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MODELACIÓN MATEMÁTICA DEL PROCESO DE LIXIVIACIÓN EN PILAS PARA LA PRODUCCIÓN DE COBRE

Tesis para optar al grado de
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MATHEMATICAL MODELLING OF COPPER HEAP LEACHING

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A mi esposa,

Patricia Elizabeth Montes Uribe.

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Abstract

In this thesis there is approached the problem that consists in the mathematical modelling of copper heap leaching. The mathematical model is formulated in the context of the macroscopic theory of porous media (isothermal and without mechanical deformation). Specifically, we consider the classical two phase problem, with liquid and gaseous phases, and a transport problem with the following components: sulphuric acid in liquid phase, and copper's ions in liquid and solid phase. Thus there spread previous works that they consider to be conditions of saturated and not saturated flow. There is assumed that the flow and transport problems are decoupled. The solution of two phase flow problem is approximated applying a numerical scheme that combines the mixed finite element method and finite volume scheme, whereas the solution of transport problem is approximated applying a finite volume scheme combined with a finite element method. In flow and transport models, a convergence analysis is realized. Finally, it's presented several computational experiments, with realistic parameters from copper industry of Chile.

Resumen

Esta tesis trata el problema de modelar matemáticamente el proceso de lixiviación en pilas de minerales de cobre. Se construye un modelo conceptual utilizando la teoría macroscópica de flujo multifásico y transporte multicomponente en medios porosos (isotermal y sin deformación mecánica). Específicamente, se considera el flujo de dos fases fluidas, una líquida y otra gaseosa, junto con el transporte de las siguientes componentes: ácido sulfúrico en la fase líquida, y cobre en las fases líquida y sólida. De este modo se extienden trabajos previos que consideran condiciones de flujo saturado y no saturado. Se asume que los problemas de flujo y de transporte están desacoplados. La solución del modelo matemático de flujo a dos fases es aproximada a través de un esquema numérico que combina el método de elementos finitos mixtos y el método de volúmenes finitos, mientras que la solución del modelo matemático de transporte es aproximada a través de un esquema de volúmenes finitos combinado con un esquema de elementos finitos. Para ambos esquemas numéricos propuestos, se efectúa el correspondiente análisis de convergencia. Finalmente, para los dos problemas considerados, se reportan diversos experimentos computacionales con parámetros, cuyos valores numéricos provienen de la industria chilena del cobre.

Para una descripción más detallada (principales resultados, aportes y conclusiones) y cuantitativa ver Capítulo 5.

Nomenclature

c_a^w	volumetric concentration of sulfuric acid in solution $[kg/m^3]$
c_c^w	volumetric concentration of copper in solution $[kg/m^3]$
c_c^s	concentration of copper in solid phase $[kg/kg]$
D	average value of D_w on $\Omega \times (0, T)$
D_m	molecular diffusion coefficient (= 0, in this thesis)
D_w	capillary diffusion coefficient
$\mathbf{D}$	tensor of hydrodynamic dispersion $[m^2/s]$
$\mathbf{G}$	auxiliary function in Model Problem ($= G_\lambda \mathbf{g}$)
f_α	fractional flow function
G_α	auxiliary functions in fractional flow formulation
G_λ	auxiliary function in fractional flow formulation
g	gravity $[m/s^2]$
$\mathbf{g}$	gravity vector ($= (0, 0, -g)$)
$\mathbf{K}$	tensor of absolute permeability ($= k\mathbf{I}$, in this thesis) $[m^2]$
k_d	equilibrium distribution constant (adsorption coefficient) $[m^3/kg]$
k_e	first-order kinetic constant (extraction coefficient) $[m^3/(kg \cdot s)]$
$k_{r\alpha}$	relative permeability of the α-phase $[-]$
m, n	van Genuchten parameters

p	global pressure $[Pa]$
p_A	atmospheric pressure $[Pa]$
p_c	capillary pressure function $[Pa]$
p_d	entry pressure $[Pa]$
p_α	pressure of α-phase $[Pa]$
$R(t)$	irrigation ratio $[m/s]$
r_α, q_α	source terms
f_α	fractional flow function $[-]$
$\mathbb{R}$	real numbers
s_{wr}	residual water saturation $[-]$
s_α	saturation of α-phase $[m^3/m^3]$
t	time $[s]$
T	total time of simulation $[s]$
$\mathbf{u}_\alpha$	flow velocity $[m/s]$
$\mathbf{u}$	total velocity $[m/s]$
$\mathbf{v}_\alpha$	volumetric (flux or Darcy's velocity) velocity of α-phase $[m/s]$
$\mathbf{x}$	spatial point

α	phase ($\alpha = w, n$)
$\alpha = w$	liquid phase
$\alpha = n$	gaseous phase
α_{VG}	van Genuchten parameter
α_L, α_T	longitudinal and transverse dispersities
λ	total mobility $[(m \cdot s)/kg]$
λ_α	phase mobility function $[(m \cdot s)/kg]$
λ_{BC}	Brooks-Corey parameter $[-]$
ρ_s	solid bulk (dry) density $[kg/m^3]$
ρ_α	density of α-phase $[kg/m^3]$
μ	first-order consumption factor (consumption coefficient) $[1/s]$
μ_α	viscosity of the α-phase $[kg/(m \cdot s)]$
ϕ	porosity of ore bed (volume of void / volumen of bed) $[m^3/m^3]$
$\partial\Omega$	boundary of Ω
Γ^{ex}	boundaries, $ex = i, o, l, r$, and $\partial\Omega = \Gamma^i \cup \Gamma^o \cup \Gamma^l \cup \Gamma^r$
θ_α	liquid content ($= \phi s_\alpha$)
θ	complementary pressure
ϕ_s	$= 1 - \phi$, (volume of solid phase / volume of bed) $[m^3/m^3]$

Introducción (In Spanish)

El objetivo de esta sección (*según el Decreto U. DE C. Nro. 2001-186, Universidad de Concepción*) es motivar el problema tratado en esta tesis, presentar su estructura, sus objetivos, y finalmente detallar las principales contribuciones realizadas.

Motivación

El cobre constituye un pilar fundamental de la economía chilena. Además, se utiliza mundialmente en una gran cantidad y variedad de productos tecnológicos. Su extracción se realiza por las vías de pirometalurgia e hidrometalurgia, siendo esta última la responsable de aproximadamente un tercio del cobre exportado por Chile (ver [25]), y es la que se considera en este trabajo de tesis.

La vía hidrometalúrgica de extracción, consiste fundamentalmente en cuatro etapas: chancado, lixiviación, extracción por solventes y electro-obtención. De las anteriores esta tesis considera el proceso de lixiviación, cuyas principales variantes son: lixiviación en pilas, lixiviación in-situ, lixiviación en vateas inundadas y lixiviación en botadero. En este sentido, el tema central de esta tesis es la modelación matemática del proceso de lixiviación en pilas de minerales de cobre en el contexto de la industria chilena, principal exportador mundial de cobre (ver [25]).

El proceso de lixiviación consiste en la disolución del cobre presente en el mineral, luego de ser atacado químicamente por un agente lixiviante, mientras que el proceso de lixiviación en pilas, consiste en un proceso de extracción del metal contenido en un mineral que ha sido previamente apilado sobre un lecho o carpeta impermeable. El mineral así

apilado es sometido a un proceso de riego en la parte superior de la pila, con una solución de ácido sulfúrico, que percola por gravedad y va reaccionando con el mineral, a partir de lo cual se obtiene una solución rica en cobre. Esta solución obtenida desde la base de la pila se colecta en estanques y se envía a las plantas de extracción por solventes y electro-obtención, en donde se obtienen cátodos de cobre metálico de alta pureza. Como subproducto se obtiene una solución agotada, la cual es acondicionada y reutilizada en el proceso de lixiviación (ver [25]).
El proceso de lixiviación en pilas corresponde a un fenómeno de flujo de fluidos y transporte de componentes en un medio poroso. Efectivamente, la pila en sí misma constituye un medio poroso, en donde coexisten fundamentalmente tres fases, dos fluidas y una estática. Las dos fases fluidas son la solución de lixiviación (cuyas principales componentes son agua, ácido sulfúrico y cobre) y la fase gaseosa (cuyas principales componentes son aire, oxígeno y vapor de agua, entre otras). Por otro lado, la tercera fase es la fase sólida (cuyas principales componentes son el cobre formando compuestos con otros elementos, más otras especies que dependerán del tipo de mineral), la cual está constituida por el mineral, que previamente ha sido chancado, aglomerado y apilado, según una disposición trapezoidal (ver [14], [25], [36], [39], y [46], por ejemplo).

Los dos fenomenos mencionados, esto es, el flujo de fluidos y el transporte de componentes, pueden suponerse acoplados o desacoplados. En esta tesis se suponen desacoplados. Por lo tanto, ambos serán tratados de manera independiente.

Flujo a Dos Fases

Respecto del fenómeno de flujo de fluidos se distinguen tres casos:

Caso 1: Flujo Saturado. En este caso el espacio de poros o vacío, está completamente lleno por la solución de lixiviación. Se dice, entonces, que la lixiviación se realiza bajo condiciones de *Flujo Saturado*. Ver [39].

Caso 2: Flujo No Saturado. En este caso en el espacio de poros o vacío, coexisten las dos fases mencionadas previamente, esto es, las fases líquida y gaseosa. Pero se supone que la fase gaseosa está estancada, esto es, posee presión y flujo constantes. Se dice, entonces,

que la lixiviación se realiza bajo condiciones de *Flujo no Saturado*. Ver [46].
Caso 3: Flujo Bifásico. En este caso el espacio de poros o vacío, coexisten las dos fases mencionadas previamente, esto es, las fases líquida y gaseosa. Pero, a diferencia del Caso 2, NO se supone que la fase gaseosa está estancada, esto es, se considera la interaccion entre ambas fases, en cuanto a su movimiento en el espacio de poros. Se dice, entonces, que la lixiviación se realiza bajo condiciones de *Flujo a Dos Fases o Bifásico*. Ver [36].

En esta tesis se desarrolla el Caso 3, constituyendo una de sus principales contribuciones desde el punto de vista de la modelación. En efecto, trabajos previos se ubican en los Casos 1 ó 2, siendo que existen situaciones de la práctica industrial, que se ubican en el Caso 3, como por ejemplo, cuando además del proceso de irrigación, se aplica aireación forzada, o el riego se realiza de manera intermitente. En relación al tipo de mineral el Caso 3 se aplica naturalmente a la lixiviación de minerales sulfurados.

Transporte de Componentes.
Respecto del segundo fenómeno mencionado, esto es, el transporte de componentes, se asume una pila formada principalmente por minerales oxidados. Se propone un modelo matemático de transporte que considera al ácido sulfúrico como una de las principales componentes en fase líquida, y al cobre como componente en las fases líquida y sólida.

En síntesis, la principal motivación de esta tesis, es desarrollar un marco teórico lo suficientemente amplio que permita modelar de manera integral el proceso de lixiviación en pilas, tanto de minerales sulfurados como de minerales oxidados. Los énfasis estarán puestos en el modelamiento conceptual, matemático y numérico. Todo lo anterior tomando como base la teoría de transporte multifásico-multicomponente en medios porosos.

Organización de la Tesis

En el **Capítulo 1** se presenta la construcción de un Modelo Conceptual (ver [5], [30], y [36], para una explicación detallada de qué es un modelo conceptual) para el proceso de lixiviación en pilas de minerales de cobre. El modelo conceptual propuesto se basa en la teoría de medios porosos, y considera los fenómenos de flujo bifásico y transporte multicomponente. El contenido de este capitulo fué publicado parcialmente en los artículos [9] y [11], esto es,

[9] E.Cariaga, F.Concha, M.Sepúlveda, Simultaneous modeling of liquid and gaseous phases in heap leaching for copper production, Proceeding of the III International Copper Hydrometallurgy Workshop, Santiago, Chile, pp.301-315, 2005.

[11] E.Cariaga, F.Concha, M.Sepúlveda, Flow and transport in leaching heaps: application of the theory of multiphase flow through porous media, Proceeding of the IV International Copper Hydrometallurgy Workshop, Viña del Mar, Chile, pp.255-261, 2007.

En el **Capítulo 2** se presenta un análisis de convergencia del esquema numérico propuesto para el modelo matemático de flujo a dos fases. Dicho esquema numérico consiste en una combinación de los métodos de elementos finitos mixtos y de volúmenes finitos. Las ecuaciones clásicas de flujo a dos fases inmiscibles e incompresibles son transformadas en una formulación equivalente del tipo flujo fraccional, que consiste en un sistema de ecuaciones en derivadas parciales del tipo elíptico-parabólico. La ecuación parabólica considerada se asume no degenerada. El análisis de convergencia se realiza calculando estimadores a priori, a través de la introducción de problemas auxiliares que permiten desacoplar el sistema original fuertemente acoplado. Se consideran un esquema semi implícito y otro completamente explícito.

El contenido de este capítulo corresponde a la corrección (*Corrigendum*) del artículo [10], en el cual se publicaron los resultados matemáticos correspondientes al Capítulo 2 original de esta tesis. Dicho capítulo contenía errores matemáticos, los cuales fueron corregidos de manera satisfactoria, debiendo ser necesario imponer una restricción adicional sobre el número de Peclet,

[10] E.Cariaga, F.Concha, M.Sepúlveda, Convergence of a MFE-FV method for two phase flow with applications to heap leaching of copper ores, Computer Methods in Applied Mechanics and Engineering, 196 (25-28), pp.2541-2554, 2007.

En este punto debemos agradecer la oportuna corrección del Profesor Dr. Mario Ohlberger, al manuscrito original de esta tesis.

En el **Capítulo 3** se presenta un análisis de convergencia del esquema numérico propuesto para el modelo matemático de transporte, el cual está constituido por un sistema de tres ecuaciones diferenciales: una ecuación diferencial parcial degenerada del tipo convección-difusión-reacción, que modela la concentración de ácido sulfúrico en la solución de lixiviación, y un subsistema formado por una ecuación del mismo tipo (que modela la concentración de cobre en la solución de lixiviación) que la ya mencionada, acoplada con una ecuacion diferencial ordinaria (que modela la concentración de cobre presente en la fase sólida de la pila). El esquema numérico se basa en el método de volúmenes finitos (para el término convectivo) combinado con el método de elementos finitos (para el término difusivo). El análisis de convergencia se basa en una aplicación del teorema de Kolmogorov de compacidad. Se considera un esquema implícito. El contenido de este capítulo corresponde al manuscrito [12], esto es,

[12] E. Cariaga, F. Concha, M.Sepúlveda, Convergence analysis of finite volume schemes for a compositional flow model in heap leaching of copper ores, submitted, 2008.

En el **Capítulo 4** se presentan distintos experimentos computacionales para los modelos matemáticos estudiados en el Capítulo 2 y en el Capítulo 3. El capítulo finaliza con un análisis de sensibilidad de las soluciones numéricas, ante pequeños cambios en los parámetros relevantes, para el modelo de transporte. El contenido de este capítulo fué publicado parcialmente en los artículos [9] y [11], ya mencionados, y en el artículo [8], que además detalla la implemetación computacional de los métodos numéricos, esto es,

[8] E.Cariaga, F.Concha, M.Sepulveda, Flow through porous media with applications to heap leaching of copper ores, Chemical Engineering Journal, 111 (2-3), pp.151-165, 2005.

Finalmente, en el **Capítulo 5** se integran los principales hallazgos de la investigacin realizada y se ubican en el contexto del conocimiento actual. Este Capítulo responde al Decreto U. DE C. Nro. 2001-186, Universidad de Concepción.

Objetivos de esta Tesis

Los objetivos de esta tesis son:

1. Construir un modelo conceptual para el proceso de lixiviación en pilas de minerales de cobre.

2. Aplicar la teoría de medios porosos bifásicos (inmiscibles e incompresibles) y multicomponentes al proceso de lixiviación en pilas de minerales de cobre.

3. Construir un modelo matemático para el fenómeno de flujo bifásico, en las fases líquida (solución de lixiviación) y gaseosa.

4. Realizar un análisis teórico de convergencia del modelo matemático de flujo bifásico aplicando teoría y técnicas estándares.

5. Realizar experimentos computacionales para el modelo de flujo a dos fases utilizando un dominio y parámetros reales tomados de la industria del cobre en Chile.

6. Construir un modelo matemático para el fenómeno de transporte de las componentes ácido sulfúrico y cobre en las fases líquida y sólida.

7. Realizar un análisis teórico de convergencia del modelo matemático de transporte de componentes, aplicando teoría y técnicas estándares.

8. Realizar experimentos computacionales para el modelo de transporte de componentes, utilizando un dominio y parámetros reales tomados de la industria del cobre en Chile.

9. Realizar un análisis de sensibilidad de las soluciones numéricas del modelo de transporte de componentes ante modificaciones en parámetros relevantes.

Principales Contribuciones de esta Tesis

Las principales contribuciones de esta tesis son la:

1. Construcción de un modelo conceptual para el proceso de lixiviación en pilas de minerales de cobre.

2. Formulación matemática del proceso de lixiviación en pilas en el contexto de la teoría macroscópica de medios porosos, con flujo a dos fases y transporte de multi-componentes.

3. Realización de un análisis teórico de convergencia para un modelo de flujo a dos fases en el contexto de modelar el flujo de la solución de lixiviación y de la fase gaseosa, al interior de una pila de lixiviación de minerales de cobre.

4. Realización de un análisis teórico de convergencia para un modelo de transporte de componentes al interior de una pila de lixiviación de minerales oxidados.

5. Generararación de código computacional para los problemas de flujo de fluidos y transporte de componentes, al interior de una pila de lixiviación.

6. Realización de un análisis de sensibilidad ante modificaciones de parámetros relevantes para el proceso de transporte en pilas de lixiviación de minerales oxidados de cobre.

Contents

Chapter 1

Conceptual Model

One of the most powerful tools in investigating phenomenon in complex systems is the *conceptual model* employed in all branches of physics, [5]. A *conceptual model* is the description of a (hydro) system, subsystem or process which is able to represent those aspects of the system behavior that are relevant for the model's application, [30]. In this chapter a *conceptual model* is developed for heap leaching of copper ores.

1.1 Introduction

Extractive metallurgy is the study and practice of separating metals from their ores and refining them to produce a pure metal. The main subareas in extractive metallurgy are hydrometallurgy, pyrometallurgy and electrometallurgy. In this thesis, the focus is on hydrometallurgy, which correspond to the extraction and recovery of metals from their ores by processes in which aqueous solutions play a predominant role. Hydrometallurgy consists in the following sequential stage (see Figure 1): dissolution or leaching (LX), solvent extraction (SX) and electrowinning (EW). The overall process of dissolution, solvent extraction and electrowinning is known as LX/SX/EW (for more details cf., v.g., [25]). In this thesis, the focus is on the leaching stage .

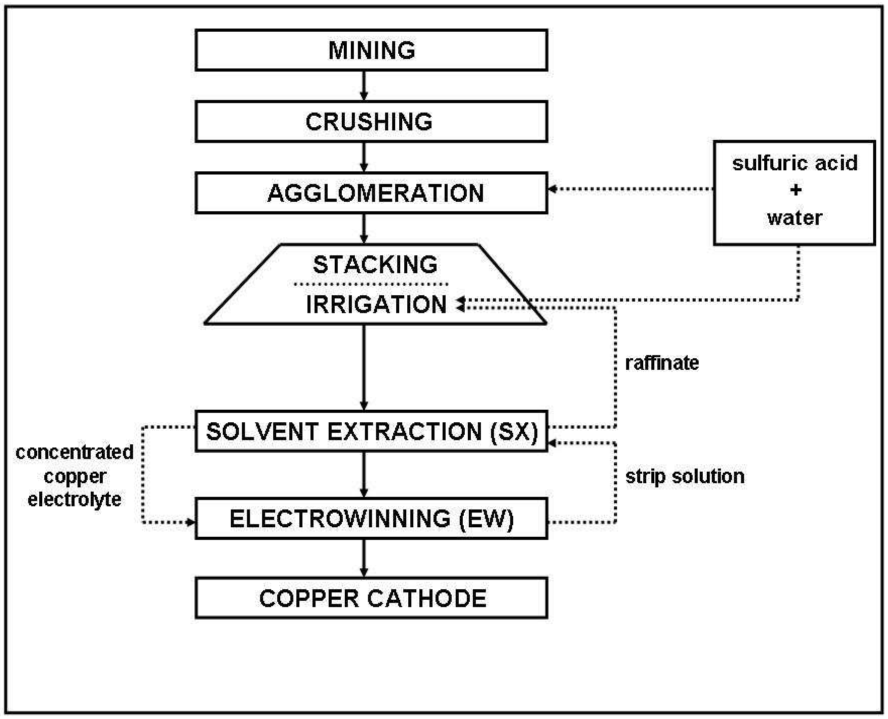

Figure 1. Recovery of copper by solvent extraction.

Leaching is a method of extraction in which a solvent is passed through a mixture to remove some desired substance from it. There are several types of leaching: heap leaching, vat leaching, dump leaching and in-situ leaching. In this thesis, the focus is on heap leaching process of copper ores.

Most companies, as a result of the favorable economics possible in heap leaching, consider heap leaching an alternative to conventional processing (flotation, agitation and vat leaching) [47]. This process is considered an integral part of most copper mining operations and should determine, along with other factors, the cutoff grade of the material sent to the mill.

Two distinct phenomena are of interest in the study of heap leaching: fluid flow (FF) and the physicochemical reactions (PR). These two phenomena can be studied separately if the extent of leaching of an element of solution that has participated in this process, and the extent of leaching that an element of the heap has undergone, does not influence the

solution flow pattern. In other words, the solution flow pattern in a heap depends only on the initial conditions of the heap. In general, researchers in heap leaching have separated the fluid flow problem from the physicochemical problem. Decoupling of the flow component from physicochemical one is possible only if the reaction is affecting neither the fluid properties (e.g. its viscosity), nor the local geometry of the medium (as it would happen in case of precipitation inside the pores of a crystal layer).
Copper ores usually contain a mixture of oxide and sulfide minerals. Oxide minerals are solubilized by acid solutions, whereas sulfide minerals are solubilized only under oxidizing conditions.
In this thesis both problems are considered, i.e., the FF and the PR problem. About the FF model proposed in this work, it is applicable to oxides and sulfide minerals of copper ores, and about the PR model proposed in this work, it is applicable to oxides minerals of copper ores.
In the following section the heap leaching process for copper ores is presented in the Porous Media Theory context.

1.2 The Porous Medium

Leaching can to be considered as a transfer process of mass between the leach solution (fluid phase) and the ore bed (solid phase) [25, 36]. Additionally, the heap leaching process can be considered as a two phase-compositional system in a porous medium. In effect, this work consider two fluid phases: the leach solution and the gaseous phase, and one static phase, the ore bed (cf. [14, 41]). This approach is applicable to oxides and sulfides minerals.

In this thesis, it is considered a simplified case of transport. En effect, the compositional model consider two component in liquid phase: sulfuric acid (H_2SO_4), as leaching agent, and copper (Cu), in liquid and solid phase (cf. [25, 39, 46]). This approach is applicable to oxides minerals which, in general terms, have the following chemical reaction of dissolution

$$MinOxCu_{(s)} + 2H^+_{(aq)} \rightarrow Cu^{2+}_{(aq)} + H_2O_{(l)},$$

where $MinOxCu_{(s)}$ represent a oxides minerals of copper, present in the ore. Therefore, this thesis consider a 2p2c model (cf. [30, 36]). On the other hand, a component can be transferred from one phase into another by the change of the thermodynamic state (e.g., by vaporization, condensation, dissolution, etc.). This phenomenon is called *phase transition*, Figure 2 illustrates the occurring phase transitions in the 2p2c model (two phase, two component) (cf. [36]).

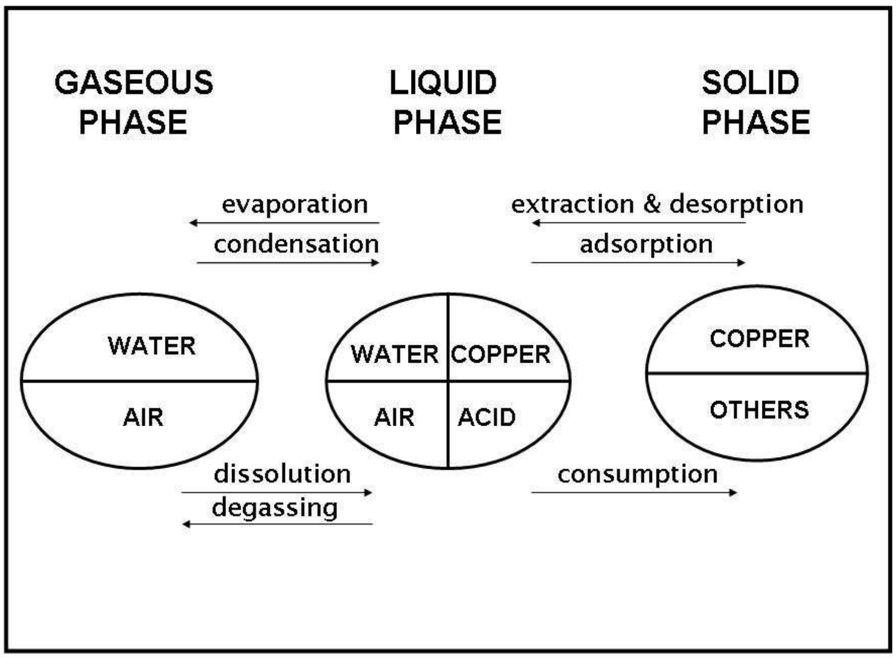

Figure 2. Phase transitions.

Let a REV (*representative elementary volume*) (see [30] for more details) in the porous medium formed by the solid matrix and both fluids phases: liquid and gaseous. The porosity of the porous medium is defined as

$$\phi(\mathbf{x}, t) := \frac{\text{volume of the pore space within the REV}}{\text{volume of REV}},$$

and the saturation of phase α is defined as

$$s_\alpha(\mathbf{x}, t) := \frac{\text{volume of fluid } \alpha \text{ within the REV}}{\text{volume of the pore space within the REV}},$$

where $\alpha \equiv w$ is the liquid phase and $\alpha \equiv n$ is the gaseous phase. It is imposed the customary property that the fluids fill the volume:

$$s_w + s_n = 1. \tag{1.2.1}$$

In order to simplify the model, it is considered a two phase flow through a porous medium with the following assumptions (see [39] for specific details):

- Flow occurs in a vertical plane 2D.
- Generalized Darcy's law for multiphase flow is valid.
- The porosity and the absolute permeability are uniform in space and constant with time.
- The porous medium is non-compressible, homogeneous and isotropic with respect to the transversal and longitudinal dispersivity coefficients.
- In the void space there are only two fluids phases: the liquid phase (leach solution) and the gaseous phase.
- The reaction between the acid and the particles of copper minerals proceeds in an instantaneous fashion and is irreversible.
- The system is isothermal.
- The regime of flow is laminar.
- The physical properties of liquid phase are constants.
- The effect of the transport of solutes on the transport of fluid is weak.

In the following section, specifically, the FF model is presented.

1.3 Two Phase Flow System

In this thesis, as mathematical domain, it is considered a 2D geometry, i.e, a transversal cut of the heap (Figure 1). The boundary of $\Omega \subset \mathbb{R}^2$, i.e., $\partial\Omega$ is expressed as $\partial\Omega = \Gamma^i \cup \Gamma^o \cup \Gamma^l \cup \Gamma^r$, where Γ^i is the input boundary (zone of irrigation), Γ^o is the output boundary (zone of drainage), Γ^l is the left boundary, Γ^r is the right boundary.

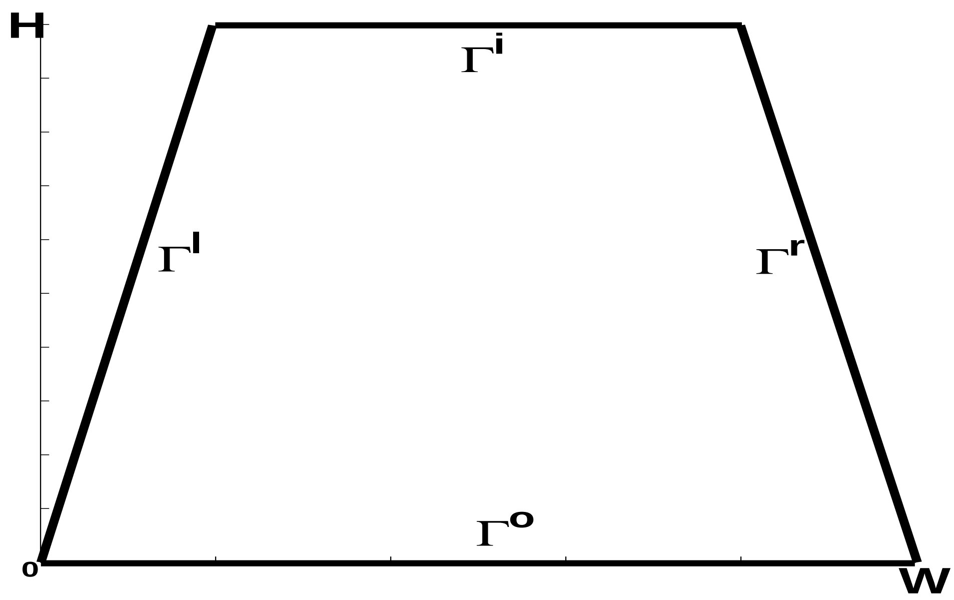

Figure 3. Mathematical domain.

The continuity equations (cf. [5] or [30]) for each phase $\alpha = w, n$ are derived from the mass balance in the REV:

$$\frac{\partial(\phi \rho_\alpha s_\alpha)}{\partial t} + div(\rho_\alpha \mathbf{v}_\alpha) = r_\alpha, \tag{1.3.1}$$

where ϕ is the porosity of the porous medium, ρ_α ,s_α, $\mathbf{v}_\alpha$, are the density, saturation, pressure, volumetric velocity of the α-phase, and r_α is the source term (by assumption: $r_\alpha = 0$, $\alpha = w, n$). As in the single-phase case, it can be shown by volume averaging or homogenization techniques that the macroscopic phase velocity can be expressed in terms of the macroscopic phase pressure by the generalized Darcy law

$$\mathbf{v}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha}\mathbf{K} \cdot (\nabla p_\alpha - \rho_\alpha \mathbf{g}), \tag{1.3.2}$$

where $\mathbf{K}$ is the absolute permeability of the porous systems, p_α, μ_α, $k_{r\alpha}$ are the pressure, viscosity and the relative permeability of the α-phase, and $\mathbf{g}$ is the gravitational, downward-pointing, constant vector. Therefore, (1.3.1) and (1.3.2) are the two-phase flow equations. The pressure at the microscopic level has a jump discontinuity when passing from one fluid phase to the other. The jump is called the *capillary pressure*. This fact is reflected by a macroscopic capillary pressure at the macroscopic level:

$$p_c(\mathbf{x},t) = p_n(\mathbf{x},t) - p_w(\mathbf{x},t).$$

The macroscopic consideration of the capillarity results in the following capillary pressure-saturation relation: $p_c(\mathbf{x},t) = f(s_w, s_n)$, but $s_w + s_n = 1$, therefore p_c is given by:

$$p_c(s_w) = p_n - p_w. \tag{1.3.3}$$

With constrains (1.2.1) y (1.3.3), equations (1.3.1) y (1.3.2), represent a coupled dynamic system of differential equations, which describes the simultaneous flow of two immiscible fluids in a variable saturation porous medium. The behavior of the system of equations is strongly nonlinear because there is a nonlinear dependence of the saturation on the capillary pressures and on the relative permeability.

1.4 Compositional Flow Model

General Mass Balance

A mass balance must be specified for each component. The mass balance equations for the transport of component κ in α-phase can be written as [3, 30]:

$$\frac{\partial\left(\theta_\alpha c_\kappa^\alpha\right)}{\partial t} + \nabla\cdot\left(c_\kappa^\alpha \mathbf{v}_\alpha - \mathbf{D}(\mathbf{v}_\alpha)\nabla c_\kappa^\alpha\right) + \Phi_\alpha = 0, \tag{1.4.1}$$

where c_κ^α is the volumetric concentration defined by

$$c_\kappa^\alpha := \frac{\text{mass of component } \kappa \text{ in phase } \alpha}{\text{volume of phase } \alpha},$$

$\theta_\alpha := \phi s_\alpha$, is the liquid content, $\mathbf{v}_\alpha$ is the *Darcy's flow of phase* α, Φ_α $[kg/m^3\cdot s]$ is the irreversible rate of solute removed (or added) from (to) the liquid solution, $\mathbf{D}$ is the dispersity-diffusion tensor given by

$$D_{ij} := \alpha_L \left|\mathbf{v}_\alpha\right| \delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{\left|\mathbf{v}_\alpha\right|} + D_m \delta_{ij},$$

where α_L and α_T are the longitudinal and transverse dispersities, respectively, $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$, and D_m is the molecular diffusion coefficient (in this thesis $D_m = 0$). In the case of sorption, (3.2.1) is modified to include a retardation factor.
On the other hand, if is assumed that there is a isotherm between the liquid phase and the solid phase $\varphi_\kappa^\alpha = \varphi_\kappa^\alpha(c_\kappa^\alpha)$, defined as

$$\varphi_\kappa^\alpha := \frac{\text{mass of component in solid phase}}{\text{mass solid phase}},$$

then (using the assumption that sorption only occurs from the liquid to the solid phase), the equation for the liquid phase can be modified to include adsorption:

$$\frac{\partial\left(\phi_s \rho_s \varphi_\kappa^\alpha\right)}{\partial t} + \frac{\partial\left(\theta_\alpha c_\kappa^\alpha\right)}{\partial t} + \nabla \cdot \left(c_\kappa^\alpha \mathbf{v}_\alpha - \mathbf{D}(\mathbf{v}_\alpha)\nabla c_\kappa^w\right) + \Phi_\alpha = 0, \tag{1.4.2}$$

where $\phi_s := 1 - \phi$, ρ_s is ore bulk density. For example, the Freundlich linear equilibrium isotherm is given by $\varphi_\kappa^\alpha := \varphi_\kappa^\alpha(c_\kappa^\alpha) = k_d c_\kappa^\alpha$, where $k_d[m^3/kg]$ is an equilibrium distribution constant that is to be determined experimentally.

Basic Chemical Reaction

In this thesis the compositional model consider two component: sulfuric acid (H_2SO_4) in liquid phase, as leaching agent, and copper (Cu) in liquid and solid phase. This approach is applicable to oxides minerals which, in general terms, have the following chemical reaction of dissolution (cf. [25, 39, 46]),

$$MinOxCu_{(s)} + 2H^+_{(aq)} \rightarrow Cu^{2+}_{(aq)} + H_2O_{(l)},$$

where $MinOxCu_{(s)}$ represent a oxides minerals of copper, present in the ore.

Remark 1.4.1 *For this Basic Chemical Reaction defined is enough to consider a not saturated flow. That is, about the fluid flow problem is enough to solve the Richard's equation (make p_n equal to a constant on $\Omega \times (0,T)$ in the two phase flow system (2.2.1)-(2.2.6).*

Sulfuric acid transport equation

During migration through the porous media (heap) sulfuric acid reacts with the different contained minerals, copper included. This reaction is an irreversible process that gives rise to a consumption (neutralization) of the acid present in the liquid solution. Acid consumption is assumed to be proportional to its concentration (μc_a^w in (3.2.3)). Additionally, and following [46], it is considered an adsorption/desorption phenomenon, which is modeled using a equilibrium isotherm ($\varphi_a^w(c_a^w)$. Therefore, from (3.2.1) with $\Phi_\alpha := \theta_w \mu c_a^w$, the transport equation of sulfuric acid in leach solution is given by

$$\frac{\partial(\phi_s \rho_s \varphi_a^w(c_a^w))}{\partial t} + \frac{\partial(\theta_w c_a^w)}{\partial t} + \nabla \cdot (c_a^w \mathbf{v}_w - \mathbf{D}(\mathbf{v}_w)\nabla c_a^w) + \theta_w \mu c_a^w = 0, \tag{1.4.3}$$

where μ is a first-order reaction constant (consumption factor) and c_a^w is the volumetric concentration of sulfuric acid in leach solution.

Copper transport equation in liquid phase

The transport of copper ions through the heap is mainly governed by two processes. The first process consists of a chemical reaction that occurs between the leaching agent and the mineral particles. The copper present in the ore is solubilized passing from the solid to the liquid phase. The kinetic involved is a the first order ($\rho_s k_e c_a^w c_c^s$ in (3.2.4)) heterogeneous reaction. Therefore, the first process is extraction of copper from the solid phase to the liquid phase. The second process in the copper adsorption/desorption phenomenon, which is modeled using a equilibrium isotherm ($\varphi_c^w(c_c^w)$ in (3.2.4)). Therefore, from (3.2.2) with $\Phi_\alpha := \phi_s \rho_s k_e c_a^w c_c^s$, the transport equation of copper in leach solution is given by

$$\frac{\partial(\phi_s \rho_s \varphi_c^w(c_c^w))}{\partial t} + \frac{\partial(\theta_w c_c^w)}{\partial t} + \nabla \cdot (c_c^w \mathbf{v}_w - \mathbf{D}(\mathbf{v}_w)\nabla c_c^w) - \theta_w \rho_s k_e c_a^w c_c^s = 0, \tag{1.4.4}$$

where k_e is a first-order kinetic constant, c_c^s is the concentration of copper associated with the solid phase (cf.(3.2.5)) and c_c^w is the volumetric concentration of copper in leach solution.

Copper transport equation in solid phase

The change in the concentration of copper in the solid phase follows the mass balance

[39]:

$$\frac{\partial c_c^s}{\partial t} + \theta_w k_e c_a^w c_c^s = \frac{\partial(\phi_s \varphi_c^w(c_c^w))}{\partial t}, \tag{1.4.5}$$

where c_c^s is the concentration of copper in solid phase, *i.e.*,

$$c_c^s := \frac{\text{mass of copper in solid phase}}{\text{mass of solid phase}}.$$

Therefore, the compositional flow model considered in this thesis, consists in to find functions c_a^w, c_c^w and c_c^s, such that (3.2.3), (3.2.4), (3.2.5), respectively.

