

Fluid Dynamics From a Theoretical and Numerical Point of View

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Abstract:

In this thesis, we present the equations governing the conservation of momentum and mass of an incompressible mixture of two fluids with different viscosities and densities contained in a vertical slab, then introduce a numerical method for approximating the velocity and pressure of said mixture, in which the velocity and pressure is updated in time by first computing a tentative update to the velocity based on a finite difference using the previous velocity and pressure, then computing a correctional pressure term used to both correct the tentative velocity so that it is divergence-free as well as update the pressure field.

Using key concepts from the theory of functional analysis, we show first the existence and uniqueness of the variational problems involved with the previously introduced methods, then the theoretic convergence of an appropriate finite volume scheme.

Lastly, we use a software implementation of the described methods and schemes to perform numerical investigations on the evolution of such a mixture. In particular, we investigate the possibility of said mixture reaching an equilibrium in which the two fluids are completely separated, with one fluid lying entirely on top of the other.

By approving submission in Digital Eksamen, each group member accepts that everyone has participated equally in the project work and that the group is collectively responsible for the contents of the report.

Preface

This report was completed during the timeframe 02.09.2022–03.06.2022 as a master thesis in Applied Mathematics at Aalborg University under guidance of Horia Cornean and Anton Evgrafov.

Citations are stated with numbers, [number], with a corresponding number in the bibliography.

When reading this report, we assume that the reader is familiar with the main concepts from Lebesgue integration theory and fundamental concepts from functional analysis, including the concepts of weak derivatives, weak solutions of partial differential equations, Sobolev spaces, and the finite element method. We refer the interested reader to [1] and [2] for a thorough exposition on these subjects.

We would like to thank our supervisors Horia and Anton for guidance throughout the project.

Notation and terminology

The following is a list of notation and terminology used throughout the project:

- We let \mathbb{R} denote the set of real numbers.
- For any positive integer d , we let \mathbb{R}^d denote the usual d -dimensional Euclidean space equipped with its usual norm, denoted by $|\cdot|$.
- Whenever $\Omega \subset \mathbb{R}^d$ is an open subset of \mathbb{R}^d , we define the following function spaces:
 - For $p \in [1, \infty)$, the space $L^p(\Omega)$ denotes the set of p -Lebesgue integrable functions $f : \Omega \rightarrow \mathbb{R}$, and $L^\infty(\Omega)$ denotes the set of essentially bounded functions $f : \Omega \rightarrow \mathbb{R}$. In both cases, we equip these spaces with the norms

$$\|f\|_{L^p(\Omega)} = \left(\int_{\Omega} |f|^p dx \right)^{1/p},$$

$$\|f\|_{L^\infty(\Omega)} = \operatorname{ess\,sup}_{\mathbf{x} \in \Omega} |f(\mathbf{x})|$$

- For any positive integer k and any $p \in [1, \infty]$, we let $W_k^p(\Omega)$ denote the Sobolev space defined by

$$W^{k,p}(\Omega) = \{f : \Omega \rightarrow \mathbb{R} : f \text{ and all its weak derivatives up to order } k \text{ belong to } L^p(\Omega)\},$$

and we equip these spaces with the Sobolev norms

$$\|f\|_{W^{k,p}(\Omega)} = \left(\sum_{|\alpha| \leq k} \|D^\alpha f\|_{L^p(\Omega)}^p \right)^{1/p}.$$

In the case $p = 2$, we also write $H^k(\Omega) = W^{k,2}(\Omega)$ in order to emphasize this space's property of being a Hilbert space.

- The space $H_0^1(\Omega)$ is defined as the closure of the set of smooth functions with compact support in Ω under the $H^1(\Omega)$ -norm. Whenever Ω has sufficiently smooth boundary, we may identify $H_0^1(\Omega)$ as the space of functions $f \in H^1(\Omega)$ whose trace vanishes at the boundary.
- Whenever $(V, \|\cdot\|_V)$ is a normed function space and d is a positive integer, we let V^d denote the set of vector-valued functions $\mathbf{f} = (f_1, \dots, f_d)$ whose components f_1, \dots, f_d belong to V . Furthermore, we endow V^d with the obvious norm

$$\|\mathbf{f}\|_{V^d} = \left(\sum_{i=1}^d \|f_i\|_V^d \right)^{1/d}.$$

Contents

1	The main problem	11
1.1	A model of the problem	11
1.1.1	The dynamic system of equations	12
1.1.2	Vanishing of the sedimentary region	12
1.1.3	Exponential convergence of h_1 to h_d	13
2	Theoretical aspects of modelling an incompressible two-phase flow	15
2.1	The governing equations of motion of a two-phase fluid	15
2.2	Variational formulation	16
2.3	Numerical experiments	23
3	Conclusion	25

1 | The main problem

In this chapter, we present the problem of interest, namely the evolution of a mixture of two fluids with distinct viscosities and densities contained in a vertical slab, then formulate a model for the evolution of said fluid. Furthermore, we also show that the mixture will reach an equilibrium after some finite amount of time, in which the two fluids are completely separated, with the fluid with lighter density resting on top of the other fluid.

1.1 A model of the problem

Let Ω be an open subset of \mathbb{R}^d with $d \in \{2, 3\}$ contained in the vertical slab $\mathbb{R}^{d-1} \times [0, H]$ for some $H > 0$, and suppose that Ω is filled with an incompressible mixture of two fluids with distinct densities ρ_1, ρ_2 and distinct viscosities μ_1, μ_2 such that the fraction of volume ϕ_0 of fluid 1 at time $t = 0$ lies strictly between 0 and 1. If we suppose that $\rho_2 < \rho_1$, then at any time $t > 0$, we can distinguish between at most four regions within the mixture:

1. A region $\Omega \cap (\mathbb{R}^{d-1} \times [h_s(t), H])$, occupied solely by fluid 2;
2. A sedimentation region $\Omega \cap (\mathbb{R}^{d-1} \times [h_d(t), h_s(t)])$;
3. A region $\Omega \cap (\mathbb{R}^{d-1} \times [h_1(t), h_d(t)])$, densely packed with spheres of fluid 2;
4. A region $\Omega \cap (\mathbb{R}^{d-1} \times [0, h_1(t)])$, occupied solely by fluid 1.

