# Modelling of fluid mixing and dynamics in curved pipelines 

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## 1 Introduction

During the Study Mathematics with Industry held in Amsterdam we worked on a challenge formulated by Shell about the mixing of fluids in curved pipelines. The question originates from a problem that can occur when transporting oil and gas through pipelines. This transportation of hydrocarbon fluids through pipelines in a safe and efficient way is a major challenge for the petrochemical industry. Especially in rough conditions like the ones that are present on the bottom of the ocean where temperatures typically lie around $4^{\circ} \mathrm{C}$. Many oil and gas fields lie beneath inland waters and offshore areas around the world, and the exploration, drilling and development of oil and gas fields in these underwater locations is called subsea. When oil and gas flow out of a subsea well the fluids are transported through pipelines on the ocean floor to offshore production platforms. These pipelines, can stretch for many kilometres, forming a large infrastructure. Because the seabed is not perfectly flat, there are segments of pipeline which will not lie horizontal but under an angle or even vertical.

When oil and gas are produced from a well, it is usually a mixture of the two which is often co-flowing with water, sand particles and other contaminants. A phenomenon related to the presence of water that can cause a lot of problems is hydrate formation, typically gas hydrates. These hydrates are solids which are crystalline water-based: they consist of a gas molecule (e.g. methane, ethane, propane and carbon dioxide) which is trapped in a water cavity composed of hydrogen bonded water molecules. Macroscopically, hydrates form a slurry which is quite similar to wet snow. Single gas hydrates can cluster together and form structures. When these structures grow, they can form a hydrate plug that blocks the full cross sectional area of the pipe.

Hydrates only form under specific circumstances, namely at low temperatures and high pressure. These circumstances arise, for instance, when an oil and gas well (re-)starts production and the pipeline is filled with cold fluids, including water. To prevent hydrates from forming the pipeline is usually flushed with a hydrate inhibitor. Such a hydrate inhibitor chemically acts the same as the antifreeze fluid one uses in a car. A common hydrate inhibitor is methanol. In general, the aim is to use as little methanol as possible, since it is both an expensive and dangerous fluid. That is one of the reasons why Shell wants to be able to better predict how methanol will mix into a pipeline filled with water.

### 1.1 Problem description

For our study, we start with a pipeline filled with water. Then, from one entrance of the pipeline, methanol is flushed into it at a constant speed. The challenge that Shell posed was:

What is the concentration of methanol along the pipeline as a function of time and space, when looking at different geometries of the pipe such as the presence of curves and sections of the pipeline under an angle?

Determining this concentration is not straightforward since there are several effects that have to be taken into account. The first one is the difference in the densities: the density of methanol is approximately $800 \mathrm{~kg} / \mathrm{m}^{3}$, whereas that of water is approximately $1000 \mathrm{~kg} / \mathrm{m}^{3}$. Because of this density difference, the methanol tends to 'float' on the water. This results in different behaviour of the methanol in the water along the various sections of the pipeline. In downward sloped sections, the density difference will result in a stable front of methanol that moves down. In horizontal or upward sloped sections a layer of methanol will form and float on top of the water. When observing a cross section of the pipe, one can see a distinct region of a 'light' fluid on top of a 'heavy' fluid. This phenomenon is called stratification.

In addition, we have to take into account that water and methanol are miscible. This means that they are able to fully dissolve in one another. This in contrary to immiscible fluids (e.g. oil and water) for which there will always exist a distinct layer between the two fluids. There are some additional effects (e.g. viscosity differences, surface tension) which will play a role in reality, but these will not be accounted for in this study.

This report is structured as follows: First, a physical background in fluid dynamics is presented with the relevant equations and their derivation. In section 3 appropriate notations and conventions are introduced. The problem is then approached from two different angles: in section 4 a 3D tranformation of coordinates is studied, intended to focus on the mixing interface of the miscible fluids. In section 5 a 1D model reduction approach is proposed, in which the along-pipeline direction is the only remaining spatial coordinate in the resulting model. This 1D model is solved numerically, as dis-
cussed in section 6. Results from simulations with this numerical model are presented in section 7 .

## 2 Navier-Stokes

In this section we provide a brief description of the Navier-Stokes equations. The contents of this section are not meant as a detailed exposition of the field but should rather be thought of as a simple and heuristic introduction to fluid dynamics. Furthermore, the idea's presented in this section are standard and no originality is claimed. The interested reader is referred to Chorin and Marsden (1979) for a more comprehensive introduction into the field of fluid dynamics.

Suppose $\Omega \subset \mathbb{R}^{3}$ is an open subset which contains a fluid with mass density $\rho(t, x)$, where $t \geq 0$ and $x \in \Omega$. Let $\mathbf{u}(t, x)$ denote the velocity of a fluid particle starting at $x \in \Omega$ at time $t$. In other words, the trajectory $t \mapsto \varphi(t, x)$ of a fluid particle starting at $x$ satisfies the differential equation

$$
\frac{d}{d t} \varphi(t, x)=\mathbf{u}(t, \varphi(t, x))
$$

The Navier-Stokes equations are based on two basic principles: conservation of mass and Newton's second law. In order for the computations in the following sections to be valid we shall henceforth assume that $\rho, \varphi$ and $\mathbf{u}$ are sufficiently smooth.

### 2.1 Conservation of mass

In this section we derive an equation for the conservation of mass. To this end, suppose $B \subset \Omega$ is an open subset. Then the rate of change of mass of the fluid contained in $B$ is given by

$$
\frac{d}{d t} \int_{B} \rho \mathrm{~d} V=\int_{B} \frac{\partial \rho}{\partial t} \mathrm{~d} V
$$

We assume that the change of mass in $B$ is only caused by fluid flowing in from $\Omega \backslash B$ or flowing out from $B$. In particular, the rate at which fluid comes in or escapes through $\partial B$ is

$$
-\int_{\partial B}\langle\rho \mathbf{u}, \mathbf{n}\rangle \mathrm{d} A=-\int_{B} \operatorname{div}(\rho \mathbf{u}) \mathrm{d} V
$$

where $\langle\cdot, \cdot\rangle$ is the standard Euclidian product on $\mathbb{R}^{3}$ and $\mathbf{n}$ is the outward (unit) normal vectorfield on $\partial B$. Therefore, conservation of mass is equivalent to

$$
\begin{equation*}
\int_{B} \frac{\partial \rho}{\partial t} \mathrm{~d} V=-\int_{B} \operatorname{div}(\rho \mathbf{u}) \mathrm{d} V \tag{1}
\end{equation*}
$$

In turn, this implies that

$$
\begin{equation*}
\frac{\partial \rho}{\partial t}+\operatorname{div}(\rho \mathbf{u})=0 \tag{2}
\end{equation*}
$$

since (2) holds for any open subset $B \subset \Omega$.

### 2.2 Newton's second law

In this section we use Newton's second law and the conservation of mass to derive an equation for the velocity field $\mathbf{u}$. The idea is straightforward: we simply compute the rate of change of momentum of the fluid, the net force acting on the fluid, and then use Newton's second law to relate the two.

