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### Thermofluidynamics of colloidal systems

**CERES** Project



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#### Abstract

The international energy agency (IEA) stated that global energy consumption in the industrial sector grew by 61% in 2004 compared to the levels recorded in the 60s. The increased energy consumption has implied a considerable increase in the levels of  $C0_2$  present in the atmosphere: the industrial activities have raised atmospheric carbon dioxide levels from 280 parts per million to 400 parts per million in the last 150 years. This rate is unprecedented in the geological record of the past 55 million years. In July 2016, global temperatures soared to the hottest in the 136 years of the instrumental record, 0.1°C warmer than previous warm Julys in 2015, 2011 and 2009. In this world context, the industrial sector is called to improve the efficiency of its production cycles in order to reduce emissions that are harmful to humans and the environment. One way is to exploit the energy that is dissipated in the environment, through waste heat recovery (WHR) systems. Most of the heat produced around the world is at low temperature, i.e. under 200  $C^{\circ}$ , and energy recovery from a source of this type is very complicated. The Colloidal EnERgEtic  $\mathbf{S}$ ystem (CERES) is an energy harvesting system aimed to the recovery of heat in this range of temperatures: the idea was born to respond directly to the challenge of NASA "Surviving extreme spatial environment" and the first step was to create the prototype known as DOUGHNUT, or rather aDatptive cOloalidal accUmulatinG / HarvestiNg UniT. This system uses an external thermal gradient (generated for example by exhaust gases), combined with a permanent magnetic field, to generate motion of convection and translation of the ferrofluid inside. With an appropriate configuration of the collection coils, using Faraday's law, it is possible to recover and store energy from these flow motions. After having described the prototype in its essential components, and having provided an overview of the fluid used, we move on to the description of the mathematical model used to describe the motions inside, with a detailed overview of all the forces that play a fundamental role in this context. Then we move on to describe the numerical method used for the discretization of the mathematical model, thanks to which we obtain the fluid dynamic views of what happens in the area of interest. Future developments of this prototype will provide for the use of these results to find the configuration of the collection coils in order to maximize energy recovery.

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# Chapter 1

### Introduction

Most climate scientists agree that main cause of the current global warming trend is human expansion of the "greenhouse effect" [1] -warming that results when the atmosphere traps heat radiating from Earth toward space.

Some gases in the atmosphere prevent heat from dissipating; some of these that remain semipermanently in the atmosphere are described as "forcing" climate change [2]. Gases that contribute to the greenhouse effect include:

- Carbon dioxide  $(CO_2)$ , not only released through natural processes like volcanic eruptions but is released into the atmosphere also by the combustion of fossil fuels. Humans have increased the concentration of  $CO_2$  in the atmosphere by more than a third since the industrial revolution began.
- Methane  $(CH_4)$  is a hydrocarbon gas produced both through natural resources and human activities, including the decomposition of waste in landfills for example. Methane is a much more active greenhouse gas than carbon dioxide, but also much less abundant in the atmosphere.
- Nitrous  $\operatorname{oxide}(N_2O)$  is a powerful greenhouse gas produced by soil cultivation practices, in particular the use of commercial and organic fertilizers, the combustion of fossil fuels, the production of nitric acid and the combustion of biomass[2].
- Chlorofluorocarbons (CFC). Synthetic compounds entirely of industrial origin capable of contributing to the destruction of the ozone layer.

In its Fifth Assessment Report, the Intergovernmental Panel on Climate Change, a group of 1,300 independent scientific experts from countries all over the world, concluded there is more than 95% probability that human activities over the past 50 years have warmed our planet.

In July 2016, global temperatures soared to the hottest in the 136 years of the instrumental record, 0.1°C warmer than previous warm Julys in 2015, 2011 and 2009. It followed a succession of rising temperatures, moving from 0.42°C above average in 2000, to 0.87°C above average by 2015.[9] The industrial activities that our modern civilization depends upon have raised atmospheric carbon dioxide levels from 280 parts per million to 400 parts per million in the last 150 years. This rate is unprecedented in the geological record of the past 55 million years, and is tracking towards the stability threshold of the Antarctic ice sheet, estimated at around 450ppm atmospheric  $CO_2$ .[9]

#### 1-Introduction



Figure 1.1: This graph, based on the comparison of atmospheric samples contained in ice cores and more recent direct measurements, provides evidence that atmospheric CO2 has increased since the Industrial Revolution. [1]

The rise in greenhouse gas levels in the atmosphere and oceans is leading to an increase in extreme weather events relative to the period 1950-60, including tropical storms such as those in Fiji, Vanuatu and the Philippines, with lives lost and damage estimated in the billions of dollars. Ice sheet melt rates have been increasing and the rate of sea-level rise has been accelerating, from roughly 1.7 mm per year over the past century to 3.2 mm per year between 1993 and 2010, and to about 3.5mm per year today. This threatens low-lying islands, deltas and lower river valleys where billions of people live a problem that is compounded by increased variability of river flows in terms of floods and droughts.[9]