At time $t = 0$, we assume that we have $h_1(0) = h_d(0) = 0$ and $h_s(0) = H$. Furthermore, we assume that the fraction of volume ϕ_d of fluid 1 within the densely packed region satisfies $0 < \phi_0 < \phi_d < 1$ and that the fraction of volume of fluid 1 in the sedimentation region is constant and equal to ϕ_0 . By the conservation of the volume of fluid 1 across regions, we obtain the relation

$$H\phi_0 = h_1(t) + (h_d(t) - h_1(t))\phi_d + (h_s(t) - h_d(t))\phi_0. \quad (1.1)$$

The goal is to write down a dynamical system of equations that models the time evolution of these four regions. In accordance with observations in physical experiments, we will show that at some finite time $T_s > 0$, the sedimentation region disappears, i.e. that $h_s(T_s) = h_d(T_s)$. For any $t \geq T_s$, the equation (1.1) remains valid if we simply discard the last term on the right-hand side. Furthermore, we will show that h_1 converges exponentially to h_d .

1.1.1 The dynamic system of equations

As stated previously, the initial conditions for the functions h_1, h_d , and h_s are given by

$$h_1(0) = h_d(0) = 0, \quad h_s(0) = H.$$

The first equation in our dynamical system, describing the evolution of h_1 , is given by

$$h'_s(t) = -K_1 t - a. \quad (1.2)$$

The second equation in our dynamical system, describing the evolution of h_d , follows directly from equation (1.1) and is given by

$$h'_d(t) = -\frac{\phi_0}{\phi_d - \phi_0} h'_s(t) - \frac{1 - \phi_d}{\phi_d - \phi_0} h'_1(t). \quad (1.3)$$

The third and final equation in our dynamical system, describing the evolution of h_1 , is given by

$$h'_1(t) = \frac{K_2(h_d(t) - h_1(t))}{1 + \frac{K_3}{D^2(t)}(h_d(t) - h_1(t))}, \quad D(t) = \sqrt{D_0^2 + bt}. \quad (1.4)$$

In the equations (1.2)-(1.4), a, b, D_0, K_1, K_2 , and K_3 are all positive constants. Notice first that the equation (1.2) combined with the initial condition $h_s(0) = H$ clearly has the solution

$$h_s(t) = H - K_1 \frac{t^2}{2} - at. \quad (1.5)$$

1.1.2 Vanishing of the sedimentary region

In order to show our desired properties, i.e. that the sedimentary region between h_d and h_s vanishes and that h_1 converges exponentially to h_d , we require a description of the solutions of equations (1.3) and (1.4). To this end, we start by introducing the new unknown function $f := h_d - h_1$. In doing so, we may combine (1.3) and (1.4) into the more “canonical” form

$$\begin{aligned} f'(t) &= \frac{\phi_0}{\phi_d - \phi_0} (K_1 t + a) - \frac{1 - \phi_0}{\phi_d - \phi_0} h'_1(t), \quad f(0) = 0, \\ h'_1(t) &= \frac{K_2 f(t)}{1 + \frac{K_3}{D^2(t)} f(t)}, \quad h_1(0) = 0, \\ h_d(t) &= h_1(t) + f(t), \quad h_d(0) = 0. \end{aligned} \quad (1.6)$$

The advantage of introducing f is that f obeys the regular ODE (1.6) near $t = 0$, hence we obtain a smooth local solution. Furthermore, $f'(0) > 0$ and $f(0) = 0$, hence $f(t) > 0$ for all $t \in (0, \varepsilon)$ for a sufficiently small $\varepsilon > 0$. However, the ODE remains regular so long as $f \geq 0$, hence we may extend the solution so long as f remains non-negative.

The key insight is that f cannot become negative at any point; indeed, if f were to become negative at some point, it follows from the intermediate value theorem that there exists some $t_1 > 0$ such that $f(t_1) = 0$. From this, we see that $f(t) > 0 = f(t_1)$ for all $t \in (0, t_1)$; however, $f'(t_1) > 0$ by (1.6), hence f is strictly increasing around t_1 , which is a contradiction.

From this argument, we conclude that $f(t) = h_d(t) - h_1(t) > 0$ for all $t > 0$, i.e. $h_1(t) < h_d(t)$ for all t . Furthermore, we can use (1.6) to obtain the following solutions of (1.3) and (1.4):

$$\begin{aligned} h_1(t) &= \frac{\phi_0}{1 - \phi_0}(K_1 t^2/2 + at) - \frac{\phi_d - \phi_0}{1 - \phi_0} f(t), \\ h_d(t) &= \frac{\phi_0}{1 - \phi_0}(K_1 t^2/2 + at) + \frac{1 - \phi_d}{1 - \phi_0} f(t). \end{aligned} \quad (1.7)$$

From (1.5) and (1.7), we see that

$$\begin{aligned} h_d(t) - h_s(t) &= \frac{\phi_0}{1 - \phi_0}(K_1 t^2/2 + at) + \frac{1 - \phi_d}{1 - \phi_0} f(t) - (H - K_1 t^2/2 - at) \\ &= \frac{1}{1 - \phi_0}(K_1 t^2/2 + at) + \frac{1 - \phi_d}{1 - \phi_0} f(t) - H \end{aligned}$$

can assume both negative and positive values for some finite $T_s > 0$, hence there exists some $T_s > 0$ such that $h_d(T_s) - h_s(T_s) = 0$, i.e. $h_s(T_s) = h_d(T_s)$.