1.5 The Decoupled Approach

The decoupled approach consists in to solve the *fluid flows* and *transport problems* in decoupled and sequential form. Specifically,

1. **Two Phase Flow Problem**.
   To solve the system formed by the equations (1.3.1), (1.3.2), (1.3.3) and (1.2.1), (or the Richard's equation (make p_n equal to a constant on $\Omega \times (0, T)$ in the two phase flow system (2.2.1)-(2.2.6)) in the oxides minerals case).

2. **Transport Problem**.
   (a) To solve the equation (3.2.3).
   (b) To solve the system formed by the equations (3.2.4)-(3.2.5).

The numerical analysis of Two Phase Problem is performed in Chapter 2, and the numerical analysis of Transport Problem is performed in Chapter 3. For both problems, several computational experiments are reported in Chapter 4. Finally, in Chapter 5 (in spanish) you can find a general discussion.

Chapter 2

Two Phase Flow Problem

In this chapter it is described error estimates for finite element approximation for partial differential systems which describe two-phase immiscible flows in porous media, with applications to heap leaching of copper ores. These approximations are based on mixed finite element (MFE) methods for pressure and velocity and finite volume (FV) for saturation. Incompressible fluids are considered.

2.1 Introduction

In this chapter it is considered the fluid flow problem only. It is used the classical two-phase flow equations, which can be rewritten in different differential formulations so that the coupling and nonlinearity are weakened. These formulations include, for example, phase, global, and weighted formulations. It is considered the global formulation, specifically, the fractional flow formulation for two-phase immiscible and incompressible fluids. It is well known that physical transport dominates diffusive effects in two-phase flow in porous media. Hence, it is important to obtain accurate approximate fluid velocities. This motivates the use of mixed finite element methods for the computation of pressure and velocity, in equations (2.2.12) and (2.2.13). Also, due to the convection-dominated feature of equation (2.2.14), efficient and accurate approximations methods should be used to solve this equation. In this thesis finite volume method is utilized for the calculation of the saturation of leaching solution in equation (2.2.14), which is capable to resolve shock fronts in a proper manner.

MFE-FV scheme for two phase flow problems were proposed in [26] and [44], but without any convergence results. Convergence results for system (2.2.12)-(2.2.14), when $f_w(s) \equiv s$, $\phi = 1$, $D_w(s) \equiv \epsilon > 0$, $G_w(s) \equiv 0$, $\varphi_1 \equiv 0$ and $s(\mathbf{x}, t) = 0, \mathbf{x} \in \Gamma, t > 0$ were proved in [40]. A fully discrete finite element analysis of multiphase flow in groundwater hydrology was given in [22] for a fractional flow formulation of system (2.2.1)-(2.2.6), in the case when ρ_w is constant and $\rho_n = \rho_n(p)$, with p global pressure. An error estimates for finite approximations of system (2.2.12)-(2.2.14), which are based on MFE methods for pressure and velocity and characteristic finite element methods for saturation was proved in [21]. A procedure which consisted in a MFE method for pressure equation and an upwind scheme was considered in [15]. It is based on a discontinuous finite element approximation associated with a slope limiter for saturation equation. In degenerate cases, i.e., when $D_w(s) = 0$, for some $s \in [0, 1]$ in equation (2.2.14), the authors of [20] consider a finite element approximation where the elliptic equation for the pressure and velocity is approximated by a mixed finite element method, while the degenerate parabolic equation for the saturation is approximated by a Galerkin finite element method. In [38] the author prove the convergence of a numerical method which combines an upwind time implicit finite volume scheme for the saturation equation (hyperbolic-parabolic type) and a centered finite volume scheme for the Chavent global pressure equation (elliptic type). Additionally, the author study the case when the diffusion term in the saturation equation is weakly degenerated. In [4] the authors formulate discontinuous Galerkin methods for the numerical computation of incompressible two-phase flow in porous media.

A more detailed and extensive review of different numerical methods for classical two phase equations, for immiscible and incompressible flow, can be found in [15], in the reservoir simulation context, and in [30], in the environmental engineering context.

In this chapter it is obtained an rigorous proof of convergence for system (2.2.12)-(2.2.14), when $D_w(s) \equiv D > 0$. This is done by proving an a priori error estimate. The proof follows the main ideas of [40]. But, additionally, the model consider a nonlinear convective term and a nonlinear gravitational term, which is very important in heap leaching, because

the flow is mainly vertical. In contrast to [40], the problem consider non homogeneous Neumann boundary conditions, which corresponds to the physical behavior of irrigation and infiltration process in Heap Leaching. Finally, it is obtained numerical results, with realistic parameters from copper industry in Chile.
The chapter is organized as follows. In section 2.2, it is stated the continuous problem. In section 2.3 it is stated the discrete problem. In section 2.4 it is presented the main results of this work. In section 2.5 it is developed some preliminary results, which will be very useful in the convergence analysis. In section 2.6 it is proved the convergence of the semi discrete scheme. Finally, in section 2.7 it is proved the convergence of the full discrete scheme.

2.2 Statement of the continuous problem

In this section it is presented the classical two phase, immiscible and incompressible flow equations for the fluid flow problem in the context of Heap Leaching. Next, it is defined a fractional flow formulation, for degenerate and non degenerate case in the weak form. Finally, it is defined a model problem for the convergence analysis.

2.2.1 Physical Problem

The flow equations of two-phase immiscible fluids in a porous media $\Omega \subset \mathbb{R}^2$, are given by equations (1.3.1), (1.3.2), (1.3.3), and (1.2.1), i.e.,

$$\begin{aligned}
\frac{\partial(\phi\rho_w s_w)}{\partial t} + \nabla\cdot(\rho_w \mathbf{v}_w) &= \rho_w q_w,\\
\frac{\partial(\phi\rho_n s_n)}{\partial t} + \nabla\cdot(\rho_n \mathbf{v}_n) &= \rho_n q_n,\\
\mathbf{v}_w &= -\frac{k_{rw}}{\mu_w}\mathbf{K}\cdot(\nabla p_w - \rho_w \mathbf{g}),\\
\mathbf{v}_n &= -\frac{k_{rn}}{\mu_n}\mathbf{K}\cdot(\nabla p_n - \rho_n \mathbf{g}),\\
p_c(s_w) &= p_n - p_w,\\
s_w + s_n &= 1.
\end{aligned}$$

In particular, in the context of heap leaching, the porosity ϕ is assumed constant, and the densities ρ_w and ρ_n are constants, there are no source terms $q_w = q_n = 0$, and $\mathbf{K} = kI$. Therefore, the Physical Problem for the fluid flow in heap leaching process is defined by

$$\phi\frac{\partial s_w}{\partial t} + \nabla\cdot\mathbf{v}_w = 0, \tag{2.2.1}$$

$$\phi\frac{\partial s_n}{\partial t} + \nabla\cdot\mathbf{v}_n = 0, \tag{2.2.2}$$

$$\mathbf{v}_w = -k\frac{k_{rw}}{\mu_w}(\nabla p_w - \rho_w \mathbf{g}), \tag{2.2.3}$$

$$\mathbf{v}_n = -k\frac{k_{rn}}{\mu_n}(\nabla p_n - \rho_n \mathbf{g}), \tag{2.2.4}$$

$$p_c(s_w) = p_n - p_w, \tag{2.2.5}$$

$$s_w + s_n = 1, \tag{2.2.6}$$

plus the initial and boundary conditions

$$
\begin{array}{rclcll}
s_w(\mathbf{x},t) & = & s_w^o & , & \mathbf{x}\in\Omega, & t=0,\\
p_n(\mathbf{x},t) & = & p_A & , & \mathbf{x}\in\Omega, & t=0,\\
(\mathbf{v}_w\cdot\mathbf{n})(\mathbf{x},t) & = & -R & , & \mathbf{x}\in\Gamma^i, & t>0,\\
(\mathbf{v}_w\cdot\mathbf{n})(\mathbf{x},t) & = & 0 & , & \mathbf{x}\in\Gamma^r\cup\Gamma^l, & t>0,\\
(\nabla p_w\cdot\mathbf{n})(\mathbf{x},t) & = & 0 & , & \mathbf{x}\in\Gamma^o, & t>0,\\
(\nabla s_n\cdot\mathbf{n})(\mathbf{x},t) & = & 0 & , & \mathbf{x}\in\Gamma^r\cup\Gamma^l\cup\Gamma^i, & t>0,\\
(\mathbf{v}_n\cdot\mathbf{n})(\mathbf{x},t) & = & 0 & , & \mathbf{x}\in\Gamma^o, & t>0,
\end{array}
\tag{2.2.7}
$$

where, as usual, $\mathbf{n}$ is the unit normal vector to $\partial\Omega$, outward to Ω, s_w^o is the initial saturation, p_A is the atmospheric pressure and $R(t)\geq 0$ is the irrigation ratio.
In what follows w will be omit in s_w.

2.2.2 Fractional Flow Formulation

Equations (2.2.1)-(2.2.6) can be rewritten in a different differential formulations so that the coupling and nonlinearity are weakened. This thesis follows the fractional flow formulation [15], i.e., a formulation in terms of a saturation and a global pressure. The main reason for this fractional flow approach is that efficient numerical methods can be devised to take advantage of many physical properties inherent in to flow equations [22]. Now it is introduced the phase mobilities $\lambda_\alpha(s):=\frac{k_{r\alpha}}{\mu_\alpha},\ \alpha=w,n$, the total mobility $\lambda(s):=\lambda_w+\lambda_n$, the fractional flow functions $f_\alpha(s):=\frac{\lambda_\alpha}{\lambda},\ \alpha=w,n$, and the total velocity $\mathbf{u}:=\mathbf{v}_w+\mathbf{v}_n$. Adding (2.2.1) and (2.2.2), and using (2.2.6), it is obtained $\nabla\cdot\mathbf{u}=0$. Additionally, following [15], it is defined the global pressure

$$
p:=p_n-\int_0^s(f_wp_c')(\mathbf{x},\xi)d\xi, \tag{2.2.8}
$$

noting that $\nabla p=\nabla p_n-f_w\nabla p_c$.

Weakly Degenerate Formulation

Summing (2.2.3) and (2.2.4), and using the gradient computation in (2.2.8), it is obtained for the total velocity

$$\mathbf{u} = \mathbf{v}_w + \mathbf{v}_n = -k\lambda(\nabla p - G_\lambda \mathbf{g}) \tag{2.2.9}$$

where $G_\lambda := \frac{\lambda_w \rho_w + \lambda_n \rho_n}{\lambda}$. On the other hand, manipulating equations (2.2.3) and (2.2.4), it is obtained $\lambda_n \mathbf{v_w} - \lambda_w \mathbf{v_n} = \lambda_n \lambda_w (\nabla p_c + (\rho_w - \rho_n)\mathbf{g})$, and using (2.2.8), it is deduced

$$\mathbf{v_w} = f_w(s)\mathbf{u} - D_w(s)\nabla s - G_w(s)\mathbf{g}, \tag{2.2.10}$$

$$\mathbf{v_n} = f_n(s)\mathbf{u} - D_n(s)\nabla s + G_n(s)\mathbf{g}, \tag{2.2.11}$$

where

$$D_w(s) := -k\lambda_n(s) f_w(s) p_c'(s) \quad G_w(s) := -k\lambda_n(s) f_w(s)(\rho_w - \rho_n)$$
$$D_n(s) := -k\lambda_w(s) f_n(s) p_c'(s) \quad G_n(s) := -k\lambda_w(s) f_n(s)(\rho_w - \rho_n).$$

Therefore, collecting (2.2.9) and (2.2.10), it is defined an alternative formulation for the system (2.2.1)-(2.2.6) which is called Fractional Flow Formulation

$$\nabla \cdot \mathbf{u} = 0, \tag{2.2.12}$$

$$\mathbf{u} = -k\lambda(s)(\nabla p - G_\lambda(s)\mathbf{g}), \tag{2.2.13}$$

$$\phi \frac{\partial s}{\partial t} + \nabla \cdot (f_w(s)\mathbf{u} - D_w(s)\nabla s - G_w(s)\mathbf{g}) = 0, \tag{2.2.14}$$

in the unknowns $\mathbf{u}$, p, and s, with initial and boundary conditions given by

$$\begin{array}{rclcll} s(\mathbf{x},t) & = & s_w^o & , & \mathbf{x}\in\Omega, & t=0, \\ p(\mathbf{x},t) & = & p_o & , & \mathbf{x}\in\Omega, & t=0, \\ (\mathbf{u}\cdot\mathbf{n})(\mathbf{x},t) & = & \varphi_1(s(\mathbf{x},t)) & , & \mathbf{x}\in\Gamma, & t>0, \\ (\mathbf{v}_w\cdot\mathbf{n})(\mathbf{x},t) & = & \varphi_2(s(\mathbf{x},t)) & , & \mathbf{x}\in\Gamma, & t>0, \end{array} \tag{2.2.15}$$

where the functions φ_1 and φ_2 are know from previous expressions.

Remark 2.2.1 *Note that the equation (2.2.14) is parabolic and weakly degenerate, because $D_w(s_{wr}) = 0$ and $D_w(1) = 0$, where s_{wr} is the residual saturation for the liquid* *phase. There is a large amount of literature written on degenerate parabolic problems, as (2.2.14). Same theoretical results about existence and uniqueness can be found in [1] and [42], for example. Furthermore, convergence results for different numerical discretization schemes are also available (cf. [43], for example). However, none of this papers are including the gravity term, or dealing with the fractional flow formulation. By another hand, the authors of [20] and [22], for example, studied the degenerate case for the fractional flow formulation. Finally, it is mentioned that in this Chapter the degenerate case is not considered.*

Non-Degenerate Formulation

Rather than a saturation, a complementary pressure was introduced in [18]. In this form, the system formally appears to be non-degenerate. In effect, the complementary pressure, i.e., the Kirchhoff Transformation, is defined as

$$\theta := -\int_0^s (\lambda_n f_w p_c^{'})(\mathbf{x}, \xi) d\xi, \tag{2.2.16}$$

where s is related to θ through $s = \mathcal{S}(\theta)$, where $\mathcal{S}(\mathbf{x}, \theta)$ is the inverse of (2.2.16) for $0 \leq \theta \leq \theta^*$ with $\theta^*(\mathbf{x}) := -\int_0^1 \lambda_n f_w p_c^{'}(\mathbf{x}, \xi) d\xi$.

Remark 2.2.2 *Note that the transformation (2.2.16) has successfully been employed for both the analysis of degenerate problems, as well as for deriving appropriate numerical schemes, v.g., cf. [1] and [42].*

From this definition it is obtained alternatives expressions for $\mathbf{u}$, $\mathbf{v}_w$ and $\mathbf{v}_n$, given by

$$\begin{aligned}
\mathbf{u} &= -k(\lambda(s)\nabla p + \gamma_1^{'}(s)), \\
\mathbf{v}_w &= -k(\nabla\theta + \lambda_w(s)\nabla p + \gamma_2^{'}(s)) = f_w(s)\mathbf{u} - k\nabla\theta - k\gamma_2(s), \\
\mathbf{v}_n &= k(\nabla\theta - \lambda_n(s)\nabla p + \gamma_3^{'}(s)),
\end{aligned}$$

where the definition of $\gamma_i^{'}, i = 1, 2, 3$ and γ_2 can be found in [18] and [20]. Therefore, it is obtained an non-degenerate alternative formulation for system (2.2.1)-(2.2.6) given by

$$\nabla \cdot \mathbf{u} = 0, \tag{2.2.17}$$

$$\mathbf{u} = -k(\lambda \nabla p + \gamma_1^{'}), \tag{2.2.18}$$

$$\phi \frac{\partial s}{\partial t} + \nabla \cdot (f_w(s)\mathbf{u} - k\nabla\theta - k\gamma_2(s)) = 0, \tag{2.2.19}$$

in the unknowns $\mathbf{u}$, p, and θ, with the initial and boundary conditions similar to (2.2.15). The differential system has a clear structure; the pressure equation is elliptic for p and the saturation equation is parabolic for θ (degenerate for s).

2.2.3 Weak Formulation

Let the spaces $\mathbf{V}(g)$, W and M be defined as $\mathbf{V}(g) := \{\mathbf{v} \in H(div; \Omega) | \mathbf{v} \cdot \mathbf{n} = g, \partial\Omega\}$, $W := \{v \in L^2(\Omega) | \int_\Omega v(\mathbf{x}, t) d\mathbf{x} = 0\}$ and $M := H^1(\Omega)$. Additionally, let the bilinear forms A and B be defined as $A(\xi; \mathbf{v}, \mathbf{w}) = \int_\Omega a(\xi)\mathbf{v}\cdot\mathbf{w}$ and $B(\mathbf{v}, \varphi) := -\int_\Omega \varphi \nabla\cdot\mathbf{v}$. It is introduced the weak form of the system (2.2.17)-(2.2.19): find $\mathbf{u} \in L^\infty(J; V(\varphi_1))$, $p \in L^\infty(J; W)$, and $\theta \in L^2(J; M)$, such that, $s = \mathcal{S}(\theta)$, $\phi\partial_t s \in L^2(J; M^{'})$, $0 \le \theta(\mathbf{x}, t) \le \theta^*(\mathbf{x})$ a.e. on Ω_T,

$$B(\mathbf{u}, v) = 0, \forall v \in L^\infty(J; W), \tag{2.2.20}$$

$$A(s; \mathbf{u}, \mathbf{v}) + B(\mathbf{v}, p) = (\gamma_1(s), \mathbf{v}), \forall \mathbf{v} \in L^\infty(J; V(0)), \tag{2.2.21}$$

$$\int_0^t (\phi\partial_t s, v) d\tau + \int_0^t (\mathbf{v}_w, \nabla v) d\tau = -\int_0^t (\varphi_2(s), v)_\Gamma \tau, \forall v \in L^2(0, t; M), t \in J, \tag{2.2.22}$$

where $a(s) := (k\lambda(s))^{-1}$ and $\gamma_1(s) := -\gamma_1^{'}(s)/\lambda(s)$.

EXISTENCE

Under the assumptions (A1)-(A10) defined in [18], the system (2.2.17)-(2.2.19) has a weak solution in the weak sense of (2.2.20)-(2.2.22), (cf. Theorem 2.1 in [18]).

UNIQUENESS

If in addition to assumptions (A1)-(A11) defined in [18], the total pressure satisfies that exists a constant $C > 0$ such that $|p(x_1, t) - p(x_2, t)| \le C|x_1 - x_2|$, for all $x_1, x_2 \in \Omega$ and for all $t \in J$, then the weak solution is unique (cf. Theorem 3.1 in [18]).

2.2.4 Model Problem for Convergence Analysis

In Heap Leaching it is physically reasonable to assume that there exits a *residual saturation* s_{wr}, an *initial saturation* s_w^o, and a *saturation of stability* s_w^e of the leaching solution, such that the capillary diffusion coefficient D_w in (2.2.14), satisfies $D_w(s_{wr}) = D_w(1) = 0$ and $D_w(s) > 0$ on the interval $[s_w^o, s_w^e]$, and $D_w \in C^o([s_w^o, s_w^e])$, where $0 < s_{wr} < s_w^o < s_w^e < 1$. Therefore, for convergence analysis the system (2.2.12)-(2.2.14) is considered, when it is **not degenerate**, that is, it's assumed the interval $[s_w^o, s_w^e]$ for the saturation of liquid phase s.

Remark 2.2.3 *The assumed bounds on D_w are depending strongly on the model. In general, the lower bound is precisely 0, as encountered, for example, in the J-Leverett model for two phase flow. Assuming that the initial and boundary data are bounded uniformly away from the residual saturation s_{wr}, respectively s_w^e, and that the medium is homogeneous, then a maximum principle holds implying the same bounds for the solution. Otherwise the diffusivity D_w degenerates to 0. (Comment of Professor I.S.Pop).*

In order to simplify the convergence analysis it is replaced the nonlinear function D_w in (2.2.14) by the constant $D > 0$ defined as

$$D := \frac{1}{|s_w^e - s_w^o|} \int_{s_w^o}^{s_w^e} D_w(u)du.$$

Additionally, it is considered a vectorial function $\mathbf{d}$ such that $\mathbf{d}(s(\mathbf{x},t)) \cdot \mathbf{n} = \varphi_1(s(\mathbf{x},t)), \mathbf{x} \in \partial\Omega$, and define the new unknown $\mathbf{w}$ as $\mathbf{w} + \mathbf{d}(s(\mathbf{x},t)) = \mathbf{u}, \mathbf{x} \in \Omega, t > 0$. Then, the homogeneous Neumann boundary condition holds for $\mathbf{w}$. Also, let $\mathbf{e}$ be a vectorial function such that $\mathbf{e}(s(\mathbf{x},t)) \cdot \mathbf{n} = \varphi_2(s(\mathbf{x},t)), \mathbf{x} \in \partial\Omega$, and define the a new unknown $\mathbf{u}_w$ as $\mathbf{u}_w + \mathbf{e}(s(\mathbf{x},t)) = \mathbf{v}_w, \mathbf{x} \in \Omega, t > 0$. Then the homogeneous Neumann boundary condition holds for $\mathbf{u}_w$. Now, it is considered this *simplifications* in the system (2.2.12)-(2.2.14) with (2.2.15) to obtain the Model Problem for the convergence analysis maintaining the notation $\mathbf{u}$ for the total velocity.

Definition 2.2.1 *Let $\Omega \subset \mathbb{R}^2$ be a convex polygonal bounded domain, $J := (0,T)$ a time interval and $\Omega_T := \Omega \times J$. A mapping $(\mathbf{u}, p, s) : \Omega_T \longrightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R}^2$ is called a Strong*

Solution (in the classical sense) of the model problem if for all $(\mathbf{x}, t) \in \Omega_T$*:*

$$\nabla \cdot \mathbf{u} = -F(s), \tag{2.2.23}$$

$$\mathbf{u} = -a(s)(\nabla p - \mathbf{G}(s)), \tag{2.2.24}$$

$$\frac{\partial s}{\partial t} + \nabla \cdot (f_w(s)\mathbf{u} - D\nabla s) = Q(s), \tag{2.2.25}$$

where $a(s) := k\lambda(s)$*. The initial and boundary conditions are given by*

$$\begin{array}{rcll} s & = & s^o & , \quad \mathbf{x} \in \Omega, \quad t = 0, \\ p & = & p_o & , \quad \mathbf{x} \in \Omega, \quad t = 0, \\ \mathbf{u} \cdot \mathbf{n} & = & 0 & , \quad \mathbf{x} \in \Gamma, \quad t > 0, \\ (f_w(s)\mathbf{u} - D\nabla s) \cdot \mathbf{n} & = & 0 & , \quad \mathbf{x} \in \Gamma, \quad t > 0. \end{array} \tag{2.2.26}$$

Remark 2.2.4 *About the Model Problem,*

1. *For the porosity it's assumed, without loss of generality, that* $\phi = 1$*.*
2. *About the gravitational term* $G_w(s)\mathbf{g}$*, this will be considered at the end of this chapter.*

Remark 2.2.5 *Let us state the following assumptions,*

(A1) Ω *is a bounded open polygonal subset of* $\mathbb{R}^2$*.*

(A2) There exits real numbers $\{s_{wr}, s_w^o, s_w^e\}$*, such that,* $0 < s_{wr} < s_w^o < s_w^e < 1$*,* $D_w(s_{wr}) = D_w(1) = 0$*,* $D_w \in C^o([s_w^o, s_w^e])$ *and* $D_w(s) > 0$ *on* $[s_w^o, s_w^e]$*.*

(A3) $a, F, Q \in L^\infty([s_w^o, s_w^e])$*.*

(A4) $\mathbf{G} \in L^\infty([s_w^o, s_w^e])$*.*

(A5) f_w *is Lipschitz continuous with constant* $K_{f_w} > 0$*.*

(A6) $f_w, f_w^{'} \in L^\infty([s_w^o, s_w^e])$*.*

(A7) $f_w(0) = 0$*.*

(A8) $Q \in L^2(\Omega)$.

(A9) $a, F, \mathbf{G}$ *are Lipschitz continuous.*

(A10) About the Peclet number Pe (cf. [5]), it is assumed that, there exits a constant $C > 0$*, such that*

$$Pe := \frac{||\mathbf{u}||_{L^\infty(J;L^\infty(\Omega))}}{D} \leq C, \tag{2.2.27}$$

where the constant $C > 0$*, is independent of* h*, and depends on the regularity of the mesh and on the constant* $K_{f_w} > 0$ *defined in (A5). For a detailed justification of this hypothesis, please to see Remark 2.5.2, and the proof of Theorem 2.6.2.*

Remark 2.2.6 *Additionally to assumptions (A1)-(A10), it is mentioned that the functions* s *and* $\mathbf{u}$ *defined in the Model Problem have the enough regularity, such that* $\nabla s \in L^\infty(\Omega_T)$*,* $\mathbf{u} \in L^\infty(\Omega_T)$*,* $\partial_t \mathbf{u} \in L^\infty(\Omega_T)$*,* $\partial_{tt} s \in L^2(\Omega)$*, and* $\partial_t s \in H^2(\Omega)$*, are satisfied. For a full analysis of regularity to see [18] and [19]. Note that this results are in general not true in the degenerate case.*

2.3 Statement of the discrete problem

2.3.1 Notation

It is follow a classical notation for unstructured grid for VF and MFE-VF methods used previously in [40, 31, 35]. Let $\mathcal{T}_h := \{T_i \mid \text{is a triangle}, i \in I \subset \mathbb{N}\}$ be a unstructured triangulation with fineness h of a bounded domain $\Omega \subset \mathbb{R}^2$. It is assumed that the following properties are satisfied:

1. $\Omega = \bigcup_{T \in \mathcal{T}_h} T$.
2. For $T_i \neq T_j \in \mathcal{T}_h$ one and only one of the following properties hold: $T_i \bigcap T_j = \emptyset$ or $T_i \bigcap T_j =$ common node of T_i, T_j or $T_i \bigcap T_j =$ common edge of T_i, T_j.
3. $h := \sup_{T \in \mathcal{T}_h} diam(T) < \infty$.

4. For any angle θ of a triangle of $\mathcal{T}_h$, one has: $0 < \theta < \pi/2$.

5. There exits $\alpha_i > 0$, $\beta_i > 0$, $i = 1, 2$, and $h > 0$ such that $\forall T \in \mathcal{T}_h$ and for any edge S_a of the mesh, $\beta_1 h^2 \leqslant |T| \leqslant \beta_2 h^2$, and $\alpha_1 h \leqslant |S_a| \leqslant \alpha_2 h$, with S_a is an edge of T.

Additionally, it is used the following notation for the unstructured triangulation:

$|T_i|$: area of T_i,

$\mathbf{x}_i$: midpoint of the ambit of T_i,

N_j: set of neighbor triangles of T_j,

$\mathbf{n}_{ij}$: outward unit normal to T_i in direction T_j, $j \in N_j$,

$\mathcal{A}$: set of all edges of $\mathcal{T}_h$,

$d(\mathbf{x}_i, S_{ij})$: distance from $\mathbf{x}_i$ to the edge S_{ij}.

If $f(\cdot, t)$ is a piecewise continuous function on $\mathcal{T}_h$ and p, $\mathbf{u}$, s is a solution of the model problem, it is defined in addition for $(\mathbf{x}, t) \in \Omega_T$:

$$f_j = \frac{1}{T_j} \int_{T_j} f(\mathbf{x}, t) d\mathbf{x},$$

$s_j(t)$: a constant approximation (average value over one triangle) of $s(\cdot, t)$ on $T_j \in \mathcal{T}_h$,

$\mathbf{n}_a(t)$: unit normal to edge $a \in \mathcal{A}$ at time t, such that $\int_a \mathbf{u}(x, t) \cdot \mathbf{n}_a(t) d\sigma \geqslant 0$,

$T_a^{\pm}$: the neighbor triangle of a, such that $\mathbf{n}_a$ is the outer (inner) normal of $T_a^{\pm}$.

$s_a^+(t)$: the upstream choice of $s(\cdot, t)$ on the edge $a \in \mathcal{A}$,

$d_a := d(\mathbf{x}_a^+, a) + d(\mathbf{x}_a^-, a)$,

$\gamma_a := l(a)/d_a$, $\kappa := \min\limits_{a \in \mathcal{A}} \gamma_a$, and $\Upsilon := \max\limits_{a \in \mathcal{A}} \gamma_a$.

For any variable π, some times it is used $\pi_a^+ = \pi_{T_a^+}$ and $\pi_a^- = \pi_{T_a^-}$ in order to lighten the notation.

Furthermore, it is used the following notation,

$$J_h := \{t^n \in J \mid t^n = n\Delta t, \text{ with } n \in \{0, ..., M\}, \text{such that } M\Delta t = T\}$$
$$f^n(\mathbf{x}) := f(\mathbf{x}, t^n), \text{ for any function } f(\mathbf{x}, t).$$

For given discrete data s_i^n let the global function $s_h(\cdot, t_n)$ be defined as $s_i^n := s_h(\mathbf{x}, t^n)|_{T_i}$ for all $T_i \in \mathcal{T}_h$ and the global function $s \in L^2(\Omega)$ it is defined the interpolation $I_h(s)$ as:

$$I_h(s(\cdot, t))\Big|_{T_i} := s(\mathbf{x}_i, t) \text{ for all } T_i \in \mathcal{T}_h.$$

The corresponding finite dimensional subspace of $L^2(\Omega)$ is defined as:

$$l^2(\Omega) := \{v \in L^2(\Omega)|v|_T = const, \quad \forall T \in \mathcal{T}_h\}$$

with the norm $\|s_h\|^2_{l^2(\Omega)} := \sum_{T_j \in \mathcal{T}_h} |T_j| s_j^2$. Finally, let $[s_h]_a := s_a^+ - s_a^-$ be the jump of s_h over an edge $a \in \mathcal{A}$.

Remark 2.3.1 *If $(\mathbf{u}, p, s)$ is a sufficiently smooth solution of the model problem, then it is have, for all $T_j \in \mathcal{T}_h$,*

$$(\partial_t s)_j + (L(\mathbf{u})s)_j = (Q(s))_j, \tag{2.3.1}$$

where $L(\mathbf{u})s := \nabla \cdot (f_w(s)\mathbf{u} - D\nabla s)$.

2.3.2 The Mixed Finite Element Part

Let $\mathbf{V}_h$ and W_h finite dimensional subspaces of $\mathbf{V} := \mathbf{V}(0)$ and W, defined as

$$W_h := \{w_h \in W \ \mid \ w_h\big|_T = const, \quad \forall T \in \mathcal{T}_h\}$$

and $\mathbf{V}_h$ is a lowest order Raviart-Thomas space.

Definition 2.3.1 *For fixed $t \in J$ let $s_h(\mathbf{x}, t)$ be given. Then the mixed finite element scheme for the equations (2.2.23) and (2.2.24) is defined as: find $(\mathbf{u}_h(t), p_h(t)) \in \mathbf{V}_h \times W_h$, such that, for all $(\mathbf{v}_h, \varphi_h) \in \mathbf{V}_h \times W_h$:*

$$B(\mathbf{u}_h(t), \varphi_h) = (F(s_h(t)), \varphi_h) \tag{2.3.2}$$
$$A(s_h(t); \mathbf{u}_h(t), \mathbf{v}_h) + B(\mathbf{v}_h, p_h(t)) = (\mathbf{G}(s_h(t)), \mathbf{v}_h). \tag{2.3.3}$$

2.3.3 The Finite Volume Part

It is considered a cell centered finite volume scheme for the equation (2.2.25) with the IBC (2.2.26), in the unknown s, *i.e.*, the level of saturation of leaching's solution. For an arbitrary triangle $T_j \in \mathcal{T}_h$

$$\begin{aligned}
\partial_t s + \nabla \cdot (f_w(s)\mathbf{u} - D\nabla s) &= Q(s), \\
\frac{1}{T_j}\int_{T_j} \partial_t s d\mathbf{x} + \frac{1}{T_j}\int_{T_j} \nabla \cdot (f_w(s)\mathbf{u} - D\nabla s) d\mathbf{x} &= \frac{1}{T_j}\int_{T_j} Q(s) d\mathbf{x}, \\
\frac{1}{T_j}\int_{T_j} \partial_t s d\mathbf{x} + \frac{1}{T_j}\sum_{l\in N_j}\int_{S_{jl}} (f_w(s)\mathbf{u} - D\nabla s)\cdot \mathbf{n} d\sigma &= \frac{1}{T_j}\int_{T_j} Q(s) d\mathbf{x}.
\end{aligned}$$

From this last equality, it is defined the discrete relation (see [34])

$$(\partial_t s_h)_j + \frac{1}{T_j}\sum_{l\in N_j} F_{jl} = (Q(s_h))_j,$$

where $F_{jl}(\mathbf{u}, s_h) := g_{jl}(\mathbf{u}; s_{hj}, s_{hl}) - D\gamma_{jl}(s_{hl} - s_{hj})$, if $S_{jl} \cap \partial\Omega = \emptyset$, $F_{jl}(\mathbf{u}, s_h) := 0$, otherwise, and $g_{jl}(\cdot)$ is a Engquist-Osher numerical flux given by

$$g_{jl}(\mathbf{u}; s_{hj}, s_{hl}) := f_w(s_{hj})u^+_{jl} + f_w(s_{hl})u^-_{jl}, \tag{2.3.4}$$

with $u^\pm_{jl} := \int_{S_{jl}} (\mathbf{u}\cdot\mathbf{n})^\pm d\sigma$. It is well know that the Engquist-Osher numerical flux $g_{jl}(\cdot)$ defined in (2.3.4), satisfies [34]: for all $r > 0$, there exists a constant $C = C(r) > 0$ such that for all x,y,x',$y' \in B_r(0)$

$$|g_{jl}(\cdot; x, y) - g_{jl}(\cdot; x', y')| \leqslant C(r)h\left(|x - x'| + |y - y'|\right), \tag{2.3.5}$$

$$g_{jl}(\cdot; x, y) = -g_{lj}(\cdot; y, x), \tag{2.3.6}$$

$$g_{jl}(\cdot; x, x) = f_w(x)\int_{S_{jl}} \mathbf{u}\cdot\mathbf{n}_{jl} d\sigma. \tag{2.3.7}$$

Note that the inequality (2.3.5) is a local Lipschitz condition, the identity (2.3.6) is the conservation property and the identity (2.3.7) is consistency. Finally, the semi discrete finite volume scheme is defined as

Definition 2.3.2 *Let* $(\mathbf{u}_h(\mathbf{x},t), p_h(\mathbf{x},t)) \in \mathbf{V}_h \times W_h$ *for* $(\mathbf{x},t) \in \Omega_T$*. Then* $s_h(\mathbf{x},t)$ *is defined by the semi discrete finite volume scheme as*

$$(\partial_t s_h)_j + (L_h(\mathbf{u}_h)s_h)_j = (Q(s_h))_j, \forall T_j \in \mathcal{T}_h \tag{2.3.8}$$

where $(L_h(\mathbf{u}_h)s_h)_j := \dfrac{1}{T_j}\sum_{l\in N_j} F_{jl}(\mathbf{u}_h, s_h)$ *and* $s_h(\cdot,0)\big|_{T_j} = (s^o(\cdot))_j$*. Additionally, the discrete inner product is defined as* $(L_h(\mathbf{u}_h)s_h, s_h)_h := \sum_j T_j s_{hj}(L_h(\mathbf{u}_h)s_{hj})_j$.

2.3.4 The Combined Schemes

The semi discrete scheme

Let $(\mathbf{u}, p, s)$ the weak solution of the Model Problem (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). It is defined the semi discrete combined and decoupled MFE-FE scheme for the model problem as follows.

Definition 2.3.3 *(Coupled) Find* $(\mathbf{u}_h, p_h, s_h) : J \longrightarrow \mathbf{V}_h \times W_h \times l^2(\Omega)$ *with:*

1. *For* $t \in J$ *fixed,* $(\mathbf{u}_h(t), p_h(t))$ *is a solution of the MFE scheme, i.e., for all* $(\mathbf{v}_h, \varphi_h) \in \mathbf{V}_h \times W_h$*:*

$$B(\mathbf{u}_h(t), \varphi_h) = (F(s_h(t)), \varphi_h) \tag{2.3.9}$$
$$A(s_h(t); \mathbf{u}_h(t), \mathbf{v}_h) + B(\mathbf{v}_h, p_h(t)) = (\mathbf{G}(s_h(t)), \mathbf{v}_h). \tag{2.3.10}$$

2. $s_h(t)$ *is a solution of the semi discrete FV scheme:*

$$(\partial_t s_h(t))_j + (L_h(\mathbf{u}_h(t))s_h(t))_j = (Q(s_h(t)))_j \tag{2.3.11}$$

with $s_h(\cdot,0)\big|_{T_j} = (s^o(\cdot))_j$.

Definition 2.3.4 *(Decoupled) Given* $t \in J$*, find* $(\widetilde{\mathbf{u}}(t), \widetilde{p}(t), \widetilde{s}(t))$ *such that:*

1. $(\widetilde{\mathbf{u}}(t), \widetilde{p}(t)) \in \mathbf{V}_h \times W_h$ *is a solution of:*

$$B(\widetilde{\mathbf{u}}(t), \varphi_h) = (F(s(t)), \varphi_h), \quad \forall \varphi_h \in W_h \tag{2.3.12}$$
$$A(s(t); \widetilde{\mathbf{u}}(t), \mathbf{v}_h) + B(\mathbf{v}_h, \widetilde{p}(t)) = (\mathbf{G}(s(t)), \mathbf{v}_h), \quad \forall \mathbf{v}_h \in \mathbf{V}_h. \tag{2.3.13}$$

2. $\widetilde{s}(\cdot,t)$ *solves:*

$$(\partial_t s(t))_j + (L_h(\mathbf{u}(t))\widetilde{s}(t))_j = (Q(s(t)))_j, \tag{2.3.14}$$

with $\widetilde{s}(\cdot,0)\big|_{T_j} = (s^o(\cdot))_j$, *for all* $T_j \in \mathcal{T}_h$,

where the functions s *and* $\mathbf{u}$, *the weak solution of the Model Problem (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22), are given.*

The full discrete scheme

Let $(\mathbf{u}, p, s)$ be the weak solution of the Model Problem (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22), which are given. It is defined the full discrete combined and decoupled MFE-FE scheme for the model problem as follows.