Actually one third of the global energy consumption is employed in industrial processes and, as reported by International Energy Agency (IEA), the industrial energy consumption had increased by 61% in 2004 with respect to the level of 1971. [3]

In the United States for example, the  $CO_2$  emission is around  $1.68 \times 10^{12} kg$  in 2015 [7] while in Europe a relative total  $CO_2$  emission is around  $0.36 \times 10^{12} kg$  in the same year. [8]

In this context, industries are challenged with the task of reducing greenhouse gas emissions and improving the efficiency of their production processes. All over the world, any industrial process presents a waste of energy or heat. It is estimated that globally, only one third of all energy usages were utilized while the remaining is rejected as waste heat.[4]

As much as 20%- 50% of energy is lost as waste heat in metal and non-metallic mineral manufacturing in United States [11], while in the European Union, it is estimated that the 70% of total energy used in industry is employed in thermal processes (furnaces, reactors, boilers and dryers) and about a third of this energy is wasted into the environment through losses: the waste heat potential in the EU has been estimated to be 300-350 TWh/year based on the energy consumption.



Figure 1.2: industrial energy consumption (Eurostat data inTWh per year) in some of the EU countries with at least moderate industrial activity. In the same graph is given the total industrial energy consumption in the EU. [5]

In this regard, the use of waste heat recovery systems (WHR) in industrial processes is one of the main research areas to reduce fuel consumption, reduce harmful emissions and improve production efficiency.[10]

The term Waste Heat Recovery (WHR) refers to the process apt to recover the heat that would otherwise be lost in the atmosphere, store it, and possibly re-use it to generate energy without combustion and without emissions: for example it is possible to directly use the waste heat to provide heating or cooling, or to convert the heat into electrical and mechanical power or to combine heating, cooling and power generation.

Any industrial process that involves the transformation of raw materials into useful products - steelworks, refineries, chemical plants, general manufacturing - generates heat that is wasted as a by-product. This residual heat is produced whenever the operation is running, often 24 hours a day, seven days a week, 365 days a year. If this heat is not recovered in any way, it is dispersed in the atmosphere, thus wasting a potential zero-emission energy source.

In this context, WHR technologies help to reduce energy costs for industrial processes. Using waste heat to generate emission-free electricity, industrial users can put the wasted energy back into the process that created it or introduce it somewhere else into the plant. The basis of these technologies are described in figure 1.3

To realize a technology of this type, different parameters are fundamentals, such as the amount of heat available, its quality, the minimum allowed temperature and so on.

Every industrial sector will have a different waste heat fraction (with respect to the total energy consumption), that is incorporated in a different thermal carrier such as gaseous streams (exhaust and flaring gases), liquid streams (hot oil, cooling water ) and solids (commodities and products, hot steel). The heat quantity is the amount of energy contained in a waste heat and it can be derived by:

$$E = m \cdot h(t) \tag{1.1}$$



Figure 1.3: The essential components necessary for the WHP energy recover technology [7].

where m is the waste stream mass [kg], h(t) is the enthalpy per unit mass [J/Kg] and E [J] represent the waste heat loss. Among all these factors, the most important one is the quality of the heat itself: the higher the temperature, the greater the potentially recoverable energy (fig.1.5). Depending on the industrial sector and the process, also the temperature at which the heat is available varies within a very wide range: in general the potential for residual heat above 1000 °C is limited and observed only in the iron and steel industries. In the temperature range between 500-1000 °C, waste heat is available, mainly in the cement, iron and steel sectors. In the range 200-500 °C the potential increases, mainly in the pulp and paper and iron and steel industries. Most of the residual heat is found in the temperature range of 100-200 °C, widespread in most industrial sectors, while below 100 °C the potential is rather limited, concentrated in the food and beverage sector, mainly from drying and preheating processes.[5]

As an example the data from the UK industry have been reported in fig.1.4

Therefore, heat loss, transferred to the atmosphere mainly through conduction, convection and radiation, can be classified into high temperature (HT), medium temperature (MT) and low temperature (LT) grades.

- Low quality:  $T < 200 \text{ }^{\circ}\text{C}$
- Medium quality: 200 °C < T < 650 °C
- High quality:  $T > 650 \ ^{\circ}C$

Compared to a heat at HT and MT, most of the heat produced (60%) is at LT and energy recovery from a source of this type is very difficult; in this perspective it is placed the CERES system concept. This device is able to produce electric potential from gradients of temperature. In the next chapter this system will be analyzed in all its main components. The purpose of this thesis is to simulate, through a Computational Fluid Dynamics (CFD) analysis, the operation of this device in order to obtain the configuration that allows to maximize energy recovery starting from the condiments previously tested in the laboratory



Figure 1.4: Waste heat fraction per industrial sector and temperature level for UK industry for the period 2000-2003.[5]



Figure 1.5: Percentages describing the amounts of technical potential (in MW) present in WHP, for different temperatures [11].