1.1.3 Exponential convergence of h_1 to h_d

Consider again the equation (1.1). Letting $f = h_d - h_1$ as in the previous subsection, we see that

$$h_1(t) = H\phi_0 - f(t)\phi_d, \quad t \geq T_s. \quad (1.8)$$

Combining (1.4) and (1.8), we see that

$$f'(t) = -\frac{K_2}{\phi_d} \frac{f(t)}{1 + \frac{K_3}{D^2(t)} f(t)}, \quad t \geq T_s. \quad (1.9)$$

Similarly to before, this equation has a unique solution so long as $f(t) > 0$. From (1.9), we see that f is decreasing for $t \geq T_s$; as $D^2(t)$ is linearly increasing, it follows that

$$\begin{aligned} 1 + \frac{K_3}{D^2(t)} f(t) &\leq 2 \max\left\{1, \frac{K_3}{D^2(T_s)} f(T_s)\right\}, \\ -\frac{1}{1 + \frac{K_3}{D^2(t)} f(t)} &\leq -\frac{1}{2} \min\left\{1, \frac{K_3}{D^2(T_s)} f(T_s)\right\} =: -K_s < 0 \end{aligned}$$

for $t \geq T_s$. Furthermore, (1.9) also implies that

$$f'(t) \leq -\frac{K_2 K_s}{\phi_d} f(t), \quad t \geq T_s,$$

from which it follows that $f(t) \exp(tK_2 K_s/\phi_d)$ is decreasing for $t \geq T_s$, hence

$$0 < f(t) \leq f(T_s) \exp(-(t - T_s)K_2 K_s/\phi_d), \quad t \geq T_s.$$

From this, we see that $f = h_d - h_1$ converges exponentially fast towards zero, but the evolution never stops in the sense that the difference never becomes exactly zero for any finite $t \geq T_s$.

2 | Theoretical aspects of modelling an incompressible two-phase flow

In this chapter, we first introduce the system of partial differential equations that govern the evolution of the pair consisting of a velocity vector field and a scalar pressure field, which together describe the flow of a mixture of two fluids such as the one considered in Chapter 1. Using these equations, we describe a classical method for approximating said velocity field and pressure field. Said method involves

2.1 The governing equations of motion of a two-phase fluid

The evolution of said mixture of fluids can be described via the velocity vector field \mathbf{u} indicating both the direction and velocity of the mixture's flow. This pair of the velocity field \mathbf{u} and the pressure field p defined on $\Omega \times [0, \infty)$ must satisfy the equations

$$\partial_t(\rho\mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho\mathbf{u}\mathbf{u}^T) = -\nabla_{\mathbf{x}}p - \rho g\mathbf{e}_3 + \nabla_{\mathbf{x}} \cdot (\mu(\nabla_{\mathbf{x}}\mathbf{u} + (\nabla_{\mathbf{x}}\mathbf{u})^T)), \quad (2.1)$$

$$\nabla_{\mathbf{x}} \cdot \mathbf{u} = 0, \quad (2.2)$$

$$\partial_t C + \mathbf{u} \cdot \nabla_{\mathbf{x}} C = 0, \quad (2.3)$$

subject to the initial conditions

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{0}, \quad p(x_1, x_2, x_3; 0) = p_{\infty} + \psi(x_1, x_2, x_3; 0) \, ds \quad (2.4)$$

for all $\mathbf{x} = (x_1, x_2, x_3) \in \Omega$ and the boundary conditions

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{0}, \quad p(x_1, x_2, x_3; t) = p_{\infty} + \psi(x_1, x_2, x_3; t) \, ds \quad (2.5)$$

for all $(\mathbf{x}, t) = (x_1, x_2, x_3; t) \in \partial\Omega \times [0, \infty)$, where C is the volume fraction function of fluid 1, $\rho = \rho(C)$ and $\mu = \mu(C)$ are the fluid density and fluid viscosity functions defined by

$$\begin{aligned} \rho(C(\mathbf{x}, t)) &= \rho_1 C(\mathbf{x}, t) + \rho_2(1 - C(\mathbf{x}, t)), \\ \mu(C(\mathbf{x}, t)) &= \mu_1 C(\mathbf{x}, t) + \mu_2(1 - C(\mathbf{x}, t)), \end{aligned}$$

p_{∞} is the atmospheric pressure, and $\psi : \Omega \times [0, \infty)$ is defined by

$$\psi(x_1, x_2, x_3; t) = \int_{x_3}^H \rho(C(x_1, x_2, s; t)) \, dx.$$

2.2 Variational formulation

Let $\Delta t > 0$ be a fixed time step. We define a sequence of points in time $\{t_n\}_{n \geq 0}$ by $t_n = n\Delta t, n \geq 0$. Furthermore, whenever f is a function defined on $\mathbb{R}^3 \times [0, \infty)$, we write $f^n = f(\cdot, t_n)$.

Taking a forward difference in time in (2.3) yields the equation

$$\frac{C^{n+1} - C^n}{\Delta t} + \mathbf{u}^n \cdot \nabla_{\mathbf{x}} C^n = 0, \quad (2.6)$$

which can be solved for C^{n+1} using a volume-of-fluid method. With the volume fraction field updated, we now turn towards updating the velocity field and the pressure field. We shall make use of a classical technique first introduced in [3] called the projection method or Chorin's method that decouples the velocity and the pressure from each other and updates both fields in three steps. Our approach to this method is based on the particular variant of the projection method called the incremental pressure correction scheme (IPCS) due to [4], and our exposition of this method is largely based on [5, sec. 3.4.2]. In the first step, we compute a tentative update for the velocity field, denoted \mathbf{u}^* , by taking a forward difference in time in (2.1), yielding the equation

$$\begin{aligned} \frac{\rho(C^{n+1}) - \rho(C^n)}{\Delta t} \mathbf{u}^n + (\mathbf{u}^n (\mathbf{u}^n)^T) \nabla_{\mathbf{x}} \rho(C^n) + \rho(C^n) \left(\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla_{\mathbf{x}}) \mathbf{u}^n - g \mathbf{e}_3 \right) \\ = (\nabla_{\mathbf{x}} \mathbf{u}^n + (\nabla_{\mathbf{x}} \mathbf{u}^n)^T) \nabla_{\mathbf{x}} \mu(C^n) + \mu(C^n) (\nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} \mathbf{u}^n) + \Delta_{\mathbf{x}} \mathbf{u}^n) - \nabla_{\mathbf{x}} p^n. \end{aligned} \quad (2.7)$$