Definition 2.3.5 *(Coupled) Find* $(\mathbf{U}_h, P_h, S_h) : J_h \longrightarrow \mathbf{V}_h \times W_h \times l^2(\Omega)$ *with:*
0. Initial values: $S_j^0 := (s^o)_j$, *for all* $T_j \in \mathcal{T}_h$.
For $n = 0$ *to* M *do:*
1. For given $S_h(\cdot,t^n)$ *let* $(\mathbf{U}_h(\cdot,t^n), P_h(\cdot,t^n)) \in \mathbf{V}_h \times W_h$ *be defined as the solution of the MFE scheme, such that, for all* $(\mathbf{v}_h, \varphi_h) \in \mathbf{V}_h \times W_h$*:*

$$B(\mathbf{U}_h(\cdot,t^n), \varphi_h) = (F(S_h(\cdot,t^n)), \varphi_h), \tag{2.3.15}$$

$$A(S_h(\cdot,t^n); \mathbf{U}_h(\cdot,t^n), \mathbf{v}_h) + B(\mathbf{v}_h, P_h(\cdot,t^n)) = (\mathbf{G}(S_h(\cdot,t^n)), \mathbf{v}_h). \tag{2.3.16}$$

2. For given $(\mathbf{U}_h(\cdot,t^n), P_h(\cdot,t^n))$ *calculate* $S_h(\cdot,t^{n+1})$ *with the full discrete FV scheme, defined as:*

$$\frac{S_{hj}^{n+1} - S_{hj}^n}{\Delta t} + (L_h(\mathbf{U}_h(\cdot,t^n))S_h(\cdot,t^n))_j = (Q(S_h(\cdot,t^n)))_j, \tag{2.3.17}$$

for all $T_j \in \mathcal{T}_h$.

Definition 2.3.6 *(Decoupled) Find* $(\widetilde{\mathbf{u}}, \widetilde{p}, \widetilde{S})$ *such that:*
1. For each $t^n \in J_h$*:* $(\widetilde{\mathbf{u}}(t^n), \widetilde{p}(t^n)) \in \mathbf{V}_h \times W_h$ *is a solution of (2.3.12) and (2.3.13).*
2. $\widetilde{S}(\cdot,t^{n+1})$ *satisfies the initial condition* $\widetilde{S}_j^o = (s^o)_j$ *for all* $T_j \in \mathcal{T}_h$ *and for* $n = 0$ *to* M*:*

$$\frac{\widetilde{S}_j^{n+1} - \widetilde{S}_j^n}{\Delta t} + (L_h(\mathbf{u}(t^n))\widetilde{S})_j = (Q(s(t^n)))_j, \tag{2.3.18}$$

where $\widetilde{S}_j^{n+1} := \widetilde{S}(t^{n+1})|_{T_j}$ *for all* $T_j \in \mathcal{T}_h$*, where* $(\mathbf{u}, p, s)$ *is the weak solution of the Model Problem (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22), which are given.*

2.4 Main Results

Under the assumptions (A1)-(A10) and regularity's conditions mentioned in Remark 2.2.6 it is proved in the rest of this chapter the Theorem 2.4.1 and Theorem 2.4.2.

2.4.1 Convergence of the semi discrete scheme

Theorem 2.4.1 *Let* $(\mathbf{u}, p, s)$ *be the weak solution of the Model Problem (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22) and* $(\mathbf{u}_h, p_h, s_h)$ *the solution of (2.3.9)-(2.3.11). Then there exits constants* $K_* > 0$ *and* $K^* > 0$*, independent of* h*, such that:*

$$||\mathbf{u} - \mathbf{u}_h||^2_{L^\infty(J;V)} + ||p - p_h||^2_{L^\infty(J;W)} + ||s - s_h||^2_{L^\infty(J;L^2(\Omega))} + \\ D\kappa \int_J \sum_{a \in \mathcal{A}} [I_h(s)(t) - s_h(t)]^2_a dt \leq h^2 K_* (1 + e^{K^* T}).$$

This Theorem will be proved at the end of section 6, after some previous results.

2.4.2 Convergence of the full discrete scheme

Theorem 2.4.2 *Let* $(\mathbf{u}, p, s)$ *be the weak solution of the Model Problem (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22) and* $(\mathbf{U}_h, P_h, S_h)$ *solution of (2.3.15)-(2.3.17). If* Δt *and* h *satisfies the conditions (2.7.1) and (2.7.2), then there exits constants* $K_*, K^*, \tilde{K} > 0$*, independent of* Δt *and* h*, such that,*

$$||\mathbf{u}(t_n) - \mathbf{U}_h^n||^2_V + ||p(t_n) - P_h^n||^2_W + ||s(t_n) - S_h^n||^2_{L^2(\Omega)} \leq K_*(h^2 + |\Delta t|^2)(K^* + e^{\tilde{K}|\Delta t|^2}).$$

This Theorem will be proved at the end of section 7, after some previous results.

2.5 Preliminary Results

It is have the following estimates from the geometric properties of an unstructured grid [31, 35, 40]:

Lemma 2.5.1 *Let $\mathcal{T}_h$ be a unstructured triangulation, $T_j, T_l \in \mathcal{T}_h$, $\mathbf{x}, \mathbf{y} \in T_j \cup T_l$, $\tilde{s}, s_h \in l^2(\Omega)$, $\partial_t s \in L^2(J; H^2(\Omega))$, $s \in H^2(\Omega)$. Then there exits constants $C_i > 0, i = 1, 2, 3, 4, 5, 6$ independent of h, such that:*

1. $|s(\mathbf{x}) - s(\mathbf{y})| \leq C_1 ||s||_{H^2(T_j \cup T_l)}$.
2. $|\partial_t s(\mathbf{x}) - \partial_t s(\mathbf{y})| \leq C_2 ||\partial_t s||_{H^2(T_j \cup T_l)}$.
3. $C_3 ||s_h||^2_{l^2(\Omega)} \leq \sum_{a \in \mathcal{A}} [s_h]^2_a \leq \frac{2}{h^2} ||s_h||^2_{l^2(\Omega)}$.
4. $||\tilde{s} - s_h||_{L^2(\Omega)} = ||\tilde{s} - s_h||_{l^2(\Omega)}$.
5. $||s - \tilde{s}||^2_{L^2(\Omega)} \leq C_4 h^2 ||s||^2_{H^2(\Omega)} + ||I_h(s) - \tilde{s}||^2_{l^2(\Omega)}$.
6. $0 < \sum_a |s^*_{ha}|^2 |S_a|^2 \leq C_5 ||s_h||^2_{l^2(\Omega)}$, $* = \pm$.
7. $\sum_a ||s||^2_{H^2(T_a^+ \cup T_a^-)} \leq C_6 ||s||^2_{H^2(\Omega)}$.

Remark 2.5.1 *For the discrete inner product $(L_h(\mathbf{w})s_h, s_h)_h$ it is have the inequality,*

$$(L_h(\mathbf{w})s_h, s_h)_h \geq D\kappa \sum_{a \in \mathcal{A}} [s_h]^2_a + \sum_{a \in \mathcal{A}} [s_h]_a g_a(\mathbf{w}; s^+_{ha}, s^-_{ha}). \tag{2.5.1}$$

The next lemma is the well-known Gronwall's inequality.

Lemma 2.5.2 *Let Φ, Ψ a continuous function in $J = (0, T)$ with $\Psi \geq 0$. Moreover let $\Phi(t) + \Psi(t) \leq \alpha + \beta \int_0^t \Phi(\tau) d\tau$ for all $t \in J$, and $\alpha, \beta \in \mathbb{R}$, $\beta > 0$. Then it is have, $\Phi(t) + \Psi(t) \leq \alpha e^{\beta t} \leq \alpha e^{\beta T}$.*

A discrete version of Gronwall's inequality is given by the next lemma.

Lemma 2.5.3 *Let $(\varphi^n)_{n=0,1,2,...}$, $(\psi^n)_{n=0,1,2,...}$ and $(\alpha^n)_{n=0,1,2,...}$ be positive sequences and let $\varphi^N + \psi^{N-1} \leq \alpha^{N-1} + (1 + \beta)\varphi^{N-1}$, for all $N = 1, 2, 3, ...$, and β a non negative real number. Then it is have, $\varphi^N + \sum_{n=0}^{N-1} \psi^n \leq (\varphi^0 + \sum_{n=0}^{N-1} \alpha^n) e^{\beta N}$.*

Remark 2.5.2 *About the Peclet number Pe (cf. [5]), it is assumed that, there exits a constant $C > 0$, such that*

$$Pe := \frac{||\mathbf{u}||_{L^\infty(J;L^\infty(\Omega))}}{D} \leq C := \frac{\kappa}{16K_{f_w}}\sqrt{\frac{C_3}{C_5}}, \tag{2.5.2}$$

where the constants $C_3, C_5 > 0$ are defined in Lemma 2.5.1, $\kappa > 0$ is defined in section 2.3.1, and $K_{f_w} > 0$ was defined in (A6). For an detailed justification of this hypothesis, please to see the proof of Theorem 2.6.2.

2.6 Convergence of the semi discrete scheme

Lemma 2.6.1 *Let $\tilde{s}$ be the solution of (2.3.14) and $(\mathbf{u}, p, s)$ the weak solution of (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Then, for all $t \in J$ there exists a constant $K > 0$, independent of h and D, such that the following estimate holds*

$$D\kappa \sum_a [\tilde{s}]_a^2 \leq \frac{4K}{D\kappa}.$$

Proof: by definition of $\tilde{s}$

$$-\frac{D}{T_j}\sum_l (\tilde{s}_l(t) - \tilde{s}_j(t))\gamma_{jl} + \frac{1}{T_j}\sum_l g_{jl}(\mathbf{u}(t); \tilde{s}_j(t), \tilde{s}_l(t)) = R_j(t),$$

where $R_j(t) := (\partial_t s(t) - Q(t))_j$. Multiplying by $T_j\tilde{s}_j$, summing up over all triangles T_j, applying $\sum_{jl} A_{jl} = \sum_a (A_{T_a^+} + A_{T_a^-})$, and inequality (2.5.1) it is obtained:

$$D\kappa \sum_a [\tilde{s}]_a^2 + \sum_a g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-)[\tilde{s}]_a \leq D\sum_a [\tilde{s}]_a^2\gamma_a + \sum_a g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-)[\tilde{s}]_a = \sum_j T_j\tilde{s}_jF_j,$$

that is,

$$D\kappa \sum_a [\tilde{s}]_a^2 \leq |\sum_a g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-)[\tilde{s}]_a| + |\sum_j T_j\tilde{s}_jF_j| \equiv H_1 + H_2.$$

About H_1,

$$\begin{aligned}
H_1 &\leq (\sum_a g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-))^{1/2} (\sum_a [\tilde{s}]_a^2)^{1/2} \\
&\leq \frac{1}{2}[\theta_1 \sum_a g_a^2(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-) + \frac{1}{\theta_1} \sum_a [\tilde{c}]_a^2] \\
&= \frac{1}{2}[\theta_1 \sum_a (f_w(\tilde{s}_a^+) u_a^+ + f_w(\tilde{s}_a^-) u_a^-)^2 + \frac{1}{\theta_1} \sum_a [\tilde{s}]_a^2] \\
&\leq \frac{1}{2}[\theta_1 \sum_a (K_1 h ||f_w||_\infty ||\mathbf{u}||_\infty)^2 + \frac{1}{\theta_1} \sum_a [\tilde{s}]_a^2] \\
&\leq \frac{1}{2}[\theta_1 K_1 ||f_w||_\infty^2 ||\mathbf{u}||_\infty^2 h^2 \frac{K_2}{h^2} + \frac{1}{\theta_1} \sum_a [\tilde{s}]_a^2].
\end{aligned}$$

About H_2,

$$\begin{aligned}
H_2 &= |\sum T_j \tilde{s}_j \frac{1}{T_j} \int_{T_j} R(x) dx| \\
&\leq \sum_j \int_{T_j} |\tilde{s}_j||R| \\
&= \int_\Omega |\tilde{c}||R| \\
&\leq ||\tilde{s}||_{L^2(\Omega)} ||R||_{L^2(\Omega)} \\
&= ||\tilde{s}||_{l^2(\Omega)} ||R||_{L^2(\Omega)} \\
&\leq \frac{1}{2}[\theta_2 ||\tilde{s}||_{l^2(\Omega)}^2 + \frac{1}{\theta_2} ||R||_{L^2(\Omega)}^2] \\
&\leq \frac{1}{2}[\theta_2 K_3 \sum_a [\tilde{s}]_a^2 + \frac{1}{\theta_2} ||R||_{L^2(\Omega)}^2].
\end{aligned}$$

Finally, it is sufficient to choose $\theta_1 = 4/D\kappa$ and $\theta_2 = D\kappa/4K_3$.□

Theorem 2.6.1 *Let* $(\mathbf{u}, p, s)$ *be the weak solution of (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). If* $p(\tau) \in H^1(\Omega)$, $\mathbf{u}(\tau) \in (H^1(\Omega))^2$ *and* $div\mathbf{u}(\tau) \in H^1(\Omega)$ *for any fixed time* $\tau \in J$, *then the scheme (2.3.12)-(2.3.13) has a unique solution* $(\widetilde{\mathbf{u}}(\tau), \widetilde{p}(\tau)) \in \mathbf{V}_h \times W_h$ *and there exists a constant* $C > 0$, *independent of* h *and* $c(\tau)$, *such that:*

$$||(\mathbf{u} - \widetilde{\mathbf{u}})(\tau)||_{H(div;\Omega)} + ||(p - \widetilde{p})(\tau)||_{L^2(\Omega)} \leq \qquad (2.6.1)$$
$$Ch(|p(\tau)|_{H^1(\Omega)} + |\mathbf{u}(\tau)|_{(H^1(\Omega))^2} + |div\mathbf{u}(\tau)|_{H^1(\Omega)}).$$

Proof: by Theorem 1.1 en [29] it is obtained that the scheme (2.3.12)-(2.3.13) has a unique solution $(\widetilde{\mathbf{u}}(\tau), \widetilde{p}(\tau)) \in \mathbf{V}_h \times W_h$ and there exits a constant $c > 0$ such that

$$\begin{aligned} ||(\mathbf{u} - \widetilde{\mathbf{u}})(\tau)||_{H(div;\Omega)} + ||(p - \widetilde{p})(\tau)||_{L^2(\Omega)} &\leq \\ c[\inf_{v_h \in V_h} ||\mathbf{u}(\tau) - \mathbf{v}_h||_{H(div;\Omega)} + \inf_{w_h \in W_h} ||p(\tau) - w_h||_{L^2(\Omega)}]. \end{aligned}$$

In effect, the bilinear form $A(s; \cdot, \cdot)$ is coercive and $B(\cdot, \cdot)$ satisfies the inf-sup condition. Finally, (2.6.1) follows from [20]. □

Theorem 2.6.2 *Let $\widetilde{s}$ be the solution of (2.3.14) and $(\mathbf{u}, p, s)$ the weak solution of (2.2.23)-(2.2.25) in the sense (2.2.20)-(2.2.22). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Let e_h be defined as $e_h := \widetilde{s} - I_h(s)$, and let the assumption 2.2.27 hold. Then, for all $t \in J$ there exists a constant $K > 0$, independent of h and D, such that the following estimate holds*

$$\frac{D\kappa}{2} \sum_a [e_h]_a^2 \leq K \frac{2h^2}{D\kappa} [||\mathbf{u}||_\infty^2 ||s||_{H^2(\Omega)}^2 + D^2 ||s||_{H^2(\Omega)}^2 + \frac{1}{(D\kappa)^2} ||\mathbf{u}||_\infty^2].$$

Proof: for $(L_h(\mathbf{u})e_h)_j$ it is have (note that it is applied the notation $s_j \equiv s(x_j^*) \equiv I(s)|_{T_j^*}$ y $\tilde{s}_j^* \equiv \tilde{s}|_{T_j^*}, * = +, -$):

$$\begin{aligned} (L_h(\mathbf{u})e_h)_j &= -\frac{D}{T_j} \sum_l (e_l - e_j)\gamma_{jl} + \frac{1}{T_j} \sum_l g_{jl}(\mathbf{u}; e_j, e_l) \\ &= (L_h(\mathbf{u})\tilde{s})_j - (L_h(\mathbf{u})I_h)_j \\ &- \frac{1}{T_j} \sum_l (-g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) + g_{jl}(\mathbf{u}; s(x_j), s(x_l)) + g_{jl}(\mathbf{u}; e_j, e_l)) \\ &= (L_h(\mathbf{u})s)_j - (L_h(\mathbf{u})I_h(s))_j \\ &- \frac{1}{T_j} \sum_l (-g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) + g_{jl}(\mathbf{u}; s(x_j), s(x_l)) + g_{jl}(\mathbf{u}; e_j, e_l)) \\ &= -(\psi_j(s) + \varphi_j(s)) \\ &- \frac{1}{T_j} \sum_l (-g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) + g_{jl}(\mathbf{u}; s(x_j), s(x_l)) + g_{jl}(\mathbf{u}; e_j, e_l)). \end{aligned}$$

Multiplying this last equality by $T_j e_j$ and summing up over all triangles T_j it is obtained

$$
\begin{aligned}
(L_h(\mathbf{u})e_h, e_h)_h &= \sum_j T_j e_j (L_h(\mathbf{u})e_h)_j \\
&= -[(\psi_h(s), e_h)_h + (\varphi_h(s), e_h)_h] \\
&+ \sum_a (-g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-) + g_a(\mathbf{u}; s(x_a^+), s(x_a^-)) + g_a(\mathbf{u}; e_a^+, e_a^-))[e_h]_a,
\end{aligned}
$$

where (cf. Lema 5.4 y Lema 5.6 in [40]), $\psi_j(s) := -\frac{D}{T_j}\sum_{l\in N_j} S_{jl}[\frac{(s_l - s_j)(t)}{d_{jl}} - \frac{1}{S_{jl}}\int_{S_{jl}} \nabla s(\cdot, t)\cdot \mathbf{n} d\sigma]$ and $\varphi_j(s) := \frac{1}{T_j}\sum_l (g_{jl}(\mathbf{u}; s_j, s_l) - \int_{S_{jl}} f_w(s)\mathbf{u}\cdot\mathbf{n}_{jl})$. Now, using the inequality 2.5.1, it is get:

$$
D\kappa \sum_a [e_h]_a^2 \leq B_1 + B_2 + B_3 + B_4 + B_5,
$$

where

$$
\begin{aligned}
B_1 &:= -(\psi_h(s), e_h)_h, \\
B_2 &:= -(\varphi_h(s), e_h)_h, \\
B_3 &:= \sum_a (g_a(\mathbf{u}; s(x_a^+), s(x_a^-)) - \int_{S_a} \mathbf{u}\cdot\mathbf{n}_a E_2)[e_h]_a, \\
B_4 &:= -\sum_a (g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-) - \int_{S_a} \mathbf{u}\cdot\mathbf{n}_a E_1)[e_h]_a, \\
B_5 &:= \sum_a (\int_{S_a} \mathbf{u}\cdot\mathbf{n}_a (E_2 - E_1))[e_h]_a,
\end{aligned}
$$

with $E_1 := f_w(\frac{\tilde{s}_a^+ + \tilde{s}_a^-}{2})$ and $E_2 := f_w(\frac{s(x_a^+)+s(x_a^-)}{2})$. About B_2, for all $\theta_2 > 0$,

$$\begin{aligned}
|B_2| &= |(\varphi_h(s), e_h)_h| \\
&= |\sum_j T_j \varphi_j(s) e_j| \\
&= |\sum_j (\sum_l (g_{jl}(\mathbf{u}; s_j, s_l) - \int_{S_{jl}} f_w(s)\mathbf{u}\cdot\mathbf{n}_{jl}))e_j| \\
&= |\sum_a ((g_a(\mathbf{u}; s_a^+, s_a^-) - \int_{S_a} f_w(s)\mathbf{u}\cdot\mathbf{n}_a))[e_h]_a| \\
&\leq \sum_a (\int_{S_a} (|f_w(s_a^+) - f_w(s)|(\mathbf{u}\cdot\mathbf{n}_a)^+ + |f_w(s_a^-) - f_w(s)|(\mathbf{u}\cdot\mathbf{n}_a)^-))|[e_h]_a| \\
&\leq \sum_a (\alpha_2 h) K_{f_w} 2C_1 ||s||_{H^2(T_a^+\cup T_a^-)} ||\mathbf{u}||_\infty |[e_h]_a| \\
&\leq \theta_2 h^2 (\alpha_2 K_{f_w} C_1 C_6 ||s||_{H^2(\Omega)} ||\mathbf{u}||_\infty)^2 + \frac{1}{\theta_2}\sum_a [e_h]_a^2.
\end{aligned}$$

About B_1, it is applied Lema 5.4 in [40]. For each $\theta_1 > 0$ it is have,

$$|B_1| \leq K_o D h ||s||_{H^2(\Omega)} (\sum_a [e_h]_a^2)^{1/2} \leq h^2 \frac{\theta_1}{2}(K_o D ||s||_{H^2(\Omega)})^2 + \frac{1}{2\theta_1}\sum_a [e_h]_a^2,$$

with $K_o > 0$ is a generic constant. About B_3 note that,

$$|f_w(s(x_a^*)) - E_2| \leq (K_{f_w}/2)|s(x_a^+) - s(x_a^-)| \leq (K_{f_w}/2)||s||_{H^2(T_a^+\cup T_a^-)}, * = \pm.$$

Therefore, for each constant $\theta_3 > 0$,

$$|B_3| \leq h^2 \frac{\theta_3}{2}(\alpha_2 K_{f_w} C_6 ||s||_{H^2(\Omega)} ||\mathbf{u}||_\infty)^2 + \frac{1}{2\theta_3}\sum_a [e_h]_a^2.$$

About B_4, it is applied the Lemma 2.6.1, and, in a similar way of B_3, it is have that for each $\theta_4 > 0$

$$|B_4| \leq \sum_a \int_{S_a} \frac{K_{f_w}}{2}|\tilde{s}_a^+ - \tilde{s}_a^-||\mathbf{u}|)[e_h]_a \leq h^2 \frac{\theta_4}{2}(\alpha_2 K_{f_w} ||\mathbf{u}||_\infty)^2 K_{\tilde{s}} + \frac{1}{2\theta_4}\sum_a [e_h]_a^2,$$

where $K_{\tilde{s}} > 0$ is from Lemma 2.6.1, that is, $K_{\tilde{s}} > 0$ is such that, $\sum_a |\tilde{s}_a^+ - \tilde{s}_a^-|^2 \leq K_{\tilde{s}}$. About B_5, note that $|E_2 - E_1| \leq (K_{f_w}/2)(|e_a^+| + |e_a^-|)$. Therefore, for all $\theta_5 > 0$ it is have

$$
\begin{aligned}
|B_5| &\leq \sum_a |S_a| ||\mathbf{u}||_\infty |E_2 - E_1| |[e_h]_a| \\
&\leq \sum_a |S_a| ||\mathbf{u}||_\infty \frac{K_{f_w}}{2} (|e_a^+| + |e_a^-|) |[e_h]_a| \\
&\leq \frac{1}{2} (\theta_5 K_{f_w}^2 ||\mathbf{u}||_\infty^2 (\sum_a |S_a|^2 |e_a^+|^2 + \sum_a |S_a|^2 |e_a^-|^2) + \frac{1}{2\theta_5} \sum_a [e_h]_a^2) \\
&\leq \frac{1}{2} (\theta_5 K_{f_w}^2 ||\mathbf{u}||_\infty^2 2C_5 ||e_h||_{l^2(\Omega)}^2 + \frac{1}{2\theta_5} \sum_a [e_h]_a^2) \\
&\leq \theta_5 K_{f_w}^2 ||\mathbf{u}||_\infty^2 C_5 ||e_h||_{l^2(\Omega)}^2 + \frac{1}{\theta_5} \sum_a [e_h]_a^2 \\
&\leq \theta_5 K_{f_w}^2 ||\mathbf{u}||_\infty^2 \frac{C_5}{C_3} \sum_a [e_h]_a^2 + \frac{1}{\theta_5} \sum_a [e_h]_a^2.
\end{aligned}
$$

Therefore, collecting previous bounds,

$$
(D\kappa - (\frac{1}{2\theta_1} + \frac{1}{\theta_2} + \frac{1}{2\theta_3} + \frac{1}{2\theta_4}) - (\frac{1}{\theta_5} + K_{f_w}^2 \frac{C_5}{C_3} ||\mathbf{u}||_\infty^2 \theta_5)) \sum_a [e_h]_a^2 \leq K h^2,
$$

where $K > 0$ is a generic constant, and $\theta_i, i = 1, 2, 3, 4$ are chosen such that, $\frac{1}{2\theta_1} + \frac{1}{\theta_2} + \frac{1}{2\theta_3} + \frac{1}{2\theta_4} = \frac{D\kappa}{8}$. On the other hand $\theta_5 > 0$, is chose such that $\frac{1}{\theta_5} + K_{f_w}^2 \frac{C_5}{C_3} ||\mathbf{u}||_\infty^2 \theta_5 = \frac{D\kappa}{8}$, which have solution $\theta_5 > 0$ if and only if $(\frac{D\kappa}{8})^2 \geq 4(K_{f_w}^2 \frac{C_5}{C_3} ||\mathbf{u}||_\infty^2)$. Please, note that this last inequality is the origin and motivation of hypothesis 2.2.27.□

Theorem 2.6.3 *Let $\widetilde{s}$ be the solution of (2.3.14) and $(\mathbf{u}, p, s)$ the weak solution of (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Let e_h be defined as $e_h := \widetilde{s} - I_h(s)$, and let the assumption 2.2.27 hold. Then, for all $t \in J$ there exists a constant $K > 0$, independent of h, such that*

$$
\frac{D\kappa}{2} \sum_a [\partial_t e_h]_a^2 \leq K h^2 \frac{8}{D\kappa}.
$$

Proof: (about the notation $s_j \equiv s(x_j^*) \equiv I(s)|_{T_j^*}$ y $\tilde{s}_j^* \equiv \tilde{s}|_{T_j^*}, * = +, -)$. About $(L_h(\mathbf{u})\partial_t e_h)_j$ it is have

$$\begin{aligned}
(L_h(\mathbf{u})\partial_t e_h)_j &= -\frac{D}{T_j}\sum_l (\partial_t e_l - \partial_t e_j)\gamma_{jl} + \frac{1}{T_j}\sum_l g_{jl}(\mathbf{u};\partial_t e_j,\partial_t e_l) \\
&= \{-\frac{D}{T_j}\sum_l (\partial_t \tilde{s}_l - \partial_t \tilde{s}_j)\gamma_{jl} + \frac{1}{T_j}\sum_l g_{jl}(\mathbf{u};\partial_t \tilde{s}_j,\partial_t \tilde{s}_l)\} \\
&- \{-\frac{D}{T_j}\sum_l (\partial_t s_l - \partial_t s_j)\gamma_{jl} + \frac{1}{T_j}\sum_l g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l)\} \\
&+ \{\frac{1}{T_j}\sum_l [-g_{jl}(\mathbf{u};\partial_t \tilde{s}_j,\partial_t \tilde{s}_l) + g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) + g_{jl}(\mathbf{u};\partial_t e_j,\partial_t e_l)]\} \\
&= (L_h(\mathbf{u})\partial_t \tilde{s})_j - (L_h(\mathbf{u})\partial_t I(s))_j \\
&+ \frac{1}{T_j}\sum_l [-g_{jl}(\mathbf{u};\partial_t \tilde{s}_j,\partial_t \tilde{s}_l) + g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) + g_{jl}(\mathbf{u};\partial_t e_j,\partial_t e_l)] \\
&= -[\psi_j(\partial_t s) + \varphi_j(\partial_t s)] + [-(div(f_w(\partial_t s)\mathbf{u}))_j + (div(\partial_t(f_w(s)\mathbf{u})))_j] \\
&+ \frac{1}{T_j}\sum_l (g_{jl}(\mathbf{u};\partial_t \tilde{s}_j,\partial_t \tilde{s}_l) - \partial_t g_{jl}(\mathbf{u};\tilde{s}_j,\tilde{s}_l)) \\
&+ \frac{1}{T_j}\sum_l [-g_{jl}(\mathbf{u};\partial_t \tilde{s}_j,\partial_t \tilde{s}_l) + g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) + g_{jl}(\mathbf{u};\partial_t e_j,\partial_t e_l)] \\
&= -[\psi_j(\partial_t s) + \varphi_j(\partial_t s)] + [-(div(f_w(\partial_t s)\mathbf{u}))_j + (div(\partial_t(f_w(s)\mathbf{u})))_j] \\
&+ \frac{1}{T_j}\sum_l [-\partial_t g_{jl}(\mathbf{u};\tilde{s}_j,\tilde{s}_l)) + g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) + g_{jl}(\mathbf{u};\partial_t e_j,\partial_t e_l)].
\end{aligned}$$

Multiplying this last equality by $T_j\partial_t e_j$ and summing up over all triangles T_j it is obtained $(L_h(\mathbf{u})\partial_t e_h, \partial_t e_h)_h = H_1 + H_2 + H_3$, where, $H_1 := -(\psi(\partial_t s), \partial_t e_h)_h$, $H_2 := -(\varphi(\partial_t s), \partial_t e_h)_h$, and $H_3 := \sum_j T_j\partial_t e_j Z_j$, with,

$$\begin{aligned}
Z_j := -(div(f_w(\partial_t s)\mathbf{u}))_j + (div(\partial_t(f_w(s)\mathbf{u})))_j] \\
+ \frac{1}{T_j}\sum_l [-\partial_t g_{jl}(\mathbf{u};\tilde{s}_j,\tilde{s}_l)) + g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) + g_{jl}(\mathbf{u};\partial_t e_j,\partial_t e_l).
\end{aligned}$$

Applying the inequality 2.5.1 it is obtained $D\kappa\sum_a[\partial_t e_h]_a^2 \leq |H_1| + |H_2| + |H_3^*|$, with $H_3^* := \sum_j T_j \partial_t e_j Z_j^*$, where,

$$Z_j^* := [-(div(f_w(\partial_t s)\mathbf{u}))_j + (div(\partial_t(f_w(s)\mathbf{u})))_j] \\ + \frac{1}{T_j}\sum_l[-\partial_t g_{jl}(\mathbf{u};\tilde{s}_j,\tilde{s}_l)) + g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l)].$$

About $|H_1|$, note that $|H_1| \leq \frac{1}{2}[\theta_1(K_o Dh||\partial_t s||_{H^2(\Omega)})^2 + \frac{1}{\theta_1}\sum_a[\partial_t e_h]_a^2]$. About $|H_2|$, note that

$$\begin{aligned}
|H_2| &= (\varphi_h(\partial_t s), \partial_t e_h)_h \\
&\leq |\sum_j(\sum_l(g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) - \int_{S_{jl}} f_w(\partial_t s)\mathbf{u}\cdot\mathbf{n}_{jl}))\partial_t e_j| \\
&= |\sum_a[g_a(\mathbf{u};\partial_t s_a^+,\partial_t s_a^-) - \int_{S_a} f_w(\partial_t s)\mathbf{u}\cdot\mathbf{n}_a][\partial_t e_h]_a| \\
&\leq \sum_a(\int_{S_a}(|f_w(\partial_t s_a^+) - f_w(\partial_t s)||(\mathbf{u}\cdot\mathbf{n}_a)^+| + |f_w(\partial_t s_a^-) - f_w(\partial_t s)||(\mathbf{u}\cdot\mathbf{n}_a)^-||[\partial_t e_h]_a|) \\
&\leq K_1 K_{f_w}\sum_a(h||\partial_t s||_{H^2(T_a^+\cup T_a^-)}||\mathbf{u}||_\infty)|[\partial_t e_h]_a| \\
&\leq \frac{1}{2}(\theta_2 K_1^2 K_{f_w}^2 h^2||\mathbf{u}||_\infty^2||\partial_t s||_{H^2(\Omega)}^2 + \frac{1}{\theta_2}\sum_a[\partial_t e_h]_a^2).
\end{aligned}$$

About $|H_3^*|$, note that

$$\begin{aligned}
H_3^* &= \sum_j T_j\partial_t e_j[\frac{1}{T_j}\sum_l g_{jl}(\mathbf{u};\partial_t s_j,\partial_t s_l) - (div(f_w(\partial_t s)\mathbf{u}))_j] \\
&- \sum_j T_j\partial_t e_j[\frac{1}{T_j}\sum_l \partial_t g_{jl}(\mathbf{u};\tilde{s}_j,\tilde{s}_l) - (div(\partial_t(f_w(s)\mathbf{u})))_j] \\
&\equiv H_{3A}^* - H_{3B}^*.
\end{aligned}$$

About $|H^*_{3A}|$,

$$\begin{aligned}
H^*_{3A} &= \sum_j T_j \partial_t e_j [\frac{1}{T_j} \sum_l g_{jl}(\mathbf{u}; \partial_t s_j, \partial_t s_l) - (div(f_w(\partial_t s)\mathbf{u}))_j] \\
&= \sum_a \{ \int_{S_a} [(f_w(\partial_t s_a^+) - f_w(\partial_t s))(\mathbf{u}\cdot\mathbf{n}_a)^+ + (f_w(\partial_t s_a^-) - f_w(\partial_t s))(\mathbf{u}\cdot\mathbf{n}_a)^-]\}[\partial_t e_h]_a \\
&\leq \sum_a \{ \int_{S_a} [|f_w(\partial_t s_a^+) - f_w(\partial_t s)||(\mathbf{u}\cdot\mathbf{n}_a)^+| + |f_w(\partial_t s_a^-) - f_w(\partial_t s)||(\mathbf{u}\cdot\mathbf{n}_a)^-|]\}|[\partial_t e_h]_a| \\
&\leq \sum_a K_{f_w} |S_a| ||\mathbf{u}||_\infty |\partial_t s_a^+ - \partial_t s| |[\partial_t e_h]_a| \\
&\leq \frac{1}{2}\{\theta_3 (K_{f_w}^2 K_3^2 h^2 ||\mathbf{u}||_\infty^2) \sum_a ||\partial_t s||^2_{H^2(T_a^+ \cup T_a^-)} + \frac{1}{\theta_3} \sum_a [\partial_t e_h]_a^2\} \\
&\leq \frac{1}{2}\{\theta_3 (K_{f_w}^2 K_3^2 h^2 ||\mathbf{u}||_\infty^2) K_4^2 ||\partial_t s||^2_{H^2(\Omega)} + \frac{1}{\theta_3} \sum_a [\partial_t e_h]_a^2\}
\end{aligned}$$

About $|H^*_{3B}|$,

$$\begin{aligned}
H^*_{3B} &= \sum_j T_j \partial_t e_j [\frac{1}{T_j} \sum_l \partial_t g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) - (div(\partial_t (f_w(s)\mathbf{u})))_j] \\
&= \sum_j \partial_t e_j [\sum_l (\partial_t f_w(\tilde{s}_j) u_{jl}^+ + \partial_t f_w(\tilde{s}_l) u_{jl}^- - \int_{S_{jl}} \partial_t f_w(s)\mathbf{u}\cdot\mathbf{n}_{jl})] \\
&+ \sum_j \partial_t e_j [\sum_l (f_w(\tilde{s}_j) \partial_t \mathbf{u}_{jl}^+ + f_w(\tilde{s}_l) \partial_t \mathbf{u}_{jl}^- - \int_{S_{jl}} f_w(s)\partial_t \mathbf{u}\cdot\mathbf{n}_{jl})] \\
&= \sum_a \{ \int_{S_a} [(\partial_t f_w(\tilde{s}_a^+) - \partial_t f_w(s))(\mathbf{u}\cdot\mathbf{n}_a)^+ + (\partial_t f_w(\tilde{s}_a^-) - \partial_t f_w(s))(\mathbf{u}\cdot\mathbf{n}_a)^-]\}[\partial_t e_h]_a \\
&+ \sum_a \{ \int_{S_a} [(f_w(\tilde{s}_a^+) - f_w(s))\partial_t(\mathbf{u}\cdot\mathbf{n}_a)^+ + (f_w(\tilde{s}_a^-) - f_w(s))\partial_t(\mathbf{u}\cdot\mathbf{n}_a)^-]\}[\partial_t e_h]_a \\
&\equiv H^*_{3Ba} + H^*_{3Bb}.
\end{aligned}$$

About H^*_{3Ba}, note that,

$$\begin{aligned}
\partial_t f_w(\tilde{s}^*_a) - \partial_t f_w(s) &= \\
f'_w(\tilde{s}^*_a)\partial_t \tilde{s}^*_a - f'_w(s)\partial_t s &= \\
f'_w(\tilde{s}^*_a)\partial_t \tilde{s}^*_a - f'_w(s)\partial_t s + f'_w(\tilde{s}^*_a)\partial_t s - f'_w(\tilde{s}^*_a)\partial_t s &= \\
f'_w(\tilde{s}^*_a)(\partial_t \tilde{s}^*_a - \partial_t s) + (\partial_t s) f'_w(\xi)(\tilde{s}^*_a - s) &= \\
f'_w(\tilde{s}^*_a)[(\partial_t \tilde{s}^*_a - \partial_t s^*_a) + (\partial_t s^*_a - \partial_t s)] + (\partial_t s) f'_w(\xi)[(\tilde{s}^*_a - s^*_a) + (s^*_a - s)] & \quad .
\end{aligned}$$