# Chapter 2 The "CERES" system

The CERES (Colloidal EneRgEtic System) system is an energy harvesting system based on a (ferro)fluid. This idea was created to respond directly to the challenge of NASA "Surviving extreme spatial environments", which aims to identify the most efficient materials, structures and solutions for developing an autonomous and energy-efficient system based on a fluid.

The first step was to create a prototype known as DOUGHNUT, or rather a**D**atptive c**O**loalidal acc**U**mulatin**G** / **H**arvesti**N**g **U**ni**T**: this system, by means of a ferrofluid enclosed within a thin shell is able to exchange only electromagnetic or thermal energy with the external environment [6]. The physical principles underlying CERES were described in the thesis work of Mattiussi [11], from now on I will describe what are the fundamental components that have been used for the first tests in the laboratory, and that are fundamental to set up the CFD simulations, after which I will describe the liquid medium used and its main properties. The following chapters will describe the equations that regulate the system inside and the discretization of the latter. The final chapter will cover the analysis of the results obtained and possible improvements

#### 2.1 "CERES" reactor

The first experimental tests were conducted using a torus-shaped device (fig.2.1) that was designed using CAD design software, in our case SOLIDWORKS. The material used was PLA, with a FDM (Fused Deposition Modeling) machine for rapid prototyping. The second prototype on which the various cases studied in this thesis work will be tested, is made of plexiglass, and it is transparent, to allow to visualize all the motions that are created inside it. In table 2.1 are reported the most relevant dimensions of the structure.

Parameters	Size
External radius	140  mm
Internal radius	110  mm
Height	$85 \mathrm{mm}$
Width	20  mm
Wall thickness	$5 \mathrm{mm}$
Bottom/lid height	20 mm

Table 2.1: Main features of CERES structure [11]



Figure 2.1: Virtual rendering of CERES system [11].

#### 2.1.1 Magnets

Permanent magnets constitute a fundamental component as they contribute to creating cyclic motions inside the reactor. They are attached to both the internal and external walls and the magnetization of each of them is parallel to the thickness.

By varying their arrangement on the walls, a magnetic field, that will have different characteristics, is created each time inside the reactor, and it will influence the motions of the fluid in a different way. This constitutes the center of the present thesis work: which configuration is optimal for our purposes. These permanent magnets are made in ALNICO, a particular alloy made by ALuminuim-NIckel-CObalt whose performance is particularly stable at high operational temperatures; they have a parallelepiped shape whose dimensions are:

$$30 \pm 0.1mm \times 15 \pm 0.1mm \times 3 \pm 0.1mm \tag{2.1}$$



Figure 2.2: One of the ALNICO magnets, successively installed all around the CERES ring[11].

#### 2.1.2 Peltier Modules

A Peltier module is a device able to transfer heat from one side to the other one by means of an electrical energy consumption.

These devices are positioned both on the external and internal walls and when they are turned on they create a thermal gradient inside the fluid giving start to the convection motions inside the CERES system



Figure 2.3: The Peltier module that is used for the CERES Project[11].

#### 2.2 Ferrofluids

#### 2.2.1 Introduction

The ferrofluid is the key element of the CERES system. To give a definition we can say that Ferrofluid(FF), also known as magnetic colloid, is a colloidal suspension of single-domain magnetic particles, with typical dimensions of about 10 nm, dispersed in a liquid carrier.[13]

A colloidal suspension is a suspension of a particle that is so small that it does not settle out (sedimentation) of solution rapidly, even in the presence of gravity. The particles are coated with a stabilizing dispersing agent (surfactant) which prevents particle agglomeration even when a strong magnetic field gradient is applied to the ferrofluid. The surfactant must overcome the attractive van der Waals and magnetic forces between the particles.[14]

The metal compounds that make up the nanoparticles are iron oxides, such as magnetite  $(Fe_3O_4)$ , magnetite  $(Fe_2O_3)$ , cobalt ferrite  $(CoFe_2O_4)$ .

The first colloids of this type were synthesized in the 1930s, but only in the 1960s, or when industrial production became possible, there was a notable interest in their applications in the technological field.