Rate of change of momentum The acceleration of a fluid particle at $x \in \Omega$ at time $t$ is given by

$$
\frac{d^{2}}{d t^{2}} \varphi(t, x)=\frac{\partial \mathbf{u}}{\partial t}(t, \varphi(t, x))+\mathbf{u} \cdot \nabla \mathbf{u}(t, \varphi(t, x))
$$

where

$$
\mathbf{u} \cdot \nabla \mathbf{u}:=\sum_{j=1}^{3} \frac{\partial \mathbf{u}}{\partial x_{j}} u_{j} .
$$

Let $B \subset \Omega$ be an open subset as before and set $B_{t}:=\varphi(t, B)$. Then the momentum of the fluid initially contained in $B$ at time $t$ is given by

$$
\int_{B_{t}} \rho \mathbf{u} \mathrm{~d} V=\int_{B}(\rho \mathbf{u}) \circ \varphi \cdot \operatorname{det} D_{x} \varphi \mathrm{~d} V .
$$

The conservation of mass (2) and a tedious (but straightforward) computation can now be used to show that the rate of change of momentum is given by

$$
\begin{equation*}
\frac{d}{d t} \int_{B_{t}} \rho \mathbf{u} \mathrm{~d} V=\int_{B_{t}} \rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u} \cdot \nabla \mathbf{u}\right) \mathrm{d} V \tag{3}
\end{equation*}
$$

Forces acting on the fluid Next, we explain how to model the forces acting on the fluid. One can separate these forces into two categories:
(i) forces which act "directly" on the fluid particles in $B_{t}$,
(ii) forces which act on $B_{t}$ through its boundary.

It is out of the scope of this text to give a detailed treatment of all the forces acting on the fluid. Instead, we have chosen to give two simple but representative examples of how to model forces of either type. We will use these examples to derive a simplified
equation for the rate of change of momentum. In the next section we will then proceed by stating the full Navier-Stokes equations with the understanding that the forces appearing in the equation are derived by using the principles presented in this section.

A simple example of a force of type $(i)$ is gravity. Indeed, gravity is a force which acts "directly" on each fluid particle in $\Omega$. In the easiest case, the force on $B_{t}$ due to gravity is given by

$$
\mathbf{F}_{g}=\int_{B_{t}} \rho g \mathrm{~d} V,
$$

where $g \approx 9.81 \mathrm{~m} / \mathrm{s}^{2}$ is the gravitational acceleration.
The general procedure for modeling forces of the second type is to derive an integral formulation of the force by using the Divergence Theorem. Let us, for example, consider the internal force $\mathbf{F}_{p}$ which corresponds to the fluid pressing on itself. One could attempt to model this force by assuming the existence of a function $p:[0, \infty) \times$ $\Omega \rightarrow \mathbb{R}$, usually called the pressure, so that the force on $\partial B_{t}$ due to the fluid outside of $B_{t}$ is given by

$$
\mathbf{F}_{p}=-\int_{\partial B_{t}} p \mathbf{n} \mathrm{~d} A=-\int_{B_{t}} \nabla p \mathrm{~d} V
$$

where $\mathbf{n}$ is the outward unit normal on $B_{t}$. We remark, however, that in reality there is also another non-tangential force acting on the boundary of $B_{t}$ which contributes to the internal force and is related to the viscosity of the fluid.

If gravity and internal pressure are the only forces acting on the fluid, i.e. $\mathbf{F}_{n e t}=$ $\mathbf{F}_{g}+\mathbf{F}_{p}$, then

$$
\begin{equation*}
\int_{B_{t}} \rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u} \cdot \nabla \mathbf{u}\right) \mathrm{d} V=\int_{B_{t}}(\rho g-\nabla p) \mathrm{d} V \tag{4}
\end{equation*}
$$

by Newton's second law and (3). Hence

$$
\begin{equation*}
\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u} \cdot \nabla \mathbf{u}\right)=\rho g-\nabla p \tag{5}
\end{equation*}
$$

since (4) holds for any open subset $B$. The latter equation is essentially an infinitesimal formulation of Newton's second law.

### 2.3 Navier-Stokes equations

In this section we combine the conservation of mass and Newton's second law to state the Navier-Stokes equations. We start with the simplified considerations from the previous section and explain why the resulting system is ill-posed. We then resolve this issue by introducing the notion of incompressiblity. Finally, we state the full set of Navier-Stokes equations for an incompressible fluid.

An ill-posed Navier-Stokes equation The equations for the conservation of mass and Newton's second law from the previous sections yield the following simplified system:

$$
\left\{\begin{array}{l}
\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u} \cdot \nabla \mathbf{u}\right)=\rho g-\nabla p  \tag{6}\\
\frac{\partial \rho}{\partial t}+\operatorname{div}(\rho \mathbf{u})=0
\end{array}\right.
$$

The unknowns in (6) are the the mass density $\rho$, the internal pressure $p$ and the three components of the velocity field $\mathbf{u}$. Note, however, that the system in (6) is underdetermined, since we have five unknowns but only four equations. A possible solution to this problem is to take the conservation of energy into account.

The total energy of the physical model consists of kinetic and internal energy. The kinetic energy of the fluid is simply the classical energy related to the motion of the fluid on a macroscopic level. More precisely, the kinetic energy of the fluid initially contained in $B$ at time $t$ is given by

$$
E_{k i n}(t, B)=\frac{1}{2} \int_{B_{t}} \rho\|\mathbf{u}\|^{2} \mathrm{~d} V
$$

where $\|\cdot\|$ denotes the Euclidian norm on $\mathbb{R}^{3}$.
The internal energy $E_{i n}$ is related to the potential energy and microscopic motion of the fluid molecules. A detailed treatment of the internal energy requires thermodynamical considerations and is out of the scope of this text. We remark, however, that it is possible to balance the number of equations and unknowns by adding a scalar equation based on the conservation of energy:

$$
\frac{d E}{d t}=0, \quad E:=E_{k i n}+E_{i n}
$$

The incompressible Navier-Stokes equations Another strategy for balancing the number of equations and unknowns is to introduce a so-called equation of state, providing an algebraic relation between the pressure and the fluid properties, the density in this case. A simple approach is to assume that the fluid is incompressible, i.e., $\varphi$ preserves volume. This is equivalent to requiring that $\operatorname{div}(\mathbf{u})=0$. It depends on the properties of the fluid whether this assumption is realistic or not. For water and methanol in liquid state, this is generally a suitable assumption.

If the velocity field is divergence free, then the equation for the conservation of mass (2) can be explicitly solved. To see this, suppose that $\operatorname{div}(\mathbf{u})=0$, then

$$
\frac{\partial \rho}{\partial t}+\operatorname{div}(\rho \mathbf{u})=\frac{\partial \rho}{\partial t}+\langle\nabla \rho, \mathbf{u}\rangle=0
$$

where $\langle\cdot, \cdot\rangle$ denotes the Euclidian inner product on $\mathbb{R}^{3}$. Consequently,

$$
\frac{d}{d t} \int_{B_{t}} \rho \mathrm{~d} V=\int_{B_{t}}\left(\frac{\partial \rho}{\partial t}+\langle\nabla \rho, \mathbf{u}\rangle\right) \mathrm{d} V=0
$$

by the same computation as in (3). In other words, if $\mathbf{u}$ is divergence free, then $\varphi$ preserves mass (the converse holds as well), i.e.,

$$
\int_{B} \rho(0, x) \mathrm{d} V=\int_{B_{t}} \rho(t, x) \mathrm{d} V=\int_{B} \rho(t, \varphi(t, x)) \operatorname{det} D_{x} \varphi(t, x) \mathrm{d} V
$$

for all $t \geq 0$. Therefore,

$$
\begin{equation*}
\rho(t, \varphi(t, x))=\frac{\rho(0, x)}{\operatorname{det} D_{x} \varphi(t, x)}=\rho(0, x), \quad t \geq 0, x \in \Omega \tag{7}
\end{equation*}
$$

since $B$ was arbitrary and $\operatorname{det} D_{x} \varphi(t, x) \equiv 1$ (because $\operatorname{div}(\mathbf{u})=0$ ). In particular, the mass density is independent of time along trajectories of the fluid.