Therefore,

$$H^*_{3Ba} = H^*_{3Ba1} + H^*_{3Ba2} + H^*_{3Ba3} + H^*_{3Ba4},$$

where,

$$\begin{aligned}
H^*_{3Ba1} &:= \sum_a \int_{S_a} f'_w(\tilde{s}^*_a)(\partial_t \tilde{s}^*_a - \partial_t s^*_a)(\mathbf{u}\cdot\mathbf{n}_a)^*[\partial_t e_h]_a, \\
H^*_{3Ba2} &:= \sum_a \int_{S_a} f'_w(\tilde{s}^*_a)(\partial_t s^*_a - \partial_t s)(\mathbf{u}\cdot\mathbf{n}_a)^*[\partial_t e_h]_a, \\
H^*_{3Ba3} &:= \sum_a \int_{S_a} (\partial_t s) f'_w(\xi)(\tilde{s}^*_a - s^*_a)(\mathbf{u}\cdot\mathbf{n}_a)^*[\partial_t e_h]_a, \\
H^*_{3Ba4} &:= \sum_a \int_{S_a} (\partial_t s) f'_w(\xi)(s^*_a - s)(\mathbf{u}\cdot\mathbf{n}_a)^*[\partial_t e_h]_a.
\end{aligned}$$

About H^*_{3Ba1},

$$\begin{aligned}
H^*_{3Ba1} &\leq \frac{1}{2}\{\theta_4 \sum_a |S_a|^2 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty |\partial_t \tilde{s}^*_a - \partial_t s^*_a|^2 + \frac{1}{\theta_4}\sum_a [\partial_t e_h]^2_a\} \\
&\leq \frac{1}{2}\{\theta_4 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_4 \sum_a T^*_a |\partial_t e^*_a|^2 + \frac{1}{\theta_4}\sum_a [\partial_t e_h]^2_a\} \\
&\leq \frac{1}{2}\{\theta_4 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_4 K_8 ||\partial_t e_h||^2_{l^2(\Omega)} + \frac{1}{\theta_4}\sum_a [\partial_t e_h]^2_a\} \\
&\leq \frac{1}{2}\{\theta_4 K^2_{f_w} ||\mathbf{u}||^2_\infty K_4 K_8 K_{12} \sum_a [\partial_t e_h]^2_a + \frac{1}{\theta_4}\sum_a [\partial_t e_h]^2_a\},
\end{aligned}$$

About H^*_{3Ba2},

$$\begin{aligned} H^*_{3Ba2} &\leq \frac{1}{2}\{\theta_5 \sum_a |S_a|^2 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty |\partial_t s^*_a - \partial_t s|^2 + \frac{1}{\theta_5}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_5 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_5 h^2 \sum_a ||\partial_t s||^2_{H^2(T_a^+ \cup T_a^-)} + \frac{1}{\theta_5}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_5 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_5 h^2 K_9 ||\partial_t s||^2_{H^2(\Omega)} + \frac{1}{\theta_5}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_5 ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty h^2 K_5 K_9 ||\partial_t s||^2_{H^2(\Omega)} + \frac{1}{\theta_5}\sum_a [\partial_t e_h]^2_a\}, \end{aligned}$$

About H^*_{3Ba3},

$$\begin{aligned} H^*_{3Ba3} &\leq \frac{1}{2}\{\theta_6 \sum_a |S_a|^2 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty |\tilde{s}^*_a - s^*_a|^2 + \frac{1}{\theta_6}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_6 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_6 \sum_a T^*_a |e^*_a|^2 + \frac{1}{\theta_6}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_6 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_6 K_{10} ||e_h||^2_{l^2(\Omega)} + \frac{1}{\theta_6}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_6 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_6 K_{10} K_{13} \sum_a [e_h]^2_a + \frac{1}{\theta_6}\sum_a [\partial_t e_h]^2_a\}, \end{aligned}$$

About H^*_{3Ba4},

$$\begin{aligned} H^*_{3Ba4} &\leq \frac{1}{2}\{\theta_7 \sum_a |S_a|^2 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty |s^*_a - s|^2 + \frac{1}{\theta_7}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_7 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_7 h^2 \sum_a ||s||^2_{H^2(T_a^+ \cup T_a^-)} + \frac{1}{\theta_7}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_7 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty K_7 h^2 K_{11} ||s||^2_{H^2(\Omega)} + \frac{1}{\theta_7}\sum_a [\partial_t e_h]^2_a\} \\ &\leq \frac{1}{2}\{\theta_7 ||\partial_t s||^2_\infty ||f'_w||^2_\infty ||\mathbf{u}||^2_\infty h^2 K_7 K_{11} ||s||^2_{H^2(\Omega)} + \frac{1}{\theta_7}\sum_a [\partial_t e_h]^2_a\}. \end{aligned}$$

About H^*_{3Bb}, note that,

$$\begin{aligned}
\sum_a \Big(\int_{S_a} (f_w(\tilde{s}_a^+) - f_w(s))\partial_t(\mathbf{u}\cdot\mathbf{n}_a)^+\Big)[\partial_t e_h]_a &\leq \\
\sum_a |S_a|||\partial_t \mathbf{u}||_\infty K_{f_w}|\tilde{s}_a^+ - s||[\partial_t e_h]_a| &\leq \\
\sum_a |S_a|||\partial_t \mathbf{u}||_\infty K_{f_w}(|\tilde{s}_a^+ - s_a^+| + |s_a^+ - s|)|[\partial_t e_h]_a| &\leq \\
\sum_a |S_a|||\partial_t \mathbf{u}||_\infty K_{f_w}|\tilde{s}_a^+ - s_a^+||[\partial_t e_h]_a| + \sum_a |S_a|||\partial_t \mathbf{u}||_\infty K_{f_w}|s_a^+ - s|[\partial_t e_h]_a| &\leq \\
\frac{1}{2}\{\theta_8(K_{14}^2 K_{f_w}^2||\partial_t \mathbf{u}||_\infty^2 ||e_h||^2_{l^2(\Omega)}) + \frac{1}{\theta_8}\sum_a [\partial_t e_h]_a^2\} &+ \\
\frac{1}{2}\{\theta_9(K_{15}^2 K_{f_w}^2 h^2 ||s||^2_{H^2(\Omega)}) + \frac{1}{\theta_9}\sum_a [\partial_t e_h]_a^2\}.&
\end{aligned}$$

Therefore, $D\kappa\sum_a[\partial_t e_h]_a^2 \leq |H_1|+|H_2|+|H^*_{3A}|+|H^*_{3Ba}|+|H^*_{3Bb}|$. Finally, it is choose the values $\theta_i = 16/(D\kappa), i = 1,2,3,5,6,7,8,9$. About $\theta_4 > 0$ it is imposed $\frac{1}{\theta_4} + \theta_4 K_{16}^2 K_{f_w}^2 ||\mathbf{u}||_\infty^2 = \frac{D\kappa}{8}$, with $K_{16}^2 := C_5/C_3$. This last equality for θ_4, has solution under the hypothesis 2.2.27. □

The next lemma, which correspond to Lemma 5.12 in [40], establishes the stability of the decoupled semi discrete schemes.

Lemma 2.6.2 *Let* $(\widetilde{\mathbf{u}}, \widetilde{p}, \widetilde{s})$ *be the solution of (2.3.12)-(2.3.14). Then exists constants* $K_*, K^* > 0$, *independent of* h, *such that for all* $t \in J$ *the following estimates hold:*

$$\begin{aligned}
||\widetilde{\mathbf{u}}(t)||_{L^\infty(\Omega)} + ||\widetilde{p}(t)||_{L^\infty(\Omega)} &\leq K_*, \\
||\widetilde{s}(t)||_{L^\infty(\Omega)} &\leq K^*.
\end{aligned}$$

The next lemma establishes the stability of the nonlinear semi discrete and full discrete schemes.

Lemma 2.6.3 *Let* $(\mathbf{u}_h, p_h, s_h)$ *be the solution of coupled semi discrete scheme defined in Definition 2.3.3, and* $(\mathbf{U}_h, P_h, S_h)$ *be the solution of coupled full discrete scheme defined in Definition 2.3.5. Assuming (A1)-(A10) and considering regularity in Remark 2.2.6.*

Then, there exists constants $K_*, K^* > 0$, independent of h and Δt, such that for all $t \in J$ the following estimates hold, $||\mathbf{u}_h(t)||_{L^\infty(\Omega_T)} \leq K_*$ and $||\mathbf{U}_h||_{L^\infty(\Omega_T)} \leq K_*$.

Proof: both discrete mixed finite element schemes, (2.3.9)-(2.3.10) and (2.3.15)-(2.3.16) can to be considered as particular cases of this discrete problem: given the function $c_h \in l^2(\Omega)$ and $t \in J$ fixed, to find $(\mathbf{w}_h, q_h) \in \mathbf{V}_h \times W_h$, such that for all $(\mathbf{v}_h, \varphi_h) \in \mathbf{V}_h \times W_h$:

$$\begin{aligned} B(\mathbf{w}_h, \varphi_h) &= (F(c_h), \varphi_h) \\ A(c_h; \mathbf{w}_h, \mathbf{v}_h) + B(\mathbf{v}_h, q_h) &= (\mathbf{G}(c_h), \mathbf{v}_h). \end{aligned}$$

This problem was studied in [7] and [17], for example. Therefore, is enough to apply inequality (4.1) of [7], or inequality (7.13) of [17], under the assumptions $a, F \in L^\infty([s_w^o, s_w^e])$ and $\mathbf{G} \in L^\infty([s_w^o, s_w^e])$, with $A(c_h; \mathbf{w}_h, \mathbf{v}_h) := \int_\Omega a(c_h)\mathbf{w}_h \cdot \mathbf{v}_h dx$.
□

Theorem 2.6.4 *Let $(\mathbf{u}_h, p_h, s_h)$ be the solution of (2.3.9)-(2.3.11), $(\widetilde{\mathbf{u}}, \widetilde{p}, \widetilde{s})$ the solution of (2.3.12)-(2.3.14)and $(\mathbf{u}, p, s)$ the weak solution of (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Then, exists a constant $K > 0$, independent of h and D, such that for all $\tau \in J$ the following estimate holds:*

$$||(\mathbf{u}_h - \widetilde{\mathbf{u}})(\tau)||_{H(div;\Omega)} + ||(p_h - \widetilde{p})(\tau)||_{L^2(\Omega)} \leq K(1 + ||\widetilde{\mathbf{u}}(\tau)||_{L^\infty(\Omega)})||(s - s_h)(\tau)||_{L^2(\Omega)}.$$

Proof: subtracting (2.3.2)-(2.3.3) from (2.3.12)-(2.3.13) it is get

$$\begin{gathered} B(\mathbf{u}_h^*, \varphi_h) = (F(s_h) - F(s), \varphi_h), \\ A(s_h; \mathbf{u}_h^*, \mathbf{v}_h) + B(\mathbf{v}_h, p_h^*) = (\mathbf{G}(s_h) - \mathbf{G}(s), \mathbf{v}_h) + A(s; \widetilde{\mathbf{u}}, \mathbf{v}_h) - A(s_h; \widetilde{\mathbf{u}}, \mathbf{v}_h), \end{gathered}$$

which is a discrete saddle point problem in $(\mathbf{u}_h^*, p_h^*) := (\mathbf{u}_h - \widetilde{\mathbf{u}}, p_h - \widetilde{p})$. Finally, the theorem follows from Remark 1.3, pp.117, in [29] and the Lipschitz continuity of $F(\cdot)$, $\mathbf{G}(\cdot)$ and $a(\cdot)$. □

Theorem 2.6.5 *Let $\widetilde{s}$ be the solution of (2.3.14) and let $(\mathbf{u}_h, p_h, s_h)$ be the solution of (2.3.9)-(2.3.11). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Then, exists constants $K_* > 0$ and $K^* > 0$, independent of h and D, such that*

$$D\kappa \int_J \sum_a [e_h]_a^2 + ||e_h||^2_{l^2(\Omega)} \leq K_* \frac{h^2}{(D\kappa)^2} \exp(\frac{K^*}{D\kappa} T),$$

where $e_h := \widetilde{s} - s_h$.

Proof: Subtracting equation (2.3.8) from equation (2.3.14) it is obtained

$$(L_h(\mathbf{u})\tilde{s})_j - (L_h(\mathbf{u}_h)s_h)_j = (-\partial_t s)_j - (-\partial_t s_h)_j,$$

that is,

$$-\frac{D}{T_j}\sum_l (e_l - e_j)\gamma_{jl} + \frac{1}{T_j}\sum_l [g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) - g_{jl}(\mathbf{u}_h; s_{hj}, s_{hl})] = (-\partial_t s)_j - (-\partial_t s_h)_j,$$

that is,

$$(L_h(\mathbf{u}_h)e_h)_j + \frac{1}{T_j}\sum_l [g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) - g_{jl}(\mathbf{u}_h; s_{hj}, s_{hl}) - g_{jl}(\mathbf{u}_h; e_j, e_l)] = (-\partial_t s)_j - (-\partial_t s_h)_j.$$

Multiplication with $e_j T_j$ and summation over all T_j yields after subtraction of $\partial_t \tilde{s}$:

$$(L_h(\mathbf{u}_h)e_h, e_h)_h + \frac{1}{2}\frac{d}{dt}\sum_j T_j e_j^2 =$$

$$-\sum_j e_j \sum_l [g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) - g_{jl}(\mathbf{u}_h; s_{hj}, s_{hl}) - g_{jl}(\mathbf{u}_h; e_j, e_l)] + \sum_j e_j T_j (-\partial_t (s - \tilde{s}))_j.$$

Applying inequality 2.5.1, it is get: $D\kappa\sum_a[e_h]_a^2 + \frac{1}{2}\frac{d}{dt}\sum_j T_j e_j^2 \leq H_1 + H_2$, where $H_1 := \sum_j e_j \sum_l [g_{jl}(\mathbf{u}_h; s_{hj}, s_{hl}) - g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l)]$ and $H_2 := \sum_j e_j T_j(-\partial_t(s-\tilde{s}))_j$. About H_2,

$$
\begin{aligned}
H_2 &\leq |\sum_j e_j T_j(-\partial_t(s-\tilde{s}))_j| \\
&= |\sum_j \int_{T_j} e_j \partial_t(s-\tilde{s})| \\
&= |\int_\Omega e_h \partial_t(s-\tilde{s})| \\
&\leq \int_\Omega |e_h||\partial_t(s-\tilde{s})| \\
&\leq ||e_h||_{L^2(\Omega)}||\partial_t(s-\tilde{s})||_{L^2(\Omega)} \\
&= ||e_h||_{l^2(\Omega)}||\partial_t(s-\tilde{s})||_{L^2(\Omega)} \\
&\leq \frac{1}{2}[\theta_1||e_h||^2_{l^2(\Omega)} + \frac{1}{\theta_1}||\partial_t(s-\tilde{s})||^2_{L^2(\Omega)}] \\
&\leq \frac{1}{2}[\theta_1||e_h||^2_{l^2(\Omega)} + \frac{1}{\theta_1}(K_1h^2||\partial_t s||^2_{H^2(\Omega)} + ||\partial_t(\tilde{s}-I_h(s))||^2_{l^2(\Omega)})] \\
&\leq \frac{1}{2}[\theta_1||e_h||^2_{l^2(\Omega)} + \frac{1}{\theta_1}(K_1h^2||\partial_t s||^2_{H^2(\Omega)} + K_2\sum_a[\partial_t(\tilde{s}-I_h(s))]^2_a)] \\
&\leq \frac{1}{2}[\theta_1 K_0\sum_a[e_h]^2_a + \frac{1}{\theta_1}(K_1h^2||\partial_t s||^2_{H^2(\Omega)} + K_2\sum_a[\partial_t(\tilde{s}-I_h(s))]^2_a)],
\end{aligned}
$$

About H_1, note that $H_1 = H_{1A} + H_{1B} + H_{1C}$, where,

$$
\begin{aligned}
H_{1A} &:= \sum_j e_j \sum_l [g_{jl}(\mathbf{u}_h; s_{hj}, s_{hl}) - \int_{S_{jl}} f_w(s)\mathbf{u}_h\cdot\mathbf{n}_{jl}] \\
H_{1B} &:= -\sum_j e_j \sum_l [g_{jl}(\mathbf{u}; \tilde{s}_j, \tilde{s}_l) - \int_{S_{jl}} f_w(s)\mathbf{u}\cdot\mathbf{n}_{jl}] \\
H_{1C} &:= -\sum_j e_j \sum_l \int_{S_{jl}} f_w(s)(\mathbf{u}-\mathbf{u}_h)\cdot\mathbf{n}_{jl}.
\end{aligned}
$$

About H_{1A},

$$
\begin{aligned}
H_{1A} &= \sum_a (g_a(\mathbf{u}_h; s_{ha}^+, s_{ha}^-) - \int_{S_a} f_w(s)\mathbf{u}_h \cdot \mathbf{n}_a)[e_h]_a \\
&\leq \sum_a [\int_{S_a} (|f_w(s_{ha}^+) - f_w(s)||(\mathbf{u}_h \cdot \mathbf{n}_a)^+| + |f_w(s_{ha}^-) - f_w(s)||(\mathbf{u}_h \cdot \mathbf{n}_a)^-|)]|[e_h]_a| \\
&\leq \sum_a [\int_{S_a} (K_{f_w}|s_{ha}^+ - s||(\mathbf{u}_h \cdot \mathbf{n}_a)^+| + K_{f_w}|s_{ha}^- - s||(\mathbf{u}_h \cdot \mathbf{n}_a)^-|)]|[e_h]_a| \\
&\leq \sum_a ||\mathbf{u}_h||_\infty |S_a| K_{f_w} |s_{ha}^* - s||[e_h]_a| \\
&\leq \sum_a ||\mathbf{u}_h||_\infty |S_a| K_{f_w} (|s_{ha}^* - \tilde{s}_a^*| + |\tilde{s}_a^* - s|)|[e_h]_a| \\
&\leq \sum_a ||\mathbf{u}_h||_\infty |S_a| K_{f_w} (|s_{ha}^* - \tilde{s}_a^*| + |\tilde{s}_a^* - s_a^*| + |s_a^* - s|)|[e_h]_a| \\
&\leq K_{f_w} ||\mathbf{u}_h||_\infty (\sqrt{\sum_a |S_a|^2 |s_{ha}^* - \tilde{s}_a^*|^2} + \sqrt{\sum_a |S_a|^2 |\tilde{s}_a^* - s_a^*|^2} \\
&+ \sqrt{\sum_a |S_a|^2 |s_a^* - s|^2)} \sqrt{\sum_a [e_h]_a^2} \\
&\leq K_{f_w} ||\mathbf{u}_h||_\infty (K_3 ||e_h||_{l^2(\Omega)} + K_4 ||\tilde{s} - I_h(s)||_{l^2(\Omega)} + K_5 h ||s||_{H^2(\Omega)}) \sqrt{\sum_a [e_h]_a^2}.
\end{aligned}
$$

Therefore, applying Lemma 2.6.3 to $||\mathbf{u}_h||_\infty$, it is get

$$
\begin{aligned}
H_{1A} \leq K_{f_w} K_6 K_3 \frac{1}{2}(\theta_2 ||e_h||_{l^2(\Omega)}^2 + \frac{1}{\theta_2} \sum_a [e_h]_a^2) + K_{f_w} K_4 \frac{1}{2}(\theta_3 ||\tilde{s} - I_h(s)||_{l^2(\Omega)}^2 \\
+ \frac{1}{\theta_3} \sum_a [e_h]_a^2) + K_{f_w} K_5 \frac{1}{2}(\theta_4 h^2 ||s||_{H^2(\Omega)}^2 + \frac{1}{\theta_4} \sum_a [e_h]_a^2),
\end{aligned}
$$

About H_{1B},

$$\begin{aligned}
H_{1B} &= -\sum_a (g_a(\mathbf{u}; \tilde{s}_a^+, \tilde{s}_a^-) - \int_{S_a} f_w(s)\mathbf{u}\cdot\mathbf{n}_a)[e_h]_a \\
&\leq \sum_a ||\mathbf{u}||_\infty |S_a| K_{f_w} |\tilde{s}_a^* - s||[e_h]_a| \\
&\leq \sum_a ||\mathbf{u}||_\infty |S_a| K_{f_w} (|\tilde{s}_a^* - s_a^*| + |s_a^* - s|)|[e_h]_a| \\
&\leq K_{f_w} ||\mathbf{u}||_\infty (\sqrt{\sum_a |S_a|^2 |\tilde{s}_a^* - s_a^*|^2} + \sqrt{\sum_a |S_a|^2 |s_a^* - s|^2}) \sqrt{\sum_a [e_h]_a^2} \\
&\leq K_{f_w} ||\mathbf{u}||_\infty (K_7 ||\tilde{s} - I_h(s)||_{l^2(\Omega)} + K_8 h ||s||_{H^2(\Omega)}) \sqrt{\sum_a [e_h]_a^2} \\
&\leq K_{f_w} K_9 K_7 \frac{1}{2} (\theta_5 ||\tilde{s} - I_h(s)||_{l^2(\Omega)}^2 + \frac{1}{\theta_5} \sum_a [e_h]_a^2) \\
&+ K_{f_w} K_9 K_8 \frac{1}{2} (\theta_6 h^2 ||s||_{H^2(\Omega)}^2 + \frac{1}{\theta_6} \sum_a [e_h]_a^2),
\end{aligned}$$

About H_{1C},

$$\begin{aligned}
H_{1C} &= -\sum_j e_j \int_{\partial T_j} f_w(s)(\mathbf{u} - \mathbf{u}_h)\cdot n_j d\sigma \\
&= -\sum_j e_j \int_{T_j} div(f_w(s)(\mathbf{u} - \mathbf{u}_h)) dx \\
&= -\sum_j e_j (\int_{T_j} f_w(s) div(\mathbf{u} - \mathbf{u}_h) dx + \int_{T_j} \nabla f_w(s) \cdot (\mathbf{u} - \mathbf{u}_h) dx) \\
&\leq \int_\Omega |e_h||f_w(s)||div(\mathbf{u} - \mathbf{u}_h)| + \int_\Omega |e_h||\nabla f_w(s)||\mathbf{u} - \mathbf{u}_h| \\
&\leq ||f_w(s)||_{L^\infty(\Omega)} ||e_h||_{L^2(\Omega)} ||div(\mathbf{u} - \mathbf{u}_h)||_{L^2(\Omega)} \\
&+ ||\nabla f_w(s)||_{L^\infty(\Omega)} ||e_h||_{L^2(\Omega)} ||\mathbf{u} - \mathbf{u}_h||_{L^2(\Omega)} \\
&\leq \frac{1}{2}(||f_w(s)||_{L^\infty(\Omega)} + ||\nabla f_w(s)||_{L^\infty(\Omega)})(\theta_7 ||e_h||_{l^2(\Omega)}^2 + \frac{1}{\theta_7} ||\mathbf{u} - \mathbf{u}_h||_{H(div;\Omega)}^2) \\
&\leq \frac{1}{2} K_{10} (\theta_7 K_{11} \sum_a [e_h]_a^2 + \frac{1}{\theta_7} ||\mathbf{u} - \mathbf{u}_h||_{H(div;\Omega)}^2),
\end{aligned}$$

Therefore,

$$
\begin{aligned}
\frac{D\kappa}{2}\sum_a [e_h]_a^2 + \frac{1}{2}\frac{d}{dt}||e_h||^2_{l^2(\Omega)} &\leq \\
\frac{1}{2}\{\frac{1}{\theta_1}(K_1h^2||\partial_t s||^2_{H^2(\Omega)} + K_2\sum_a[\partial_t(\tilde{s}-I_h(s))]_a^2) &+ \\
K_{f_w}[\theta_3K_4+\theta_5K_9K_7]||\tilde{s}-I_h(s)||^2_{l^2(\Omega)} + K_{f_w}h^2[\theta_4K_5+\theta_6K_9K_8]||s||^2_{H^2(\Omega)} &+ \\
\frac{K_{10}}{\theta_7}||\mathbf{u}-\mathbf{u}_h||^2_{H(div;\Omega)} + K_{f_w}K_6K_3\theta_2||e_h||^2_{l^2(\Omega)}\},
\end{aligned}
$$

where $\theta_1 := (\frac{D\kappa}{14})(\frac{2}{K_0})$, $\frac{1}{\theta_2} := (\frac{D\kappa}{14})(\frac{2}{K_{f_w}K_3K_6})$, $\frac{1}{\theta_3} := (\frac{D\kappa}{14})(\frac{2}{K_{f_w}K_4})$, $\frac{1}{\theta_4} := (\frac{D\kappa}{14})(\frac{2}{K_{f_w}K_5})$, $\frac{1}{\theta_5} := (\frac{D\kappa}{14})(\frac{2}{K_{f_w}K_7K_9})$, $\frac{1}{\theta_6} := (\frac{D\kappa}{14})(\frac{2}{K_{f_w}K_8K_9})$, $\theta_7 := (\frac{D\kappa}{14})(\frac{2}{K_{10}K_{11}})$.
About the term $||\mathbf{u}-\mathbf{u}_h||^2_{H(div;\Omega)}$ note that

$$
\begin{aligned}
||\mathbf{u}-\mathbf{u}_h||_{H(div;\Omega)} &= \\
||\mathbf{u}-\mathbf{u}_h+\tilde{\mathbf{u}}-\tilde{\mathbf{u}}||_{H(div;\Omega)} &\leq \\
||\mathbf{u}-\tilde{\mathbf{u}}||_{H(div;\Omega)} + ||\tilde{\mathbf{u}}-\mathbf{u}_h||_{H(div;\Omega)} &\leq \\
K_{12}h + K_{13}||s-s_h||_{L^2(\Omega)} &\leq \\
K_{12}h + K_{13}(||s-\tilde{s}||_{L^2(\Omega)} + ||s_h-\tilde{s}||_{L^2(\Omega)}) &\leq \\
K_{12}h + K_{13}[(K_{14}h||s||_{H^2(\Omega)} + ||\tilde{s}-I_h(s)||_{l^2(\Omega)}) + ||e_h||_{l^2(\Omega)}]. &
\end{aligned}
$$

Collecting the constants gives:

$$
\frac{D\kappa}{2}\sum_a [e_h(t)]_a^2 + \frac{1}{2}\frac{d}{dt}||e_h(t)||^2_{l^2(\Omega)} \leq \frac{K_{14}}{(D\kappa)^2}h^2 + \frac{K_{15}}{D\kappa}||e_h(t)||^2_{l^2(\Omega)}.
$$

After integration with respect to time it is get the statement of the proof by applying Gronwall's Lemma 2.5.2 and using $e_h(0) \equiv 0$:

$$
D\kappa\int_J\sum_a [e_h]_a^2 + ||e_h||^2_{l^2(\Omega)} \leq \frac{K_{14}}{(D\kappa)^2}h^2|J| + \frac{K_{15}}{D\kappa}\int_J ||e_h||^2_{l^2(\Omega)}.
$$

□

Proof of the Theorem 2.4.1. Applying the triangle inequality, Theorem 2.6.1 and

Theorem 2.6.4 it is get:

$$\begin{aligned}
&||\mathbf{u}-\mathbf{u}_h||_{H(div;\Omega)}(t) + ||p-p_h||_{L^2(\Omega)}(t) \leq \\
&||\mathbf{u}-\widetilde{\mathbf{u}}||_{H(div;\Omega)}(t) + ||\widetilde{\mathbf{u}}-\widetilde{\mathbf{u}}_h||_{H(div;\Omega)}(t) + ||p-\widetilde{p}||_{L^2(\Omega)}(t) + ||\widetilde{p}-p_h||_{L^2(\Omega)}(t) \leq \\
&K_1 h + K_2||s-s_h||_{L^2(\Omega)}(t),
\end{aligned}$$

where, using triangle inequality, Lemma 2.5.1, Theorem 2.6.2 and Theorem 2.6.5,

$$\begin{aligned}
&||s-s_h||^2_{L^2(\Omega)}(t) \leq \\
&2(||s-I_h(s)||^2_{L^2(\Omega)}(t) + ||I_h(s)-s_h||^2_{L^2(\Omega)}(t)) \leq \\
&2\{(K_3h^2||s||^2_{H^2(\Omega)} + ||I_h(s)-I_h(s)||^2_{l^2(\Omega)}) + (||I_h(s)-\widetilde{s}||^2_{l^2(\Omega)} + ||\widetilde{s}-s_h||^2_{l^2(\Omega)})\} \leq \\
&2\{K_3h^2||s||^2_{H^2(\Omega)} + (\sum_a [I_h(s)-\widetilde{s}]^2_a + ||\widetilde{s}-s_h||^2_{l^2(\Omega)})\} \leq \\
&2\{K_3h^2||s||^2_{H^2(\Omega)} + [K_4h^2 + (TK_ah^2)exp(2K_bT)]\} \leq \\
&K_5h^2 + (TK_ah^2)exp(2K_bT)].
\end{aligned}$$

Since this holds for all $t \in J$, it is have proved the L^∞-estimate in time. Finally, with Theorem 2.6.2 and Theorem 2.6.5,

$$\begin{aligned}
&D\kappa \int_J \sum_{a\in\mathcal{A}} [I_h(s)(t) - s_h(t)]^2_a dt \leq \\
&2[D\kappa \int_J \sum_{a\in\mathcal{A}} [\widetilde{s}(t) - s_h(t)]^2_a dt + D\kappa \int_J \sum_{a\in\mathcal{A}} [I_h(s)(t) - \widetilde{s}(t)]^2_a dt] \leq \\
&K_6h^2 + (TK_{\mathbf{u}}h^2)exp(2K_wT)]. \ \square
\end{aligned}$$

2.7 Convergence of the full discrete scheme

Lemma 2.7.1 *Let* $\mathbf{w} \in L^\infty(\Omega) \cap H(div;\Omega)$*, with* $div(\mathbf{w}) = 0$ *and let* s_h*, and* z_h *be piecewise constant functions on* Γ_h*. Then,*

$$(L_h(\mathbf{w})s_h, z_h)_h \leq [D\Upsilon(\sum_a [s_h]^2_a)^{1/2} + 2K_{f_w}\sqrt{C_5}||\mathbf{w}||_\infty||s_h||_{l^2(\Omega)}](\sum_a [z_h]^2_a)^{1/2},$$

where C_5 *is from Lemma 2.5.1.*

Proof: by definition

$$(L_h(\mathbf{w})s_h, z_h)_h \le [D\Upsilon(\sum_a [s_h]_a^2)^{1/2} + (\sum_a g_a^2(\mathbf{w}; s_a^+, s_a^-))^{1/2}](\sum_a [z_h]_a^2)^{1/2}.$$

Therefore, is enough to show that

$$\begin{aligned}(\sum_a g_a^2(\mathbf{w}; s_a^+, s_a^-))^{1/2} &= (\sum_a (f_w(s_a^+)w_a^+ + f_w(s_a^-)w_a^-)^2)^{1/2} \\ &\le 2||\mathbf{w}||_\infty(\sum_a (|f_w(s_a^*)||S_a|)^2)^{1/2} \\ &\le 2K_{f_w}||\mathbf{w}||_\infty(\sum_a |s_a^*|^2|S_a|^2)^{1/2} \\ &\le 2K_{f_w}||\mathbf{w}||_\infty\sqrt{C_5}||s_h||_{l^2(\Omega)}.\end{aligned}$$

□

Lemma 2.7.2 *Let $\tilde{S}$ the solution of (2.3.18), $\tilde{s}$ the solution of (2.3.14) and $(\mathbf{u}, p, s)$ the weak solution of (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Define moreover $e_h^n := \tilde{S}^n - \tilde{s}(t_n)$, $0 \le n \le M$. Then there exits a constant $K > 0$, independent of h and Δt, such that*

$$\begin{aligned}||e_h^{n+1} - e_h^n||_{l^2(\Omega)} &\le \sqrt{2}\frac{\Delta t}{h}[D\Upsilon(\sum_a [e_h^n]_a^2)^{1/2} + 2K_{f_w}C_5^{1/2}||\mathbf{u}(t_n)||_\infty||e_h^n||_{l^2(\Omega)}] \\ &+ \Delta t\int_{t_n}^{t_{n+1}} ||\frac{\partial^2 s}{\partial t^2}(x)||_{L^2(\Omega)}dx + h\Delta t(K + C_4^{1/2}||\partial_t s||_{L^\infty(J;H^2(\Omega))}) \\ &+ 8C_5^{1/2}\frac{\Delta t}{h}K_{f_w}||\mathbf{u}||_\infty||e_h||_{l^2(\Omega)},\end{aligned}$$

where the constant $K > 0$ is from Theorem 2.6.3 and the constants $C_4 > 0$ and $C_5 > 0$, are from Lemma 2.5.1.

Proof: let $0 \le n \le M$. Subtracting eq. (2.3.14) from eq. (2.3.18) it is have

$$e_j^{n+1} - e_j^n = -\Delta t(L_h(\mathbf{u}(t_n))e_h^n)_j - \frac{\Delta t}{T_j}\sum_l G_{jl} + \int_{t_n}^{t_{n+1}} [(\partial_t s)(t_n) - \partial_t\tilde{s}(\sigma)]d\sigma,$$

with

$$G_{jl} := g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - g_{jl}(\mathbf{u}(t_n); \tilde{s}_j^n, \tilde{s}_l^n) - g_{jl}(\mathbf{u}(t_n); e_j^n, e_l^n).$$

Multiplying by $T_j(e_j^{n+1}-e_j^n)$, and summing up over j, this yields:

$$||e_h^{n+1}-e_h^n||^2_{l^2(\Omega)} \leq H_1+H_2+H_3+H_4,$$

where,

$$\begin{aligned} H_1 &:= \Delta t|(L_h(\mathbf{u}(t_n))e_h^n, e_h^{n+1}-e_h^n)| \\ H_2 &:= |\int_{t_n}^{t_{n+1}}\int_{t_n}^{\sigma}(\frac{\partial^2 s}{\partial t^2}(s), e_h^{n+1}-e_h^n))dsd\sigma| \\ H_3 &:= |\int_{t_n}^{t_{n+1}}(\partial_t\tilde{s}_j(\sigma)-\partial_t s(\sigma), e_h^{n+1}-e_h^n))| \\ H_4 &:= \Delta t|\sum_j (e_h^{n+1}-e_h^n)\sum_l G_{jl}|. \end{aligned}$$

About H_1, note that applying Lemmas 2.5.1 and 2.7.1 it is get

$$\begin{aligned} H_1 &\leq \Delta t[D\Upsilon(\sum_a [e_h^n]_a^2)^{1/2} + 2K_{f_w}\sqrt{C_5}||\mathbf{u}(t_n)||_\infty ||e_h^n||_{l^2(\Omega)}](\sum_a [e_h^{n+1}-e_h^n]_a^2)^{1/2} \\ &\leq \sqrt{2}\frac{\Delta t}{h}[D\Upsilon(\sum_a [e_h^n]_a^2)^{1/2} + 2K_{f_w}\sqrt{C_5}||\mathbf{u}(t_n)||_\infty ||e_h^n||_{l^2(\Omega)}]||e_h^{n+1}-e_h^n||_{l^2(\Omega)}. \end{aligned}$$

About H_2 : $H_2 \leq \Delta t\int_{t_n}^{t_{n+1}}||\frac{\partial^2 s}{\partial t^2}(x)||_{L^2(\Omega)}dx||e_h^{n+1}-e_h^n||_{l^2(\Omega)}$. About H_3, note that applying Theorem 2.6.3 and Lemma 2.5.1 it is get

$$\begin{aligned} H_3 &\leq \Delta t||\partial_t\tilde{s}-\partial_t s||_{L^\infty(J;L^2(\Omega))}||e_h^{n+1}-e_h^n||_{l^2(\Omega)} \\ &\leq \Delta t(||\partial_t\tilde{s}-\partial_t I_h(s)||_{L^\infty(J;l^2(\Omega))} + ||\partial_t I_h(s)-\partial_t s||_{L^\infty(J;L^2(\Omega))})||e_h^{n+1}-e_h^n||_{l^2(\Omega)} \\ &\leq h\Delta t(K+C_4^{1/2}||\partial_t s||_{L^\infty(J;H^2(\Omega))})||e_h^{n+1}-e_h^n||_{l^2(\Omega)}, \end{aligned}$$

where the constant $K>0$ is from Theorem 2.6.3. About H_4 note that, $H_4 = H_{4A}+H_{4B}$, where $H_{4A} := \Delta t\sum_a(g_a(\mathbf{u}(t_n);\tilde{S}_a^{n,+},\tilde{S}_a^{n,-}) - g_a(\mathbf{u}(t_n);\tilde{s}_a^{n,+},\tilde{s}_a^{n,-}))[e_h^{1+n}-e_h^n]_a$, and $H_{4B} := -\Delta t\sum_a g_a(\mathbf{u}(t_n);e_a^{n,+},e_a^{n,-})[e_h^{1+n}-e_h^n]_a$. About H_{4A}, in first place note that,

$$\begin{aligned} |g_a(\mathbf{u}(t_n);\tilde{S}_a^{n,+},\tilde{S}_a^{n,-}) - g_a(\mathbf{u}(t_n);\tilde{s}_a^{n,+},\tilde{s}_a^{n,-})| &= \\ |(f_w(\tilde{S}_a^{n,+})u_a^+ + f_w(\tilde{S}_a^{n,-})u_a^-) - (f_w(\tilde{s}_a^{n,+})u_a^+ + f_w(\tilde{s}_a^{n,-})u_a^-)| &= \\ |f_w(\tilde{S}_a^{n,+}) - f_w(\tilde{s}_a^{n,+})||u_a^+| + |f_w(\tilde{S}_a^{n,-}) - f_w(\tilde{s}_a^{n,-})||u_a^-| &= \\ K_{f_w}(|e_a^{n,+}||u_a^+| + |e_a^{n,-}||u_a^-|) &\leq \\ K_{f_w}||\mathbf{u}||_\infty|S_a|(|e_a^{n,+}|+|e_a^{n,-}|). \end{aligned}$$

Therefore,

$$\begin{aligned} H_{4A} &\leq \Delta t(\sum_a [K_{f_w}||\mathbf{u}||_\infty |S_a|(|e_a^{n,+}| + |e_a^{n,-}|)]^2)^{1/2} (\sum_a [e_h^{1+n} - e_h^n]_a^2)^{1/2} \\ &\leq 2\Delta t K_{f_w}||\mathbf{u}||_\infty (\sum_a |S_a|^2 (|e_a^{n,+}|^2 + |e_a^{n,-}|^2))^{1/2} \frac{\sqrt{2}}{h} ||e_h^{1+n} - e_h^n||_{l^2(\Omega)} \\ &\leq 2\Delta t K_{f_w}||\mathbf{u}||_\infty (2C_5||e_h||^2_{l^2(\Omega)})^{1/2} \frac{\sqrt{2}}{h} ||e_h^{1+n} - e_h^n||_{l^2(\Omega)}. \end{aligned}$$

On the other hand, about H_{4B}, and analogously to H_{4A},

$$\begin{aligned} H_{4B} &\leq \Delta t(\sum_a (||\mathbf{u}||_\infty K_{f_w} |S_a|(|e_a^{n,+}| + |e_a^{n,-}|))^2)^{1/2} (\sum_a [e_h^{1+n} - e_h^n]_a^2)^{1/2} \\ &\leq 2\Delta t K_{f_w}||\mathbf{u}||_\infty (2C_5||e_h||^2_{l^2(\Omega)})^{1/2} \frac{\sqrt{2}}{h} ||e_h^{1+n} - e_h^n||_{l^2(\Omega)}. \end{aligned}$$

The proof is ending with dividing by $||e_h^{1+n} - e_h^n||_{l^2(\Omega)}$.