The appeal of this special material derives from the fact that its flow and properties can be significantly altered by the influence of magnetic fields; in the absence of the latter, the magnetic moments of the particles are randomly distributed and the fluid has no net magnetization. When a magnetic field is applied to a FF, the magnetic moments of the particles orient along the field lines almost instantly. The magnetization of the FF responds immediately to the changes in the applied magnetic field and when the applied field is removed, the moments randomize quickly. In a gradient field the whole fluid responds as a homogeneous magnetic liquid which moves to the region of highest flux. This means that FF can be precisely positioned and controlled by an external magnetic field. The forces holding the magnetic fluid in place are proportional to the gradient of the external field and the magnetization value of the fluid. [14]

The presence of ferromagnetic nanoparticles with magnetic moments that are  $10^3 - 10^4$  times larger than those of ions of paramagnetic materials allows to obtain a FF magnetization up to  $\approx 100 kA/m$  using external magnetic fields created by ordinary permanent magnets.[15] Taking into account the fact that the strength and direction of magnetic fields and field gradients can be adapted to a specific need, one can imagine the variety of possibilities that arise. The interaction of the fluid with external field is studied in a special division of hydrodynamics which is known as ferrohydrodynamics.

The possibility of exerting an externally controllable force in a fluid obviously also opens up a wide range of possibilities in the search for basic fluid dynamics; the magnetic force enters directly into the Navier-Stokes equation and can therefore be used to control and guide flows in the fluid. The main motivating factor for the rapid development of this research area is a wide range of FF applications including: vibration damping, magnetic sealing, species separation and use in various sensors, laser radiation actuator modulators and cancer treatment to name a few.

However, the significant discrepancy between successful applications on the one hand, the potential and scientific activities on the other hand, emerges mainly from the complexity of fluids and the description of their behavior in a magnetic field.



Figure 2.4: Schematic representation not in scale of the magnetic particles and of the surfactant. [16]

#### 2.2.2 Magnetism and Properties of ferrofluids

In the presence of a magnetic field different materials show different behaviors depending on their atomic structure. Elementary particles, like electrons, have an intrinsic magnetic moment (spin) that allows them to rotate around their own axis. The magnetic properties of the materials derive above all from the movement of the orbitals and the variation of the spins of their electrons while the other contributions, like the magnetic one of the nucleus, are negligible with respect to these effects.

If spins are paired, their magnetic moments are canceled; if they are not balanced, the atom behaves like a permanent dipole.

Magnetic materials can be classified, based on their response to an external magnetic field, in:

- diamagnetic
- ferromagnetic /ferrimagnetic
- antiferromagnetic / antiferrimagnetic
- paramagnetic

Diamagnetic materials such as water, organic substances and some metals are substances that are weakly rejected by a magnetic field.

Paramagnetic materials are formed by atoms that have unpaired electrons and have a zero magnetization in the absence of the external field. The application of an external magnetic field leads instead to align the elementary moments along its direction giving rise to a resulting magnetization of concordance and intensity proportional to the field itself.

Ferromagnetic and ferrimagnetic materials, under the action of an external magnetic field, have the ability to maintain the magnetization induced by the field, through the alignment (parallel or antiparallel) of their magnetic moments, even when this is canceled.

The antiferromagnetic materials show an alignment of the antiparallel moments, with zero magnetization resulting. In figure 2.5, the different situations are reported.



Figure 2.5: Different types of magnetism in materials: A) In paramagnetism the magnetic moments are randomly aligned in absence of a magnetic field (this is also the case of ferromagnets above T C); B) Ferromagnetism show all moments aligned and with the same intensity in absence of a magnetic field (or is the case of paramagnets in presence of an external magnetic field); C) Antiferromagnetism presents magnetic domains aligned in opposite direction, but with the same intensity, so that the total resulting magnetization is null; D) Ferrimagnetism is similiar to antiferrimagnetism, but in this case the opposite magnetic moments have different amplitudes, and consequently the resulting magnetization is not zero. [11]

The typical characteristic of ferromagnetic materials is that when the magnetic field H is removed, a residual magnetization remains  $M_r$ . The figure 2.6 clarifies this concept by showing the typical hysteresis curve for magnetization and highlighting the saturation magnetization  $M_{max}$  and the coercive field  $H_c$ .



Figure 2.6: Typical hysteresis curve of ferromagnetic materials.[16]

When a ferromagnetic material is subjected to a temperature higher than a limit, called Curie temperature, it loses the orderly arrangement of the electrons and becomes paramagnetic (figure 2.7).



Figure 2.7: Magnetic susceptibility trend with temperature variation. [16]

A ferromagnetic sample subjected to a magnetic field retains its magnetic properties until it reaches the Curie temperature. Beyond this limit, the sample becomes paramagnetic. The consequence of this phenomenon is that the sample cancels its own magnetization and becomes insensitive to a further action of the field. In the first laboratory tests the FF used consisted of solid magnetite particles  $(T_c = 948K)$ , and considering that the temperatures in our case are of the order of 323K - 333K, our system will never become paramagnetic.

Following what was written in Mattiussi's thesis work [11], we can give some information about the ferrofluid used.