Note that

$$\begin{aligned} \frac{\rho(C^{n+1}) - \rho(C^n)}{\Delta t} &= (\rho_1 - \rho_2) \frac{C^{n+1} - C^n}{\Delta t}, \\ \nabla_{\mathbf{x}} \rho(C^n) &= (\rho_1 - \rho_2) \nabla_{\mathbf{x}} C^n, \\ (\mathbf{u}^n (\mathbf{u}^n)^T) \nabla_{\mathbf{x}} \rho(C^n) &= \mathbf{u}^n ((\mathbf{u}^n)^T \nabla_{\mathbf{x}} \rho(C^n)) = (\rho_1 - \rho_2) (\mathbf{u}^n \cdot \nabla_{\mathbf{x}} C^n) \mathbf{u}^n, \end{aligned}$$

hence we may reduce (2.7) to

$$\begin{aligned} \rho(C^n) \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + \rho(C^n) (\mathbf{u}^n \cdot \nabla_{\mathbf{x}}) \mathbf{u}^n + \nabla_{\mathbf{x}} p^n + \rho(C^n) g \mathbf{e}_3 \\ = (\nabla_{\mathbf{x}} \mathbf{u}^n + (\nabla_{\mathbf{x}} \mathbf{u}^n)^T) \nabla_{\mathbf{x}} \mu(C^n) + \mu(C^n) (\nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} \mathbf{u}^n) + \Delta_{\mathbf{x}} \mathbf{u}^n). \end{aligned} \quad (2.8)$$

by applying the calculations above and (2.6). Rearranging terms, we may restate (2.8) as

$$\begin{aligned} \mathbf{u}^* = \mathbf{u}^n + \Delta t \left((\mathbf{u}^n \cdot \nabla_{\mathbf{x}}) \mathbf{u}^n - g \mathbf{e}_3 + \frac{1}{\rho(C^n)} [(\nabla_{\mathbf{x}} \mathbf{u}^n + (\nabla_{\mathbf{x}} \mathbf{u}^n)^T) \nabla_{\mathbf{x}} \mu(C^n) - \nabla_{\mathbf{x}} p^n \right. \\ \left. + \mu(C^n) (\nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} \mathbf{u}^n) + \Delta_{\mathbf{x}} \mathbf{u}^n) \right]. \end{aligned} \quad (2.9)$$

By taking a dot product with a test function \mathbf{v} belonging to a function space to be defined,

then integrating over Ω on both sides of (2.9), we obtain the equation

$$\begin{aligned} \int_{\Omega} \mathbf{u}^* \cdot \mathbf{v} \, dx &= \int_{\Omega} \mathbf{u}^n \cdot \mathbf{v} \, dx + \Delta t \left(\int_{\Omega} (\mathbf{u}^n \cdot \nabla_{\mathbf{x}}) \mathbf{u}^n \cdot \mathbf{v} \, dx - \int_{\Omega} g \mathbf{e}_3 \cdot \mathbf{v} \, dx \right. \\ &\quad + \int_{\Omega} \frac{1}{\rho(C^n)} [(\nabla_{\mathbf{x}} \mathbf{u}^n + (\nabla_{\mathbf{x}} \mathbf{u}^n)^T) \nabla_{\mathbf{x}} \mu(C^n)] \cdot \mathbf{v} \, dx \\ &\quad \left. + \int_{\Omega} \frac{1}{\rho(C^n)} [\mu(C^n) (\nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} \mathbf{u}^n) + \Delta_{\mathbf{x}} \mathbf{u}^n) - \nabla_{\mathbf{x}} p^n] \cdot \mathbf{v} \, dx \right). \end{aligned} \quad (2.10)$$

Notice that (2.10) makes sense whenever \mathbf{u}^* and \mathbf{v} belong to the space $H_0^1(\Omega)^3$, the previous velocity field \mathbf{u}^n belongs to the space

$$V(\Omega) := H^2(\Omega)^3 \cap \{\mathbf{f} \in H_0^1(\Omega)^3 : \nabla_{\mathbf{x}} \cdot \mathbf{f} = 0 \text{ a.e. in } \Omega\},$$

and the previous pressure field p^n belongs to the space

$$P^n(\Omega) := \{f \in H^1(\Omega) : f = p_{\infty} + \psi^n \text{ on } \partial\Omega\}.$$

Defining a bilinear form $a_1 : H^1(\Omega)^3 \times H^1(\Omega)^3 \rightarrow \mathbb{R}$ by

$$a_1(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \mathbf{u} \cdot \mathbf{v} \, dx \quad (2.11)$$

and a linear functional $\ell_1 : H^1(\Omega)^3 \rightarrow \mathbb{R}$ by

$$\begin{aligned} \ell_1(\mathbf{v}) &= \int_{\Omega} \mathbf{u}^n \cdot \mathbf{v} \, dx + \Delta t \left(\int_{\Omega} (\mathbf{u}^n \cdot \nabla_{\mathbf{x}}) \mathbf{u}^n \cdot \mathbf{v} \, dx - \int_{\Omega} g \mathbf{e}_3 \cdot \mathbf{v} \, dx \right. \\ &\quad + \int_{\Omega} \frac{1}{\rho(C^n)} [(\nabla_{\mathbf{x}} \mathbf{u}^n + (\nabla_{\mathbf{x}} \mathbf{u}^n)^T) \nabla_{\mathbf{x}} \mu(C^n)] \cdot \mathbf{v} \, dx \\ &\quad \left. + \int_{\Omega} \frac{1}{\rho(C^n)} [\mu(C^n) (\nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} \mathbf{u}^n) + \Delta_{\mathbf{x}} \mathbf{u}^n) - \nabla_{\mathbf{x}} p^n] \cdot \mathbf{v} \, dx \right), \end{aligned} \quad (2.12)$$

we obtain the following variational problem from (2.10):

$$\text{find } \mathbf{u}^* \in H_0^1(\Omega)^3 \text{ such that } a_1(\mathbf{u}^*, \mathbf{v}) = \ell_1(\mathbf{v}) \quad \forall \mathbf{v} \in H_0^1(\Omega)^3 \quad (2.13)$$

Whenever a variational problem such as (2.13) is introduced, it makes sense to ask whether said problem has a weak solution, and whether said solution is unique. The following proposition gives an affirmative answer to both of these questions.