□

Theorem 2.7.1 *Let* $\mathbf{u}$, $\tilde{s}$ *and* $\tilde{S}$, *defined as in Lemma 2.7.2. Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Moreover let* Δt, *with the assumptions of Lemma 2.7.2, satisfy the condition:*

$$\frac{1}{D}(16\frac{\Delta t}{h^2} + \frac{4\sqrt{2}}{h}) \leq \frac{\kappa}{\max\{K[(D\Upsilon)^2 + 20K_{f_w}^2 C_5||\mathbf{u}||_\infty^2], \sqrt{C_5}K_{f_w}||\mathbf{u}||_\infty\}}, \tag{2.7.1}$$

where, the constant $K > 0$ *is from Theorem 2.6.3 and* $C_i > 0, i = 4, 5$ *is from Lemma 2.5.1. Then it is have for* $e_h^n := \tilde{S}^n - \tilde{s}(t_n), 0 \leq n, N \leq M$:

$$||e_h^N||^2_{l^2(\Omega)} \leq (1 + \frac{2}{D\kappa})[(\Delta t)^2 (\int_0^{t_N} ||\frac{\partial^2 s}{\partial t^2}||)^2 + T\Delta t h^2 (K^2 + C_4||\partial_t s||^2_{L^\infty(J;H^2(\Omega))})].$$

Proof: following the same ideas of Lemma 2.7.2 it is get

$$e_j^{n+1} - e_j^n + \Delta t(L_h(\mathbf{u}(t_n))e_h^n)_j = -\frac{\Delta t}{T_j}\sum_l G_{jl} + \int_{t_n}^{t_{n+1}} [(\partial_t s)(t_n) - \partial_t \tilde{s}(\sigma)]d\sigma,$$

where

$$G_{jl} := g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - g_{jl}(\mathbf{u}(t_n); \tilde{s}_j^n, \tilde{s}_l^n) - g_{jl}(\mathbf{u}(t_n); e_j^n, e_l^n).$$

Multiplying with $T_j e_j^n$ and summing up over j yields with $a^2 - b^2 - (a-b)^2 = 2(ab - b^2)$:

$$\begin{aligned} \frac{1}{2}(||e_h^{n+1}||^2_{l^2(\Omega)} - ||e_h^n||^2_{l^2(\Omega)}) + \Delta t(L_h(\mathbf{u}(t_n))e_h^n, e_h^n) &= \frac{1}{2}||e_h^{n+1} - e_h^n||^2_{l^2(\Omega)} \\ - \int_{t_n}^{t_{n+1}} (\partial_t \tilde{s}_j(\sigma) - \partial_t s(\sigma), e_h^n) d\sigma - \int_{t_n}^{t_{n+1}} \int_{t_n}^{\sigma} (\frac{\partial^2 s}{\partial t^2}(s), e_h^n)) ds d\sigma &- \Delta t \sum_j e_h^n \sum_l G_{jl}, \end{aligned}$$

but, by inequality 2.5.1, and eliminating $\sum_a g_a(\mathbf{u(t_n)}, e_a^+, e_a^-)[e_h^n]_a$, it is get

$$\begin{aligned} \frac{1}{2}(||e_h^{n+1}||^2_{l^2(\Omega)} - ||e_h^n||^2_{l^2(\Omega)}) + \Delta t D\kappa \sum_a [e_h^n]_a^2 &\leq \frac{1}{2}||e_h^{n+1} - e_h^n||^2_{l^2(\Omega)} \\ - \int_{t_n}^{t_{n+1}} (\partial_t \tilde{s}_j(\sigma) - \partial_t s(\sigma), e_h^n) d\sigma - \int_{t_n}^{t_{n+1}} \int_{t_n}^{\sigma} (\frac{\partial^2 s}{\partial t^2}(x), e_h^n)) dx d\sigma &- \Delta t \sum_j e_h^n \sum_l \tilde{G}_{jl}, \end{aligned}$$

with,

$$\tilde{G}_{jl} := g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - g_{jl}(\mathbf{u}(t_n); \tilde{s}_j^n, \tilde{s}_l^n).$$

Therefore,

$$\begin{aligned} ||e_h^{n+1}||^2_{l^2(\Omega)} - ||e_h^n||^2_{l^2(\Omega)} + 2\Delta t D\kappa \sum_a [e_h^n]_a^2 &\leq \\ ||e_h^{n+1} - e_h^n||^2_{l^2(\Omega)} + 2\Delta t ||\partial_t \tilde{s} - \partial_t s||_{L^\infty(J; L^2(\Omega))} ||e_h^n||_{l^2(\Omega)} &+ \\ 2\Delta t \int_{\Delta t} ||(\frac{\partial^2 s}{\partial t^2})(x)||_{L^2(\Omega)} dx ||e_h^n||_{l^2(\Omega)} + 2\Delta t |\sum_j e_j^n \sum_l \tilde{G}_{jl}|. & \end{aligned}$$

About to the last term in the last inequality,

$$\begin{aligned} 2\Delta t |\sum_j e_j^n \sum_l \tilde{G}_{jl}| &= \\ 2\Delta t |\sum_a \tilde{G}_a [e_h^n]_a| &= \\ 2\Delta t |\sum_a |g_a(\mathbf{u}(t_n); \tilde{S}_a^{n,+}, \tilde{S}_a^{n,+}) - g_a(\mathbf{u}(t_n); \tilde{s}_a^{n,+}, \tilde{s}_a^{n,-})| [e_h^n]_a| &\leq \\ 2\Delta t \sum_a (|S_a| ||\mathbf{u}||_\infty K_{f_w} (|e_a^{n,+}| + |e_a^{n,-}|)) |[e_h^n]_a| &\leq \\ 2\Delta t K_{f_w} ||\mathbf{u}||_\infty \{\sum_a |S_a|^2 (|e_a^{n,+}| + |e_a^{n,-}|)^2\}^{1/2} (\sum_a [e_h^n]_a^2)^{1/2} &\leq \\ 4\Delta t K_{f_w} ||\mathbf{u}||_\infty C_5^{1/2} ||e_h^n||_{l^2(\Omega)} \frac{\sqrt{2}}{h} ||e_h^n||_{l^2(\Omega)}. & \end{aligned}$$

Therefore, applying Lemma 2.7.2 and Hölder's inequality, where $K > 0$ is a constant from Theorem 2.6.3,

$$\begin{aligned}||e_h^{n+1}||^2_{l^2(\Omega)} - ||e_h^n||^2_{l^2(\Omega)} &\leq ||e_h^{n+1}||^2_{l^2(\Omega)} - ||e_h^n||^2_{l^2(\Omega)} + \Delta t D\kappa \sum_a [e_h^n]_a^2 \\ &\leq (\Delta t)^2(1+\theta_2)(\int_{t_n}^{t_{n+1}} ||\frac{\partial^2 s}{\partial t^2}(x)||_{L^2(\Omega)} dx)^2 \\ &+ (h\Delta t)^2(K^2 + C_4||\partial_t s||^2_{L^\infty(J;H^2(\Omega))}) \\ &+ (\Delta t)^2\theta_1||\partial_t\tilde{s} - \partial_t s||^2_{L^\infty(J;L^2(\Omega))}\end{aligned}$$

if

$$4(\frac{\Delta t}{h})^2[4(D\Upsilon)^2 + 80K_{f_w}^2 C_5||\mathbf{u}||^2_\infty] + 4\sqrt{2}\frac{\Delta t}{h}K_{f_w}||\mathbf{u}||_\infty\sqrt{C_5} \leq 2\Delta t D\kappa - \Delta t(\frac{1}{\theta_1} + \frac{1}{\theta_2})$$

with $\theta_1 = \theta_2 = \frac{2}{D\kappa}$. Additionally, note that applying Theorem 2.6.3 and Lemma 2.5.1 it is get

$$||\partial_t\tilde{s} - \partial_t s||^2_{L^2(\Omega)} \leq C_4h^2||\partial_t s||^2_{H^2(\Omega)} + ||I_h(\partial_t s) - \partial_t\tilde{s}||^2_{l^2(\Omega)} \leq C_4h^2||\partial_t s||^2_{H^2(\Omega)} + Kh^2,$$

where $K > 0$ is from Theorem 2.6.3. Finally, summing up over n from 0 to $N-1$ it is get the statement of the theorem.

□

Theorem 2.7.2 *Let* $(\mathbf{U}_h, P_h, S_h)$ *be the solution of (2.3.15)-(2.3.17),* $(\widetilde{\mathbf{u}}, \widetilde{p}, \widetilde{S})$ *the solution of (2.3.12)-(2.3.13)-(2.3.18) and* $(\mathbf{u}, p, s)$ *the weak solution of (2.2.23)-(2.2.25) in the sense of (2.2.20)-(2.2.22). Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Then there exits a constant* $K > 0$*, independent of* h *and* D*, such that*

$$||\mathbf{U}_h^n - \widetilde{\mathbf{u}}_h^n||_{H(div;\Omega)} + ||P_h^n - \widetilde{p}^n||_{L^2(\Omega)} \leq K(||\widetilde{\mathbf{u}}^n||_{L^\infty(\Omega)} + 1)||s(t^n) - S_h^n||_{L^2(\Omega)}.$$

Proof: the proof is completely the same as the proof of Theorem 2.6.4 if $(\mathbf{u}_h, p_h, s_h)$ is replaced by $(\mathbf{U}_h, P_h, S_h)$. □

Lemma 2.7.3 *Let S_h the solution of 2.3.17 and $\tilde{S}$ the solution of 2.3.18. Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Then it is have for the error $e_h^n := \tilde{S}^n - S_h^n, 0 \leq n, N \leq M$:*

$$\begin{aligned}
||e_h^{n+1} - e_h^n||_{l^2(\Omega)} &\leq \sqrt{2}\frac{\Delta t}{h}[D\Upsilon(\sum_a [e_h^n]_a^2)^{1/2} + 2K_{f_w}\sqrt{C_5}||\mathbf{u}||_\infty ||e_h^n||_{l^2(\Omega)}] \\
&+ 2\sqrt{2}K_{f_w}\sqrt{C_5}\frac{\Delta t}{h}||\mathbf{u}||_\infty(||\tilde{S}^n - \tilde{s}(t_n)||_{l^2(\Omega)} + ||s - I_h(s)||_{l^2(\Omega)} \\
&+ ||I_h(s) - \tilde{s}(t_n)||_{l^2(\Omega)}) + 2\sqrt{2}K_{f_w}\sqrt{C_5}\frac{\Delta t}{h}||\mathbf{U}_h^n||_\infty(||\tilde{S}^n - \tilde{s}(t_n)||_{l^2(\Omega)} \\
&+ ||s - I_h(s)||_{l^2(\Omega)} + ||I_h(s) - \tilde{s}(t_n)||_{l^2(\Omega)} + ||e_h^n||_{l^2(\Omega)}) \\
&+ \Delta t||\mathbf{u} - \mathbf{U}_h^n||_{H(div;\Omega)}(||f_w||_\infty + ||\nabla f_w(s)||_\infty) \\
&+ 4\frac{\Delta t}{h}K_{f_w}\sqrt{C_5}||\mathbf{u}||_\infty ||e_h^n||_{l^2(\Omega)},
\end{aligned}$$

where $||\mathbf{U}_h^n||_\infty$ is bounded from Lemma 2.6.3.

Proof: Following the ideas of proof of Lemma 2.7.2, $||e_h^{1+n} - e_h^n||^2_{l^2(\Omega)} = H_1 + H_2$ where $H_1 := -\Delta t(L_h(\mathbf{u}(t_n))e_h^n, e_h^{1+n} - e_h^n)_h$ and $H_2 := \Delta t\sum_j(e_j^{1+n} - e_j^n)\sum_l \tilde{G}_{jl}$, with $\tilde{G}_{jl} := g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - g_{jl}(\mathbf{U}_h^n; S_j^n, S_l^n) - g_{jl}(\mathbf{u}(t_n); e_j^n, e_l^n)$. On the other hand, note that $H_2 = H_{21} + H_{22}$, where $H_{21} := \Delta t\sum_j(e_j^{1+n} - e_j^n)\sum_l(g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - g_{jl}(\mathbf{U}_h^n; S_j^n, S_l^n))$, and $H_{22} := -\Delta t\sum_j(e_j^{1+n} - e_j^n)\sum_l g_{jl}(\mathbf{u}(t_n); e_j^n, e_l^n)$. About H_{21} note that, $H_{21} = H_{21a} - H_{21b} + H_{21c}$, where

$$\begin{aligned}
H_{21a} &:= \Delta t\sum_j(e_j^{1+n} - e_j^n)\sum_l(g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - \int_{S_{jl}} f_w(s)\mathbf{u}(t_n)\cdot\mathbf{n}_{ij}) \\
H_{21b} &:= \Delta t\sum_j(e_j^{1+n} - e_j^n)\sum_l(g_{jl}(\mathbf{U}_h^n; S_j^n, S_l^n) - \int_{S_{jl}} f_w(s)\mathbf{U}_h^n\cdot\mathbf{n}_{ij}) \\
H_{21c} &:= \Delta t\sum_j(e_j^{1+n} - e_j^n)\sum_l\int_{S_{jl}} f_w(s)(\mathbf{u}(t_n) - \mathbf{U}_h^n)\cdot\mathbf{n}_{jl}.
\end{aligned}$$

About H_{21a} note that

$$\begin{aligned}
g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_l^n) - \int_{S_{jl}} f_w(s)\mathbf{u}(t_n)\cdot\mathbf{n}_{ij} &= \\
(f_w(\tilde{S}_j^n) - f_w(s))u_a^+ + (f_w(\tilde{S}_l^n) - f_w(s))u_a^- &\leq \\
K_{f_w}|\tilde{S}_j^n - s||S_a|||\mathbf{u}||_\infty + K_{f_w}|\tilde{S}_l^n - s||S_a|||\mathbf{u}||_\infty,&
\end{aligned}$$

and

$$\tilde{S}_j^n - s = (\tilde{S}_j^n - \tilde{s}(t_n)) - [(s - I_h(s)) + (I_h(s) - \tilde{s}(t_n))].$$

Therefore, applying Hölder's inequality and Lemma 2.5.1 it is get,

$$H_{21a} \leq 2\sqrt{2}K_{f_w}\sqrt{C_5}\frac{\Delta t}{h}||\mathbf{u}||_\infty(||\tilde{S}^n - \tilde{s}(t_n)||_{l^2(\Omega)} + ||s - I_h(s)||_{l^2(\Omega)} + ||I_h(s) - \tilde{s}(t_n)||_{l^2(\Omega)})||e_h^{1+n} - e_h^n||_{l^2(\Omega)}.$$

About H_{21b}, in a similar way of H_{21a}, and applying the identity

$$S_j^n - s = (\tilde{S}_j^n - \tilde{s}(t_n)) - (s - I_h(s)) - (I_h(s) - \tilde{s}(t_n)) - e_j^n,$$

it is get

$$H_{21b} \leq 2\sqrt{2}K_{f_w}\sqrt{C_5}\frac{\Delta t}{h}||\mathbf{U}_h^n||_\infty(||\tilde{S}^n - \tilde{s}(t_n)||_{l^2(\Omega)} + ||s - I_h(s)||_{l^2(\Omega)} + ||I_h(s) - \tilde{s}(t_n)||_{l^2(\Omega)} + ||e_h^n||_{l^2(\Omega)})||e_h^{1+n} - e_h^n||_{l^2(\Omega)}.$$

About H_{21c} note that

$$\begin{aligned}
H_{21c} &= \Delta t \sum_j (e_j^{1+n} - e_j^n) \int_{T_j} div(f_w(s)(\mathbf{u} - \mathbf{U}_h^n))dx \\
&= \Delta t \int_\Omega (e_j^{1+n} - e_j^n) f_w(s) div(\mathbf{u} - \mathbf{U}_h^n)dx + \Delta t \int_\Omega (e_j^{1+n} - e_j^n)\nabla f_w(s) \cdot (\mathbf{u} - \mathbf{U}_h^n)dx \\
&\leq \Delta t||\mathbf{u} - \mathbf{U}_h^n||_{H(div;\Omega)}(||f_w||_\infty + ||\nabla f_w(s)||_\infty)||e_h^{1+n} - e_h^n||_{l^2(\Omega)}.
\end{aligned}$$

About H_{22} note that, applying Hölder's inequality and Lemma 2.5.1 it is get

$$|H_{22}| \leq 4\frac{\Delta t}{h}K_{f_w}\sqrt{C_5}||\mathbf{u}||_\infty||e_h^n||_{l^2(\Omega)}||e_h^{1+n} - e_h^n||_{l^2(\Omega)}.$$

Finally, about H_1 applying Lemma 2.7.1, it is get

$$H_1 \leq \Delta t[D\Upsilon(\sum_a [e_h^n]_a^2)^{1/2} + 2K_{f_w}\sqrt{C_5}||\mathbf{u}||_\infty||e_h^n||_{l^2(\Omega)}]\frac{\sqrt{2}}{h}||e_h^{1+n} - e_h^n||_{l^2(\Omega)}.$$

□

Theorem 2.7.3 *Let S_h the solution of 2.3.17 and $\tilde{S}$ the solution of 2.3.18. Assuming (A1)-(A10) and considering regularity in Remark 2.2.6. Then it is have with the condition,*

$$\frac{\Delta t}{h^2} \leq \frac{D\kappa}{2[10(D\Upsilon)^2 + 84K_{f_w}^2 \frac{C_5}{C_3}(||\mathbf{u}(t_n)||_\infty^2 + ||\mathbf{U}_h^n||_\infty^n)]}, \tag{2.7.2}$$

where the constants $C_i, i = 4, 5$ are from Lemma 2.5.1. Then it is have for the error $e_h^n := \tilde{S}^n - S_h^n, 0 \leq n, N \leq M$:

$$\sum_{n=0}^{N-1} \frac{\Delta t D\kappa}{2} \sum_a [e_h^n]_a^2 + \frac{1}{2}||e_h^N||_{l^2(\Omega)}^2 \leq K^*(h^2 + (\Delta t)^2)e^{K_*}e^{\tilde{K}(\Delta t)^2},$$

where the constants K^*, K_*, and $\tilde{K}$, are independent of parameters h and Δt.

Proof: subtracting 5.19(2.) y 4.8(2.) it is get: $\frac{1}{2}(||e_h^{1+n}||_{l^2(\Omega)}^2 - ||e_h^n||_{l^2(\Omega)}^2) + \Delta t D\kappa \sum_a [e_h^n]_a^2 \leq H_1 + H_2$, where $H_1 := \frac{1}{2}||e_h^{1+n} - e_h^n||_{l^2(\Omega)}^2$ and $H_2 := -\Delta t \sum_j e_j^n \sum_l G_{jl}$, with $G_{jl} := g_{jl}(\mathbf{u}(t_n); \tilde{S}_j^n, \tilde{S}_j^n) - g_{jl}(\mathbf{U}_h^n; S_j^n, S_j^n)$. Applying Lemma 2.7.3 to H_1, following the same ideas of Lemma 2.7.3's proof to H_2, and considering that

$$\begin{aligned}
||\mathbf{u}(t_n) - \mathbf{U}_h^n||_{H(div;\Omega)}^2 &\leq \\
2(||\mathbf{u}(t_n) - \tilde{\mathbf{u}}(t_n)||_{H(div;\Omega)}^2 + ||\tilde{\mathbf{u}}(t_n) - \mathbf{U}_h^n||_{H(div;\Omega)}^2) &\leq \\
2(K_1 h^2 + K_2||s(t_n) - S_h^n||_{L^2(\Omega)}^2) &\leq \\
2(K_1 h^2 + 2K_2(||s(t_n) - I_h(s)||_{L^2(\Omega)}^2 + ||S_h^n - I_h(s)||_{L^2(\Omega)}^2)) &\leq \\
2(K_1 h^2 + 2K_2[||s(t_n) - I_h(s)||_{L^2(\Omega)}^2 + 2(||S_h^n - \tilde{S}^n||_{L^2(\Omega)}^2 + ||I_h(s) - \tilde{S}^n||_{L^2(\Omega)}^2)]) &\leq \\
2(K_1 h^2 + 2K_2[C_4 h^2||s||_{H^2(\Omega)}^2 + 2(||e_h^n||_{l^2(\Omega)}^2 + K_3(h^2 + \Delta t^2))]) &\leq \\
K_4(h^2 + \Delta t^2) + K_5||e_h^n||_{l^2(\Omega)}^2, &
\end{aligned}$$

$||\tilde{S}^n - \tilde{s}(t_n)||_{l^2(\Omega)}^2 \leq K_6(h^2 + \Delta t^2)$, and $||I_h(s) - \tilde{s}(t_n)||_{l^2(\Omega)}^2 \leq K_7 h^2$, it is get (applying Lemma 2.6.3 to $||\mathbf{U}_h^n||_\infty$)

$$\frac{1}{2}(||e_h^{1+n}||_{l^2(\Omega)}^2 - ||e_h^n||_{l^2(\Omega)}^2) + \frac{\Delta t D\kappa}{2} \sum_a [e_h^n]_a^2 \leq K_7(h^2 + (\Delta t)^2) + (K_8 + K_9(\Delta t)^2)||e_h^n||_{l^2(\Omega)}^2,$$

if

$$\Delta t D\kappa - (\frac{\Delta t}{h})^2[10(D\Upsilon)^2 + 84K_{f_w}^2 \frac{C_5}{C_3}(||\mathbf{u}(t_n)||_\infty^2 + ||\mathbf{U}_h^n||_\infty^n)] \geq \frac{\Delta t D\kappa}{2}.$$

Finally, it is applied the Gronwall's inequality in Lemma 2.5.3 to finish the proof. □

Proof of Theorem 2.4.2. The proof of this result will be given in the same way as in Theorem 2.4.1. Applying Theorems 2.6.1 and 2.7.2, it is get that for all $t^n \in J_h$, exits constants $K_1, K_2 > 0$, such that

$$\begin{aligned}
||\mathbf{u}(t^n) - \mathbf{U}_h^n||^2_{H(div;\Omega)} + ||p(t^n) - P_h^n||^2_{L^2(\Omega)} \leq \\
(||\mathbf{u}(t^n) - \mathbf{U}_h^n||_{H(div;\Omega)} + ||p(t^n) - P_h^n||_{L^2(\Omega)})^2 \leq \\
(||\mathbf{u}(t^n) - \widetilde{\mathbf{u}}^n||_{H(div;\Omega)} + ||\widetilde{\mathbf{u}}^n - \mathbf{U}_h^n||_{H(div;\Omega)} + ||p(t^n) - \widetilde{p}^n||_{L^2(\Omega)} + ||\widetilde{p}^n - P_h^n||_{L^2(\Omega)})^2 \leq \\
4(K_1 h^2 + K_2||s(t^n) - S_h^n||^2_{L^2(\Omega)}),
\end{aligned}$$

but,

$$||s(t^n) - S_h^n||^2_{L^2(\Omega)} \leq 3(||s(t^n) - I_h(s)(t^n)||^2_{L^2(\Omega)} + ||I_h(s)(t^n) - \widetilde{S}^n||^2_{L^2(\Omega)} + ||\widetilde{S}^n - S_h^n||^2_{L^2(\Omega)}).$$

In this last inequality, about $||s(t^n) - I_h(s)(t^n)||^2_{L^2(\Omega)}$, applying Lemma 2.5.1, it is get that exits a constant $K_3 > 0$, such that $||s(t^n) - I_h(s)(t^n)||^2_{L^2(\Omega)} \leq C_4 h^2 ||s||^2_{H^2(\Omega)} \leq K_3 h^2$. About $||I_h(s)(t^n) - \widetilde{S}^n||^2_{L^2(\Omega)}$, applying Lemma 2.5.1, Theorem 2.6.2 and Theorem 2.7.1, it is get that exits constants $K_4, K_5 > 0$, such that

$$\begin{aligned}
||I_h(s)(t^n) - \widetilde{S}^n||^2_{L^2(\Omega)} \leq \\
2(||I_h(s)(t^n) - \widetilde{s}(t^n)||^2_{L^2(\Omega)} + ||\widetilde{s}(t^n) - \widetilde{S}^n||^2_{L^2(\Omega)}) = \\
2(||I_h(s)(t^n) - \widetilde{s}(t^n)||^2_{l^2(\Omega)} + ||\widetilde{s}(t^n) - \widetilde{S}^n||^2_{l^2(\Omega)}) \leq \\
2[K_4 h^2 + K_5((\Delta t)^2 + h^2)].
\end{aligned}$$

About $||\widetilde{S}^n - S_h^n||^2_{L^2(\Omega)}$, applying Lemma 2.5.1 and Theorem 2.7.3, it is get that exits constants $K_7, K_8 > 0$, such that

$$||\widetilde{S}^n - S_h^n||^2_{L^2(\Omega)} = ||\widetilde{S}^n - S_h^n||^2_{l^2(\Omega)} \leq K_7((\Delta t)^2 + h^2)e^{K_8(\Delta t)^2}.$$

This completes the proof. □

Remark 2.7.1 *The error estimates in Theorem 2.4.2 are obtained under high regularity assumptions for the solution of the continuous model. This regularity holds in the situation under consideration here, since the problem is assumed regular non degenerate. As the lower bound for the diffusivity approaches 0, the estimates blow up. (Comment of Professor I.S.Pop).*

In Chapter 4 you can find computational experiments for the fluid flow problem in heap leaching.

Chapter 3

Transport Problem

In this chapter a solute transport model, from copper heap leaching industry, is considered. The mathematical model consists in a differentials equations's system: two diffusion-convection-reaction equations with Neumann boundary conditions, and one ordinary differential equation. The numerical scheme consists in a combination of finite volume and finite element methods. A Godunov scheme is used for the convection term and an P1-FEM for the diffusion term. The convergence analysis is based on standard compactness results in L^2.

3.1 Introduction

Leaching is a mass transfer process between the leaching solution (fluid phase) and the ore bed (solid phase) [25, 39]. The heap leaching process, for copper production, can be considered as a *flow of two fluids phases* (liquid and gaseous) and *components transport* (sulfuric acid, copper's ions, water, air, oxigen, for example) in a porous medium (the heap) [14, 36, 41, 47]. Therefore, the two phenomena of interest are: the fluids flow and the physicochemical reactions. In this work it is follow the *decoupled approach*, where these two phenomena can be studied separately if the extent of leaching does not influence the flow pattern. In other words, the flow pattern in a heap depends on the initial conditions of the heap only.

The first problem, i.e., the fluids's flow in heap leaching has been studied in [9, 10, 36, 46], for example. Specifically, Cariaga et.al., in [9], studied the application of classical two phase flow equations (cf. [15, 30], for an study of this equations in a more general context) to heap leaching. On the other hand, the components's transport problem, i.e., the physicochemical reactions phenomena, has been studied in [8, 36, 39, 46], for example. Specifically, [8] and [36] studied this problem in the two phase context, but without any theoretical convergence analysis. In the present work, it is studied the convergence of a numerical scheme for the transport model proposed in [8], which consists in the system formed by the equations (3.2.3), (3.2.4) and (3.2.5). In the model the nonlinearity of diffusion term is relevant and cannot be neglected. Additionally, this diffusion term degenerates in one point: when the volumetric concentration is equal to zero. The main difficulties related to the convergence of the approximate solution of such equations is the degeneracy of the diffusion term, the solution then lacks regularity. By this reason, the convergence analysis is done by means of a priori estimates in L^∞ and L^2 estimates without any CFL conditions.

The numerical scheme consists in an combined approach, i.e, for the convective term it is applied a finite volume scheme, upwind Godunov, and for the diffusive term it is applied a P_1 finite element method. This combined approach was applied by in [2], where their mathematical problem consists in a nonlinear, degenerate, and convection-diffusion equation, and without reaction term. The mathematical problem considers a reactive term, a system formed by a convection-diffusion-reaction equation and an ordinary differential equation, non homogeneous Neumann boundary conditions, which corresponds to the physical behavior of the irrigation and infiltration processes in heap leaching.

The chapter is organized as follows. In section 3.2, it is stated the compositional flow model for the volumetric concentration of sulfuric acid in liquid phase and for the copper's ions in liquid and solid phase. In section 3.3, it is stated the finite volume scheme, where a Godunov's scheme is used for the approximation of the convective term. Additionally, for the diffusive term, let us consider a standard P_1-FEM. In sections 3.4 and 3.5 it is presented the main convergence results, for sulfuric acid equation and for the copper system, respectively. It is derived L^∞ and L^2 estimates.

3.2 Compositional Flow Model.

It is considered a two phase (liquid and gaseous phase)-two component (sulfuric acid and copper) system 2p2c, in the porous medium formed by the heap. Let a REV (*representative elementary volume*) (see [5, 30] for more details). The porosity ϕ of the porous medium is defined as the ratio between the *volume of the pore space within the* REV and *the volume of* REV, and the saturation of phase $\alpha = w, n$ (where $\alpha = w$ is the liquid phase and $\alpha = n$ is the gaseous phase), s_α, is defined as the ratio between the *volume of fluid α within the* REV and the *volume of the pore space within the* REV. It is imposed the customary property that the fluids fill the volume: $s_w + s_n = 1$. A mass balance must be specified for each component. The mass balance equations for the transport of component κ ($\kappa = a$ for the sulfuric acid, and $\kappa = c$ for the copper) in α-phase can be written as [3], [30]:

$$\frac{\partial\left(\theta_\alpha c_\kappa^\alpha\right)}{\partial t} + \nabla\cdot\left(c_\kappa^\alpha \mathbf{v}_\alpha - \mathbf{D}(\mathbf{v}_\alpha)\nabla c_\kappa^\alpha\right) + \Phi_\alpha = 0, \tag{3.2.1}$$

where c_κ^α is the volumetric concentration defined as the ratio between the *mass of component κ in phase α* and the *volume of phase α*, $\theta_\alpha := \phi s_\alpha$, is the liquid content, $\mathbf{v}_\alpha$ is the *Darcy's flow of phase α*, Φ_α $[kg/m^3 \cdot s]$ is the irreversible rate of solute removed (or added) from (to) the liquid solution, $\mathbf{D}$ is the dispersity-diffusion tensor given by $D_{ij} := \alpha_L\left|\mathbf{v}_\alpha\right|\delta_{ij} + (\alpha_L - \alpha_T)\frac{u_i u_j}{|\mathbf{v}_\alpha|} + D_m\delta_{ij}$, where α_L and α_T are the longitudinal and transverse dispersities, respectively, $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$, and D_m is the molecular diffusion coefficient (in this paper $D_m = 0$).

On the other hand, if is assumed that there is a isotherm between the liquid phase and the solid phase $\varphi_\kappa^\alpha = \varphi_\kappa^\alpha(c_\kappa^\alpha)$, defined as the ratio between the *mass of component in solid phase* and *mass of solid phase*, then (using the assumption that sorption only occurs from the liquid to the solid phase), the equation for the liquid phase can be modified to include adsorption:

$$\frac{\partial\left(\phi_s\rho_s\varphi_\kappa^\alpha\right)}{\partial t} + \frac{\partial\left(\theta_\alpha c_\kappa^\alpha\right)}{\partial t} + \nabla\cdot\left(c_\kappa^\alpha \mathbf{v}_\alpha - \mathbf{D}(\mathbf{v}_\alpha)\nabla c_\kappa^w\right) + \Phi_\alpha = 0, \tag{3.2.2}$$

where $\phi_s := 1 - \phi$, ρ_s is ore bulk density. Note that the most common sorption isotherms (cf. [32]) are *Langmuir* type: $\varphi_\kappa^\alpha(w) := \frac{k_1 w}{1+k_2 w}$, or *Freundlich* type: $\varphi_\kappa^\alpha(w) := k_3 w^p, 0 < p$, or *mixed* type: $\varphi_\kappa^\alpha := \frac{k_4 w^p}{1+k_5 w^p}$.

Decoupled Approach. In the general transport equation (3.2.1) it is **suppose** that, for $\alpha = w, n$, the functions $\theta_\alpha = \phi s_\alpha$ and $\mathbf{v}_\alpha$, are known from the classical two phase flow equations (cf. system (2.2.1)-(2.2.6) and related analysis):

$$\begin{aligned}
\phi\frac{\partial s_w}{\partial t} + \nabla\cdot\mathbf{v}_w &= 0,\\
\phi\frac{\partial s_n}{\partial t} + \nabla\cdot\mathbf{v}_n &= 0,\\
\mathbf{v}_w &= -k\frac{k_{rw}}{\mu_w}(\nabla p_w - \rho_w\mathbf{g}),\\
\mathbf{v}_n &= -k\frac{k_{rn}}{\mu_n}(\nabla p_n - \rho_n\mathbf{g}),\\
p_c(s_w) &= p_n - p_w,\\
s_w + s_n &= 1,
\end{aligned}$$

where k is the absolute permeability of the porous medium, p_α, μ_α, $k_{r\alpha}$ are the pressure, viscosity and the relative permeability of the α-phase, respectively, and $\mathbf{g}$ is the gravitational, downward-pointing, constant vector, and p_c is the capillary pressure.

Remark 3.2.1 *The nonlinearities $k_{rw}(\cdot)$ and $p_c(\cdot)$ are chosen such that the functions s_w and $\mathbf{u} = \mathbf{v}_w + \mathbf{v}_n$ are the weak solution of system (2.2.23)-(2.2.25), in the sense of (2.2.20)-(2.2.22).*

Basic Chemical Reaction

In this thesis, and in this chapter it is considered oxide's minerals only, which in general terms, have the following chemical reaction of dissolution (cf. [25, 39, 46]),

$$MinOxCu_{(s)} + 2H^+_{(aq)} \rightarrow Cu^{2+}_{(aq)} + H_2O_{(l)},$$

where $MinOxCu_{(s)}$ represent a oxides minerals of copper, present in the ore.

Remark 3.2.2 *For this Basic Chemical Reaction defined is enough to consider a not saturated flow. That is, about the fluid flow problem is enough to solve the Richard's* *equation (make p_n equal to a constant on $\Omega \times (0,T)$ in the two phase flow system (2.2.1)-(2.2.6).*

3.2.1 Sulfuric acid transport equation

From (3.2.1) with $\Phi_\alpha := \theta_w \mu c_a^w$, the transport equation of sulfuric acid in leach solution is given by (cf. Chapter 1, for more details)

$$\frac{\partial(\phi_s \rho_s \varphi_a^w(c_a^w))}{\partial t} + \frac{\partial(\theta_w c_a^w)}{\partial t} + \nabla \cdot (c_a^w \mathbf{v}_w - \mathbf{D}(\mathbf{v}_w)\nabla c_a^w) + \theta_w \mu c_a^w = 0, \tag{3.2.3}$$

where μ is a first-order reaction constant (consumption factor) and c_a^w is the volumetric concentration of sulfuric acid in leach solution.

3.2.2 Copper transport equation in liquid phase

From (3.2.2) with $\Phi_\alpha := \phi_s \rho_s k_e c_a^w c_c^s$, the transport equation of copper in leach solution is given by (cf. Chapter 1, for more details)

$$\frac{\partial(\phi_s \rho_s \varphi_c^w(c_c^w))}{\partial t} + \frac{\partial(\theta_w c_c^w)}{\partial t} + \nabla \cdot (c_c^w \mathbf{v}_w - \mathbf{D}(\mathbf{v}_w)\nabla c_c^w) - \theta_w \rho_s k_e c_a^w c_c^s = 0, \tag{3.2.4}$$

where k_e is a first-order kinetic constant, c_c^s is the concentration of copper associated with the solid phase (cf.(3.2.5)) and c_c^w is the volumetric concentration of copper in leach solution.