We are now ready to state the incompressible Navier-Stokes equations:

$$
\left\{\begin{array}{l}
\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u} \cdot \nabla \mathbf{u}\right)=-\nabla p+\mu \Delta \mathbf{u}+\rho g  \tag{8}\\
\operatorname{div}(\mathbf{u})=0
\end{array}\right.
$$

where $(t, x) \in[0, T] \times \Omega$ and

- $p:[0, \infty) \times \Omega \rightarrow \mathbb{R}$ is the internal pressure,
- $\mu$ is the dynamic viscosity of the fluid,
- $g \approx 9.81$ is the acceleration of gravity,
- $T>0$ is a prescribed integration time.

The unknowns in (8) are the internal pressure $p$ and the velocity field $\mathbf{u}$. The mass density $\rho$ is explicitly given by the initial and boundary conditions, as can be inferred from (7). Therefore, the number of unknowns and equations in (8) is balanced. Finally, the system should be supplemented with an initial condition $\mathbf{u}_{0}: \Omega \rightarrow \mathbb{R}^{3}$ and suitable boundary conditions. These are dictated by the physical model under consideration.

## 3 Notation and conventions

Here we introduce the coordinates/variables as seen in Figure 1. The pipeline is fully described using the following coordinates:

- $s$ is tangential to the central line of the pipeline. It is oriented along the flow, which we chose to be from left to right (water flowing in from the left entrance)
- $w$ is the vertical direction starting from the the central line. It is normal to the central line and the radial direction $q$ but not to the mixing layer.
- $q$ is normal to both $s$ and $w$. It is pointing out of the paper in the sketch shown in Figure 1. We will ignore this coordinate in all our subsequent transformations since we assume that the liquid is homogeneously distributed along a vertical cross section (the mixing layer is horizontal).
- $\alpha$ denotes the angle that the central line makes with the horizontal. It is positive in case the pipeline is sloping downwards and negative in case the pipeline is sloping upwards (see sketch).
- $c$ and $A$ denote the concentration of methanol in the fluid and the area of the fluid (see Figure 1), respectively. Since we only have two components, the concentration of water $\tilde{c}$ satisfies $\tilde{c}=1-c$.
- The subscripts $u$ and $l$ denote the upper and lower regions, with respect to the vertical position of the fluids.
- $D_{w}$ is the normal diffusion coefficient in the $w$-direction.
- $\psi$ is a mixing term that will be used in the 1D model in section 5 .


Figure 1: Sketch of the 3D pipeline and a cross-section of the pipeline in the vertical direction.

## 4 3D Approach: Coordinate transformation along the central line

### 4.1 3D co-moving frame

The non-trivial curvature of pipelines makes it difficult to model the flow of different fluids and the change in concentration. To account for this, we suggest to perform a coordinate transformation that allows us to focus on the specific needs: computing the concentration in the case of miscible fluids. In this section we discuss how such a transformation can be carried out. Although not fully complete at this point, the ideas presented in this section may provide a useful approach when worked out in more detail. We leave a more detailed exploration of these ideas for future study.

The performed coordinate transformation follows the fluid interface and allows for a stretching in the direction normal to the flow (so where the diffusion is highest between the two fluids), a method also known as asymptotics. We assume that the fluids are evenly distributed along a vertical cross-section, as depicted in Figure 1. Therefore, the $y$-direction can be omitted when it comes to the spatial distribution of the fluids. Therefore, our 3D model reduces to a 2 D model, centred along the central line of the pipe $s$. The height of the interface between the fluids, can be parametrized as a (non-trivial) function of position and time. Define $h(s, t)$ as the height of the interface surface, oriented along the $w$-direction, which is defined to be normal to the interface surface. Then, for any time $t$, the interface at point $s_{0}$ has height $h\left(s_{0}, t\right)$.

For immiscible fluids, the concentration of methanol is represented by a Heaviside function, with changing point at $h(s, t)$ :

$$
c_{0}(s, t)=\left\{\begin{array}{lll}
0 & \text { if } & w<h(s, t)  \tag{9}\\
1 & \text { if } & w>h(s, t)
\end{array}\right.
$$

Note that the immiscible solution has a discontinuous volume fraction $c_{0}$. The mass fraction can only be 1 or 0 , because there is no mixing. The velocity and pressure fields are continuous, but there may be discontinuities in their derivatives.

Due to the discontinuity in the volume fractions, the advection-diffusion equations only hold in integrated form.

### 4.2 Immiscible and miscible solutions

We will try to find the solution of the miscible system

$$
\begin{align*}
\rho \frac{\partial \vec{v}}{\partial t} & +\rho \vec{v}^{T} \nabla \vec{v}=\mu \nabla^{2} \vec{v}-\nabla p+\rho \vec{g},  \tag{10}\\
\nabla \cdot \vec{v} & =0,  \tag{11}\\
\frac{\partial c}{\partial t} & +\nabla \cdot c \vec{v}=D \nabla^{2} c . \tag{12}
\end{align*}
$$

where $D$ is small. The first two equations are the incompressible Navier-Stokes equations (8) discussed before. The third equation is the advection-diffusion equations for
$c$, with the flow velocity $\vec{v}$ from (10)-(11).

Because the interface moves with the fluid, the time derivative of the water height is given by the kinematic boundary condition for the interface in two dimensions. :

$$
\begin{equation*}
\left(0,0, \frac{\partial h}{\partial t}\right) \cdot \vec{n}=\vec{v} \cdot \vec{n} \quad \Leftrightarrow \quad \frac{\partial h}{\partial t}+\frac{\partial h}{\partial s} v_{0, s}=v_{0, w} . \tag{13}
\end{equation*}
$$

A (non-unit) upward normal vector $\vec{m}$ to the interface is given by

$$
\begin{equation*}
\vec{m}:=\left(-\frac{\partial h}{\partial s}, 1\right) . \tag{14}
\end{equation*}
$$

The unit upward normal vector $\vec{n}$ is found by scaling $\vec{m}$ :

$$
\begin{equation*}
\vec{n}:=\frac{\vec{m}}{|\vec{m}|} . \tag{15}
\end{equation*}
$$

The directions parallel to the interface are called $\vec{a}$ and $\vec{b}$ :

$$
\begin{equation*}
\vec{a}:=\frac{\left(1, \frac{\partial h}{\partial s}\right)}{\left|\left(1, \frac{\partial h}{\partial s}\right)\right|} \quad, \quad \vec{b}:=\vec{n} \times \vec{a} . \tag{16}
\end{equation*}
$$

