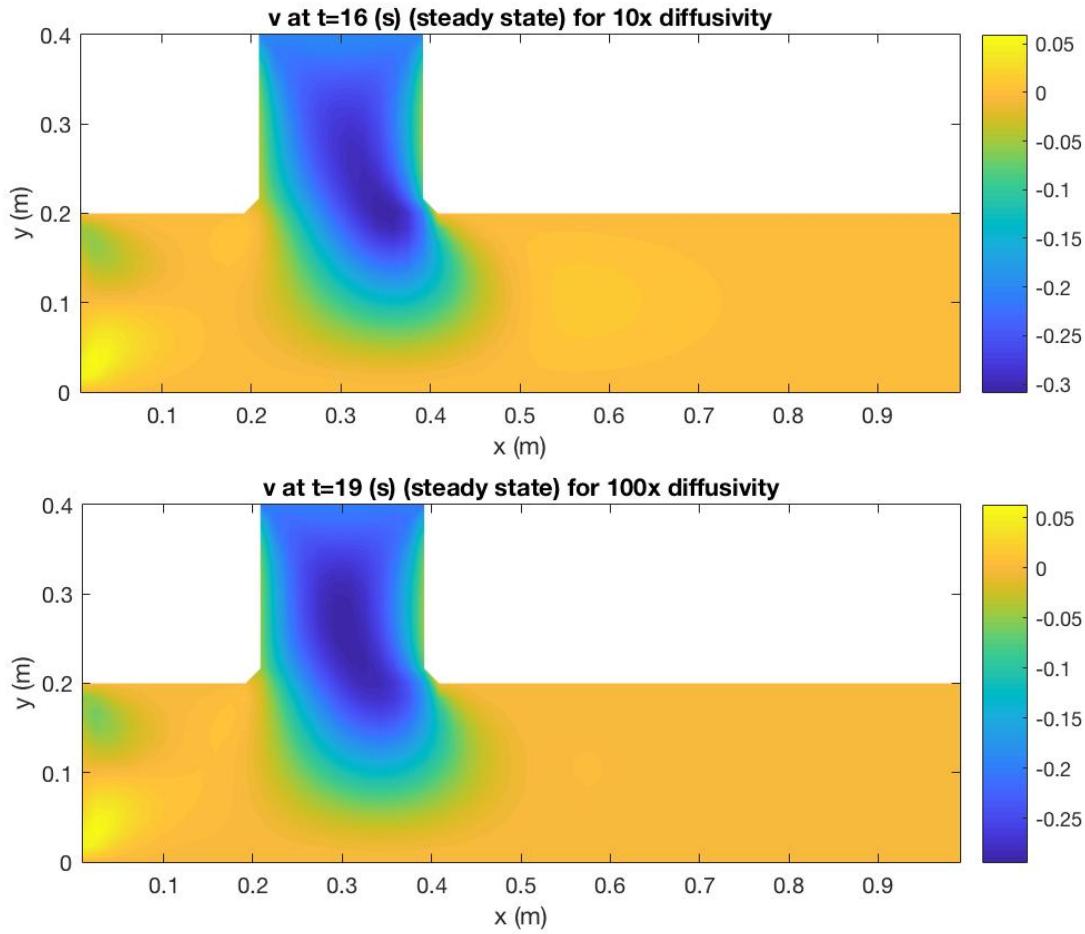
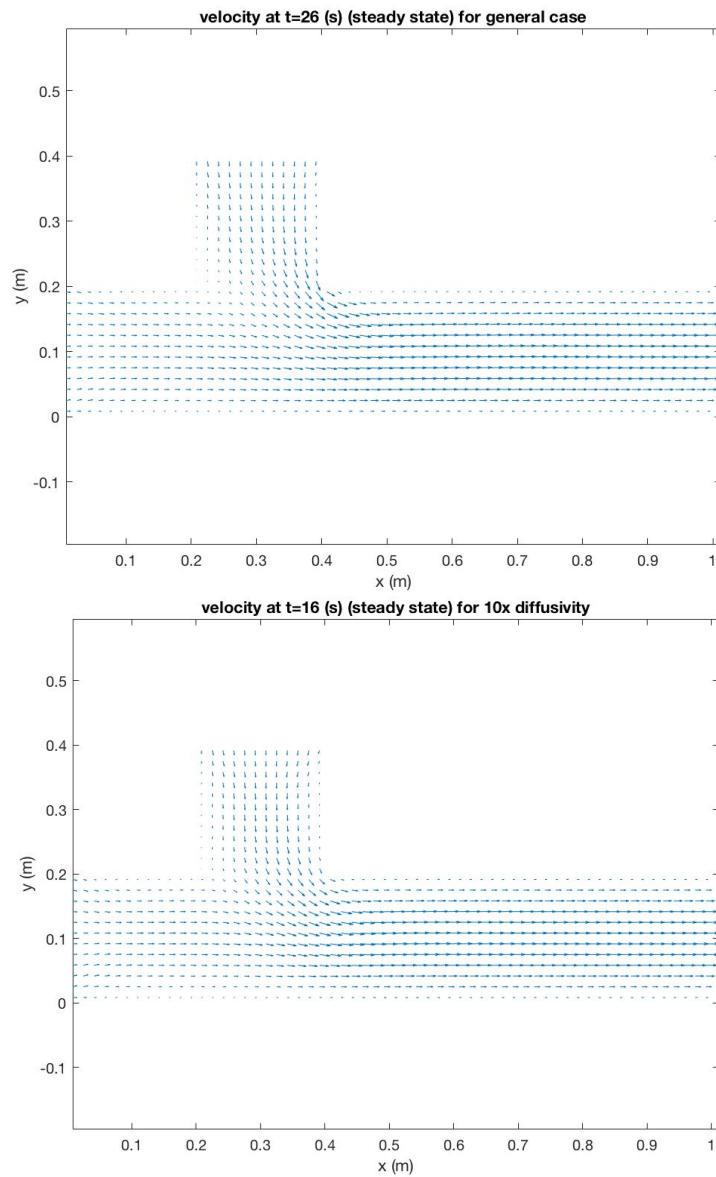