3.2.3 Copper transport equation in solid phase

The change in the concentration of copper in the solid phase follows the mass balance [39]:

$$\frac{\partial c_c^s}{\partial t} + \theta_w k_e c_a^w c_c^s = \frac{\partial(\phi_s \varphi_c^w(c_c^w))}{\partial t}, \tag{3.2.5}$$

where c_c^s is the concentration of copper in solid phase, *i.e.*,

$$c_c^s := \frac{\text{mass of copper in solid phase}}{\text{mass of solid phase}}.$$

3.2.4 Initial and boundary conditions

It is considered a 2D geometry, i.e, a transversal cut of the heap (cf. Figure 3, p.6). The boundary of $\Omega \subset \mathbb{R}^2$, i.e., $\partial\Omega$ is expressed as $\partial\Omega = \Gamma^i \cup \Gamma^o \cup \Gamma^t$, where Γ^i is the input boundary (zone of irrigation), Γ^o is the output boundary (zone of drainage), and Γ^t is the atmospheric boundary:

$$
\begin{array}{rclll}
(c_a^w \mathbf{v}_w - \mathbf{D}\nabla c_a^w) \cdot \mathbf{n} & = & c_a^i \mathbf{v}_w \cdot \mathbf{n} & \mathbf{x} \in \Gamma^i & t \geq 0 \\
(c_{a,c}^w \mathbf{v}_w - \mathbf{D}\nabla c_{a,c}^w) \cdot \mathbf{n} & = & 0 & \mathbf{x} \in \Gamma^t & t \geq 0 \\
(c_{a,c}^w \mathbf{v}_w - \mathbf{D}\nabla c_{a,c}^w) \cdot \mathbf{n} & = & (c_{a,c}^w - c_{a,c}^o)\mathbf{v}_w \cdot \mathbf{n} & \mathbf{x} \in \Gamma^o & t \geq 0 \\
(c_c^w \mathbf{v}_w - \mathbf{D}\nabla c_c^w) \cdot \mathbf{n} & = & 0 & \mathbf{x} \in \Gamma^i & t \geq 0 \\
c_{a,c}^w(\mathbf{x}, t) & = & c_{a,c}^o & \mathbf{x} \in \Omega & t = 0 \\
c_c^s(\mathbf{x}, t) & = & c_c^{so} & \mathbf{x} \in \Omega & t = 0,
\end{array}
\tag{3.2.6}
$$

where, as usual, $\mathbf{n}$ is the unit normal vector to $\partial\Omega$, outward to Ω, $c_{a,c}^i$ concentration of sulfuric acid and copper in the irrigation solution, $c_c^{so} := \lambda_c^s G_c^s$, with λ_c^s is the leachable fraction of the total copper contained in the heap and G_c^s is the grade of the ore.

3.2.5 Model problem for convergence analysis

By simplicity in the notation it is considered a change. In effect, c_a^w will be denoted as u_1, c_c^w as u_2, c_c^s as u_3, $\mathbf{v}_w$ as $\mathbf{v}$, φ_a^w as φ_1, and φ_c^w as φ_2. Therefore, the compositional flow model, in simplified notation, consists in to find functions (u_1, u_2, u_3) such that

$$
\begin{array}{rcl}
\dfrac{\partial(\theta_s \varphi_1(u_1))}{\partial t} + \dfrac{\partial(\theta_w u_1)}{\partial t} + \nabla \cdot (u_1 \mathbf{v} - \mathbf{D}(\mathbf{v})\nabla u_1) & = & -\theta_w \mu u_1 \\
\dfrac{\partial(\theta_s \varphi_2(u_2))}{\partial t} + \dfrac{\partial(\theta_w u_2)}{\partial t} + \nabla \cdot (u_2 \mathbf{v} - \mathbf{D}(\mathbf{v})\nabla u_2) & = & \theta_w \rho_s k_e u_1 u_3 \\
\dfrac{\partial u_3}{\partial t} + \theta_w k_e u_1 u_3 & = & \dfrac{\partial(\phi_s \varphi_2(u_2))}{\partial t},
\end{array}
$$

where $\theta_s = \phi_s \rho_s$. However, note that if, for $i = 1, 2$, it is introduced the auxiliary function

$$
U_i(x, t) := \psi_i(u_i(x, t)) := \theta_s \varphi_i(u_i(x, t)) + \theta_w(x, t) u_i(x, t),
$$

such that $\alpha_i(U_i) := \psi_i^{-1}(U_i) = u_i$ is well defined, then the **Model Problem A** (in the unknown U_1) for convergence analysis is defined as

$$\partial_t U_1 + \nabla \cdot (\alpha_1(U_1)\mathbf{v} - \mathbf{D}(\mathbf{v})\nabla\alpha_1(U_1)) = -\theta_w \mu \alpha_1(U_1), \tag{3.2.7}$$

and the **Model Problem B** (in the unknowns U_2 and u_3) as

$$\partial_t U_2 + \nabla \cdot (\alpha_2(U_2)\mathbf{v} - \mathbf{D}(\mathbf{v})\nabla\alpha_2(U_2)) = \theta_w \rho_s k_e \alpha_1(U_1) u_3 \tag{3.2.8}$$

$$\frac{\partial u_3}{\partial t} + \theta_w k_e \alpha_1(U_1) u_3 = \frac{\partial(\phi_s \varphi_2(\alpha_2(U_2)))}{\partial t}. \tag{3.2.9}$$

Note that the Model Problem A and Model Problem B are decoupled. By another hand, in the Model Problem B, both equations are coupled in the reactive term.

Remark 3.2.3 *About the diffusive term $\nabla\alpha_i(U_i) = \alpha_i^{'}\nabla U_i, i = 1, 2$, in the equations (3.2.7) and (3.2.8), note that, for example, for a Freundlich isotherm $\varphi_i(u_i) := cu_i^p, c > 0$, with $0 < p < 1$, it is have that if $u_i \longrightarrow 0$, then $\varphi_i^{'} \longrightarrow \infty$, i.e.,*

$$\alpha_i^{'} = \frac{1}{\psi_i^{'}} = \frac{1}{\theta_s \varphi_i^{'}(u_i) + (\theta_w u_i)^{'}} \longrightarrow 0,$$

i.e., the transport equations (3.2.7) and (3.2.8) are degenerate (cf. [2, 32, 45]). This mathematical property is in according with the physical behavior of u_1 and u_2 in heap leaching operations.

3.2.6 Weak formulation

Model Problem A

A weak solution U_1 of the model problem A is a function $U_1 :]0, T[\rightarrow W$, with $\partial_t U_1 \in L^2(0, T; H^{-1}(\Omega))$ and $\alpha_1 \in L^2(0, T; H^1(\Omega))$, such that, for all $\phi \in V$

$$\begin{aligned} \int_{Q_T} (U_1 \partial_t \phi &+ (\alpha_1(U_1)\mathbf{v} - \mathbf{D}(\mathbf{v})\nabla\alpha_1(U_1)) \cdot \nabla\phi - \mu\theta_w \alpha_1(U_1)\phi) \\ &+ \int_\Omega U_1^o \phi^o - \int_0^T < \phi, U_1^i \mathbf{v}\cdot\mathbf{n} >_{\Gamma^i} - \int_0^T < \phi, (U_1 - U_1^o)\mathbf{v}\cdot\mathbf{n} >_{\Gamma^o} = 0, \end{aligned}$$

where $V := \{v \in C^1(0,T;C^2(\overline{\Omega})); v(\cdot;T) = 0\}$, $W := \{w \in L^2(\Omega); \alpha_i(w) \in H^1(\Omega), i = 1,2\}$ and $H^{-1}(\Omega)$ is the dual space of $H^1(\Omega)$.

Existence and Uniqueness for Model Problem A. A mathematical analysis of Model Problem A can be found, v.g. in [1] and [15]. For an existence and uniqueness analysis for Model Problem A, in the context of entropy solutions, to see the classical paper [13].

Model Problem B

A weak solution (U_2, u_3) of the model problem B is a function $U_2 :]0,T[\to W$, with $\partial_t U_2 \in L^2(0,T;H^{-1}(\Omega))$ and $\alpha_2 \in L^2(0,T;H^1(\Omega))$, such that, for all $\phi \in V$

$$\begin{aligned}\int_{Q_T}(U_2\partial_t\phi \quad &+ \quad (\alpha_2(U_2)\mathbf{v} - \mathbf{D}(\mathbf{v})\nabla\alpha_2(U_2))\cdot\nabla\phi + k_e\rho_s\theta_w\alpha_1(U_1)u_3\phi)\\ &+ \quad \int_\Omega U_2^o\phi^o - \int_0^T < \phi, U_2^i\mathbf{v}\cdot\mathbf{n} >_{\Gamma^i} - \int_0^T < \phi, (U_2 - U_2^o)\mathbf{v}\cdot\mathbf{n} >_{\Gamma^o} = 0,\end{aligned}$$

and a function $u_3 :]0,T[\to W$, with $\partial_t u_3 \in L^2(0,T;H^{-1}(\Omega))$, such that, for all $\psi \in V$

$$\int_{Q_T}\frac{\partial u_3}{\partial t}\psi + \int_{Q_T}\theta_w k_e\alpha_1(U_1)u_3\psi = \int_{Q_T}\frac{\partial(\phi_s\varphi_2(\alpha_2(U_2)))}{\partial t}\psi. \tag{3.2.10}$$

Existence and Uniqueness for Model Problem B. For existence analysis of Model Problem B to see [32], and for uniqueness analysis of Model Problem B to see [33]. By another hand, a similar model to Model Problem B was studied in [45] with an operator splitting scheme.

3.3 Finite volume discretization

Now it is presented the definition of *admissible mesh*, which is taken from [28] (cf. Definition 9.1, p.762 in [28]). In this chapter an admissible mesh is considered.

Definition 3.3.1 *(Admissible Mesh). Let Ω be an open bounded polygonal subset of $\mathbb{R}^d, d = 2,3$. An admissible finite volume mesh of Ω, denoted by $\mathcal{T}$, is given by a family of "control* *volumes", which are open polygonal convex subset of* Ω, *a family of subsets of* $\overline{\Omega}$ *contained in hyperplanes of* $\mathcal{R}^d$, *denoted by* $\mathcal{E}$ *(these are the edges* $(d = 2)$ *or sides* $(d = 3)$ *of the control volumes), with strictly positive* $(d-1)$*-dimensional measure, and a family of points of* Ω *denoted by* $\mathcal{P}$ *satisfying the following properties:*

1. *The closure of the union of all the control volumes is* $\overline{\Omega}$.

2. *For any* $M \in \mathcal{T}$, *there exists a subset* $\mathcal{E}_M$ *of* $\mathcal{E}$ *such that* $\partial M = \overline{M} \backslash M = \cup_{\sigma \in \mathcal{E}_M} \overline{\sigma}$. *Furthermore,* $\mathcal{E} = \cup_{M \in \mathcal{T}} \mathcal{E}_M$.

3. *For any* $(M, L) \in \mathcal{T}^2$ *with* $M \neq L$, *either the* $(d-1)$*-dimensional Lebesgue measure of* $\overline{M} \cap \overline{L}$ *is* 0 *or* $\overline{M} \cap \overline{L} = \overline{\sigma}$ *for some* $\sigma \in \mathcal{E}$, *which then be denoted by* $M|L$ *or* l.

4. *The family* $\mathcal{P} = (x_M)_{M \in \mathcal{T}}$ *is such that* $x_M \in \overline{M}$ *(for all* $M \in \mathcal{T}$*) and, if* $\sigma = M|L = l$, *it is assumed that* $x_M \neq x_L$, *and that the straight line* $\mathcal{D}_{M,L}$ *going through* x_M *and* x_L *is orthogonal to* $M|L = l$.

5. *For any* $\sigma \in \mathcal{E}$ *such that* $\sigma \subset \partial\Omega$, *let* M *be the control volume such that* $\sigma \in \mathcal{E}_M$. *If* $x_M \notin \sigma$, *let* $\mathcal{D}_{M,\sigma}$ *be the straight line going through* x_M *and orthogonal to* σ, *then the condition* $\mathcal{D}_{M,\sigma} \cap \sigma \neq \emptyset$ *is assumed; let* $y_\sigma = \mathcal{D}_{M,\sigma} \cap \sigma$.

Remark 3.3.1 *In this chapter, it is considered as admissible mesh (cf. Definition 3.3.1):* $\mathcal{T}$, *a* Donald Dual *mesh (cf. [34], p.158, Figure 3.2.2), generated by an finite element triangulation (cf. [23], p.38):* $\Lambda := \{T_i, i = 1, ..., N_e\}$. *Note that* x_T, *the barycenter of* $T \in \Lambda$, *is such that* $x_T = \cap_{M \cap T \neq \varnothing} \partial M \in T$, $x_M := \cap_{T \cap M \neq \varnothing} \partial T \in M$, *a node in the triangulation,* $l := \partial M_i \cap \partial M_j \cap T$ *the line segment between the points* x_T *and the midpoint of* (x_{M_i}, x_{M_j}) *and let* $\pounds_h := \{l \in \partial M \backslash \Gamma, M \in \mathcal{T}\}$.

Remark 3.3.2 *The time discretization may be performed with a variable time step; in order to simplify the notations, it is considered a constant time step* $\Delta t \in (0, T)$. *Let* $N_{\Delta t} \in \mathbb{N}^*$ *such that* $N_{\Delta t} := \max\{n \in \mathbb{N}, nk < T\}$, *and it is denoted* $t_n = n\Delta t$, *for* $n \in \{0, ..., N_{\Delta t+1}\}$.

In the sequel, the following notations is used. The mesh size is defines by: h:=size($\mathcal{T}$)=sup{diam(M),$M \in \mathcal{T}$}. For any $M \in \mathcal{T}$, $m(M) \equiv |M|$ is the d-dimensional Lebesgue measure of M (it is the area of M if $d = 2$). The set of neighbours of M is denoted by $\mathcal{N}(M)$, i.e., $\mathcal{N}(M) = \{L \in \mathcal{T}; \exists \sigma \in \mathcal{E}_M, \overline{\sigma} = \overline{M} \cap \overline{L}\}$.

It is denoted by $\{w_M^n, M \in \mathcal{T}, n \in \{0, ..., N_{\Delta t} + 1\}\}$ the discrete unknowns; the value w_M^n is an expected approximation of $w(x_M, n\Delta t)$, where $w \equiv U_1$, $w \equiv U_2$, or $w \equiv u_3$.

Definition 3.3.2 *Let $X(\mathcal{T}, \Delta t)$ be the set of functions w from $\Omega \times (0, (N_{\Delta t} + 1)\Delta t)$ to $\mathbb{R}$ such that there exists a family of real values $\{w_M^n, M \in \mathcal{T}, n \in \{0, ..., N_{\Delta t} + 1\}\}$, with $w(x, t) = w_M^n$ for a.e. $x \in M, M \in \mathcal{T}$ and for a.e. $t \in [n\Delta t, (n + 1)\Delta t), n \in \{0, ..., N_{\Delta t}\}$.*

3.3.1 Discretization of equation (3.2.7)

Integrating (3.2.7) over the set $M \times [t_n, t_{n+1}]$ with $M \in \mathcal{T}$, it is obtained

$$\int_M (U_1(\cdot, t_{n+1}) - U_1(\cdot, t_n)) + T_c - T_d = T_r, \tag{3.3.1}$$

where $T_c := \sum_{l \in \partial M} \int_{t_n}^{t_{n+1}} \int_l \alpha_1(U_1)\mathbf{v} \cdot \mathbf{n}_{M,l}$, $T_d := \sum_{l \in \partial M} \int_{t_n}^{t_{n+1}} \int_l \mathbf{D}(\mathbf{v})\nabla\alpha_1(U_1) \cdot \mathbf{n}_{M,l}$ and $T_r := -\mu \int_M \int_{t_n}^{t_{n+1}} \theta_w \alpha_1(U_1)$, are the convective, diffusive and reactive term, respectively, and $\mathbf{n}_{M,l}$ is the outward normal to $l \in \partial M$. The advection term T_c is approximated by an upwind Godunov scheme (cf. [34])

$$T_c \approx \sum_l |\Delta t||l|\alpha_1(U_{1,l}^{n+1})\mathbf{v}_l^n \cdot \mathbf{n}_{M,l} = -\sum_l |\Delta t||l|(\alpha_1(U_{1,M_l}^{n+1}) - \alpha_1(U_{1,M}^{n+1}))(-\mathbf{v}_l^n \cdot \mathbf{n}_{M,l})^+, \tag{3.3.2}$$

where

$$\alpha_1(U_{1,l}^{n+1}) := \{ \begin{array}{lll} \alpha_1(U_{1,M}^{n+1}) & if & \mathbf{v}_l^n \cdot \mathbf{n}_{M,l} \geq 0 \\ \alpha_1(U_{1,M_l}^{n+1}) & if & \mathbf{v}_l^n \cdot \mathbf{n}_{M,l} < 0. \end{array}$$

On the other hand, the diffusive term T_d, is approximated by an P1-FEM scheme. In effect, let us considers the standard P1 finite element basis functions satisfying $\chi_{M_i}(M_j) = \delta_{ij}$. Therefore,

$$T_d \approx \sum_l D_{M,l}(\alpha_1(U_{1,M_l}^{n+1}) - \alpha_1(U_{1,M}^{n+1})), \tag{3.3.3}$$

where $D_{M,l} := -|T|\nabla\chi_{M_l,T} \cdot \mathbf{D}(\mathbf{v}_T^n)\nabla\chi_{M,T}$, and T is such that $M \cap T \neq \emptyset$ and $l \in \partial M \cap T$. Finally, about the reactive term T_r

$$\int_M \int_{t_n}^{t_{n+1}} \theta_w \alpha_1(U_1) \approx |\Delta t||M|\theta_{w,M}^{1+n}\alpha_1(U_{1,M}^{1+n}), \tag{3.3.4}$$

where $\theta_{w,M}^{1+n}$ is the mean value of θ_w over $M \times [t_n, t_{n+1}]$.
Therefore, using (3.3.2), (3.3.3) and (3.3.4) in (3.2.7), the finite volume scheme for (3.2.7) is defined as

$$|M|(U_{1j}^{n+1} - U_{1j}^n) + \hat{T}_{1c} - \hat{T}_{1d} = \hat{T}_{1r}, \tag{3.3.5}$$

where

$$\hat{T}_{1c} := -|\Delta t| \sum_l |l|(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+,$$

$$\hat{T}_{1d} := |\Delta t| \sum_l (\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))D_{jl},$$

and

$$\hat{T}_{1r} := -\mu|\Delta t||M|\theta_{w,M}^{1+n}\alpha_1(U_{1,M}^{1+n}).$$

About the notation note that $j \equiv M \equiv M_j$, $l \equiv M_l$.

3.3.2 Discretization of system (3.2.8)-(3.2.9)

In a similar way to (3.3.5) it is defined a finite volume scheme for system (3.2.8)-(3.2.9) as follow

$$|M|(U_{2j}^{n+1} - U_{2j}^n) + \hat{T}_{2c} - \hat{T}_{2d} = \hat{T}_{2r}, \tag{3.3.6}$$

$$\frac{u_{3j}^{n+1} - u_{3j}^n}{|\Delta t|} + k_e\theta_{wj}^n\alpha_1(U_{1j}^n)u_{3j}^n = \phi_s\frac{(\varphi_2 \circ \alpha_2)(U_{2j}^{n+1}) - (\varphi_2 \circ \alpha_2)(U_{2j}^n)}{|\Delta t|}, \tag{3.3.7}$$

where

$$\hat{T}_{2c} := -|\Delta t| \sum_l |l|(\alpha_2(U_{2l}^{n+1}) - \alpha_2(U_{2j}^{n+1}))(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+,$$

$$\hat{T}_{2d} := |\Delta t| \sum_l (\alpha_2(U_{2l}^{n+1}) - \alpha_2(U_{2j}^{n+1}))D_{jl},$$

and

$$\hat{T}_{2r} := k_e\rho_s|\Delta t||M|\theta_{wj}^n\alpha_1(U_{1j}^n)u_{3j}^n.$$

3.4 Convergence Analysis for Model Problem A

In this section the equation (3.2.7) and its corresponding numerical scheme (3.3.5) are considered. The convergence analysis follows the main ideas of [2], [27] and [28].

Let us state the following assumptions:

(A1) Ω is a bounded open polygonal subset of $\mathbb{R}^2$.

(A2) $\theta_w(x,t) \in L^\infty(\Omega \times (0,T))$ is such that $0 < \theta_w^- \leq \theta_w(x,t) \leq \theta_w^+ < 1$.

(A3) $\mathbf{D}$ is a bounded, uniformly positive definite symmetric tensor on $\Omega \times (0,T)$.

(A4) $U_i(x,t=0), u_3(x,t=0) \in L^\infty(\Omega \times (0,T)), i = 1,2$.

(A5) $\alpha_i \in C^1[0,\infty[$, such that $\alpha_i^{'}(0) = 0$ y $\alpha_i^{'}(s) > 0$, $\forall s > 0$, $i = 1,2$.
$\alpha_i, \alpha_i^{'} \in L^\infty(\Omega \times (0,T)), i = 1,2$.

(A6) $\mathbf{v}_w \in (L^\infty(\Omega \times (0,T))^2$, $\nabla \cdot \mathbf{v}_w = 0$, $\mathbf{v}_w^n \to \mathbf{v}_w$ in $L^2(\Omega \times (0,T))$.

(A7) $\varphi_i, \alpha_i, i = 1,2$ are Lipschitz continuous with constant $K_{\varphi_i}, L_{\alpha_i}, i = 1,2$, respectively.

By assuming (A5), the class of problems under investigation can be assimilated to the slow diffusion case, in particular to the porous medium equation.

3.4.1 L^∞ Stability

Proposition 3.4.1 *Under the assumptions (A1)-(A7) the scheme (3.3.5) is L^∞ stable without any CFL condition.*

Proof. In first place note that there exists $\xi = \xi(U_{1j}^{1+n})$ such that

$$\alpha_1(U_{1l}^{1+n}) - \alpha_1(U_{1j}^{1+n}) = \alpha_1^{'}(\xi)(U_{1l}^{1+n} - U_{1j}^{1+n}).$$

Therefore, the scheme (3.3.5) can be written as

$$\begin{aligned} U_{1j}^{1+n} &- U_{1j}^{n} - \frac{|\Delta t|}{|M|}\sum_{l}|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{jl})^{+}\alpha_1^{'}(\xi)(U_{1l}^{1+n}-U_{1j}^{1+n}) \\ &- \frac{|\Delta t|}{|M|}\sum_{l}D_{jl}\alpha_1^{'}(\xi)(U_{1l}^{1+n}-U_{1j}^{1+n}) + \mu|\Delta t|\theta_{wj}^{1+n}\alpha_1(U_{1j}^{1+n}) = 0, \end{aligned}$$

that is,

$$\begin{aligned} U_{1j}^{1+n}\{1 &+ \frac{|\Delta t|}{|M|}\sum_{l}\alpha_1^{'}(\xi)(|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{jl})^{+}+D_{jl})\} \\ &- \frac{|\Delta t|}{|M|}\sum_{l}\alpha_1^{'}(\xi)(|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{jl})^{+}+D_{jl})U_{1l}^{1+n} \\ &+ \mu|\Delta t|\theta_{wj}^{1+n}\alpha_1(U_{1j}^{1+n}) = U_{1j}^{n}. \end{aligned}$$

This last scheme can be written as system of equations,

$$A(\mathbf{U}_1^{1+n})\mathbf{U}_1^{1+n} + \mathbf{b}(\mathbf{U}_1^{1+n}) = \mathbf{U}_1^{n}, n \geq 0,$$

where, for all $i \neq j \in \{0, ..., N_s\}$:

$$\begin{aligned} A_{ii} &:= 1 + \frac{|\Delta t|}{|M|}\sum_{l\in\partial M_i}\alpha_1^{'}(\xi)(|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{il})^{+}+D_{il}), \\ A_{ij} &:= -\frac{|\Delta t|}{|M|}\sum_{l\in\partial M_i\cap\partial M_j}\alpha_1^{'}(\xi)(|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{il})^{+}+D_{il}), \\ b_i &:= \mu|\Delta t|\theta_{wj}^{1+n}\alpha_1(U_{1j}^{1+n}), \end{aligned}$$

and

$$\mathbf{U}_1^{1+n} := [U_{11}^{1+n}, U_{12}^{1+n}, ..., U_{1j}^{1+n}, ..., U_{1N_s}^{1+n}]^T.$$

Therefore, the auxiliary non linear problem is given by: given the applications $\mathbf{b}(\cdot)$ and $A(\cdot)$, and the vector $\mathbf{c}$, to find $\mathbf{x}$ such that,

$$\mathbf{F}(\mathbf{x}) := A(\mathbf{x})\mathbf{x} + \mathbf{b}(\mathbf{x}) = \mathbf{c}.$$

Let the sequence of vectors $\{\mathbf{x}^k\}, k \geq 0$, and $\mathbf{x}^0 := \mathbf{c} = \mathbf{U}^n$, defined as

$$A(\mathbf{x}^k)\mathbf{x}^{1+k} + \mathbf{b}(\mathbf{x}^k) = \mathbf{c}, k \geq 0$$

Existence: in first place note that the matrix A is a monotone matrix, i.e., it is have $A_{ij}^{-1} \geq 0$, furthermore $(A_{ij} - \sum_{i \neq j} |A_{ij}|) \geq 1$, then $||A^{-1}||_\infty \leq 1$, where $||\cdot||_\infty$ is the l_∞ matrix norm, hence there exists a generic constant $C > 0$, independent of h, $|\Delta t|$ and k, such that,

$$\begin{aligned} ||\mathbf{x}^{1+k}||_\infty &= ||A^{-1}(\mathbf{x}^k)\mathbf{c} - A^{-1}(\mathbf{x}^k)\mathbf{b}(\mathbf{x}^k)|| \\ &\leq ||A^{-1}(\mathbf{x}^k)||_\infty(||\mathbf{c}||_\infty + ||\mathbf{b}(\mathbf{x}^k)||_\infty) \\ &\leq ||\mathbf{U}_1^n||_\infty + \mu|\Delta t|||\theta_w^{1+n}||_\infty||\alpha_1||_\infty \\ &\leq C, \end{aligned}$$

because an induction argument on $n \geq 0$. Therefore, the sequence $\{\mathbf{x}^m, m \geq 0\}$, is bounded, then it is extracted a subsequence, still denoted as $\{\mathbf{x}^m, m \geq 0\}$, such that $\tilde{\mathbf{x}} = \lim_{m \to \infty} \mathbf{x}^m$, then from the continuity of the application $\mathbf{F} : \mathbf{x} \mapsto A(\mathbf{x})\mathbf{x} + \mathbf{b}(\mathbf{x})$, the limit $\tilde{\mathbf{x}}$ is a solution of $\mathbf{F}(\tilde{\mathbf{x}}) = \mathbf{c}$. Therefore, $\mathbf{U}_1^{1+n} := \tilde{\mathbf{x}}$.

Uniqueness: let $\mathbf{U}_1^{1+n}$ and $\mathbf{V}_1^{1+n}$ be two solutions of the implicit scheme (3.4.1), i.e., for $i = 0, ..., N_s$,

$$\begin{aligned} U_{1j}^{1+n} &- U_{1j}^n - \frac{|\Delta t|}{|M|}\sum_l |l|(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+(\alpha_1(U_{1l}^{1+n}) - \alpha_1(U_{1j}^{1+n})) \\ &- \frac{|\Delta t|}{|M|}\sum_l D_{jl}(\alpha_1(U_{1l}^{1+n}) - \alpha_1(U_{1j}^{1+n})) + \mu|\Delta t|\theta_{wj}^{1+n}\alpha_1(U_{1j}^{1+n}) = 0, \end{aligned}$$

$$\begin{aligned} V_{1j}^{1+n} &- V_{1j}^n - \frac{|\Delta t|}{|M|}\sum_l |l|(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+(\alpha_1(V_{1l}^{1+n}) - \alpha_1(V_{1j}^{1+n})) \\ &- \frac{|\Delta t|}{|M|}\sum_l D_{jl}(\alpha_1(V_{1l}^{1+n}) - \alpha_1(V_{1j}^{1+n})) + \mu|\Delta t|\theta_{wj}^{1+n}\alpha_1(V_{1j}^{1+n}) = 0, \end{aligned}$$

By subtracting, and applying similar arguments to existence case, it is obtained for $W_{1q}^{1+n} := U_{1q}^{1+n} - V_{1q}^{1+n}, q = j, l$,

$$\begin{aligned} W_{1j}^{1+n}\{1 &+ \frac{|\Delta t|}{|M|}\sum_l \alpha_{1j}'(\xi_j)(|l|(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+ + D_{jl} + \mu|\Delta t|\theta_{wj}^{1+n})\} \\ &- \frac{|\Delta t|}{|M|}\sum_l \alpha_{1l}'(\xi_l)(|l|(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+ + D_{jl})W_{1l}^{1+n} = 0, \end{aligned}$$

where, $\alpha'_{1q}(\xi_q) := \alpha'_{1q}(U_q^{1+n}, V_q^{1+n}), q = j, l$. This last scheme can be written as system of equations,

$$\tilde{A}(\mathbf{U}_1^{1+n}, \mathbf{V}_1^{1+n})\mathbf{W}_1^{1+n} = \mathbf{0},$$

where following a similar argument to existence case, it is have that the matrix $\tilde{A}$ is non singular. Therefore, $\mathbf{W}_1^{1+n} = \mathbf{U}_1^{1+n} - \mathbf{V}_1^{1+n} = \mathbf{0}$.

□

Proposition 3.4.2 *Under the assumptions (A1)-(A7), it is have for the scheme (3.3.5) that there exits constants* $C_i > 0, i = 1, 2,$ *independent of* h *and* Δt*, such that*

$$\begin{aligned} \Delta t \sum_{n,l} |l|(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 |\mathbf{v}_l^n \cdot \mathbf{n}_{jl}| &\leq C_1 \\ \Delta t \sum_{n,l} (\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 D_{jl} &\leq C_2. \end{aligned}$$

Proof. Multiplying (3.3.5) by U_{1j}^{n+1} and using $\sum_j$ it is get

$$\sum_j |M| U_{1j}^{n+1}(U_{1j}^{n+1} - U_{1j}^n) = -\sum_j U_{1j}^{n+1}\hat{T}_{1c} + \sum_j U_{1j}^{n+1}\hat{T}_{1d} + \sum_j U_{1j}^{n+1}\hat{T}_{1r}.$$

With respect to the left side it is used the identity $\frac{a^2-b^2}{2} = a(a-b) - \frac{(a-b)^2}{2}$, that is $0 \leq \frac{(a-b)^2}{2} = a(a-b) - \frac{a^2-b^2}{2}$, that is, for each real numbers a, b,

$$a(a-b) \geq \frac{a^2 - b^2}{2}.$$

Therefore,

$$\frac{1}{2}\sum_j |M|[(U_{1j}^{n+1})^2 - (U_{1j}^n)^2] \leq -\sum_j U_{1j}^{n+1}\hat{T}_{1c} + \sum_j U_{1j}^{n+1}\hat{T}_{1d} + \sum_j U_{1j}^{n+1}\hat{T}_{1r},$$

that is,

$$\sum_j U_{1j}^{n+1}\hat{T}_{1c} - \sum_j U_{1j}^{n+1}\hat{T}_{1d} \leq -\frac{1}{2}\sum_j |M|[(U_{1j}^{n+1})^2 - (U_{1j}^n)^2] + \sum_j U_{1j}^{n+1}\hat{T}_{1r}.$$

In this last inequality note that,

about the convective term in the left hand side,

$$\begin{aligned}\sum_j U_{1j}^{n+1}\hat{T}_{1c} &= \sum_j U_{1j}^{n+1}\{-|\Delta t|\sum_l |l|(\alpha_1(U_{1l}^{n+1})-\alpha_1(U_{1j}^{n+1}))(-\mathbf{v}_l^n\cdot\mathbf{n}_{jl})^+\}\\ &\geq \frac{|\Delta t|}{2\sup(\alpha_1^{'})}\sum_{j,l}|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{jl})^+(\alpha_1(U_{1j}^{1+n})-\alpha_1(U_{1l}^{1+n}))^2,\end{aligned}$$

about the diffusive term in the left hand side,

$$\begin{aligned}-\sum_j U_{1j}^{n+1}\hat{T}_{1d} &= \sum_j U_{1j}^{n+1}\{|\Delta t|\sum_l(\alpha_1(U_{1l}^{n+1})-\alpha_1(U_{1j}^{n+1}))D_{jl}\}\\ &\geq \frac{|\Delta t|}{2\sup(\alpha_1^{'})}\sum_{l\in\pounds_h}D_{j,l}(\alpha_1(U_{1j}^{1+n})-\alpha_1(U_{1l}^{1+n}))^2,\end{aligned}$$

about the reactive term in the right hand side,

$$\begin{aligned}\sum_j U_{1j}^{n+1}\hat{T}_{1r} &= \sum_j U_{1j}^{n+1}\{-\mu|\Delta t||M|\theta_{w,M}^{1+n}\alpha_1(U_{1,M}^{1+n})\}\\ &\leq \mu|\Delta t|||\theta_w||_\infty||\alpha_1^{'}||_\infty||\mathbf{U}_1^{1+n}||_\infty|\Omega|.\end{aligned}$$

Then by summing over $n = 0, ..., N_{\Delta t}$, it is have that there exits a constant $C > 0$, independent of h and Δt, such that

$$\begin{aligned}\frac{|\Delta t|}{2\sup(\alpha_1^{'})}\sum_{n,j,l}|l|(-\mathbf{v}_l^n\cdot\mathbf{n}_{jl})^+(\alpha_1(U_{1j}^{1+n})-\alpha_1(U_{1l}^{1+n}))^2 &\quad +\\ \frac{|\Delta t|}{2\sup(\alpha_1^{'})}\sum_{n,l\in\pounds_h}D_{j,l}(\alpha_1(U_{1j}^{1+n})-\alpha_1(U_{1l}^{1+n}))^2 &\quad \leq\\ \frac{1}{2}\sum_j|M|((U_{1j}^0)^2-(U_{1j}^{N_{\Delta t}+1})^2)+\mu T||\theta_w||_\infty||\alpha_1^{'}||_\infty||\mathbf{U}_1^{1+n}||_\infty|\Omega| &\quad \leq \quad C.\end{aligned}$$

□

3.4.2 Convergence results

Lemma 3.4.1 *Let the scheme (3.3.5). There exits a constant $C > 0$, independent of h and Δt, such that*

$$\sum_{n,j}\Delta t|M|(\alpha_1(U_{1j}^{n+1})-\alpha_1(U_{1j}^n))^2+\sum_{n,l}\Delta t|l|(\alpha_1(U_{1l}^n)-\alpha_1(U_{1j}^n))^2\leq C(h+|\Delta t|). \quad (3.4.1)$$

Proof. Multiplying (3.3.5) by $\alpha_1(U_{1j}^{n+1}) - \alpha_1(U_{1j}^n)$, using $\sum_j$, and reordering, it is get

$$\sum_j |M|(\alpha_1(U_{1j}^{n+1}) - \alpha_1(U_{1j}^n))(U_{1j}^{n+1} - U_{1j}^n) = C_{1+n} - C_n + D_{1+n} - D_n - R_{1+n}, \quad (3.4.2)$$

where for $s \in \{n, n+1\}$,

$$C_s := |\Delta t| \sum_{M_j} \sum_{l \in \partial M_j} |l|(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))\alpha_1(U_{1j}^s)(-\mathbf{v}_l^n \cdot \mathbf{n}_{jl})^+,$$

$$D_s := |\Delta t| \sum_{M_j} \sum_{l \in \partial M_j} (\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))\alpha_1(U_{1j}^s) D_{jl},$$

and

$$R_{1+n} := \mu |\Delta t| \sum_{M_j} |M_j| \theta_{wj}^{1+n} \alpha_1(U_{1j}^{1+n}).$$

About of the terms C_s and D_s, with $s \in \{n, n+1\}$, and following to [2], note that there exits constants $C_1 > 0$ and $C_2 > 0$, independent of h and Δt, such that, $\sum_n |C_s| \leq C_1$ and $\sum_n |D_s| \leq C_2$.