Proposition 2.1. The variational problem (2.13) has a unique weak solution $\mathbf{u}^* \in H_0^1(\Omega)^3$.

Proof:

Using the definitions of a_1 and ℓ_1 as given in (2.11) and (2.12), respectively, it suffices to prove that a_1 is continuous and coercive and that ℓ_1 is bounded, i.e. that there exist constants $C_1, C_2, C_3 > 0$ such that

$$\begin{aligned} |a_1(\mathbf{u}, \mathbf{v})| &\leq C_1 \|\mathbf{u}\|_{H^1(\Omega)^3} \|\mathbf{v}\|_{H^1(\Omega)^3}, \\ a_1(\mathbf{u}, \mathbf{u}) &\geq C_2 \|\mathbf{u}\|_{H^1(\Omega)^3}^2, \\ \ell_1(\mathbf{v}) &\leq C_3 \|\mathbf{v}\|_{H^1(\Omega)^3} \end{aligned}$$

for all $\mathbf{u}, \mathbf{v} \in H^1(\Omega)^3$. Once these properties have been verified, we may invoke the Lax-Milgram theorem to directly obtain both existence and uniqueness of a weak solution \mathbf{u}^* of (2.13). The proof naturally splits into three parts, each concerned with verifying one of the three properties listed above.

Let $\mathbf{u} = (u_1, u_2, u_3)^T, \mathbf{v} = (v_1, v_2, v_3)^T \in H^1(\Omega)^3$. We start by showing continuity of a_1 . Using the definition of a_1 and Hölder's inequality along with the obvious inequalities $\|u_i\|_{L^2(\Omega)} \leq \|\mathbf{u}\|_{H^1(\Omega)^3}, i = 1, 2, 3$, it follows that

$$\begin{aligned} |a_1(\mathbf{u}, \mathbf{v})| &= \left| \int_{\Omega} \sum_{i=1}^3 u_i v_i \, dx \right| \leq \sum_{i=1}^3 \int_{\Omega} |u_i v_i| \, dx \\ &\leq \sum_{i=1}^3 \|u_i\|_{L^2(\Omega)} \|v_i\|_{L^2(\Omega)} \leq \|\mathbf{u}\|_{H^1(\Omega)^3} \sum_{i=1}^3 \|v_i\|_{L^2(\Omega)} \\ &\leq \|\mathbf{u}\|_{H^1(\Omega)^3} \|\mathbf{v}\|_{H^1(\Omega)^3}, \end{aligned}$$

hence a_1 is continuous with $C_1 = 1$. Next, we turn to coercivity of a_1 . We start by writing

$$a_1(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^3 \int_{\Omega} u_i v_i \, dx = \sum_{i=1}^3 a_{1,i}(u_i, v_i),$$

where $a_{1,i} : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}$ is the bilinear form defined by

$$a_{1,i}(u, v) = \int_{\Omega} uv \, dx, \quad i = 1, 2, 3.$$

Each of the bilinear forms $a_{1,i}$ can be shown to be coercive over $H^1(\Omega) \times H^1(\Omega)$ by using the Poincaré-Friedrichs inequality; for a proof of this, see [6, pp.12-22]. Using this fact, we obtain coefficients $C_i > 0, i = 1, 2, 3$ such that

$$C_i \|u\|_{H^1(\Omega)}^2 \leq a_{1,i}(u, u)$$

for all $u \in H^1(\Omega)$. Letting $C^* = \min \left\{ \frac{1}{C_i} : i = 1, 2, 3 \right\}$, we see that

$$\|\mathbf{u}\|_{H^1(\Omega)^3}^2 = \sum_{i=1}^3 \|u_i\|_{H^1(\Omega)}^2 \leq C^* \sum_{i=1}^3 a_{1,i}(u_i, u_i) = C^* a_1(\mathbf{u}, \mathbf{u}),$$

hence a_1 is coercive with constant $C_2 = \frac{1}{C^*}$. Finally, to prove continuity of ℓ_1 , note that