Introduce the coordinate transformation:

$$
\begin{align*}
\tilde{s}(s, \chi, t) & =s-\frac{\partial h(s, t)}{\partial s} \chi \delta  \tag{17}\\
w(s, \chi, t) & =h(s, t)+\chi \delta \tag{18}
\end{align*}
$$

where $\chi$ represents the stretching along the $w$-axis. Then the derivatives in terms of
the new coordinates become:

$$
\begin{align*}
\frac{\partial c}{\partial s} & =\frac{\partial \chi}{\partial \tilde{s}} \frac{\partial \tilde{s}}{\partial s} \frac{\partial c}{\partial \chi}+\frac{\partial \tilde{s}}{\partial s} \frac{\partial c}{\partial \tilde{s}}  \tag{19}\\
& =\left(-\frac{\partial h}{\partial s} \delta\right)^{-1}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial c}{\partial \chi}+\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial c}{\partial \tilde{s}}  \tag{20}\\
\frac{\partial c}{\partial w} & =\frac{\partial \chi}{\partial w} \frac{\partial c}{\partial \chi}+\frac{\partial \tilde{s}}{\partial \chi} \frac{\partial \chi}{\partial w} \frac{\partial c}{\partial \tilde{s}}  \tag{21}\\
& =\delta^{-1} \frac{\partial c}{\partial \chi}-\frac{\partial h}{\partial s} \frac{\partial c}{\partial \tilde{s}}  \tag{22}\\
\frac{\partial^{2} c}{\partial s^{2}} & =\frac{\partial^{2} h}{\partial s^{2}} \delta\left(\frac{\partial h}{\partial s} \delta\right)^{-2}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial c}{\partial \chi}+\left(-\frac{\partial h}{\partial s} \delta\right)^{-1}\left(-\frac{\partial^{3} h}{\partial s^{3}} \chi \delta\right) \frac{\partial c}{\partial \chi}  \tag{23}\\
& +\left(\frac{\partial h}{\partial s} \delta\right)^{-2}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right)^{2} \frac{\partial^{2} c}{\partial \chi^{2}}-\frac{\partial^{3} h}{\partial s^{3}} \chi \delta \frac{\partial c}{\partial \tilde{s}}  \tag{24}\\
& +2\left(\frac{\partial h}{\partial s} \delta\right)^{-1}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial^{2} c}{\partial \chi \partial \tilde{s}}+\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial^{2} c}{\partial \tilde{s}^{2}}  \tag{25}\\
\frac{\partial^{2} c}{\partial w^{2}} & =\delta^{-2} \frac{\partial^{2} c}{\partial \chi^{2}}+\left(\frac{\partial h}{\partial s}\right)^{2} \frac{\partial^{2} c}{\partial \tilde{s}^{2}}-2 \delta^{-1} \frac{\partial h}{\partial s} \frac{\partial^{2} c}{\partial \chi \partial \tilde{s}} \tag{26}
\end{align*}
$$

Then the LHS of equation (12) for the concentration becomes:

$$
\begin{align*}
\frac{\partial c}{\partial t}+\nabla \cdot c \vec{v} & =\frac{\partial c(\tilde{s}, \tilde{w}, t)}{\partial t}+\nabla \cdot c(\tilde{s}, \tilde{w}, t) \vec{v}  \tag{28}\\
& =\frac{\partial c(\tilde{s}, \tilde{w}, t)}{\partial t}+\frac{\partial c(\tilde{s}, \tilde{w}, t)}{\partial s} \cdot v_{s}+\frac{\partial c(\tilde{s}, \tilde{w}, t)}{\partial w} \cdot v_{w}  \tag{29}\\
& =\frac{\partial c(\tilde{s}, \tilde{w}, t)}{\partial t}+\left(\left(-\frac{\partial h}{\partial s} \delta\right)^{-1}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial c}{\partial \chi}\right.  \tag{30}\\
& \left.+\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial c}{\partial \tilde{s}}\right) \cdot v_{s}+\left(\delta^{-1} \frac{\partial c}{\partial \chi}-\frac{\partial h}{\partial s} \frac{\partial c}{\partial \tilde{s}}\right) \cdot v_{w} \tag{31}
\end{align*}
$$

Furthermore, the RHS of (12) becomes:

$$
\begin{align*}
D_{w} \nabla^{2} c & =D_{w}\left(\frac{\partial^{2} c(\tilde{s}, \tilde{w}, t)}{\partial s^{2}}+\frac{\partial^{2} c(\tilde{s}, \tilde{w}, t)}{\partial w^{2}}\right)  \tag{32}\\
& =D_{w} \cdot\left(\frac{\partial^{2} h}{\partial s^{2}} \delta\left(\frac{\partial h}{\partial s} \delta\right)^{-2}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial c}{\partial \chi}\right.  \tag{33}\\
& +\left(-\frac{\partial h}{\partial s} \delta\right)^{-1}\left(-\frac{\partial^{3} h}{\partial s^{3}} \chi \delta\right) \frac{\partial c}{\partial \chi}  \tag{34}\\
& +\left(\frac{\partial h}{\partial s} \delta\right)^{-2}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right)^{2} \frac{\partial^{2} c}{\partial \chi^{2}}-\frac{\partial^{3} h}{\partial s^{3}} \chi \delta \frac{\partial c}{\partial \tilde{s}}  \tag{35}\\
& +2\left(\frac{\partial h}{\partial s} \delta\right)^{-1}\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial^{2} c}{\partial \chi \partial \tilde{s}}+\left(1-\frac{\partial^{2} h}{\partial s^{2}} \chi \delta\right) \frac{\partial^{2} c}{\partial \tilde{s}^{2}}  \tag{36}\\
& \left.+\delta^{-2} \frac{\partial^{2} c}{\partial \chi^{2}}+\left(\frac{\partial h}{\partial s}\right)^{2} \frac{\partial^{2} c}{\partial \tilde{s}^{2}}-2 \delta^{-1} \frac{\partial h}{\partial s} \frac{\partial^{2} c}{\partial \chi \partial \tilde{s}}\right)
\end{align*}
$$

These expressions can lead to the advection-diffusion equation in the new coordinates. Further work is needed to apply a similar approach, using the same coordinate stretching, to equations (10)-(11). As mentioned at the start of this section, such a further exploration is beyond the scope of this report, and is left for future study.

## 5 1D approach: Averaging over the concentrations

### 5.1 A two-layer model with one space dimension

In this section we discuss a simple model for mixing and diffusion of fluids in a pipeline. We consider a situation with two layers with different fluid mixtures, one above the other. This vertical stratification can be the result of e.g. density differences, with the heaviest mixture in the lower layer and the lightest in the upper layer. Furthermore, we assume that each layer contains a mixture of two fluids, methanol and water. We remark that two natural extensions of this simple set-up are (i) to model more than two layers in the vertical, or even consider a situation of continuous vertical stratification, and (ii) to let each mixture consist of more than two fluids. Clearly, the number of layers and the number of mixture components need not be the same.

The fluid mixtures in the upper and lower layers have different horizontal velocities. The time evolution of the fluid mixtures are governed by 1-dimensional advectiondiffusion equations for the upper and lower layer separately. The spatial coordinate in these advection-diffusion equations is $s$, the coordinate along the central line of the pipe. The two layers exchange fluid at the layer interface, modelled with source/sink terms in the horizontal advection-diffusion equations. These source/sink terms are derived from a vertical diffusion equation. For simplicity, we ignore here the angle of the pipeline, and assume that the pipeline is oriented horizontally so that a vertical
cross-section forms a perfect circle in a plane orthogonal to the direction of $s$. The circle has the diameter of the pipe, denoted $D$, so we have $0 \leq w \leq D$ for the vertical coordinate $w$. We denote by $h$ the height of the layer interface, i.e. the lower layer extends from $w=0$ to $w=h$, and the upper layer from $w=h$ to $w=D$.