About the reactive term, note that there exits a constant $C_3 > 0$, independent of h and Δt, such that,

$$\sum_n |R_{1+n}| \leq \mu ||\theta_w||_\infty ||\alpha_1||_\infty \sum_n |\Delta t| \sum_j |M_j| \leq \mu ||\theta_w||_\infty ||\alpha_1||_\infty T|\Omega| \leq C_3.$$

About the left hand side in (3.4.2) note that for each real numbers a and b:

$$\begin{aligned} (\alpha_1(b) - \alpha_1(a))^2 &= \\ \frac{\alpha_1(b) - \alpha_1(a)}{b-a}(\alpha_1(b) - \alpha_1(a))(b-a) &= \\ \alpha_1'(\cdot)(\alpha_1(b) - \alpha_1(a))(b-a) &\leq \\ \sup|\alpha_1'|(\alpha_1(b) - \alpha_1(a))(b-a). \end{aligned}$$

Therefore, there exists a constant $C_4 > 0$, such that

$$\sum_{n,j} |M_j|(\alpha_1(U_{1j}^{n+1}) - \alpha_1(U_{1j}^n))^2 \leq C_4,$$

that is,

$$\sum_{n,j} |\Delta t||M_j|(\alpha_1(U_{1j}^{n+1}) - \alpha_1(U_{1j}^{n}))^2 \leq C_4|\Delta t|.$$

Finally, by Proposition 3.4.2, it is know that, there exits a constant $C_5 > 0$, such that

$$|\Delta t|\sum_{n,l}(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 D_- \leq |\Delta t|\sum_{n,l}(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 D_{jl} \leq C_5,$$

that is,

$$|\Delta t|D_-\sum_{n,l}(C_6|l|)(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 \leq |\Delta t|\sum_{n,l} h(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 D_- \leq hC_5.$$

Therefore, there exits a constant $C_7 > 0$ such that

$$\begin{aligned} |\Delta t|\sum_{n,j}|M_j|(\alpha_1(U_{1j}^{n+1}) - \alpha_1(U_{1j}^{n}))^2 + |\Delta t|\sum_{n,l}|l|(\alpha_1(U_{1l}^{n+1}) - \alpha_1(U_{1j}^{n+1}))^2 &\leq \\ C_4|\Delta t| + \frac{hC_5}{(D_-)C_6} &\leq \\ (|\Delta t| + h)C_7. \end{aligned}$$

□

Lemma 3.4.2 *Under Assumptions (A1) to (A7), let $\mathcal{T}$ be an admissible mesh in the sense of Definition 3.3.1 and $\Delta t \in (0, T)$. Let $U_{1,\mathcal{T},\Delta t} \in X(\mathcal{T}, \Delta t)$ be given by Definition 3.3.2. Let $B_1 := ||U_{1,\mathcal{T},\Delta t}||_{L^\infty(\Omega\times(0,T))}$ and L_{α_1} be the Lipschitz constant of α_1 on $[-B_1, B_1]$. One defines $\tilde{U}_1$ by $\tilde{U}_1 = U_{1,\mathcal{T},\Delta t}$ a.e. on $\Omega \times (0,T)$, and $\tilde{U}_1 = 0$ a.e. on $\mathbb{R}^{2+1} \setminus \Omega \times (0,T)$. Then, there exits a constant $C > 0$, independent of τ, h and Δt, such that*

$$||\alpha_1(\tilde{U}_1(\cdot, \cdot + \tau)) - \alpha_1(\tilde{U}_1(\cdot, \cdot))||^2_{L^2(\mathbb{R}^{2+1})} \leq C|\tau|, \forall \tau \in \mathbb{R}.$$

Proof. This proof follows the main ideas of Lemma 18.7 in [28]. Let $\tau \in (0, T)$. Since L_{α_1} is the Lipschitz constant of α_1 and α_1 is non decreasing, the following inequality holds:

$$\int_{\Omega\times(0,T-\tau)}(\alpha_1(U_{1,\mathcal{T},\Delta t}(x, t + \tau)) - \alpha_1(U_{1,\mathcal{T},\Delta t}(x, t)))^2 dxdt \leq L_{\alpha_1}\int_0^{T-\tau} A(t)dt,$$

where, for almost every $t \in (0, T-\tau)$,

$$A(t) = \int_{\Omega} (\alpha_1(U_{1,\mathcal{T},\Delta t}(x,t+\tau)) - \alpha_1(U_{1,\mathcal{T},\Delta t}(x,t)))(U_{1,\mathcal{T},\Delta t}(x,t+\tau) - U_{1,\mathcal{T},\Delta t}(x,t))dx.$$

Note that the function $A(t)$ may be written as (for more details cf. proof of Lemma 18.7 in [28]):

$$A(t) = \sum_{M\in\mathcal{T}} (\alpha_1(U_{1M}^{n_1(t)}) - \alpha_1(U_{1M}^{n_0(t)}))(\sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau) m(M)(U_{1M}^{n} - U_{1M}^{n-1})), \qquad (3.4.3)$$

where $n_0(t), n_1(t) \in \{0, ..., N_{\Delta t}\}$ such that $n_0(t)\Delta t \leq t < (n_0(t)+1)\Delta t$ and $n_1(t)\Delta t \leq t < (n_1(t)+1)\Delta t$, and $\chi_n(t,t+\tau) = 1$ if $n\Delta t \in (t, t+\tau]$ and $\chi_n(t,t+\tau) = 0$ if $n\Delta t \notin (t,t+\tau]$. In (3.4.3), the order of summation between n and M is changed and the scheme (3.3.5) is used. Hence,

$$\begin{aligned} A(t) &= \Delta t \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau)[\sum_{M\in\mathcal{T}} (\alpha_1(U_{1M}^{n_1(t)}) - \alpha_1(U_{1M}^{n_0(t)}))(\sum_{l\in\mathcal{N}(M)} |l|(\alpha_1(U_{1L}^{n}) \\ &- \alpha_1(U_{1M}^{n}))(-\mathbf{v}_l^{n-1}\cdot \mathbf{n}_l)^+) + \sum_{l\in\mathcal{N}(M)} (\alpha_1(U_{1L}^{n}) - \alpha_1(U_{1M}^{n}))D_{jl} - \mu|M|\theta_{wj}^{n}\alpha_1(U_{1j}^{n})] \\ &= A_1(t) + A_2(t) + A_3(t), \end{aligned}$$

where

$$\begin{aligned} A_1(t) &:= \Delta t \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau) \sum_{M,l} |l|(\alpha_1(U_{1M}^{n_1(t)}) - \alpha_1(U_{1M}^{n_0(t)}))(\alpha_1(U_{1L}^{n}) - \alpha_1(U_{1M}^{n}))(-\mathbf{v}_l^{n-1}\cdot \mathbf{n}_l)^+ \\ A_2(t) &:= \Delta t \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau) \sum_{M,l} (\alpha_1(U_{1M}^{n_1(t)}) - \alpha_1(U_{1M}^{n_0(t)}))(\alpha_1(U_{1L}^{n}) - \alpha_1(U_{1M}^{n}))D_{jl} \\ A_3(t) &:= \Delta t \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau) \sum_{M} (\alpha_1(U_{1M}^{n_1(t)}) - \alpha_1(U_{1M}^{n_0(t)}))(-\mu|M|\theta_{wj}^{n}\alpha_1(U_{1j}^{n})). \end{aligned}$$

About the $A_3(t)$ term note that

$$\begin{aligned} \int_0^{T-\tau} A_3(t)dt &\leq \mu \sum_{n=1}^{N_{\Delta t}} \Delta t(\sum_{M\in\mathcal{T}} 2B_1 L_{\alpha_1}|M|||\theta_w||_\infty||\alpha_1||_\infty) \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\ &\leq \tau\mu T|\Omega|2B_1 L_{\alpha_1}||\theta_w||_\infty||\alpha_1||_\infty. \end{aligned}$$

About the $A_2(t)$ term note that gathering by edges, and using the inequality $2ab \leq a^2+b^2; a,b \in \mathbb{R}$, this yields

$$\begin{aligned}
\int_0^{T-\tau} A_2(t)dt &\leq \sum_{n=1}^{N_{\Delta t}} \Delta t \sum_l (\alpha_1(U_{1L}^{n_0(t)}) - \alpha_1(U_{1M}^{n_0(t)}))(\alpha_1(U_{1L}^n) - \alpha_1(U_{1M}^n))D_{jl} \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\
&+ \sum_{n=1}^{N_{\Delta t}} \Delta t \sum_l (\alpha_1(U_{1L}^{n_1(t)}) - \alpha_1(U_{1M}^{n_1(t)}))(\alpha_1(U_{1L}^n) - \alpha_1(U_{1M}^n))D_{jl} \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\
&\leq \frac{1}{2}\sum_{n,l} \Delta t(\alpha_1(U_{1L}^{n_0(t)}) - \alpha_1(U_{1M}^{n_0(t)}))^2 D_{jl} \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\
&+ \frac{1}{2}\sum_{n,l} \Delta t(\alpha_1(U_{1L}^{n_1(t)}) - \alpha_1(U_{1M}^{n_1(t)}))^2 D_{jl} \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\
&+ \sum_{n,l} \Delta t(\alpha_1(U_{1L}^{n}) - \alpha_1(U_{1M}^{n}))^2 D_{jl} \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\
&\leq \frac{1}{2}C\tau + \frac{1}{2}C\tau + C\tau,
\end{aligned}$$

where the constant $C > 0$, which is independent of τ, k, and h, is from Proposition 3.4.2. Finally, and applying similar arguments, about the $A_1(t)$ term note that gathering by edges and using the inequality $2ab \leq a^2+b^2; a,b \in \mathbb{R}$, this yields

$$\begin{aligned}
\int_0^{T-\tau} A_1(t)dt &\leq \frac{1}{2}[\sum_{n=1}^{N_{\Delta t}} \Delta t \sum_{l \in \mathcal{N}(M)} |l|(\alpha_1(U_{1M}^{n_1(t)}) - \alpha_1(U_{1M}^{n_0(t)}))^2(-\mathbf{v}_l^{n-1} \cdot \mathbf{n}_{jl})^+ \\
&+ \sum_{n=1}^{N_{\Delta t}} \Delta t \sum_{l \in \mathcal{N}(M)} |l|(\alpha_1(U_{1L}^{n_1(t)}) - \alpha_1(U_{1L}^{n_0(t)}))^2(\mathbf{v}_l^{n-1} \cdot \mathbf{n}_{jl})^+ \\
&+ \sum_{n=1}^{N_{\Delta t}} \Delta t \sum_{l \in \mathcal{N}(M)} |l|(\alpha_1(U_{1L}^{n}) - \alpha_1(U_{1M}^{n}))^2|\mathbf{v}_l^{n-1} \cdot \mathbf{n}_{jl}|] \int_0^{T-\tau} \chi_n(t,t+\tau)dt \\
&\leq \frac{1}{2}(C_1+C_2+C_3)\tau,
\end{aligned}$$

where $C_i > 0, i = 1,2,3$, are constants, independent of τ, Δt and h.

□

It is used the Kolmogorov (in the version of [28], Theorem 14.1, p.833) compactness theorem in $L^2(\Omega)$ which it is now recall. The essential part of the proof of this theorem can be found in [6].

Theorem 3.4.3 ***(Fréchet-Kolmogorov)*** *Let ω be an open bounded set of $\mathbb{R}^N$, $N \geq 1$, $1 \leq q \leq \infty$ and $A \subset L^q(\omega)$. Then, A is relatively compact in $L^q(\omega)$ if and only if there exits $\{p(u), u \in A\} \subset L^q(\mathbb{R}^N)$ such that*

1. *$p(u) = u$ a.e. on ω, for all $u \in A$.*
2. *$\{p(u), u \in A\}$ is bounded in $L^q(\mathbb{R}^N)$.*
3. *$||p(u)(\cdot + \zeta) - p(u)||_{L^q(\mathbb{R}^N)} \longrightarrow 0$, as $\zeta \longrightarrow 0$, uniformly with respect to $u \in A$.*

Now it is proved the main result of this section.

Theorem 3.4.4 *Under the assumptions (A1)-(A7) the approximate solution U_{1h} given by the scheme (3.3.5), without any CFL condition, converges to U_1 in $L^2(Q_T)$ as h and Δt go to zero.*

Proof. In order to show the convergence of $U_{1h} := U_{1h}(x,t) := U_{1M}^n$ in $M \times [t_n, t_{n+1}]$ toward the weak solution defined in section 3.2.6, it is passed to the limit in the scheme (3.3.5).

Let us set $\tilde{\alpha}_{1h} := \alpha_1(U_{1h})$ on Q_T and $\tilde{\alpha}_{1h} := 0$ on $\mathbb{R}^3 \backslash Q_T$. From Propositions 3.4.1 and 3.4.2, and Lemma 3.4.1, $(\tilde{\alpha}_{1h}) \subseteq L^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Then, applying the Theorem 3.4.3, (with $N = d+1, d = 2$, $q = 2$, and $\omega = \Omega \times (0,T)$) note that the first and second items of Theorem 3.4.3 are clearly satisfied. About the third hypothesis, note that for $\eta \in \mathbb{R}^2$ and $\tau \in \mathbb{R}$,

$$\begin{aligned} ||\tilde{\alpha}_{1h}(\cdot + \eta, \cdot + \tau) - \tilde{\alpha}_{1h}(\cdot, \cdot)||_{L^2(\mathbb{R}^{2+1})} &\leq \\ ||\tilde{\alpha}_{1h}(\cdot + \eta, \cdot) - \tilde{\alpha}_{1h}(\cdot, \cdot)||_{L^2(\mathbb{R}^{2+1})} &+ ||\tilde{\alpha}_{1h}(\cdot, \cdot + \tau) - \tilde{\alpha}_{1h}(\cdot, \cdot)||_{L^2(\mathbb{R}^{2+1})}. \end{aligned}$$

About the term $||\tilde{\alpha}_{1h}(\cdot + \eta, \cdot) - \tilde{\alpha}_{1h}(\cdot, \cdot)||_{L^2(\mathbb{R}^{2+1})}$, in this last inequality, note that by Lemma 18.3 in [28], p.851, there exits a bound $C(|\eta|) > 0$, such that $||\tilde{\alpha}_{1h}(\cdot + \eta, \cdot) - \tilde{\alpha}_{1h}(\cdot, \cdot)||_{L^2(\mathbb{R}^{2+1})} \leq C(|\eta|)$, and $C(|\eta|) \to 0$ if $|\eta| \to 0$.

(About the applicability of Lemma 18.3 from [28], p.851, in this proof, note that its hypothesis are satisfied, i.e., the mesh $\mathcal{T}$ is admissible and $\tilde{\alpha}_1 \in X(\mathcal{T}, \Delta t)$. Additionally, the proof of Lemma 18.3 is based on arguments strictly geometrics (cf. proof of Lemma 9.3 in [28], p.770), i.e., is not depend on the numerical scheme utilized.)

By another hand, about the term $||\tilde{\alpha}_{1h}(\cdot,\cdot+\tau)-\tilde{\alpha}_{1h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})}$ note that by Lemma 3.4.2, there exits a constant $C>0$, independent of η and τ, such that $||\tilde{\alpha}_{1h}(\cdot,\cdot+\tau)-\tilde{\alpha}_{1h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})}\leq C\tau$.
This yields the compactness of the sequence $(\tilde{\alpha}_{1h})$ in $L^2(Q_T)$. Therefore, there exits a subsequence, still denoted by $(\tilde{\alpha}_{1h})$, and there exits $\alpha_1^*\in L^2(Q_T)$ such that $(\tilde{\alpha}_{1h})$ converges to α_1^* in $L^2(Q_T)$. Indeed, since $(\tilde{\alpha}_{1h})\subseteq L^\infty(Q_T)$, this convergence holds in $L^q(Q_T)$ for all $1\leq q<\infty$. Furthermore, since α_1 is nondecreasing, Theorem 18.2 in [28] gives that $\alpha_1^*=\alpha_1(U_1^*)$, that is $U_1^*=\alpha_1^{-1}(\alpha_1^*)$. Therefore, (α_{1h}) converges to $\alpha_1(U_1^*)$ in $L^1(Q_T)$ (and even in $L^p(Q_T)$ for all $p\in[0,\infty)$.)
It remains to be shown that U_1^* is a weak solution (see definition in Section 3.2.6). For this, let $v\in V$ be a test function and denote $v_j^n\equiv v(x_{M_j},t_n)$. Multiply by v_j^n in the scheme (3.3.5), it is obtain by summation

$$\sum_{n,j}|M||\Delta t|v_j^n\frac{U_{1j}^{n+1}-U_{1j}^n}{|\Delta t|}+\sum_{n,j}v_j^n\hat{T}_{1c}=\sum_{n,j}v_j^n\hat{T}_{1d}+\sum_{n,j}v_j^n\hat{T}_{1r},$$

that is, $H_1+H_2=H_3+H_4$, where

$$\begin{aligned}
H_1 &:= -\sum_j|M|v_j^oU_{1j}^o+\sum_{n,j}|\Delta t||M|U_{1j}^{n+1}\frac{v_j^n-v_j^{n+1}}{|\Delta t|},\\
H_2 &:= \sum_{n,j}|\Delta t|v_j^n\sum_{l\in\partial M}\alpha_1(U_1)|_l^{n+1}\mathbf{v}_l^n\cdot\mathbf{n}_{j,l}|l|,\\
H_3 &:= \sum_{n,j}|\Delta t|v_j^n\sum_{l\in\partial M}(\alpha1(U_{1l}^{n+1})-\alpha_1(U_{1j}^{n+1}))D_{j,l},\\
H_4 &:= -\sum_{n,j}v_j^n(\mu|\Delta t||M|\theta_{w,j}^{n+1}\alpha_1(U_{1j}^{n+1})).
\end{aligned}$$

Taking into account the assumptions on the data and using the Lebesgue theorem, it follows that as h and Δt go to 0 (and following the main ideas of theorem 4.2's proof in [2]). In first place, note that about H_1 is enough to mention that

$$H_1\longrightarrow-\int_\Omega U_1^ov(x,0)-\int_{Q_T}U_1^*\partial_tv.$$

About H_2 note that, $H_2 = H_{2a} + H_{2b}$, where

$$H_{2a} := \sum_{n,j} \Delta t \sum_{l \in \partial M} (\alpha_1(U_1) - \alpha_1(U_{1j}^{n+1}))\mathbf{v}_l^n \cdot \mathbf{n}_{jl}|l|(v_j^n - v_l^n),$$

and

$$H_{2b} := -\sum_{n,j} |\Delta t| \alpha_1(U_{1j}^{n+1}) \sum_{l \in \partial M} \int_l v^n \mathbf{v}_l^n \cdot \mathbf{n}_{jl} d\sigma.$$

About H_{2a} note that there exits a constant $C > 0$, independent of h and Δt, such that, $|H_{2a}| \leq Ch^{1/2}$, that is, $\lim_{h \to 0} |H_{2a}| = 0$. By another hand, about H_{2b} note that,

$$H_{2b} = -\sum_{n,j} |\Delta t| \int_{M_j} \alpha_1(U_j^{n+1}) div(\mathbf{v}_l^n v^n) dx = -\sum_{n,j} |\Delta t| \int_{M_j} \alpha_1(U_j^{n+1}) \mathbf{v}_l^n \cdot \nabla v^n dx.$$

Therefore, $H_2 \longrightarrow -\int_{Q_T} \alpha_1(U_1^*)\mathbf{v} \cdot \nabla v$.

About H_3 note that,

$$\begin{aligned} H_3 &= -\sum_{n,j} \Delta t \alpha_1(U_{1j}^{n+1}) \sum_{l \in \partial M \setminus \Gamma} (v_l^n - v_j^n) D_{j,l} \\ &= -\sum_{n,j} \Delta t \alpha_1(U_{1j}^{n+1}) \sum_{T \cap M \neq \emptyset} \sum_{l \in \partial M \cap T \setminus \Gamma} (D_T \nabla v_T^n \cdot \mathbf{n}_{j,l}|l|) \\ &= -\sum_{n,j} \Delta t \alpha_1(U_{1j}^{n+1}) \sum_{l \in \partial M \setminus \Gamma} (D_l \nabla v_l^n \cdot \mathbf{n}_{j,l}|l|) \\ &= \sum_{n,j} \Delta t \alpha_1(U_{1j}^{n+1}) \sum_{l \in \partial M \cap \Gamma} (D_l \nabla v_l^n \cdot \mathbf{n}_{j,l}|l|) - \sum_{n,j} \Delta t \alpha_1(U_{1j}^{n+1}) \sum_{l \in \partial M} (D_l \nabla v_l^n \cdot \mathbf{n}_{j,l}|l|). \end{aligned}$$

Therefore,

$$H_3 \longrightarrow \int_J \int_\Gamma \alpha_1(U_1^*)\mathbf{D}(\mathbf{v})\nabla v \cdot \mathbf{n} ds dt - \int \int_{Q_T} \alpha_1(U_1^*) div(\mathbf{D}(\mathbf{v})\nabla v) dt dx,$$

that is, $H_3 \longrightarrow -\int_{Q_T} \mathbf{D}(\mathbf{v})\nabla \alpha_1(U_1^*) \cdot \nabla v$.

About H_4 is enough to mention that $H_4 \longrightarrow -\mu \int_{Q_T} \theta_w \alpha_1(U_1^*) v$. Finally, passing to the limit in (3.4.2) yields

$$[-\int_\Omega U_1^o v(x,0) - \int_{Q_T} U_1^* \partial_t v] - \int_{Q_T} \alpha_1(U_1^*)\mathbf{v} \cdot \nabla v = -\int_{Q_T} \mathbf{D}(\mathbf{v})\nabla \alpha_1(U_1^*) \cdot \nabla v - \mu \int_{Q_T} \theta_w \alpha_1(U_1^*) v.$$

Then, U_1^* is a weak solution of problem (3.2.7) which only admits a unique solution U_1. Thus the entire sequence (U_{1h}^n) converges to U_1, which ends the proof. □

3.5 Convergence Analysis for Model Problem B

In this section the system (3.2.8)-(3.2.9) and its numerical scheme (3.3.6)-(3.3.7) are considered.

3.5.1 L^∞ Stability

Proposition 3.5.1 *Under the assumptions (A1)-(A7) the scheme (3.3.7) is L^∞ stable without any CFL condition.*

Proof. From (3.3.7), and by an induction argument, is enough to mention that

$$\begin{aligned} |u_{3j}^{n+1}| &\leq |u_{3j}^n|(1 - k_e|\Delta t|\theta_{wj}^n \alpha_1(U_{1j}^n)) + \phi_s|(\varphi_2 \circ \alpha_2)(U_{2j}^{n+1}) - (\varphi_2 \circ \alpha_2)(U_{2j}^n)| \\ &\leq (k_e \tau \phi_s ||\theta_w||_\infty ||\alpha_1||_\infty ||\varphi_2 \circ \alpha_2||_\infty)|u_{3j}^n|, \end{aligned}$$

where $|u_{3j}^o| \leq C$. □

Proposition 3.5.2 *Under the assumptions (A1)-(A7) the scheme (3.3.6) is L^∞ stable without any CFL condition.*

Proof. In this case, the scheme (3.3.6) can be written as system of equations, namely

$$A(\mathbf{U}_2^{n+1})\mathbf{U}_2^{n+1} = \mathbf{U}_2^n + \tilde{\mathbf{b}}(\mathbf{U}_1^n, \mathbf{v}_3^n),$$

with $\tilde{b}_i := k_e \rho_s |\Delta t| \theta_{wi}^n \alpha_1(U_{1i}^n) u_{3i}^n$, the matrix A is the same of Proposition 3.4.1, and the vectors $\mathbf{U}_2^n$ and $\tilde{\mathbf{b}}(\mathbf{U}_1^n, \mathbf{v}_3^n)$ are given. In this case the approximating sequence is defined as

$$A(\mathbf{x}^k)\mathbf{x}^{1+k} = \mathbf{c}, k \geq 0.$$

The proof follows the same lines that Proposition 3.4.1. □

Proposition 3.5.3 *Under the assumptions (A1)-(A7), it is have for the scheme (3.3.6) that there exists constants $C_i > 0, i = 1, 2$, independent of h and Δt, such that*

$$\begin{aligned} \Delta t \sum_{n,l} |l|(\alpha_2(U_{2l}^{n+1}) - \alpha_2(U_{2j}^{n+1}))^2 |\mathbf{v}_l^n \cdot \mathbf{n}_{jl}| &\leq C_1 \\ \Delta t \sum_{n,l} (\alpha_2(U_{2l}^{n+1}) - \alpha_2(U_{2j}^{n+1}))^2 D_{jl} &\leq C_2. \end{aligned}$$

Proof. In a similar way to Proposition 3.4.2 it is get

$$\frac{1}{2}\sum_j |M|[(U_{1j}^{n+1})^2 - (U_{1j}^n)^2] \leq -\sum_j U_{1j}^{n+1}\hat{T}_{1c} + \sum_j U_{1j}^{n+1}\hat{T}_{1d} + \sum_j U_{1j}^{n+1}\hat{T}_{1r},$$

or equivalently,

$$\sum_j U_{1j}^{n+1}\hat{T}_{1c} - \sum_j U_{1j}^{n+1}\hat{T}_{1d} \leq -\frac{1}{2}\sum_j |M|[(U_{1j}^{n+1})^2 - (U_{1j}^n)^2] + \sum_j U_{1j}^{n+1}\hat{T}_{1r}.$$

About the reactive term, there exits a constant $C > 0$, independent of h and Δt such that,

$$\begin{aligned}\sum_{n,j} U_{1j}^{n+1}\hat{T}_{1r} &= \sum_{n,j} U_{1j}^{n+1}(k_e\rho_s|\Delta t||M_j|\theta_{wj}^n\alpha_1(U_{1j}^n)u_{3j}^n) \\ &\leq k_e\rho_s||\mathbf{U}_1^{1+n}||_\infty||\theta_w||_\infty||\alpha_1||_\infty||\mathbf{v}_3^n||_\infty\sum_{n,j}|\Delta t||M_j| \\ &\leq C.\end{aligned}$$

In this point the proof follow the same line of Proposition 3.4.2. □

3.5.2 Convergence results

Lemma 3.5.1 *The following estimate is valid for scheme (3.3.6). There exists a constant $C > 0$, independent of h and Δt, such that*

$$\sum_{n,j}\Delta t|M|(\alpha_2(U_{2j}^{n+1}) - \alpha_2(U_{2j}^n))^2 + \sum_{n,l}\Delta t|l|(\alpha_2(U_{2l}^n) - \alpha_2(U_{2j}^n))^2 \leq C(h + |\Delta t|). \quad (3.5.1)$$

Proof. The proof follow the same lines of Lemma 3.4.1. Only is enough to mention about the reactive term that, there exits a constant $C_1 > 0$, independent of h and Δt such that,

$$\begin{aligned}\sum_{n,j}|M_j|(\alpha_2(U_{2j}^{1+n}) - \alpha_2(U_{2j}^n))\hat{T}_{1r} &= \sum_{n,j}|M_j|(\alpha_2(U_{2j}^{1+n}) - \alpha_2(U_{2j}^n))(k_e\rho_s|\Delta t|\theta_{wj}^n\alpha_1(U_{1j}^n)u_{3j}^n) \\ &\leq k_e\rho_s||\mathbf{U}_1^{1+n}||_\infty||\theta_w||_\infty||\alpha_1||_\infty||\alpha_2||_\infty||\mathbf{v}_3^n||_\infty\sum_{n,j}|\Delta t||M_j| \\ &\leq C_1.\end{aligned}$$

□

Proposition 3.5.4 *Under the assumptions (A1)-(A7), it is have for the scheme (3.3.7) that exits a constant $C > 0$, independent of h and Δt, such that*

$$\sum_{n,j} |\Delta t||M|(u_{3j}^{1+n} - u_{3j}^{n})^2 \leq C(|\Delta t| + h). \tag{3.5.2}$$

Proof. From scheme (3.3.7)

$$\sum_{n,j} |\Delta t||M|(u_{3j}^{1+n} - u_{3j}^{n})^2 \leq T_1 + T_2,$$

where

$$\begin{aligned} T_1 &:= \phi_s \sum_{n,j} |\Delta t||M||(\varphi_2 \circ \alpha_2)(U_{2j}^{n+1}) - (\varphi_2 \circ \alpha_2)(U_{2j}^{n})||u_{3j}^{n+1} - u_{3j}^{n}| \\ &\leq \phi_s \sum_{n,j} |\Delta t||M|[\epsilon|(\varphi_2 \circ \alpha_2)(U_{2j}^{n+1}) - (\varphi_2 \circ \alpha_2)(U_{2j}^{n})|^2 + \frac{1}{4\epsilon}|u_{3j}^{n+1} - u_{3j}^{n}|^2] \\ &\leq \phi_s \sum_{n,j} |\Delta t||M|[\epsilon K_{\varphi_2}|\alpha_2(U_{2j}^{n+1}) - \alpha_2(U_{2j}^{n})|^2 + \frac{1}{4\epsilon}|u_{3j}^{n+1} - u_{3j}^{n}|^2], \end{aligned}$$

(is enough to choose $\epsilon := \phi_s/2$), and

$$T_2 := k_e \sum_{n,j} |\Delta t|^2|M|\theta_{wj}^{n}\alpha_1(U_{1j}^{n})|u_{3j}^{n}||u_{3j}^{n+1} - u_{3j}^{n}| \leq k_e|\Delta t|C_2. \square$$

Proposition 3.5.5 *Under the assumptions (A1)-(A7), it is have for the scheme (3.3.7), that there exists a constant $C > 0$, independent of h and Δt, such that*

$$\frac{1}{2}\sum_{n,l} |\Delta t||l|(u_{3j}^{n} - u_{3l}^{n})^2 \leq C(|\Delta t| + h). \tag{3.5.3}$$

Proof. From equation (3.2.9)

$$u_{3j}(t) = -tk_e\theta_{wj}(t)\alpha_1(U_{1j}(t))u_{3j}(t) + \phi_s(\varphi_2 \circ \alpha_2)(U_{2j})(t) + u_{3j}(0) - \phi_s(\varphi_2 \circ \alpha_2)(U_{2j})(0).$$

Hence,

$$\sum_{n,l} |\Delta t||l||u_{3j}(t) - u_{3l}(t)|^2 = T_1 + T_2,$$

where

$$T_1 := \phi_s \sum_{n,l} |\Delta t||l|((\varphi_2 \circ \alpha_2)(U_{2j}) - (\varphi_2 \circ \alpha_2)(U_{2l}))(u_{3j} - u_{3l}),$$

and

$$T_2 := -k_e \sum_{n,l} t|\Delta t||l|(\theta_{wj}\alpha_1(U_{1j})u_{3j} - \theta_{wl}\alpha_1(U_{1l})u_{3l})(u_{3j} - u_{3l}).$$

About T_1,

$$\begin{aligned} T_1 &\leq \phi_s \sum_{n,l} |\Delta t||l|[\epsilon_1|(\varphi_2 \circ \alpha_2)(U_{2j}) - (\varphi_2 \circ \alpha_2)(U_{2l})|^2 + \frac{1}{4\epsilon_1}|u_{3j} - u_{3l}|^2] \\ &\leq \phi_s \sum_{n,l} |\Delta t||l|[\epsilon_1 K_{\varphi_2}|\alpha_2(U_{2j}) - \alpha_2(U_{2l})|^2 + \frac{1}{4\epsilon_1}|u_{3j} - u_{3l}|^2]. \end{aligned}$$

About T_2 note that if it is applied the equality:

$$ab - cd = (ab - cd) + (bc - bc) = (ab - bc) + (bc - cd) = b(a - c) + c(b - d),$$

for each real numbers a, b, c, d, then

$$\begin{aligned} (\theta_{wj}\alpha_1(U_{1j})u_{3j} - \theta_{wl}\alpha_1(U_{1l})u_{3l})(u_{3j} - u_{3l}) &= \\ u_{3j}\alpha_1(U_{1j})(\theta_{wj} - \theta_{wl}) + u_{3j}\theta_{wl}(\alpha_1(U_{1j}) - \alpha_1(U_{1l})) + \theta_{wl}\alpha_1(U_{1l})(u_{3j} - u_{3l}). \end{aligned}$$

Therefore, if it is supposed that for each j, l: $\theta_{wj} = \theta_{wl}$, then for T_2 it is get

$$\begin{aligned} T_2 &= -k_e \sum_{n,l} t|\Delta t||l|\{u_{3j}\theta_w(\alpha_1(U_{1j}) - \alpha_1(U_{1l})) + \theta_w\alpha_1(U_{1l})(u_{3j} - u_{3l})\}(u_{3j} - u_{3l}) \\ &= -k_e \sum_{n,l} t|\Delta t||l|u_{3j}\theta_w(\alpha_1(U_{1j}) - \alpha_1(U_{1l}))(u_{3j} - u_{3l}) \\ &- k_e \sum_{n,l} t|\Delta t||l|\theta_w\alpha_1(U_{1l})(u_{3j} - u_{3l})^2. \end{aligned}$$

If, in this last equality, the second term in the right hand side is exchanged to lest hand side, it is get

$$\begin{aligned} \sum_{n,l} |l||\Delta t|(u_{3j} - u_{3l})^2 &\leq \sum_{n,l} |l||\Delta t|(1 + k_e t\theta_w\alpha_1(U_{1l}))(u_{3j} - u_{3l})^2 \\ &\leq \phi_s \sum_{n,l} |\Delta t||l|[\epsilon_1 K_{\varphi_2}|\alpha_2(U_{2j}) - \alpha_2(U_{2l})|^2 + \frac{1}{4\epsilon_1}|u_{3j} - u_{3l}|^2] \\ &+ \sum_{n,l} |\Delta t||l|[\epsilon_2|u_{3j}||\theta_w||\alpha_1(U_{1j}) - \alpha_1(U_{1l})|^2 + \frac{1}{4\epsilon_2}|u_{3j} - u_{3l}|^2]. \end{aligned}$$

Therefore is enough to choose $\epsilon_1 = \epsilon_2 = 1$.
□

Lemma 3.5.2 *Under Assumptions (A1) to (A7), let* $\mathcal{T}$ *be an admissible mesh in the sense of Definition 3.3.1 and* $\Delta t \in (0,T)$*. Let* $u_{3,\mathcal{T},\Delta t} \in X(\mathcal{T},\Delta t)$ *be given by Definition 3.3.2. One defines* $\tilde{u}_3$ *by* $\tilde{u}_3 = u_{3,\mathcal{T},\Delta t}$ *a.e. on* $\Omega\times(0,T)$*, and* $\tilde{u}_3 = 0$ *a.e. on* $\mathbb{R}^{2+1}\backslash\Omega\times(0,T)$*. Then, there exits a constant* $C > 0$*, independent of* τ*,* h *and* Δt*, such that*

$$||\tilde{u}_3(\cdot,\cdot+\tau) - \tilde{u}_3(\cdot,\cdot)||^2_{L^2(\mathbb{R}^{2+1})} \leq C|\tau|, \forall\tau \in \mathbb{R}.$$

Proof.

$$\int_{\Omega\times(0,T-\tau)} (\tilde{u}_3(x,t+\tau) - \tilde{u}_3(x,t))^2 dt = \int_0^{T-\tau} A(t)dt,$$

where

$$\begin{aligned}
A(t) : &= \int_\Omega (\tilde{u}_3(x,t+\tau) - \tilde{u}_3(x,t))^2 dx \\
&= \sum_{M\in\mathcal{T}} |M|(u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)})^2 \\
&= \sum_{M\in\mathcal{T}} |M|(u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)})(u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)}) \\
&= \sum_{M\in\mathcal{T}} (u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)}) \sum_{n=n_0(t)+1}^{n_1(t)} |M|(u_{3j}^{n} - u_{3j}^{n-1}) \\
&= \sum_{M\in\mathcal{T}} (u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)}) \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau)|M|(u_{3j}^{n} - u_{3j}^{n-1}) \\
&= A_1(t) + A_2(t),
\end{aligned}$$

with

$$\begin{aligned}
A_1(t) : &= \sum_{M\in\mathcal{T}} (u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)}) \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau)|M|[-\Delta t k_e \theta_{wj}^n \alpha_1(U_{1j}^n) u_{3j}^n] \\
A_2(t) : &= \sum_{M\in\mathcal{T}} (u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)}) \sum_{n=1}^{N_{\Delta t}} \chi_n(t,t+\tau)|M|\phi_s[(\varphi_2\circ\alpha_2)(U_{2j}^{n+1}) - (\varphi_2\circ\alpha_2)(U_{2j}^n)].
\end{aligned}$$

About the $A_1(t)$ term note that

$$\begin{aligned}\int_0^{T-\tau} A_1(t)dt &\leq \sum_{n=1}^{N_{\Delta t}} \Delta t[\sum_{M\in(T)} (u_{3j}^{n_1(t)} - u_{3j}^{n_0(t)})|M|k_e\theta_{wj}^n\alpha_1(U_{1j}^n)u_{3j}^n \int_0^{T-\tau} \chi_n(t,t+\tau)dt] \\ &\leq (2T||u_3||_\infty|\Omega|k_e||\theta_w||_\infty||\alpha_1||_\infty||u_3||_\infty)\tau \\ &\leq C\tau.\end{aligned}$$

Finally, with the same argument, it is obtained that there exits a constant $C > 0$ such that, $\int_0^{T-\tau} A_2(t)dt \leq C\tau$.
□

Theorem 3.5.6 *Under the assumptions (A1)-(A7) the approximate solution* (U_{2h}, u_{3h}) *given by the scheme (3.3.6)-(3.3.7), without any CFL condition, converges to* (U_2, u_3) *in* $L^2(Q_T) \times L^2(Q_T)$ *as* h *and* Δt *go to zero.*

Proof. The proof follow the same lines of Theorem 3.4.4. In order to show the convergence of $U_{2h} := U_{2h}(x,t) := U_{2M}^n$ and $u_{3h} := u_{3h}(x,t) := u_{3M}^n$, in $M \times [t_n, t_{n+1}]$, toward the weak solution defined in section 3.2.6, it is passed to the limit in the scheme (3.3.6)-(3.3.7).

About U_{2h}**.** Let us set $\tilde{\alpha}_{2h} := \alpha_2(U_{2h})$ on Q_T and $\tilde{\alpha}_{2h} := 0$ on $\mathbb{R}^3 \backslash Q_T$. From Propositions 3.5.2 and 3.5.3, and Lemma 3.5.1, $(\tilde{\alpha}_{2h}) \subseteq L^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Then, applying Theorem 3.4.3 and Lemma 3.5.1 it is get (following the same lines of Theorem 3.4.4's proof) that $(\tilde{\alpha}_{2h})$ is relatively compact in $L^2(Q_T)$. Therefore, there exits a subsequence, still denoted by $(\tilde{\alpha}_{2h})$, and there exits $\alpha_2^* \in L^2(Q_T)$ such that $(\tilde{\alpha}_{2h})$ converges to α_2^* in $L^2(Q_T)$. Indeed, since $(\tilde{\alpha}_{2h}) \subseteq L^\infty(Q_T)$, this convergence holds in $L^q(Q_T)$ for all $1 \leq q < \infty$. Furthermore, since α_2 is nondecreasing, Theorem 18.2 in [28] gives that $\alpha_2^* = \alpha_2(U_2^*)$, that is $U_2^* = \alpha_2^{-1}(\alpha_2^*)$. Therefore, (α_{2h}) converges to $\alpha_2(U_2^*)$ in $L^1(Q_T)$ (and even in $L^p(Q_T)$ for all $p \in [0, \infty)$).

About u_{3h}**.** Let us set $\tilde{u}_{3h} := u_{3h}$ on Q_T and $\tilde{u}_{3h} := 0$ on $\mathbb{R}^3 \backslash Q_T$. From Propositions 3.5.1 and 3.5.4, and Lemma 3.5.5, $(\tilde{u}_{3h}) \subseteq L^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$.