For example the FF volume subject to the thermal gradient can be considered constant since the  $\alpha$  thermal expansion coefficient is very small and constant for a temperature range between 100 K and 300 K.

$$\alpha = (1.2 \pm 2) \times 10^{-4} K^{-1} \tag{2.2}$$

The speech is different for the density of the magnetite nanoparticles which decreases as the temperature increases as shown in the table 2.2

Temperature[C]	<b>Density</b> $[kg/m^3]$
10	2462
20	2458
30	2453
40	2448
50	2443
60	2439
70	2434
80	2429

Table 2.2: Density values for magnetite/oleic acid aggregates for different increasing temperatures [11]

The FF considered in this thesis work is the EMG 901 produced by Ferrotec, whose main characteristics are summarized in the table 2.3

Properties	EMG 901
Appearence	Black-brown fluid
Carrier liquid	light hydrocarbon oil
Nominal particle diameter	10 nm
Magnetic particle concentration	11.8% vol
Saturation magnetization	66  mT
Viscosity @ 27C	8 mPas
Initial magnetic susceptibilit y	6.79
Density	$1.43 \times 10^3 kg/m^3$

Table 2.3: Properties of EMG 901 by Ferrotec [14]

#### 2.3 Extraction System

Since this device is designed as a WHP, its primary objective is certainly to store energy by exploiting the properties and flow motions that develop inside it thanks to the thermal gradient provided by Peltier cells and thanks to the external magnetic field induced by permanent magnets. When FF particles are introduced into the reactor, they are affected by the magnetic field, instantaneously magnetizing; they are dragged by the convective motions that are established and their movement produces fluctuations in the magnetic field: the latter can be exploited with a suitable extraction system.

The device is therefore comparable to a sort of solenoid: the variation of the magnetic field will produce an EMF (Electro $\mathbf{M}$ otive Force) at the output of the system. The charge thus acquired can be stored in electrical systems for example.

#### 2.3.1 The Faraday's Law

The phenomenon of electromagnetic induction was discovered in 1831 by Michael Faraday and can be summarized as follows:

" The electromotive force around a closed path is equal to the negative of the time rate of change of magnetic flux enclosed by the path [12]"

This law was demonstrated for the first time in that same year with a simple experiment. Faraday built a system consisting of a toroidal iron ring with two coils wrapped around it.



Figure 2.8: The apparatus realized by Faraday. The left side wire is connected to a battery, while the right one is plugged to a voltmeter, in order to measure the induced EMF on the right wire [11]

When the battery is disconnected from the left coil, no phenomenon is observed, but when the connection is activated, the current flows in the left loop, inducing a transient in the current (and in the voltage), in the right wire. This phenomenon is generated by the variation in the magnetic flux  $\Phi$  that occurs when the battery is connected or disconnected. From a mathematical point of view, the Faraday's law can be expressed as follow:

$$\epsilon = -\frac{d\Phi}{dt} \tag{2.3}$$

where  $\epsilon$  represent de EMF induced in the circuit and  $\Phi$  is the magnetic flux. [11] The magnetic flux is defined as:



Figure 2.9: The magnetic flux  $\boldsymbol{\Phi}$  across a closed surface  $\Sigma$ . [11]

We know that  $B = \mu_0(H + M)$  where M si the magnetization of FF particles and H is the external magnetic field.

The magnetic field H will not be uniform, as we will see later, therefore particles will be subject to different magnetization depending on the area in which they pass. Fluid dynamics simulations serve to understand exactly how these particles move dragged by the flow and therefore how their magnetization varies inside the reactor. A variation of magnetization involves a variation of B. If the trajectory along which the variation of B takes place, is wound with coils, according to Faraday's law, it will generate electromotive force induced inside them and therefore current induced in the circuit.

The main objective of this thesis is therefore to be able to define the motion of dispersed ferromagnetic particles. Future developments, even from an experimental point of view, will be based on these results to obtain the best possible configuration in order to maximize the current induced in the circuit.

### Chapter 3

### Mathematical model

#### 3.1 Classification on multiphase flow

In the previous chapter we have described the main characteristics of a ferrofluid; its composition given by solid particles dispersed in a carrier liquid push us to consider this fluid as biphasic. Moreover, for our simulations, not only FF is introduced into the CERES reactor, but it is diluted with water. When we derive the mathematical model of the system, the keyword is multiphase fluid.

A multiphase system is characterized by two or more phases that flow simultaneously in the mixture that have phase separation above the molecular level. In fluid mechanics, multi-phase flow is simultaneous flow of (a) materials with different states or phases (i.e. gas, liquid or solid), or (b) materials with different chemical properties but in the same state or phase (i.e. liquid-liquid systems such as oil droplets in water). This type of flow is an ubiquitous feature of our environment, whether it is rain, snow, fog, avalanches, mud slides, sediment transport, debris flows and countless other natural phenomena. Even very critical biological and medical flows are multiphase, such as blood flow. Countless industrial processes have to do with fluids of this type and, clearly, the ability to predict the flow behavior of these processes is fundamental for the efficiency and effectiveness of the latter.