From here on, we use notations with subscripts $u$ and $l$ to denote quantities for the upper and lower layer, respectively. The cross-sectional area of the upper layer is $A_{u}$, and that of the lower layer is $A_{l}$. Clearly $A_{u}+A_{l}=A$ with $A$ the total cross-sectional area $A=\pi R^{2}$ and $R=D / 2$ the pipe radius. Given the layer interface height $h$, we have

$$
\begin{equation*}
A_{u}=R^{2} \cos ^{-1}((h-R) / R)+(R-h) \sqrt{2 h R-h^{2}} \quad \text { and } \quad A_{l}=\pi R^{2}-A_{u} \tag{37}
\end{equation*}
$$

### 5.2 Coupled advection-diffusion equations

We denote by $c_{u}$ the volume fraction of methanol in the upper layer. By construction, the volume fraction of water in the upper layer, denoted by $\tilde{c}_{u}$, satisfies $\tilde{c}_{u}=1-c_{u}$. Likewise, the lower layer methanol and water fractions are denoted $c_{l}$ and $\tilde{c}_{l}$, satisfying $c_{l}+\tilde{c}_{l}=1$. Furthermore, let $u_{u}$ and $u_{l}$ be the fluid velocities (in the $s$-direction) in the upper and lower layer. We model the time evolution of the fractions $c_{u}(s, t)$ and $c_{l}(s, t)$ with advection-diffusion equations coupled by a source/sink term:

$$
\begin{align*}
\partial_{t}\left(c_{u} A_{u}\right)+\partial_{s}\left(u_{u} c_{u} A_{u}\right) & =\partial_{s}\left(D_{u} \partial_{s}\left(c_{u} A_{u}\right)\right)+\psi  \tag{38a}\\
\partial_{t}\left(c_{l} A_{l}\right)+\partial_{s}\left(u_{l} c_{l} A_{l}\right) & =\partial_{s}\left(D_{l} \partial_{s}\left(c_{l} A_{l}\right)\right)-\psi \tag{38b}
\end{align*}
$$

We denote partial derivatives with respect to $s$ and $t$ by $\partial_{s}$ and $\partial_{t}$, respectively. The velocity fields $u_{u}(s, t)$ and $u_{l}(s, t)$ are given. We assume that the effective axial diffusion coefficients ( $D_{u}$ and $D_{l}$ ) are constant in $s$ and $t$, and that they are identical in the upper and lower layer, i.e. $D_{u}=D_{l}$. Finally, the term $\psi$ is a source $/ \operatorname{sink}$ term that accounts for the exchange/mixing of fluids between the two layers. Below, we derive an expression for $\psi$ based on a diffusion equation in the vertical direction.

As can be seen, the volume fractions $c_{u}, c_{l}$ depend only on $(s, t)$ in our model set-up here. Thus, these fractions are assumed constant over the upper ( $w>h$ ) and lower $(w<h)$ parts of the pipe cross-section. Any exchange of fluids between the layers, as modelled by $\psi$, is assumed to be mixed instantaneously within each layer in the directions perpendicular to $s$. This will guide the derivation of $\psi$.

### 5.3 Exchange between layers: a source/sink term from the heat equation

In our model set-up, there is no advection in the vertical direction, only diffusion. We start our derivation of $\psi$ by considering the methanol volume fraction in a pipe cross-section (i.e., $s$ is fixed) to be a function of both the vertical coordinate $w$ and time $t$, so $c=c(w, t)$. The time evolution is governed by the diffusion equation

$$
\begin{equation*}
\partial_{t} c=\partial_{w}\left(D_{w} \partial_{w} c\right) \tag{39}
\end{equation*}
$$

with diffusion coefficient $D_{w}$. Let the initial state of $c$ be the piecewise-constant (in $w$ ) profile with $c_{u}$ in the upper layer and $c_{l}$ in the lower layer. Thus, $c(w, 0)=$ $c_{l}+H(w-h)\left(c_{u}-c_{l}\right)$ with $h$ the interface height and $H($.$) the Heaviside function.$ We assume $c_{u}>c_{l}$ so that the lower layer fluid mixture is heavier than the mixture in the upper layer (as water is heavier than methanol).

If $D_{w}$ is independent of $w,(39)$ reduces to the heat equation in 1-d. Below, we use a simple analytical solution for the heat equation on $\mathbb{R}$, although strictly speaking, the domain for our problem is finite since $w$ is bounded by the pipe wall. A more refined treatment, beyond the scope of this report, would be to take account of this finite domain size (note that the curvature of the pipe wall makes the characterization of the finite domain complicated). We remark that our primary interest is in diffusion over small time intervals, so that most of the exchange is (very) close to the layer interface and effects of finite domain size may not have much impact.

Consider the following standard initial value problem for the heat equation on $\mathbb{R}$ :

$$
\partial_{t} v=\kappa \partial_{x}^{2} v, \quad x \in \mathbb{R}, \quad v(x, 0)= \begin{cases}1 & \text { if } x>0  \tag{40}\\ 0 & \text { if } x<0\end{cases}
$$

with diffusion constant $\kappa>0$. The solution at time $t>0$ is

$$
\begin{equation*}
v(x, t)=\frac{1}{2}+\frac{1}{2} \operatorname{erf}\left(\frac{x}{\sqrt{4 \kappa t}}\right) \tag{41}
\end{equation*}
$$

with $\operatorname{erf}($.$) the error function Temme (1996). From the solution at t$ we can calculate the amount of exchange over the time interval $[0, t]$ across the interface at $x=0$ in this standard problem:

$$
\begin{align*}
\int_{0}^{\infty}[v(x, t)-v(x, 0)] d x & =\lim _{x^{*} \rightarrow \infty} \frac{1}{2} \int_{0}^{x^{*}}\left[\operatorname{erf}\left(\frac{x}{\sqrt{4 \kappa t}}\right)-1\right] d x \\
& =\lim _{x^{*} \rightarrow \infty} \frac{1}{2}\left[\sqrt{\frac{4 \kappa t}{\pi}}\left(e^{-\left(x^{*}\right)^{2} /(4 \kappa t)}-1\right)-x^{*}+x^{*} \operatorname{erf}\left(\frac{x^{*}}{\sqrt{4 \kappa t}}\right)\right] \\
& =-\sqrt{\frac{\kappa t}{\pi}} \tag{42}
\end{align*}
$$

where we have used that $\operatorname{erf}(x) \rightarrow 1-\frac{\exp \left(-x^{2}\right)}{x \sqrt{\pi}}$ as $x \rightarrow+\infty$ Oldham et al. (2009).
Transforming the standard problem above to the diffusion equation (39) of interest to us, we obtain for the exchange over a time interval $d t$ the following:

$$
\begin{equation*}
\int_{h}^{\infty}[c(w, d t)-c(w, 0)] d w=-\left(c_{u}-c_{l}\right) \sqrt{\frac{D_{w} d t}{\pi}} \tag{43}
\end{equation*}
$$

To obtain an expression for the source/sink term $\psi$ from this, we must take into account that the vertical exchange takes place over the layer interface with length $2 \sqrt{2 h R-h^{2}}$, hence it should be proportional to this length.

Furthermore, an important assumption is that the amount of exchanged fluid is instantaneously mixed throughout the upper and lower parts of the pipe cross-section, with cross-sectional areas $A_{u}$ and $A_{l}$, respectively. Thus, if we consider the upper layer at location $s$ and time $t$, the change in $c_{u}$ over a time interval $d t$ due to fluid exchange between the layers is

$$
\begin{align*}
c_{u}(s, t+d t) & =\frac{c_{u}(s, t) A_{u}(s, t)+\text { exchange }}{A_{u}(s, t)} \\
& =c_{u}(s, t)-\frac{\left[c_{u}(s, t)-c_{l}(s, t)\right] \sqrt{D_{w} d t / \pi} 2 \sqrt{2 h(s, t) R-h^{2}(s, t)}}{A_{u}(s, t)} \\
& =c_{u}(s, t)-\frac{\left[c_{u}(s, t)-c_{l}(s, t)\right] F(s, t) \sqrt{D_{w} d t}}{A_{u}(s, t)} \tag{44}
\end{align*}
$$

where $F$ is dependent on the interface height $h(s, t)$ :

$$
\begin{equation*}
F(s, t)=2 \sqrt{\frac{2 h(s, t) R-h^{2}(s, t)}{\pi}} \tag{45}
\end{equation*}
$$

We note that $A_{u}$ depends on $(s, t)$ through $h(s, t)$, see (37). Also, we neglect the (presumably small) change in $h(s, t)$ (and thus $A_{u}$ ) over the time interval $d t$.