$$\begin{aligned}
 |\ell_1(\mathbf{v})| &\leq \int_{\Omega} \sum_{i=1}^3 |u_i^n v_i| \, dx + \Delta t \left(\int_{\Omega} \sum_{i,j=1}^3 |u_i^n \partial_{x_i} u_j^n v_j| \, dx + \int_{\Omega} |g v_3| \, dx \right. \\
 &\quad + \int_{\Omega} \left| \frac{1}{\rho(C^n)} \right| \sum_{i,j=1}^3 (|\partial_{x_j} u_i^n| + |\partial_{x_i} u_j^n|) |\partial_{x_i} \mu(C^n)| |v_i| \, dx \\
 &\quad \left. + \int_{\Omega} \left| \frac{1}{\rho(C^n)} \right| \sum_{i,j=1}^3 \left(|\mu(C^n)| (|\partial_{x_j x_i}^2 u_j^n| + |\partial_{x_j^2} u_i^n|) + |\partial_{x_i} p^n| \right) |v_i| \, dx \right) \\
 &\leq \sum_{i=1}^3 \|u_i^n\|_{L^2(\Omega)} \|v_i^n\|_{L^2(\Omega)} + \Delta t \left(\sum_{i,j=1}^3 \|u_i^n\|_{L^4(\Omega)} \|\partial_{x_i} u_j^n\|_{L^4(\Omega)} \|v_j\|_{L^2(\Omega)} \right. \\
 &\quad + \frac{|\mu_1 - \mu_2|}{\min\{\rho_1, \rho_2\}} \sum_{i,j=1}^3 (\|\partial_{x_j} u_i^n\|_{L^2(\Omega)} + \|\partial_{x_i} u_j^n\|_{L^2(\Omega)}) \|\partial_{x_i} C^n\| \|v_i\|_{L^2(\Omega)} \\
 &\quad + \sum_{i,j=1}^3 \frac{\max\{\mu_1, \mu_2\}}{\min\{\rho_1, \rho_2\}} \left(\|\partial_{x_j x_i}^2 u_j^n\|_{L^2(\Omega)} + \|\partial_{x_j^2} u_i^n\|_{L^2(\Omega)} \right) \|v_i\|_{L^2(\Omega)} \\
 &\quad \left. + g \sqrt{\lambda(\Omega)} \|v_3\|_{L^2(\Omega)} + \frac{1}{\min\{\rho_1, \rho_2\}} \sum_{i=1}^3 \|\partial_{x_i} p^n\|_{L^2(\Omega)} \|v_i\|_{L^2(\Omega)} \right) \\
 &\leq C_3 \|\mathbf{v}\|_{H^2(\Omega)^3},
 \end{aligned}$$

where $C_3 > 0$ is a constant depending on Ω , \mathbf{u}^n , $\rho(C^n)$, and $\mu(C^n)$. In order to obtain the second inequality, we have made the following observations:

- The term $\int_{\Omega} \sum_{i,j=1}^3 |u_i^n \partial_{x_i} u_j^n v_j| \, dx$ can be bounded upwards using the generalized Hölder inequality, yielding the estimate

$$\int_{\Omega} \sum_{i,j=1}^3 |u_i^n \partial_{x_i} u_j^n v_j| \, dx \leq \sum_{i,j=1}^3 \|u_i^n\|_{L^4(\Omega)} \|\partial_{x_i} u_j^n\|_{L^4(\Omega)} \|v_j\|_{L^2(\Omega)}.$$

This is due to the fact that u_i^n and $\partial_{x_j} u_i^n$ belonging to $H^2(\Omega)$ implies that they belong to $L^6(\Omega)$ by the Sobolev embedding theorem, since $q = 6$ satisfies $\frac{1}{q} = \frac{1}{p} - \frac{1}{d} = \frac{1}{6}$. By the Riesz-Thorin interpolation theorem, it follows that u_i^n and $\partial_{x_j} u_i^n$ in particular belongs to the intermediate space $L^4(\Omega)$ for $i, j = 1, 2, 3$. As v_j belongs to $L^2(\Omega)$ for $j = 1, 2, 3$ and $\frac{1}{4} + \frac{1}{4} + \frac{1}{2} = 1$, the generalized Hölder inequality implies that each term $u_i^n \partial_{x_i} u_j^n v_j$ belongs to $L^1(\Omega)$ and yields the estimate

$$\int_{\Omega} |u_i^n \partial_{x_i} u_j^n v_j| \, dx \leq \|u_i^n\|_{L^4(\Omega)} \|\partial_{x_i} u_j^n\|_{L^4(\Omega)} \|v_j\|_{L^2(\Omega)}, \quad i, j = 1, 2, 3.$$

- The partial derivatives $\partial_{x_i} C^n$ are bounded on Ω , hence the partial derivatives $\partial_{x_i} \mu(C^n) = (\mu_1 - \mu_2) \partial_{x_i} C^n$ are also bounded on Ω .
- Every term on the right-hand side of the first inequality besides the term mentioned in the first point can be bounded upwards by applying Hölder's inequality.

Having shown the desired properties of a_1 and ℓ_1 , we are now in a position to invoke the Lax-Milgram theorem and obtain a unique solution \mathbf{u}^* of (2.13). \square

The tentative velocity \mathbf{u}^* obtained from the variational problem (2.13) has one defect, namely that there is no guarantee that it satisfies the divergence-free condition (2.2). In order to ensure the next velocity field satisfies (2.2), we will compute a correctional pressure term that will be used to modify the tentative vector field \mathbf{u}^* such that the new vector field is divergence-free.

We obtain this correctional pressure term as follows: By taking a forward difference in time in (2.1) at the n th time step and using the pressure field p^{n+1} , we obtain the equation

$$\begin{aligned} & \frac{\rho(C^{n+1}) - \rho(C^n)}{\Delta t} \mathbf{u}^n + (\mathbf{u}^n (\mathbf{u}^n)^T) \nabla_{\mathbf{x}} \rho(C^n) + \rho(C^n) \left(\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla_{\mathbf{x}}) \mathbf{u}^n - g \mathbf{e}_3 \right) \\ & = (\nabla_{\mathbf{x}} \mathbf{u}^n + (\nabla_{\mathbf{x}} \mathbf{u}^n)^T) \nabla_{\mathbf{x}} \mu(C^n) + \mu(C^n) (\nabla_{\mathbf{x}} (\nabla_{\mathbf{x}} \cdot \mathbf{u}^n) + \Delta_{\mathbf{x}} \mathbf{u}^n) - \nabla_{\mathbf{x}} p^n. \end{aligned} \quad (2.14)$$

Notice here that we use the actual velocity field \mathbf{u}^{n+1} in the forward difference instead of the tentative velocity \mathbf{u}^* . Subtracting (2.14) from (2.7) and dividing through by $\rho(C^n)$ yields

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} + \frac{\nabla_{\mathbf{x}} p^{n+1} - \nabla_{\mathbf{x}} p^n}{\rho(C^n)} = 0. \quad (2.15)$$