Two general typologies of multi-phase flow can be usefully identified at the outset:

- **Disperse flows** are those consisting of finite particles, drops or bubbles (the disperse phase) distributed in a connected volume of the continuous phase
- **Separeted flows** consist of two or more continuous streams of different fluids separated by interfaces.

In a disperse flow, the characteristics of the movement of the solid particles are strongly dependent on the size of the individual elements and on the motions of the associated fluids. Very small particles follow the fluid motions, whereas larger particles are less responsive.

Such a premise was necessary to clarify the way in which the flow within the CERES reactor was considered: as a first approximation, the overall mixture of FF and water was considered as biphasic; this means that the carrier liquid of ferrofluid and the water were considered as two miscible liquids and the equations obtained in the next chapter reflect this configuration.

To know the amount of dispersed solid phase it is essential to clarify what are the proportions that are created inside the device: in the tests conducted previously, 8 mL of FF were placed in 0.5 L of water, which means that the mixture was composed by 1.6% of FF.

Knowing that the volumetric concentration is 11.8%, the concentration in the mixture is 0.188%. Although this model is very simplified with respect to the great complexity of the mixture used, future developments of the prototype involve the use of undiluted ferrofluid alone, thus finding agreement with the equations obtained for a two-phase mixture.



Figure 3.1: Classification of gas-liquid flows. [17]

#### **3.2** Modeling approaches

Nowadays, for the numerical calculation of multiphase flows, there are two different types of approaches: the Euler-Lagrange approach and the Euler-Euler approach.

In the Euler-Euler approach, the different phases are treated mathematically as interpenetrating continua. Since the volume of a phase cannot be occupied by the other phases, the concept of phasic volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information, or, in the case of granular flows, by application of kinetic theory[18].

In the Euler-Lagrange approach, the fluid phase is treated as a continuum by solving the timeaveraged Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles, bubbles, or droplets. The dispersed phase can exchange momentum, mass, and energy with the fluid phase. A fundamental assumption made in this model is that the dispersed second phase occupies a low volume fraction. The particle or droplet trajectories are computed individually at specified intervals during the fluid phase calculation. The model is appropriate to simulate spraydryers, coal and liquid fuel combustion, but it's inappropriate to model liquid-liquid mixtures, fluidizedbeds, or any application where the volume fraction of the second phase is not negligible.[18]

Having in mind the main differences between the two models, we have used an Euler-Euler approach to derive the mathematical model of our system.

Following what is written on the theoretical rules of most CFD calculation software, three different

Euler-Euler multiphase models are implemented: the VOF model, the mixture model and the Eulerian model.

Without going into the details of all these three models, we will focus only on the **mixture model**, which is the one adopted in the present thesis work. The mixture model uses a single-fluid approach:

- Allows the phases to be interpenetrating. The volume fractions  $\varphi_d$  and  $\varphi_f$  for a control volume can therefore be equal to any value between 0 and 1, depending on the space occupied by phase d(dispersed) and phase f(fluid).
- Allows the phases to move at different velocities, using the concept of slip velocities.

The mixture model solves the continuity, momentum and energy equation for the mixture, and the volume fraction equation for the secondary phases, as well as algebraic expressions for the relative velocities (if the phases are moving at different velocities)[17]: the equations just described are obtained in the following chapters.

#### 3.3 Mixture continuity equation

The mixture continuity equation, that is referred to the whole fluid system plus dispersed phase, expresses the physical principle for which the mass within an infinitesimal and fixed control volume, is conserved.

We can say that the net flux of mass coming out from the control volume through control surfaces is equal to the time rate of reduction of the mass contained inside the control volume. Referring to the fig. 3.2 we can derive, for example the net mass flux perpendicular to the x- direction.



Figure 3.2: mass flow that crosses every single face of the control volume [19]

The the mass flux across the left surface, is:

$$\begin{array}{c} (\rho u)dydz \\ 25 \end{array} \tag{3.1}$$

whereas, for the right surface, we have:

$$\left[(\rho u) + \frac{\partial(\rho u)}{dx}dx\right]dydz \tag{3.2}$$

Since in our convention the velocity components u,v,w are positive in the x,y and z- directions, respectively, the net flux of mass coming out from the considered surfaces will be:

$$\left[(\rho u) + \frac{\partial(\rho u)}{dx}dx\right]dydz - (\rho u)dydz = \frac{\partial(\rho u)}{dx}dxdydz$$
(3.3)

following the same reasoning the net flows in the y and z -direction are easily obtained. The global mass flux that passes through the infinitesimal control volume will be:

$$\left[\frac{\partial(\rho u)}{dx} + \frac{\partial(\rho v)}{dy} + \frac{\partial(\rho w)}{dz}\right] dx dy dz \tag{3.4}$$