The advection-diffusion equations (38) describe the time evolution of $c_{u} A_{u}$ and $c_{l} A_{l}$ rather than $c_{u}$ and $c_{l}$. As a result, the factor $A_{u}$ in (44) drops out and we obtain for the source/sink term

$$
\begin{equation*}
\psi(s, t)=\lim _{d t \downarrow 0}-\left[c_{u}(s, t)-c_{l}(s, t)\right] F(s, t) \sqrt{\frac{D_{w}}{d t}} \tag{46}
\end{equation*}
$$

Note that $\psi$ diverges in the $d t \rightarrow 0$ limit, a consequence of our set-up with a sharp layer interface at which the mixture fractions are discontinuous. It implies that $\psi$ should be interpreted in a weak or distributional sense. For numerical time integration with time step $\Delta t$ we will use $\psi(s, t) \Delta t \approx-\left[c_{u}(s, t)-c_{l}(s, t)\right] F(s, t) \sqrt{D_{w} \Delta t}$.

We conclude this section with some remarks about the vertical diffusion coefficient $D_{w}$. Above, we assumed it to be independent of $w$ to obtain an expression for $\psi$ from the 1-dimensional heat equation. It would make sense to let $D_{w}$ depend on the (local) shear, i.e. the horizontal velocity difference between the two layers, $\left|u_{u}(s, t)-u_{l}(s, t)\right|$. A large shear may generate small-scale turbulence at the layer interface, enhancing the effective vertical diffusivity. We leave further exploration of this issue for future study.

## 6 Implementation

In this section we provide a concise description of the numerical method employed to approximate solutions of the coupled 1-d advection-diffusion equations presented in the previous section. For notational convenience, we will replace the subscripts $u$ and
$l$ by the integers 1 and 2 , respectively, and refer to the upper and lower region as the first and second region, respectively.

The system of equations to be solved is

$$
\left\{\begin{array}{l}
\frac{\partial}{\partial t}\left(A_{i} c_{i}\right)+\frac{\partial}{\partial s}\left(u_{i} A_{i} c_{i}\right)=\frac{\partial}{\partial s}\left(D_{i} \frac{\partial}{\partial s}\left(A_{i} c_{i}\right)\right)+(-1)^{i+1} \psi  \tag{47}\\
c_{i}(t, 0)=\alpha_{i}, \quad \frac{\partial c_{i}}{\partial s}(t, L)=\beta_{i} \\
c_{i}(0, s)=c_{i}^{0}(s)
\end{array}\right.
$$

for $1 \leq i \leq 2$, where

- $T>0$ is the integration time,
- $L>0$ is the length of the pipe,
- $u_{i}:[0, T] \times[0, L] \rightarrow \mathbb{R}$ is the prescribed speed of the mixture in the $i$-th region in the direction of the pipe,
- $D_{i} \in \mathbb{R}$ is the diffusion coefficient of methanol in the $i$-th region,
- $\psi:[0, T] \times[0, L] \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ models the diffusion across the interface,
- $c_{i}^{0}:[0, L] \rightarrow \mathbb{R}$ is the initial concentration of methanol,
- $\alpha_{i}, \beta_{i} \in \mathbb{R}_{\geq 0}$.

The Dirichlet-boundary conditions at $s=0$ correspond to a constant stream of methanol being pumped into the pipe. The Neumann-boundary conditions at $s=L$ are used to model the outward flux of methanol at the end of the pipe.

The strategy is to first discretize (47) in space by using the Finite Volume Method (FVM). This results in a system of nonlinear ODEs. The solution of this ODE is then approximated by using the so-called $\theta$-method. Both methods are discussed in more detail below.

### 6.1 Discretization in space

In this section we explain how to discretize (47) in space by using the FVM. The main idea of the FVM is to approximate the averages of $\left(c_{i}\right)_{i=1}^{2}$ instead of the pointwise values. To this end, partition $[0, L]$ into $N \in \mathbb{N}$ subdomains of equal size and let $\left\{s_{j}:=\delta_{s}\left(j-\frac{1}{2}\right): 1 \leq j \leq N\right\}$ denote the midpoints of these subdomains, where $\delta_{s}=\frac{L}{N}$ (see Figure 2). The objective is to approximate the averages

$$
\bar{c}_{i, j}(t):=\frac{1}{\delta_{s}} \int_{s_{j-\frac{1}{2}}}^{s_{j+\frac{1}{2}}} c_{i}(t, s) \mathrm{d} s, \quad 1 \leq i \leq 2,1 \leq j \leq N
$$



Figure 2: The interval $[0, L]$ is subdivided into $N$ subdomains of size $\delta_{s}=\frac{L}{N}$. The boundaries of these subdomains are depicted as black vertical lines. The red dots correspond to the associated midpoints $\left(s_{j}\right)_{j=1}^{N}$. The additional grid-points $s_{0}=-\frac{\delta_{s}}{2}$ and $s_{N+1}=L+\frac{\delta_{s}}{2}$ are needed to approximate $\frac{\partial c_{i}}{\partial s}(t, 0)$, and $\frac{\partial c_{i}}{\partial s}(t, L)$, respectively, with central differences.
on each subdomain at some prescribed points in time $\left\{0=t_{0}<t_{1} \ldots<t_{m}=T\right\}$. Observe that if $\delta_{s}$ is sufficiently small and $c_{i}$ is sufficiently regular, the averages $\bar{c}_{i, j}$ constitute accurate approximations of the point-values $\left(c_{i}\left(t, s_{j}\right)\right)_{j=1}^{N}$.

Let $1 \leq i \leq 2,1 \leq j \leq N$ and take the average of (47) around $s_{j}$ to obtain the following equation:

$$
\begin{align*}
A_{i} & {\left[\frac{d \bar{c}_{i, j}}{d t}+\frac{\left(u_{i} c_{i}\right)\left(t, s_{j+\frac{1}{2}}\right)-\left(u_{i} c_{i}\right)\left(t, s_{j-\frac{1}{2}}\right)}{\delta_{s}}\right] } \\
= & \frac{A_{i} D_{i}}{\delta_{s}}\left[\frac{\partial c_{i}}{\partial s}\left(t, s_{j+\frac{1}{2}}\right)-\frac{\partial c_{i}}{\partial s}\left(t, s_{j-\frac{1}{2}}\right)\right] \\
& \quad+\frac{(-1)^{i+1}}{\delta_{s}} \int_{s_{j-\frac{1}{2}}}^{s_{j+\frac{1}{2}}} \psi\left(t, s, c_{1}(t, s), c_{2}(t, s)\right) \mathrm{d} s . \tag{48}
\end{align*}
$$

We will now explain how to discretize the latter equation in space for fixed time $t$. In order for the following arguments to make sense, we will henceforth assume that $\delta_{s}$ is sufficiently small.