Taking the divergence of both sides of (2.15) and requiring that the $(n+1)$ th velocity field \mathbf{u}^{n+1} satisfies the divergence-free condition (2.2), the equation

$$\frac{1}{\rho(C^n)} \Delta_{\mathbf{x}} p^* - \frac{\rho_1 - \rho_2}{(\rho(C^n))^2} (\nabla_{\mathbf{x}} C^n) \cdot (\nabla_{\mathbf{x}} p^*) = \frac{1}{\Delta t} \nabla_{\mathbf{x}} \cdot \mathbf{u}^* \quad (2.16)$$

follows, where $p^* = p^{n+1} - p^n$ and we used the fact that

$$\begin{aligned} \nabla_{\mathbf{x}} \cdot \left(\frac{1}{\rho(C^n)} \nabla_{\mathbf{x}} p^* \right) & = \left(\nabla_{\mathbf{x}} \frac{1}{\rho(C^n)} \right) \cdot (\nabla_{\mathbf{x}} p^*) + \frac{1}{\rho(C^n)} \nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} p^*) \\ & = \frac{1}{\rho(C^n)} \Delta_{\mathbf{x}} p^* - \frac{\rho_1 - \rho_2}{(\rho(C^n))^2} (\nabla_{\mathbf{x}} C^n) \cdot (\nabla_{\mathbf{x}} p^*). \end{aligned}$$

Multiplying both sides of (2.16) by $\rho(C^n)$ and a scalar test function $q \in H_0^1(\Omega)$, then integrating over Ω yields

$$\int_{\Omega} (\Delta_{\mathbf{x}} p^*) q \, dx - \int_{\Omega} \frac{\rho_1 - \rho_2}{\rho(C^n)} (\nabla_{\mathbf{x}} C^n) \cdot (\nabla_{\mathbf{x}} p^*) q \, dx = \frac{1}{\Delta t} \int_{\Omega} \rho(C^n) (\nabla_{\mathbf{x}} \cdot \mathbf{u}^*) q \, dx. \quad (2.17)$$

Using integration by parts on the first integral on the left hand side of (2.17) and recalling that q vanishes on $\partial\Omega$, we obtain

$$\begin{aligned} \int_{\Omega} (\Delta_{\mathbf{x}} p^*) q & = \int_{\partial\Omega} q (\nabla_{\mathbf{x}} p^* \cdot \mathbf{n}_{\partial\Omega}) \, dS - \int_{\Omega} (\nabla_{\mathbf{x}} p^*) \cdot (\nabla_{\mathbf{x}} q) \, dx \\ & = - \int_{\Omega} (\nabla_{\mathbf{x}} p^*) \cdot (\nabla_{\mathbf{x}} q) \, dx; \end{aligned}$$

using this equation, we may restate (2.17) as

$$\int_{\Omega} (\nabla_{\mathbf{x}} p^*) \cdot (\nabla_{\mathbf{x}} q) + \frac{\rho_1 - \rho_2}{\rho(C^n)} (\nabla_{\mathbf{x}} C^n) \cdot (\nabla_{\mathbf{x}} p^*) q \, dx + \int_{\Omega} \frac{\rho(C^n)}{\Delta t} (\nabla_{\mathbf{x}} \cdot \mathbf{u}^*) q \, dx = 0. \quad (2.18)$$

Similarly to (2.10), the equation (2.18) makes sense when the correctional pressure field p^* belongs to the space

$$\tilde{P}^n(\Omega) := \{f \in H^1(\Omega) : f = \psi^{n+1} - \psi^n \text{ on } \partial\Omega\}.$$

Defining a bilinear form $a_2 : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}$ by

$$a_2(p, q) = \int_{\Omega} (\nabla_{\mathbf{x}} p) \cdot (\nabla_{\mathbf{x}} q) \, dx + \int_{\Omega} \frac{\rho_1 - \rho_2}{\rho(C^n)} (\nabla_{\mathbf{x}} C^n) \cdot (\nabla_{\mathbf{x}} p) q \, dx \quad (2.19)$$

and a linear functional $\ell_2 : H^1(\Omega) \rightarrow \mathbb{R}$ by

$$\ell_2(q) = -\frac{1}{\Delta t} \int_{\Omega} \rho(C^n) (\nabla_{\mathbf{x}} \cdot \mathbf{u}^*) q \, dx, \quad (2.20)$$

we obtain the following variational problem:

$$\text{find } p^* \in \tilde{P}^n(\Omega) \text{ such that } a_2(p^*, q) = \ell_2(q) \quad \forall q \in H_0^1(\Omega). \quad (2.21)$$

Similarly to Proposition 2.1, we are able to show existence and uniqueness of a weak solution of (2.21):

Proposition 2.2. The variational problem (2.21) has a unique weak solution $\mathbf{u}^* \in (H^2(\Omega) \cap H_0^1(\Omega))^3$.

Proof:

As in the proof of Proposition 2.1, it is enough to show that the bilinear form a_2 defined by (2.19) is continuous and coercive and the linear functional ℓ_2 defined by (2.20) is continuous. Once we have shown these properties, we may finish the proof by directly invoking the Lax-Milgram theorem. To this end, let $p, q \in H^1(\Omega)$. Recalling that $\frac{1}{\rho(C^n)}$ and the partial derivatives $\partial_{x_i} C^n$ are bounded, applying Hölder's inequality directly to (2.19) shows that

$$\begin{aligned} |a_2(p, q)| &\leq \int_{\Omega} \sum_{i=1}^3 |\partial_{x_i} p \partial_{x_i} q| \, dx + \int_{\Omega} \left| \frac{\rho_1 - \rho_2}{\rho(C^n)} \right| |q| \sum_{i=1}^3 |\partial_{x_i} C^n \partial_{x_i} p| \, dx \\ &\leq \sum_{i=1}^3 \|\partial_{x_i} p\|_{L^2(\Omega)} \|\partial_{x_i} q\|_{L^2(\Omega)} + C \|q\|_{L^2(\Omega)} \sum_{i=1}^3 \|\partial_{x_i} p\|_{L^2(\Omega)} \\ &\leq C' \|q\|_{H^1(\Omega)} \sum_{i=1}^3 \|\partial_{x_i} p\|_{L^2(\Omega)} \\ &\leq C'' \|p\|_{H^1(\Omega)} \|q\|_{H^1(\Omega)}, \end{aligned}$$

hence a_2 is continuous. Furthermore, by arguing as in [6, pp.12-22], we obtain coercivity of a_2 .