The time-rate of reduction of the mass of fluid that is present inside the infinitesimal control volume is:

$$-\frac{\partial\rho}{\partial t}dxdydz\tag{3.5}$$

Putting togheter eq.(3.4) and eq.(3.5), the continuity equation written in conservative and differential form became:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{3.6}$$

Developing in terms of derivation in space and applying the definition of a Lagrangian derivative <sup>1</sup>we obtain:

$$\frac{D\rho}{Dt} + \nabla \cdot \mathbf{v} = 0 \tag{3.7}$$

what has been written so far is identical to the case in which we have a single phase of density  $\rho$  inside the control volume, but now the global density of the mixture  $\rho_m$  must take into account the contribution of the dispersed phase( $\rho_d$ ) and of the phase fluid( $\rho_f$ ): we will write that:

$$\rho_m = \varphi_d \rho_d + \varphi_f \rho_f$$

where  $\varphi_d$  and  $\varphi_f$  are the volumetric concentration of particles and fluid respectively; being dimensionless, the following law will be applied

$$\varphi_d + \varphi_f = 1 \tag{3.8}$$

Following what is written in [20], we apply the Boussinesq approximation for which the flux

 $<sup>{}^{1}\</sup>partial(\cdot)/\partial t + \mathbf{v}\nabla(\cdot) = D(\cdot)/Dt$ 

density will change, if there is a variation in the temperature inside the fluid that can be caused by a different temperature on the walls of the control volume, as in our case.

However, this density variation is neglected everywhere except in the buoyancy term as we shall see later.

Following this approximation, we can write:

$$\rho_f = \rho_0 (1 - \alpha \Delta T) \tag{3.9}$$

where  $\rho_0$  is the fluid density at  $T_0$  and  $\alpha$  is the thermal diffusion coefficient. If  $\Delta T < 10K$  the term  $\alpha(\Delta T)$  is much lower than 1 and it is therefore negligible; because of what has been said, being  $\rho_f = \rho_0 = cost$  and  $\rho_d = cost$  the global continuity equation becomes

$$\nabla \cdot \mathbf{v} = 0 \tag{3.10}$$

#### 3.4 Mixture momentum equation

The momentum equation, based on Newton's second law, releates the fluid mass acceleration to the surface and volumetric forces experienced by the fluid.

Volumetric forces "act at a distance" and they act directly on the mass that is contained in the control volume: in our case we have gravitational and magnetic force.

Surface forces, instead, act directly on the surface of the control volume and they are: pressure imposed by the external field and shear and normal stresses imposed by the external field through friction. We can now consider an infinitesimal control volume that moves with the flow, we will obtain the equation for only x-component and, after that, we will analyze the volumetric forces. Following the fig.3.3 we can observe how the surface forces act and we can develop the balance of forces along the x-axis as an example.

The net pressure force in the x-direction is written as:

$$\left[p - \left(p + \frac{\partial p}{\partial x}dx\right)\right]dydz \tag{3.11}$$

The shear and normal stresses in a fluid are related to the time-rate-of-change of the deformation of the fluid element.

The shear stress, denoted by  $\tau_{ij}$   $(i \neq j)$  is related to the time rate-of-change of the shearing deformation of the fluid element, whereas the normal stress, denoted by  $\tau_{ij}$  (i = j), is related to the time-rate-of-change of volume of the fluid element: both shear and normal stresses depend on velocity gradients in the flow. [21]

For our convention,  $\tau_{ij}$  denotes a stress in the j-direction exerted on a plane perpendicular to the i-axis. Note the directions of the shear force on faces "abcd" and "efgh" for example; on the bottom face,  $\tau_{yx}$  is to the left (the negative x-direction), whereas on the top face,  $\tau_{yx} + (\partial \tau_{yx}/\partial y)dy$ ] is to the right (the positive x-direction).

These directions reflect the convention that positive increases in all three velocity components occur in the positive directions of the axes.

Explaining it more clearly, referring to the figure 3.3, u increases in the positive y-direction, therefore, concentrating on the top face, u is higher just above the face than on the face itself:



Figure 3.3: Infinitesimally small, moving fluid element. Only the forces in the x- direction are shown [21]



Figure 3.4: Illustration of shear and normal stresses [21]

this causes the fluid element to be pulled to the right (positive x-direction).

Concentrating on the bottom face instead, u is lower just beneath the face than on the face itself: this causes a dragging action on the fluid element, which acts in the negative x-direction (to the left) [21].