Discretization of the spatial derivatives To approximate the spatial derivatives in the righthand-side of (48) we would like to use the (second order) central difference approximation

$$
\begin{equation*}
\frac{\partial c_{i}}{\partial s}\left(t, s_{j+\frac{1}{2}}\right) \approx \frac{c_{i}\left(t, s_{j+1}\right)-c_{i}\left(t, s_{j}\right)}{\delta_{s}} \approx \frac{\bar{c}_{i, j+1}(t)-\bar{c}_{i, j}(t)}{\delta_{s}} \tag{49}
\end{equation*}
$$

for $0 \leq j \leq N$. However, the latter approximation only makes sense for $1 \leq j \leq N-1$, since $\bar{c}_{i, 0}$ and $\bar{c}_{i, N+1}$ are undefined. In order to make sense of (49) for $j=0$ and $j=N$ we formally introduce additional ghost nodes $s_{0}=-\frac{\delta_{s}}{2}$ and $s_{N+1}=L+\frac{\delta_{s}}{2}$, see Figure 2.

The value of $\bar{c}_{i, 0}$ is determined by taking an average over the two neighboring nodes and using the boundary condition at $s=0$. In other words, since

$$
\alpha_{i}=c_{i}(t, 0) \approx \frac{c_{i}\left(t, s_{1}\right)+c_{i}\left(t, s_{0}\right)}{2}
$$

we set $\bar{c}_{i, 0}:=2 \alpha_{i}-\bar{c}_{i, 1}$. Similarly, the value of $\bar{c}_{i, N+1}$ is determined by using the Neumann-boundary condition at $s=L$. That is, since

$$
\beta_{i}=\frac{\partial c_{i}}{\partial s}(t, L) \approx \frac{c_{i}\left(t, s_{N+1}\right)-c_{i}\left(t, s_{N}\right)}{\delta_{s}},
$$

we set $\bar{c}_{i, N+1}:=\delta_{s} \beta_{i}+\bar{c}_{i, N}$. We can now use (49) to approximate the spatial derivatives for $0 \leq j \leq N$.

Approximation of the nonlinearity If the map $s \mapsto \psi\left(t, s, c_{1}(t, s), c_{2}(t, s)\right)$ is sufficiently regular (at the very least $L^{1}$ ), then

$$
\begin{align*}
& \frac{1}{\delta_{s}} \int_{s_{j-\frac{1}{2}}}^{s_{j+\frac{1}{2}}} \psi\left(t, s, c_{1}(t, s), c_{2}(t, s)\right) \mathrm{d} s \\
& \quad \approx \psi\left(t, s_{j}, c_{1}\left(t, s_{j}\right), c_{2}\left(t, s_{j}\right)\right) \\
& \quad \approx \psi\left(t, s_{j}, \bar{c}_{1, j}(t), \bar{c}_{2, j}(t)\right), \tag{50}
\end{align*}
$$

for $0 \leq j \leq N$. Alternatively, one could use numerical quadrature to approximate the integral. The latter could potentially yield more accurate approximations provided $s \mapsto \psi\left(t, s, c_{1}(t, s), c_{2}(t, s)\right)$ is sufficiently smooth.

Approximation of the advection term To approximate the advection term in (48) we simply approximate the average of $c_{i}$, as before, by using its values at the neighboring nodes:

$$
\begin{align*}
\left(u_{i} c_{i}\right)\left(t, s_{j+\frac{1}{2}}\right) & \approx u_{i}\left(t, s_{j+\frac{1}{2}}\right) \frac{c_{i}\left(t, s_{j+1}\right)+c_{i}\left(t, s_{j}\right)}{2} \\
& \approx u_{i}\left(t, s_{j+\frac{1}{2}}\right) \frac{\bar{c}_{i, j+1}(t)+\bar{c}_{i, j}(t)}{2} \tag{51}
\end{align*}
$$

for $0 \leq j \leq N$. Recall that we are assuming that $u_{i}$ is known, in the sense that we can evaluate it at any $(t, s) \in[0, T] \times[0, L]$ on the computer.

### 6.2 Discretization in time

In this section we explain how the spatial discretizations from the previous section can be used to approximate solutions of (47). Substitution of (49), (50), and (51)
into (48) yields a system of nonlinear equations of the form

$$
\begin{cases}\frac{d \bar{c}_{i}}{d t}=Q \cdot \bar{c}_{i}+(-1)^{i+1} \Psi\left(t, \bar{c}_{1}, \bar{c}_{2}\right), t \in[0, T], & 1 \leq i \leq 2  \tag{52}\\ \bar{c}_{i}(0)=\left[c_{i}^{0}\left(s_{j}\right)\right]_{j=0}^{N}\end{cases}
$$

where $\bar{c}_{i}:=\left[\begin{array}{lll}\bar{c}_{i, 0} & \ldots & \bar{c}_{i, N}\end{array}\right]^{T}, Q$ is the $(N+1) \times(N+1)$ matrix which encodes the linear part of the equations (i.e. it is the discretization of the advection and diffusion term), and $\Psi:[0, L] \times \mathbb{R}^{N+1} \times \mathbb{R}^{N+1} \rightarrow \mathbb{R}^{N+1}$ corresponds to the nonlinear part associated to (50).

For notational convenience, we introduce the map $F:[0, T] \times \mathbb{R}^{2(N+1)} \rightarrow \mathbb{R}^{2(N+1)}$ defined by

$$
F(t, \bar{c}):=\left[\begin{array}{l}
Q \cdot \bar{c}_{1}+\Psi\left(t, \bar{c}_{1}, \bar{c}_{2}\right) \\
Q \cdot \bar{c}_{2}-\Psi\left(t, \bar{c}_{1}, \bar{c}_{2}\right)
\end{array}\right],
$$

where $\bar{c}:=\left[\begin{array}{l}\bar{c}_{1} \\ \bar{c}_{2}\end{array}\right]$. Then (52) can be rewritten as

$$
\left\{\begin{array}{l}
\frac{d \bar{c}}{d t}=F(t, \bar{c}), \quad t \in[0, T]  \tag{53}\\
\bar{c}(0)=c^{0}
\end{array}\right.
$$

where

$$
c^{0}=\left[\begin{array}{llllll}
c_{1}^{0}\left(s_{0}\right) & \ldots & c_{1}^{0}\left(s_{N}\right) & c_{2}^{0}\left(s_{0}\right) & \ldots & c_{2}^{0}\left(s_{N}\right)
\end{array}\right]^{T} .
$$

Finally, the solution of (53) is approximated at the times $\left(t_{k}\right)_{k=0}^{m}$ by using the $\theta$ method:

$$
\bar{c}\left(t_{k+1}\right)=\bar{c}\left(t_{k}\right)+\delta_{k}\left[\theta F\left(t_{k}, \bar{c}\left(t_{k}\right)\right)+(1-\theta) F\left(t_{k+1}, \bar{c}\left(t_{k+1}\right)\right)\right],
$$

where $0 \leq k \leq m-1, \delta_{k}=t_{k+1}-t_{k}$, and $\theta \in[0,1]$ is a fixed parameter.

## 7 Numerical results

In this section we investigate the behavior of the 1-d model developed in Section 5 with the aid of numerical simulations. There are many interesting aspects of the proposed model to investigate; both from a numerical point of view and from a modeling point of view. Here we restrict our attention to studying the influence of the coupling term $\psi$. More precisely, we investigate the dependence of the model on the height $h \in(0, D)$ of the layer interface for two different scenarios. To accomplish this, we fix all other parameters throughout this section. We note that there are many more interesting parameter dependencies to investigate and leave this as a topic of future research.