Fig 23

Results are similar to the u -velocities. The more laminar cases (higher viscosities) lead to a more stable mixing where the two flows are not diverted that much due to the effect of each other. So here, the v -velocity is not pushed to the right that much which leads to the lower velocities at the right edge of the junction.

Velocity quivers



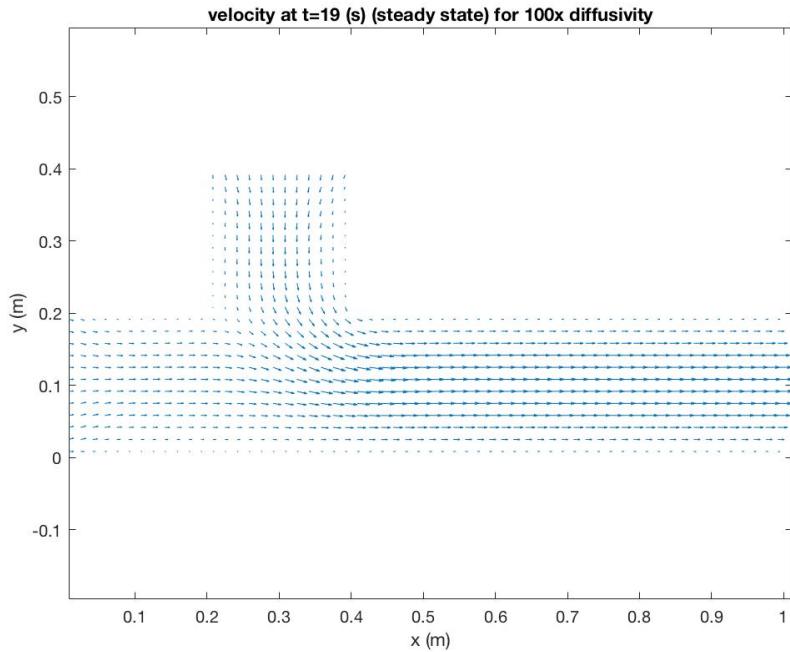
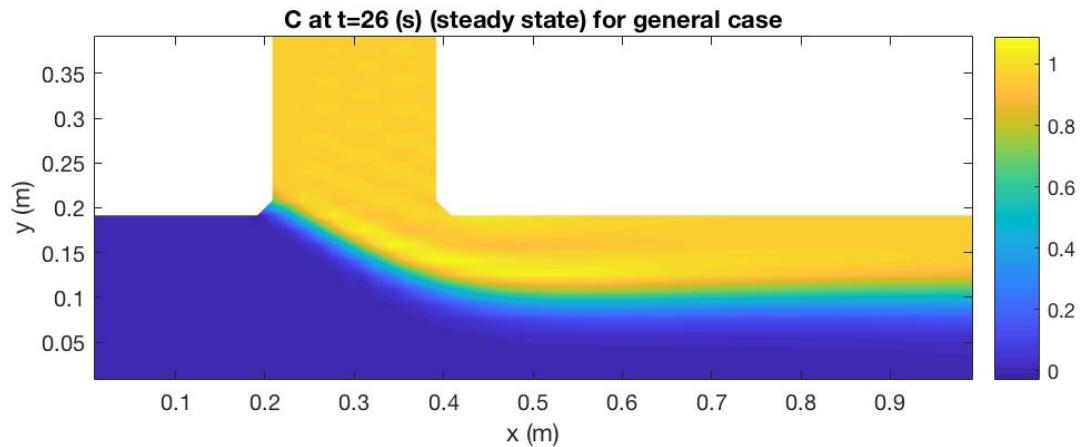


Fig 24

Flows not diverting each other to the sides, as discussed in u- and v-velocity sections, is visible. We can also clearly see the lower velocities at the right edge since the flows are not pushed to the edge.