It remains to show that ℓ_2 is continuous. Recalling that \mathbf{u}^* belongs to $H_0^1(\Omega)^3$, an appli-

cation of Hölder's inequality shows that

$$\begin{aligned} |\ell_2(q)| &\leq \frac{1}{\Delta t} \int_{\Omega} |\rho(C^n)| |q| \sum_{i=1}^3 |\partial_{x_i} u_i^*| \, dx \\ &\leq \frac{1}{\Delta t} \|q\|_{L^2(\Omega)} \sum_{i=1}^3 \|\partial_{x_i} u_i^*\|_{L^2(\Omega)} \\ &\leq \frac{1}{\Delta t} \|q\|_{H^1(\Omega)} \sum_{i=1}^3 \|\partial_{x_i} u_i^*\|_{L^2(\Omega)}, \end{aligned}$$

hence ℓ_2 is continuous. □

With the correctional pressure term p^* obtained from (2.21), we are ready to update both the velocity field \mathbf{u}^n and the pressure field p^n in time. We obtain the $(n + 1)$ th pressure field p^{n+1} simply by recalling that $p^{n+1} = p^n + p^*$ by the very definition of p^* . To obtain the $(n + 1)$ th velocity field \mathbf{u}^{n+1} , consider the equation (2.15). Taking a scalar product with a vector test function $\mathbf{v} \in H_0^1(\Omega)^3$ and integrating over Ω on both sides, we obtain the equation

$$\int_{\Omega} \mathbf{u}^{n+1} \cdot \mathbf{v} \, dx = \int_{\Omega} \mathbf{u}^* \cdot \mathbf{v} \, dx - \Delta t \int_{\Omega} \frac{1}{\rho(C^n)} \nabla_{\mathbf{x}} p^* \cdot \mathbf{v} \, dx. \quad (2.22)$$

Similarly to the previous steps, we define a bilinear functional a_3 by

$$a_3(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \mathbf{u} \cdot \mathbf{v} \, dx \quad (2.23)$$

and a linear functional ℓ_3 by

$$\ell_3(\mathbf{v}) = \int_{\Omega} \mathbf{u}^* \cdot \mathbf{v} \, dx - \Delta t \int_{\Omega} \frac{1}{\rho(C^n)} \nabla_{\mathbf{x}} p^* \cdot \mathbf{v} \, dx, \quad (2.24)$$

then consider the following variational problem based on (2.22):

$$\text{find } \mathbf{u}^{n+1} \in E(\Omega) \text{ such that } a_3(\mathbf{u}^{n+1}, \mathbf{v}) = \ell_3(\mathbf{v}) \quad \forall \mathbf{v} \in H_0^1(\Omega)^3, \quad (2.25)$$

As with the previous variational problems, we start by ensuring existence and uniqueness of a weak solution:

Proposition 2.3. The variational problem (2.25) has a unique weak solution $\mathbf{u}^* \in E(\Omega)$.

Proof:

As before, we wish to show that a_3 as defined by (2.23) is continuous and coercive and that ℓ_3 as defined by (2.24) is continuous in order to invoke the Lax-Milgram theorem to directly obtain the existence of a weak solution of (2.25).

The continuity and coercivity of a_3 follows by analogous arguments to the ones made for the same properties of the bilinear form a_1 in the proof of Proposition 2.1, since the two bilinear forms are defined by the same expression. As for the continuity of ℓ_3 , we recall

that $\mathbf{u}^* \in H^1(\Omega)^3$ and $p^* \in H^1(\Omega)$, hence we may once again apply Hölder's inequality to show that for any $\mathbf{v} \in H^1(\Omega)$,

$$\begin{aligned} |\ell_3(\mathbf{v})| &\leq \int_{\Omega} \sum_{i=1}^3 |u_i^* v_i| \, dx + \Delta t \int_{\Omega} \left| \frac{1}{\rho(C^n)} \right| \sum_{i=1}^3 |\partial_{x_i} p^* v_i| \, dx \\ &\leq \sum_{i=1}^3 \|u_i^*\|_{L^2(\Omega)} \|v_i\|_{L^2(\Omega)} + C \sum_{i=1}^3 \|\partial_{x_i} p^*\|_{L^2(\Omega)} \|v_i\|_{L^2(\Omega)} \\ &\leq C' \|\mathbf{v}\|_{H^1(\Omega)}, \end{aligned}$$

hence ℓ_3 is continuous. □

2.3 Numerical experiments

Hvaing introduced the IPCS, we now turn back to the original problem presented in Chapter 1, i.e. the question of whether a two-phase flow reaches an equilibrium in which the two fluids are separated. To this end, we have conducted a range of numerical experiments using an implementation of the IPCS in the open-source computing platform FeNICSx [7, 8, 9, 10, 11, 12, 13, 14, 15]. In the appended Python script “num_exp.py”, we have created a scripts which implements the IPCS in order to simulate a mixture of water and oil in the slab $\Omega = [0, 1]^2 \times [0, 5]$.

3 | Conclusion

Through this thesis, we have managed to show theoretical properties of the evolution of a two-phase flow in a vertical slab and managed to verify them numerically as well. However, the field still contains several open questions, including but not limited to:

- Investigating more general subsets $\Omega \subset \mathbb{R}^3$ and their effects on the stability of the methods
- Incorporating several more concepts from the theory of finite element analysis and finite volume analysis in order to achieve new results, e.g. a priori estimates on the error committed in the approximations
- Conducting more numerical experiments.

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