Physically relevant parameters We set the length of the pipe and the radius of its cross-sections equal to $L=2$ and $R=1$, respectively. The constant volume fractions of methanol pumped into the upper and lower regions of the pipe are set to $\alpha_{1}=1$ and $\alpha_{2}=\frac{1}{10}$, respectively. For the sake of simplicity, we choose the initial distribution of methanol in both the upper and lower part of the pipe to be constant throughout the pipe, i.e., $c_{1}^{0}, c_{2}^{0}:[0, L] \rightarrow \mathbb{R}$ are constant. Therefore, due to the Dirichlet boundary conditions at the left-end of the pipe, we must necessarily set $c_{i}^{0} \equiv \alpha_{i}$. We impose a Neumann boundary condition at the right end of the pipe by setting $\beta_{1}=\beta_{2}=0$. Finally, we choose the horizontal and vertical diffusion coefficients to be the same in each coordinate direction: $D_{w}=D_{1}=D_{2}=10^{-2}$.

Computational parameters We use the same computational parameters in all numerical simulations (see Section 6 for the implementation details). The parameters associated to the discretization sizes in time and space are set to $\delta_{k} \equiv \delta=10^{-3}$ and $N=200$, respectively. The latter corresponds to a uniform spatial discretization of size $\frac{L}{N}$. Furthermore, we use $\theta=0$ to perform the time integration, which corresponds to a backward Euler scheme. Finally, in each numerical simulation, we set the integration time to $T=10$. This particular choice was motivated by the observation that in all numerical experiments the solutions approached a steady state within this time frame.

We consider the following two scenarios:
(i) The velocity in the upper part of the pipe is smaller than in the lower part: $u_{1}=\frac{1}{10}, u_{2}=1$.
(ii) The velocity in the upper part of the pipe is larger than in the lower part: $u_{1}=1, u_{2}=\frac{1}{10}$.

For each scenario, we have performed numerical simulations for different choices of the height of the layer interface; we have considered

$$
h \in \Delta:=\left\{h_{j}:=\frac{5+j}{100}: 0 \leq j \leq 95\right\} .
$$

### 7.1 Case (i)

We start with the case in which $u_{1}<u_{2}$. In all scenarios, i.e., for all $h \in \Delta$, the volume concentrations of methanol in the upper and lower part of the pipe converged to a steady state. We have shown the typical behavior of $c_{1}$ and $c_{2}$ in Figure 3 for three different choices of $h$. The results show that the volume fractions of methanol in the upper part of the pipe evolved into a decreasing function of $s$ as time progressed. In particular, the concentration profiles transitioned more quickly into these decreasing "states" as the height of the layer interface increased. Furthermore, the time in which $c_{1}$ approached a steady state decreased as $h$ increased.

The volume fraction of methanol in the lower part of the pipe evolved into an increasing function of $s$ as time progressed. For relatively small $t$, the fractions were relatively high "near" the right-end of the pipe (the part of the pipe which corresponds to the green regions in Figures 3d, 3e and 3f). Furthermore, the fractions in these regions decreased as time progressed. In particular, the rate at which this decrease occurred (with respect to time) slightly decreased as $h$ increased.

We have depicted the steady states to which $c_{1}$ and $c_{2}$ converged in Figure 4 for $h \in \Delta$. In all scenarios the steady states were constant in a relatively large region of the pipe. Furthermore, the size of these regions increased as $h$ increased. Moreover, the "final" volume fractions of methanol in these parts of the pipe were (approximately) the same in both the upper and lower region and increased as $h$ increased from $h=0.05$ to $h=1$.


Figure 3: Case $(i)$ : (a), (b), (c) The values of $c_{1}$ on $[0, T] \times[0, L]$ for various choices of $h$. (d), (e), (f) The values of $c_{2}$ on $[0, T] \times[0, L]$ for various choices of $h$.

To quantify the assertion that $c_{1}$ and $c_{2}$ approached a steady state more quickly as $h$ increased, recall that we approximated the volume fractions at the following discrete moments in time: $t \in \mathcal{T}:=\left\{k \delta: 0 \leq k \leq 10^{4}\right\}$, where $\delta=10^{-3}$. Let $\varepsilon>0$ be a given tolerance and set

$$
T_{i}(h):=\min \left\{t \in \mathcal{T}:\left\|c_{i}(t, \cdot)-\hat{c}_{i}\right\|_{L^{2}([0, L])}<\varepsilon\right\}, \quad i \in\{1,2\}, h \in \Delta
$$



Figure 4: Case ( $i$ ): numerical approximations of the steady states to which $c_{1}$ and $c_{2}$ converged for various values of $h \in \Delta$. (a) The steady states associated to the upper part of the pipe. For $h$ close to $h_{0}=0.05$, we have colored the corresponding steady states in light blue. As $h$ increased to 1 , we have used increasingly darker shades of blue. (b) The steady states associated to the lower part of the pipe. For $h$ close to $h_{0}=0.05$, we have colored the corresponding steady states in orange. As $h$ increased to 1 , the color of the steady states transitioned from orange to red.
where $\hat{c}_{i}:[0, L] \rightarrow \mathbb{R}$ is a numerical approximation of the steady state to which $c_{i}$ converged. In practice, we set $\hat{c}_{i}=c_{i}(T, \cdot)$. We remark that it would be more accurate to determine an approximation $\hat{c}_{i}$ by directly solving the steady state equation (an $\mathrm{ODE})$. In any case, if $\hat{c}_{i}$ is a sufficiently accurate approximation of the steady state in question (which we are assuming) and $\varepsilon>0$ is sufficiently small (but not too small), then $T_{i}$ can be used to substantiate the above assertion. More specifically, if $T_{i}\left(h_{1}\right)<T_{i}\left(h_{2}\right)$, then we have numerical evidence for the claim that the solution associated to $h_{1}$ approached a steady state more quickly than the solution associated to $h_{2}$.

We have depicted the points $\left\{\left(h, T_{i}(h)\right): h \in \Delta\right\}$ on the graph of $T_{i}$ for $\varepsilon=10^{-5}$ and $i \in\{1,2\}$ in Figure 5. The results support our claim and show that $c_{1}$ and $c_{2}$ approached a steady state more quickly as $h$ increased.

### 7.2 Case (ii)

Finally, we consider the case in which $u_{1}>u_{2}$. The typical behavior of the fractions is shown in Figure 6. In each scenario, the observed behavior was similar (but not entirely the same) as in the previous case. In particular, $c_{1}$ and $c_{2}$ both approached a steady state as time progressed. The steady state associated to the upper part of the pipe was decreasing in $s$ and the one associated to the lower part was increasing. Furthermore, both steady states were constant in a relatively large part of the pipe.


Figure 5: The dependence of $T_{i}$ on the height of the interface for $i \in\{1,2\}$. The depicted curves were obtained by sampling $T_{i}$ on $\Delta$.

A key difference in this case is that the volume fraction of methanol "near" the right-end of the pipe (the "upper" green regions in Figure 6) increased as time progressed, whereas in the previous case it decreased. Furthermore, on average, the methanol fraction throughout the pipe was higher than in the previous case. Another noticeable difference is that the values of the steady state solutions decreased as $h$ increased in those regions of the pipe where the "final" fractions were constant, see Figure 7.

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Figure 6: Case (ii) (a), (b), (c) The values of $c_{1}$ on $[0, T] \times[0, L]$ for various choices of $h$. (d), (e), (f) The values of $c_{2}$ on $[0, T] \times[0, L]$ for various choices of $h$.


Figure 7: Case (ii): numerical approximations of the steady states to which $c_{1}$ and $c_{2}$ converged for various values of $h \in \Delta$. (a) The steady states associated to the upper part of the pipe. For $h$ close to $h_{0}=0.05$, we have colored the corresponding steady states in light blue. As $h$ increased to 1 , we have used increasingly darker shades of blue. (b) The steady states associated to the lower part of the pipe. For $h$ close to $h_{0}=0.05$, we have colored the corresponding steady states in orange. As $h$ increased to 1 , the color of the steady states transitioned from orange to red.