Concentration plots



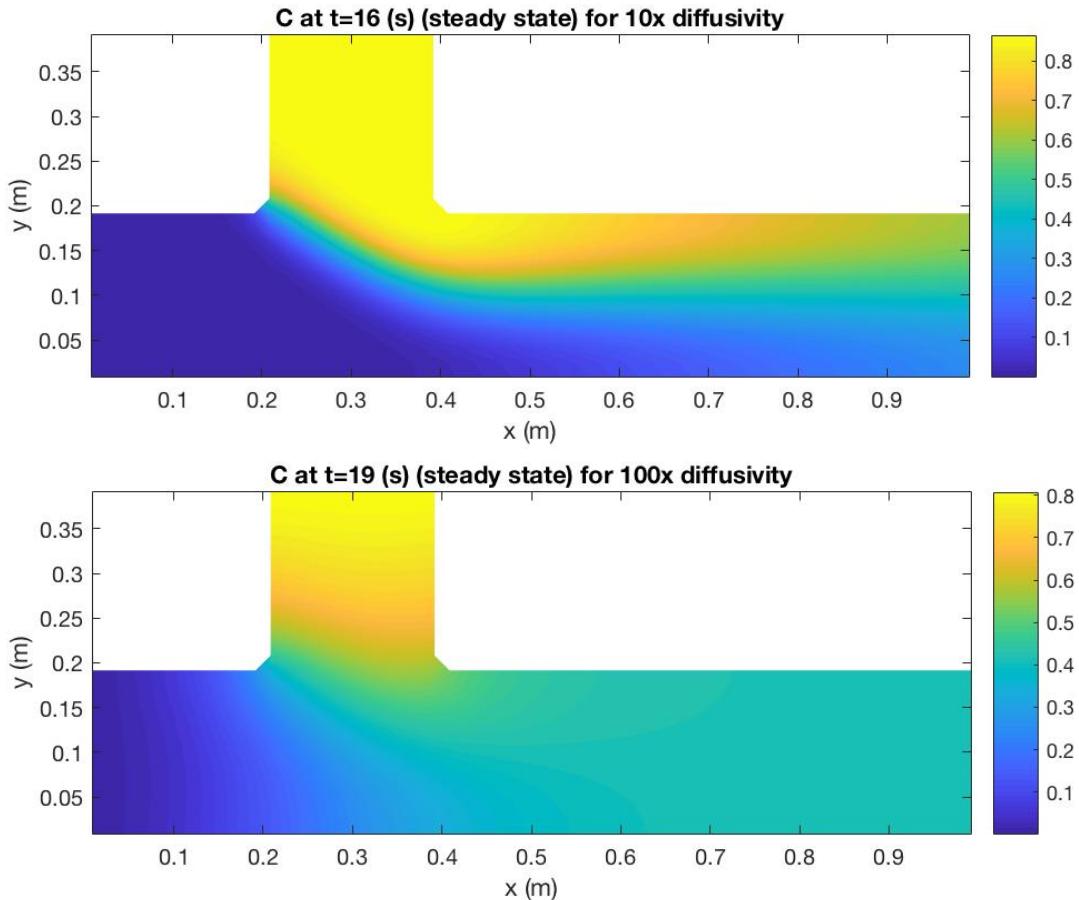


Fig 25

The effect of diffusion is clear in the concentration plots. In the general case, since the mass diffusion is low, the flows move on top of each other and the concentration doesn't get dispersed along the channel width. But with higher diffusivity, higher concentration starts to be diffused to the lower flow and a more uniform outlet flow is observed. In the last case, the flows are perfectly mixed at outlet, and the diffusion is big enough that we can see the effect of diffusion in the upstream direction in the inlet channels. The second case shows the effect of longer outlet channel on the better mixing of the two flows.

Conclusion

By running the code for different conditions, a good understanding of the problems and contributing factors is achieved. The entrance length, diffusive parameters, and relative velocities, all have a contribution to the resulting velocity and concentration fields. As discussed in the results section, the relative influx will determine the percentage of the outlet channel that is taken by each flow; the diffusive term and outlet length govern the dissipation of the concentration between the two flows; and the entrance length affects the velocity and pressure distributions and results in a more laminar mixing. The code is flexible to simulate different geometries (different lengths shown in fig 4) and different mesh spacing in x- and y-directions. The explicit staggered scheme makes this code a fast tool to get the fields, but due to the explicit scheme, there are limitations to the time step set by Courant number from convective and diffusive terms. These values are checked at every time step along with the Reynolds number to make sure that flow is laminar and the solution is stable.

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