Then, applying the Theorem 3.4.3, (with $N = d+1, d = 2$, $q = 2$, and $\omega = \Omega \times (0,T)$) note that the first and second items of Theorem 3.4.3 are clearly satisfied. About the third hypothesis, note that for $\eta \in \mathbb{R}^2$ and $\tau \in \mathbb{R}$,

$$\begin{aligned} ||\tilde{u}_{3h}(\cdot+\eta,\cdot+\tau) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})} &\leq \\ ||\tilde{u}_{3h}(\cdot+\eta,\cdot) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})} &+ ||\tilde{u}_{3h}(\cdot,\cdot+\tau) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})}. \end{aligned}$$

About the term $||\tilde{u}_{3h}(\cdot+\eta,\cdot) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})}$, in this last inequality, note that by Lemma 18.3 in [28], p.851, there exits a bound $C(|\eta|) > 0$, such that $||\tilde{u}_{3h}(\cdot+\eta,\cdot) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})} \leq C(|\eta|)$, and $C(|\eta|) \to 0$ if $|\eta| \to 0$.
By another hand, about the term $||\tilde{u}_{3h}(\cdot,\cdot+\tau) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})}$ note that by Lemma 3.5.2, there exits a constant $C > 0$, independent of η and τ, such that $||\tilde{u}_{3h}(\cdot,\cdot+\tau) - \tilde{u}_{3h}(\cdot,\cdot)||_{L^2(\mathbb{R}^{2+1})} \leq C\tau$.
This yields the compactness of the sequence $(\tilde{u}_{3h})$ in $L^2(Q_T)$, that is, $(\tilde{u}_{3h})$ is relatively compact in $L^2(Q_T)$. Therefore, there exits a subsequence, still denoted by $(\tilde{u}_{3h})$, and there exits $u_3^* \in L^2(Q_T)$ such that (u_{3h}) converges to u_3^* in $L^2(Q_T)$. Indeed, since $(u_{3h} \subseteq L^\infty(Q_T)$, this convergence holds in $L^q(Q_T)$ for all $1 \leq q < \infty$. Therefore, (u_{3h}) converges to u_3^* in $L^1(Q_T)$ (and even in $L^p(Q_T)$ for all $p \in [0,\infty)$).
It remains to be shown that (U_2^*, u_3^*) is a weak solution. Because, the proof follows the same lines of Theorem 3.4.4, is enough to mention that

$$\sum_{n,j} v_j^n \hat{T}_{2r} = \sum_{n,j} v_j^n \{k_e\rho_s|\Delta t||M|\theta_{wj}^n \alpha_1(U_{1j}^n)u_{3j}^n\} \to \int_{Q_T} k_e\rho_s\theta_w\alpha_1(U_1)u_3 v.$$

□

In Chapter 4 you can find computational experiments for the transport problem in heap leaching.

Chapter 4

Computational Experiments

The objective of this chapter is to show several computational experiments based in the models presented in the chapters 2 and 3.

4.1 Introduction

The chapter is organized as follows. In section 4.2 are reported numerical experiments for the two phase fluid problem, and in section 4.3, are reported numerical experiments for the compositional transport problem.

4.2 The Two Phase Flow Problem

In this section is considered the fractional flow formulation (*fff*), (2.2.12)-(2.2.14), given by (for more details cf. Chapter 2, section 2.2.2)

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0, \\ \mathbf{u} &= -k\lambda(s)(\nabla p - G_\lambda \mathbf{g}), \\ \phi \frac{\partial s}{\partial t} + \nabla \cdot (f_w(s)\mathbf{u} - D_w(s)\nabla s - G_w(s)\mathbf{g}) &= 0, \end{aligned}$$

in the unknowns $\mathbf{u}$, p and $s \equiv s_w$.

4.2.1 Parameters

The numerical solution of system *fff* require an explicit definition for $p_c(\cdot)$ and $k_{r\alpha}(\cdot), \alpha = w, n$. In this sense the most usual correlations for a two-phase gas-water system are defined in Table 1,

Model	$p_c(s_w)$	$k_{rw}(s_w)$	$k_{rn}(s_w)$
BC	$p_d S_e^{-1/\lambda}$	$S_e^{\frac{2+3\lambda}{\lambda}}$	$(1-S_e)^2(1-S_e^{\frac{2+\lambda}{\lambda}})$
VG	$\frac{1}{\alpha}(S_e^{-1/m}-1)^{1/n}$	$S_e^{\varepsilon}(1-(1-S_e^{1/m})^m)^2$	$(1-S_e)^{\gamma}(1-S_e^{1/m})^{2m}$

Table 1. Brooks-Corey (BC) and van Genuchten (VG) models, [30].

where $S_e(s_w) := \frac{s_w - s_{wr}}{1-s_{wr}}$ is the effective saturation, with s_{wr} is the residual water saturation. The BC-parameters are the entry pressure $p_d > 0$ and λ, which usually lies between 0.2 and 3.0. The VG-parameters are $\alpha > 0$ and $m = 1 - \frac{1}{n}$, with $0 < m < 1$. The parameters ε and γ are form parameters which describe the connectivity of the pores. Generally, $\varepsilon = \frac{1}{2}$ and $\gamma = \frac{1}{3}$. For an analysis of BC and VG parameters, in the heap leaching context, cf. [9]. The numerical values of model's parameters are in in Table 2 (cf. [36]):

name	**symbol**	**value**	**unit**
absolute permeability	k	$1.78 \cdot 10^{-11}$	$[m^2]$
liquid density	ρ_w	1011	$[kg/m^3]$
gas density	ρ_n	1.16	$[kg/m^3]$
porosity	ϕ	0.33	$[-]$
liquid viscosity	μ_w	10^{-3}	$[kg/m \cdot s]$
gas viscosity	μ_n	$1.85 \cdot 10^{-5}$	$[kg/m \cdot s]$
residual water saturation	s_{wr}	0	$[-]$
initial water saturation	s_w^o	0.4343	$[-]$
VG-parameter	n	1.411	$[-]$
VG-parameter	α	$1.35 \cdot 10^{-4}$	$[1/Pa]$
heap slope	θ	$\pi/4$	*radians*
heap width	W	25	$[m]$
heap height	H	5	$[m]$

Table 2. Numerical values for physical parameters.

4.2.2 Characterization of functions p_c, $k_{r\alpha}$, f_w, G_w and D_w

The behavior of these functions is very important in the mathematical and numerical analysis of the system (2.2.12)-(2.2.14). In this subsection it is showed their plots according Table 2. The plot of p_c function is given in Figure 4.

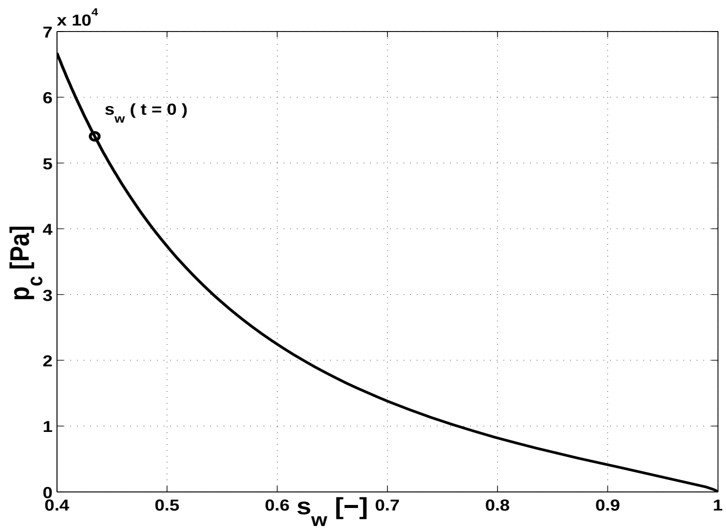

Figure 4. Capillary pressure for VG model.

The plot of $k_{r\alpha}$ function is given in Figure 5.

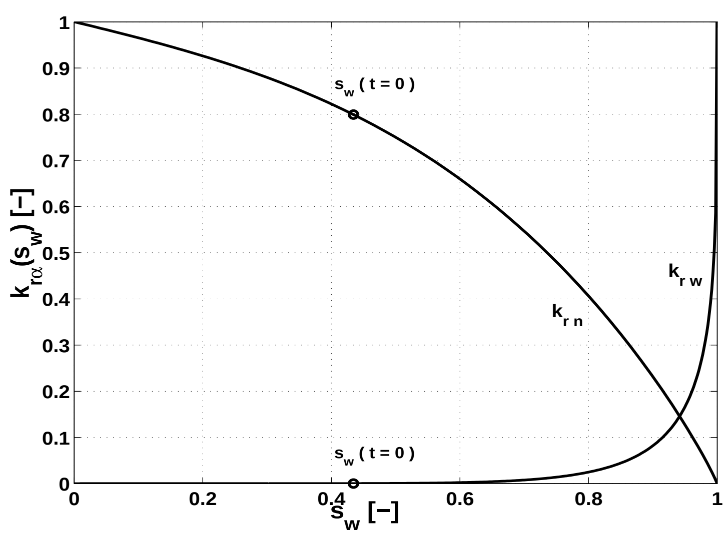

Figure 5. Relative permeability for VG model.

The plot of f_w function is given in Figure 6.

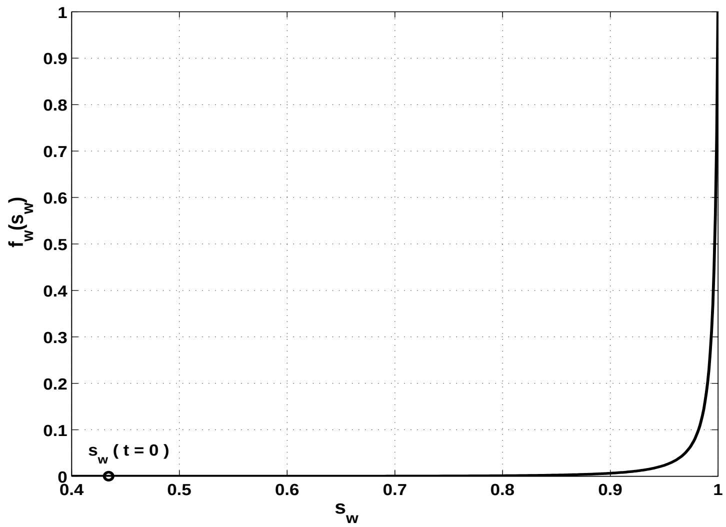

Figure 6. Fractional flow function for VG model.

The plot of G_w function is given in Figure 7.

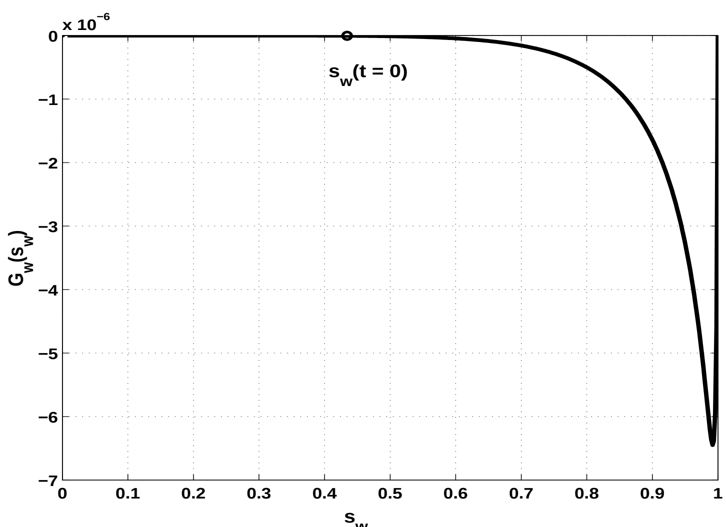

Figure 7. Gravitational function for VG model.

The plot of D_w function is given in Figure 8.

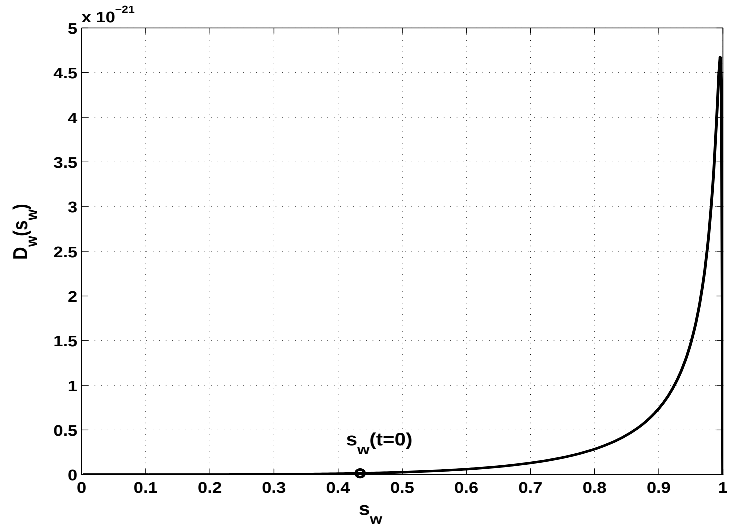

Figure 8. Capillary diffusion coefficient for VG model.

4.2.3 Solution of MFE-FV scheme

The computational code consider an implicit scheme for MFE method to obtain an approximation of $p(\mathbf{x}, t^{n+1})$ and $\mathbf{u}(\mathbf{x}, t^{n+1})$, where the liquid saturation s_w is replaced by an approximation of $s_w(\mathbf{x}, t^n)$, while that the saturation equation is solved by a cell centered FV implicit scheme to obtain an approximation of $s_w(\mathbf{x}, t^{n+1})$, where the total velocity $\mathbf{u}$ is replaced by an approximation of $\mathbf{u}(\mathbf{x}, t^{n+1})$, [8], [16]. It is used a damped inexact Newton algorithm for solving the nonlinear system of equations, [3], [30].
A plot of evolution of s_w in two points $P1 = (13.57, 5.00)$ and $P2 = (13.17, 2.95)$ in the heap Ω is given in Figure 9, for an irrigation ratio $R = 5.34[lt/hr/m^2]$.

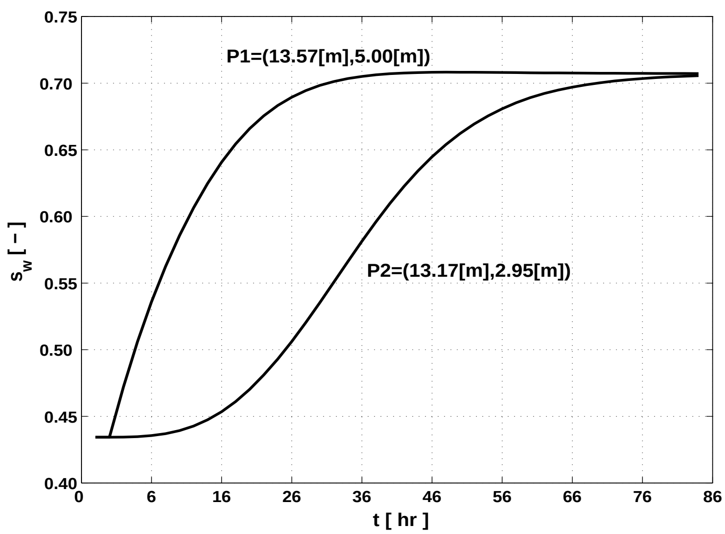

Figure 9. Evolution of s_w in two points of Ω.

A plot of 2D-evolution of s_w in $t = 22, 42, 64, 84[hr]$ is given in Figure 10, for an irrigation ratio $R = 5.34[lt/hr/m^2]$.

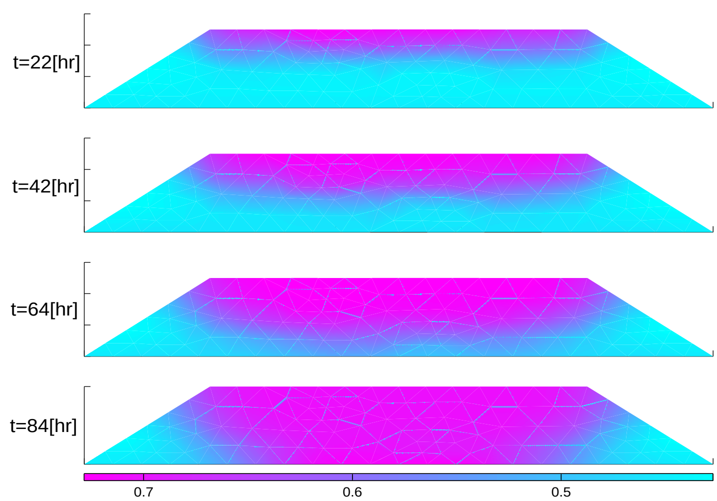

Figure 10. 2D-evolution of s_w.

4.3 The Transport Problem

In this section, it is reported numerical results in 2-D based on the scheme presented in this paper for sulfuric acid (cf. equation (3.2.7)) and copper in liquid and solid phase (cf. system (3.2.8)-(3.2.9)). Additionally, a sensitivity study has to be conducted. From qualitative point of view, the numerical results are in according with physical behavior (cf. [39, 46]).

4.3.1 Initial Set of Parameters

It is considered a heap where height is equal to 3[m] and the bottom weight is equal to 15[m]. Additionally, in this simulation it is considered one isotherm only for the copper in liquid phase, which is given by $\varphi_2 = k_d c_c^w$. The irrigation rate on the top boundary (Γ^i) is given by $R = 18[l/hr/m^2]$. The another parameters are given by: $\mathbf{u}_w = (18/36)\cdot 10^{-5}[m/s]$, $s_w = 0.7[-]$, $\phi = 0.33[-]$, $\mu = 10^{-5}[1/s]$, $k_e = 8.3\cdot 10^{-7}[m^3/kg\cdot s]$, $k_d = 8.67\cdot 10^{-5}[m^3/kg]$, $\rho_s = 1800[kg/m^3]$, $\lambda_c^s = 0.62[-]$, $G_c^s = 2.9\cdot 10^{-3}[kg/kg]$, $c_a^o = 10[kg/m^3]$, $c_c^o = 0[kg/m^3]$, and $c_a^i = 40[kg/m^3]$. In figures 11, 12 and 13, it is showed the concentration's evolution on 19 days, where P1 is a generic point on Γ^i, P2 is in the middle of Ω, and P3 is on Γ^o.

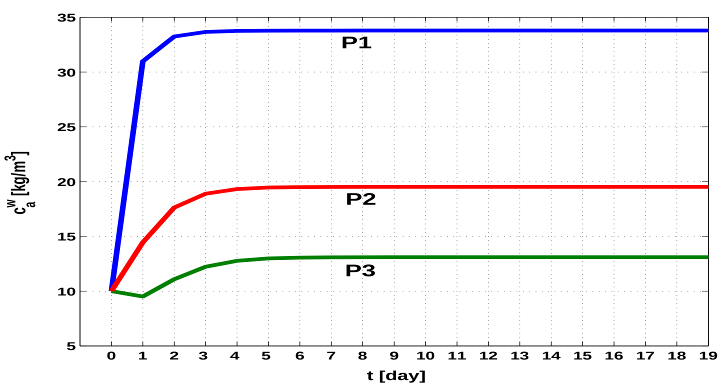

Figure 11. Sulfuric Acid in Liquid Phase: c_a^w.

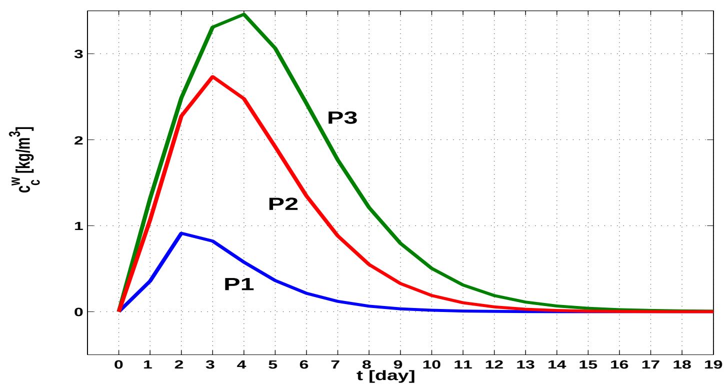

Figure 12. Copper in Liquid Phase: c_c^w.

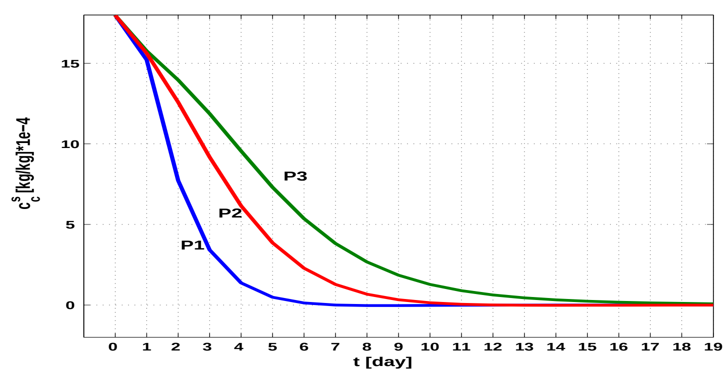

Figure 13. Copper in Solid Phase: c_c^s.

4.3.2 Sensitivity Test

In order to test the ability and performance of the model to simulate the leaching process under different conditions, and also to provide a basis for optimization of operation conditions, some sensitivity tests are carried out by changing the parameters of importance one by one.

In figures 14, 15, 16, 17, 18, 19, it is presented some sensitivity tests. The reference's parameters are the initial set defined in before section and the parameters under investigation are: (i) the volumetric concentration of sulfuric acid in the irrigation solution: c_a^i (see Figures 14, 15 and 16 and cf. subsection 3.2.4), (ii) the consumption factor, a first-order reaction constant: μ (see Figure 17 and cf. subsection 3.2.1), (iii) equilibrium distribution constant: k_d (see Figure 18 and cf. subsection 1.4) and (iv) first-order kinetic constant: k_e (see Figure 19 and cf. subsection 3.2.2).

In all following plots, it is showed the evolution on the point P2, which is a generic point in the middle of heap Ω, specifically, P2=(6.9[m],1.6[m]).

Influence of c_a^i. The reference's value is $c_a^i = 40[kg/m^3]$. In Figure 14, 15 and 16, it is showed the evolution of sulfuric acid in liquid solution c_a^w, the copper in liquid solution c_c^w, and copper in solid phase, c_c^s, respectively; when the reference's value is amplified to $c_a^i = 60[kg/m^3]$ and reduced to $c_a^i = 20[kg/m^3]$.

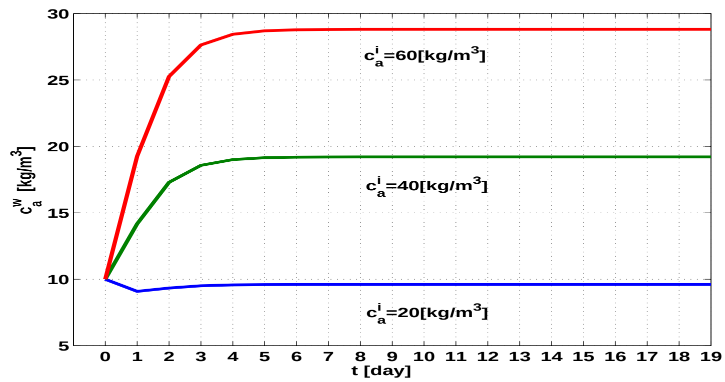

Figure 14. Influence of c_a^i on c_a^w.

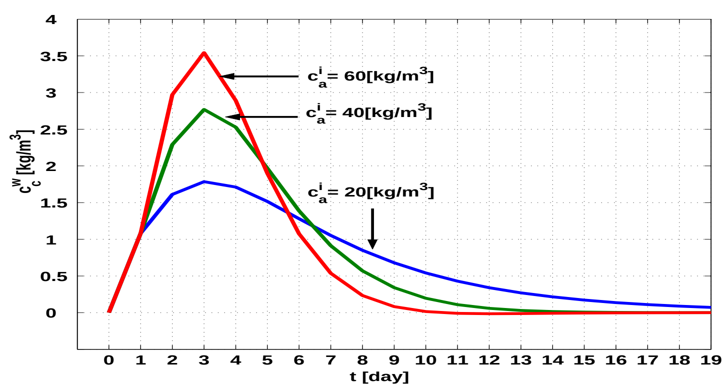

Figure 15. Influence of c_a^i on c_c^w.

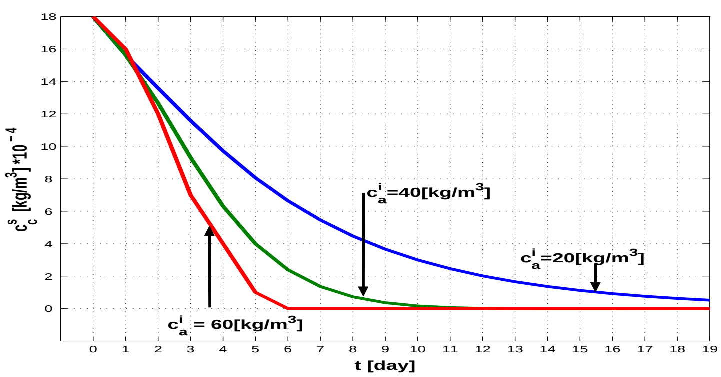

Figure 16. Influence of c_a^i on c_c^s.

The figures 14, 15, y 16, show that if the level of c_a^w increase, the level of copper in liquid phase c_c^w too.

Influence of μ. The reference's value is $\mu = 10^{-5}[1/s]$. In Figure 17 it is the evolution of sulfuric acid in liquid solution c_a^w; when the reference's value is amplified to $\mu = 10^{-4}[1/s]$ and reduced to $\mu = 10^{-6}[1/s]$.

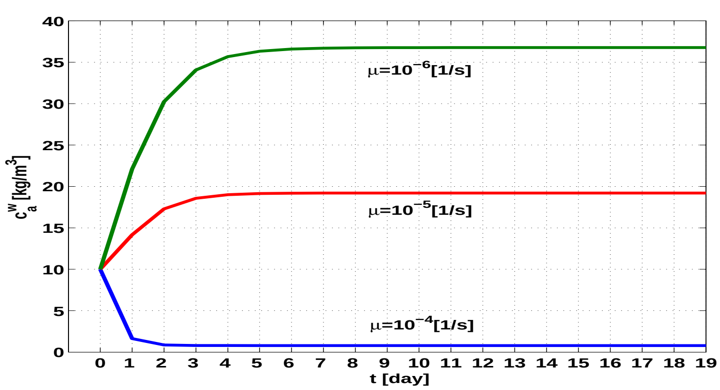

Figure 17. Influence of μ on c_a^w.

The figure 17, show that if the value of μ increase, the level of sulfuric acid in liquid phase c_a^w diminish.

Influence of k_d. The reference's value is $k_d = 8.67 \cdot 10^{-5}[m^3/kg]$. In Figure 18 it is the evolution of copper in liquid solution c_c^w; when the reference's value is reduced to $k_d = 8.67 \cdot 10^{-6}[m^3/kg]$.

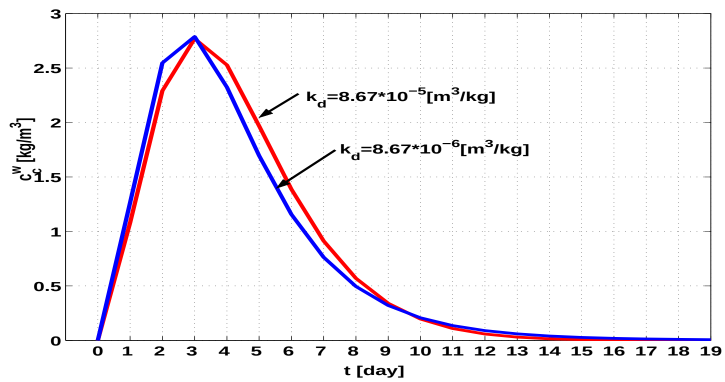

Figure 18. Influence of k_d on c_c^w.

The figure 18 show that if the value of k_d is less, then you have the same concentration of copper in liquid phase c_c^w in less time.

Influence of k_e. The reference's value is $k_e = 8.3 \cdot 10^{-7}[m^3/kg \cdot s]$. In Figure 19 it is the evolution of copper in liquid solution c_c^w; when the reference's value is reduced to $k_e = 8.3 \cdot 10^{-8}[m^3/kg \cdot s]$.

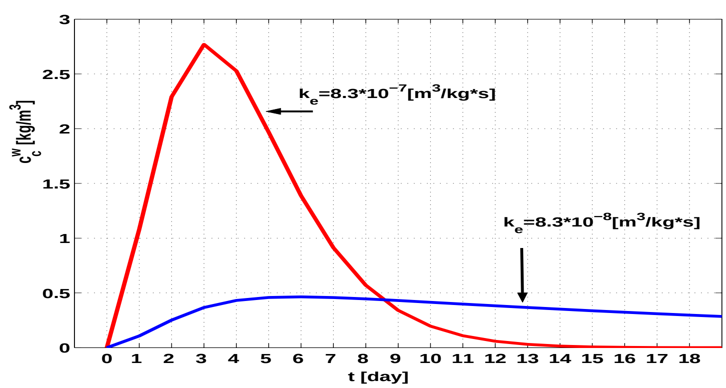

Figure 19. Influence of k_e on c_c^w.

The figure 19 show that if the value of k_e is less, the concentration of copper in liquid phase c_c^w too.

Chapter 5

Discusión General (In Spanish)

El objetivo principal de este capítulo (*según el Decreto U. DE C. Nro. 2001-186, Universidad de Concepción*) es integrar los principales hallazgos de la investigación realizada y ponerlos en el contexto del conocimiento actual.

5.1 Resultados v/s Estado del Arte

En esta sección se comparan los principales resultados obtenidos en esta tesis con los resultados publicados por otros autores. El análisis comparativo se desglosa en tres ámbitos: modelo conceptual, análisis numérico y experimentos computacionales.

5.1.1 Modelo Conceptual.

La construcción de un modelo conceptual del proceso de lixiviación en pilas, utilizando la teoría de flujos multifásicos-multicomponentes en medios porosos, es un aporte inédito de esta tesis (hasta donde alcanza el conocimiento del autor). En efecto, la formulación del problema de flujo quitando la hipótesis de una fase gaseosa estática, está enunciado para el caso 1D en [37], pero sin ningún tipo de desarrollo computacional ni teórico. Especificamente en [37] se menciona que: *desde el punto de vista práctico este modelo permitiría controlar y manipular los procesos de lixiviación que dependen de la cantidad de aire en la pila en un determinado momento y a una determinada altura.* Otro trabajo en donde sí se postula un modelamiento similar al propuesto en esta tesis es [36], el cual se desarrolló bajo las indicaciones del autor de esta tesis. La diferencia es que en [36] el modelo matemático a dos fases se resuelve íntegramente usando el método numérico de volúmenes finitos y el modelo de transporte no considera el consumo del ácido sulfúrico. Además el autor de [36] utiliza un ambiente computacional ya construido, esto es, no desarrolla código computacional propio ni realiza análisis teórico alguno. Finalmente, y para mayor completitud, se menciona [24], en donde se discuten las ventajas del modelamiento conceptual seguido en esta tesis, y se reportan algunos experimentos computacionales.

5.1.2 Analisis Numérico.

Ver la Introducción a los Capítulos 2 y 3, que tratan el análisis numérico de los modelos de flujo y transporte, respectivamente, para una comparación con distintas alternativas reportadas en la literatura y una especificación de las contribuciones de esta tesis.

5.1.3 Experimentos Computacionales.

Los experimentos computacionales reportados en el Capítulo 4 tienen como finalidad mostrar la capacidad de los modelos propuestos, tanto de flujo como de transporte, de generar resultados físicamente coherentes con la práctica industrial y otras simulaciones reportadas en la literatura. El análisis que sigue se divide en tres partes: (i) Modelo de flujo a dos fases, (ii) Modelo de transporte, (iii) Análisis de sensibilidad.

Modelo de Flujo a Dos Fases

El flujo de una fase fluida líquida, al interior de un medio poroso, puede ocurrir fundamentalmente de tres formas: **(i)** flujo saturado, **(ii)** flujo no saturado, y **(iii)** flujo a dos fases. En el caso (i) el espacio de poros está completamente lleno con la fase líquida, en el caso (ii) el espacio de poros está parcialmente lleno con la fase líquida, esto es, coexisten las fases líquida y gaseosa, pero la fase gaseosa se supone estática, o sea, se descarta una interacción e influencia mutuas entre ambas, y el caso (iii) coincide con el caso (ii) pero se considera que ambas fases interactúan de manera significativa, influenciándose mutuamente en su evolución a través del espacio de poros.

Respecto del caso (i), en el ámbito de la lixiviación, se puede citar [39], por ejemplo. En el caso (ii) se puede citar a [14], [37] y [46], por ejemplo, en donde, la fase de interés en [14] es la fase gaseosa, pues se trata de una pila de mineral sulfurado, y el estudio se realiza en el ámbito de la biolixiviación. En [37] y [46] se utilizó la ecuación de Richards para aproximar la humedad o el nivel de saturación de la fase líquida.

Esta tesis aborda el caso (iii), esto es, se formulan las ecuaciones clásicas de flujo a dos fases para el proceso de lixiviación en pilas de minerales de cobre. Los únicos trabajos conocidos por el autor de esta tesis, en esta dirección, son los ya mencionados, esto es, [8], [24], y [36]. Como se sabe, la ecuación de Richards es una caso particular de las ecuaciones de flujo a dos fases, por lo que esta tesis se ubica en el nivel más alto de generalización, la cual se hace necesaria cuando se lleva a cabo, por ejemplo, un proceso de aireación forzada o riego intermitente en una pila de minerales principalmente sulfurados. Los experimentos computacionales reportan la implementación del modelo de flujo a dos fases para pilas de lixiviación con parámetros físico-químicos tomados de la práctica industrial y de otros experimentos similares reportados en la literatura (ver Figuras 9 y 10, sección 4.2.3).

Modelo de Transporte

Se considera una pila de lixiviación formada principalmente por minerales oxidados. Los antecedentes del modelo de transporte estudiado en esta tesis se encuentran en [39] y [46]. Consiste en dos submodelos: **(i)** una ecuación diferencial parcial del tipo convección-difusión-reacción, que modela el consumo de ácido sulfúrico, y **(ii)** un sistema de ecuaciones diferenciales formado por una ecuación del mismo tipo mencionado en (i), más una ecuación diferencial ordinaria. En este sistema la primera ecuación modela la extracción de cobre desde la fase sólida a la fase líquida, y la segunda ecuación modela la evolución de la concentración de cobre en fase sólida.

Las figuras 11, 12 y 13, en la sección 4.3.1, reportan la solución de los dos submodelos mencionados anteriormente, para el conjunto de valores numéricos de los parámetros indicados. La Figura 11 muestra la evolución del ácido sulfúrico para tres puntos en la pila.

Se observan distintos valores de estabilidad, con una mayor concentración de ácido en los niveles superiores de la pila (punto P1), lo que se traduce en una mayor extracción de cobre. Este hecho se ve reflejado, también, en la Figura 13, en que para el mismo punto P1, el cobre en fase sólida decrece más rápido. Se observa una mayor concentración de cobre en fase líquida en los niveles inferiores de la pila (ver Figura 12, punto P3) producto del cobre proveniente de los niveles superiores. Los resultados numericos mencionados son cualitativamente similares a los reportados por [39] y [46].

Análisis de Sensibilidad

Se realizó un análisis de sensibilidad, de la solución del modelo de transporte descrito en la sección anterior, ante variaciones de los siguientes parámetros: **(i)** c_a^i : concentración de ácido sulfúrico de la solución de riego en la superficie de la pila (ver Figuras 14,15 y 16), **(ii)** μ : factor de consumo de ácido sulfúrico (ver Figura 17), **(iii)** k_d : constante de distribución en equilibrio, presente en la isoterma (ver Figura 18), y **(iv)** k_e : la constante de extracción de cobre (ver Figura 19). El único estudio similar, según el conocimiento del autor de esta tesis, es el realizado en [46], pero no exactamente al mismo conjunto de parámetros elegido. Los resultados obtenidos son cualitativamente similares a [46], y muestran la capacidad del modelo propuesto y de la solución numérica implementada computacionalmente, de dar cuenta de la física del fenómeno de transporte bajo distintas condiciones.

5.2 Conclusiones Generales

1. La teoría macroscópica de medios porosos, que considera el flujo de las fases fluidas líquida y gaseosa, junto con el transporte e intercambio de especies o componentes entre las fases líquida, gaseosa y sólida, constituye el marco teórico natural para modelar el proceso de lixiviación en pilas de minerales de cobre (ver Capítulo 1).

2. La solución numérica de las ecuaciones clásicas de flujo a dos fases utilizando un esquema que combina el método de elementos finitos mixtos con el método de volúmenes finitos, en el caso de que la ecuación de saturación incluya un término convectivo no lineal, y se consideren condiciones de contorno más generales, es convergente (ver Capítulo 2).

3. La solución numérica de un sistema de tres ecuaciones diferenciales del tipo convección-difusión-reacción utilizando un esquema que combina el método de volúmenes finitos para el término convectivo, con el método de elementos finitos para el término difusivo, es convergente (ver Capítulo 3).

4. Los resultados de los experimentos computacionales realizados para los modelos de flujo a dos fases y de transporte de componentes, utilizando parámetros tomados de la práctica industrial, son físicamente coherentes con la observacion experimental (ver Capítulo 4).

5.3 Futuros Desarrollos

1. **Modelo Conceptual:** (i) incorporar los fenómenos de transporte en pilas de minerales sulfurados, considerando la concentración e intercambio de oxígeno, junto con condiciones no isotermales, (ii) considerar la deformación mecánica que sufre la pila de lixiviación durante el proceso de riego, (iii) considerar la disminución en la porosidad producto del consumo de ácido sulfúrico.

2. **Análisis Numérico:** (i) realizar el análisis matemático y numérico de los modelos de transporte que surgan del punto anterior, (ii) considerar un modelo acoplado de flujo y transporte, (iii) estudiar los mismos modelos con nuevos métodos numéricos.

3. **Experimentación Computacional:** optimizar el código desarrollado por el autor de esta tesis y el uso del recurso computacional, a través del desarrollo de un mallado adaptivo, por ejemplo. Esto permitiría realizar simulaciones con un intervalo temporal de mayor longitud, y efectuar un mallado espacial más fino.

4. **Parámetros:** quitar la hipótesis utilizada en esta tesis de que la porosidad y la permeabilidad absoluta son constantes. Esto puede dar origen a problemas matemáticos y numéricos relevantes.

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