All other viscous stresses, including those normal to the surface, are justified in this way. Remembering what has just been written, for the moving fluid element, the net surface force in the x-direction is written as:

$$\left[-\tau_{xx} + \left(\tau_{xx} + \frac{\partial \tau_{xx}}{\partial x}dx\right)\right]dydz + \left[-\tau_{yx} + \left(\tau_{yx} + \frac{\partial \tau_{yx}}{\partial y}dy\right)\right]dxdz + \left[-\tau_{zx} + \left(\tau_{zx} + \frac{\partial \tau_{zx}}{\partial z}dz\right)\right]dxdy$$
(3.12)

The left-hand side of the dynamical equation is the rate of change of the momentum: the

mass of the fluid element is fixed and is equal to  $\rho dx dy dz$ . The acceleration of the fluid element is the time-rate-of-change of its velocity. Hence, the component of acceleration in the x-direction, is simply the time-rate-of-change of u; since we are following a moving fluid element, this time-rate-of-change is given by the substantial derivative. The left-hand side term is written as:

$$\rho dx dy dz \frac{Du}{Dt} \tag{3.13}$$

Putting togheter (3.11) and (3.12) with the left-hand written just above, we obtain the Navier-Stokes equation in x-direction with only the contributions of surface forces.

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}$$
(3.14)

In a similar fashion, the y and z components can be obtained as:

$$\rho \frac{Dv}{Dt} = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}$$
(3.15)

$$\rho \frac{Dw}{Dt} = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}$$
(3.16)

The three equation above are the x-,y- and z-components respectively of the mixture momentum equation.

When shear stress in a fluid is proportional to the time-rate-of-strain, i.e. velocity gradients, we are dealing with a Newtonian fluid. (Fluids in which  $\tau$  is not proportional to the velocity gradients are non-Newtonian fluids; blood flow is one example)[21]. For such fluids, Stokes, in 1845, obtained:

$$\tau_{xx} = \lambda \nabla \cdot \mathbf{v} + 2\mu \left(\frac{\partial u}{\partial x}\right) \tag{3.17}$$

$$\tau_{yy} = \lambda \nabla \cdot \mathbf{v} + 2\mu \left(\frac{\partial v}{\partial y}\right) \tag{3.18}$$

$$\tau_{zz} = \lambda \nabla \cdot \mathbf{v} + 2\mu \left(\frac{\partial w}{\partial z}\right) \tag{3.19}$$

$$\tau_{xy} = \tau_{yx} = \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)$$
(3.20)

$$\tau_{xz} = \tau_{zx} = \mu \left( \frac{\partial u}{\partial x} + \frac{\partial w}{\partial x} \right)$$
(3.21)

$$\tau_{yz} = \tau_{zy} = \mu \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)$$
(3.22)

where  $\mu$  is the molecular viscosity coefficient and  $\lambda$  is the bulk viscosity coefficient.[22] The stokes hypothesis says that

$$\lambda = -\frac{2}{3}\mu \tag{3.23}$$

However, for the continuity equation,  $\nabla \cdot \mathbf{v} = 0$ . If, additionally,  $\mu$  is taken to be constant, the global Navier-Stokes equation written for all three directions in compact form becomes

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{v} + F_{buoyancy} + F_{magnetic}$$
(3.24)

Let's change the differential and non-conservative form into the conservative form; to do it, we have to use the definition of Lagrangian derivative. Explicating in all three directions, you get the following system:

$$\rho\left(\frac{\partial u}{\partial t} + \nabla \cdot (u\mathbf{v})\right) = -\frac{\partial p}{\partial x} + \mu \nabla^2 u + F_{x,buoyancy} + F_{x,magnetic} 
\rho\left(\frac{\partial v}{\partial t} + \nabla \cdot (v\mathbf{v})\right) = -\frac{\partial p}{\partial y} + \mu \nabla^2 v + F_{y,buoyancy} + F_{y,magnetic} 
\rho\left(\frac{\partial w}{\partial t} + \nabla \cdot (w\mathbf{v})\right) = -\frac{\partial p}{\partial x} + \mu \nabla^2 w + F_{z,buoyancy} + F_{z,magnetic}$$
(3.25)

We will focus, in the following chapters, to define which are the volumetric forces that act a "distance" on our control volume and finally we will write the Navier-Stokes equation completely.

#### 3.4.1 Buoyancy

There are two definitions for buoyancy:

- the tendency of a body to float or to rise when submerged in a fluid
- the power of a fluid to exert an upward force on a body placed in it.

The components that are at stake in the evaluation of this force are therefore a mass, a surrounding fluid and the force of gravity. The density difference is fundamental to the development of this force; for example, inside our planet, density difference, with other phenomenon, generates the motion of magma.

When we talk about fluids, the density differences are usually small and their influence on the inertia of a fluid can often be neglected, but in our case, the ferromagnetic particles have a much higher density than the surrounding fluid and therefore this contribution cannot be ignored.

As we said previously, the Boussinesq approximation consists in neglecting density differences in the equations except if they are multiplied by g which is usually much bigger than the vertical accelerations within the fluid; in a multiplase flow we can say that:

$$\rho_m = \rho_f(\varphi_f) + \rho_d \varphi_d \tag{3.26}$$

$$\varphi_f + \varphi_d = 1 \tag{3.27}$$

where  $\varphi$  is the volume concentration of particles. The subscripts f and d differentiate the fluid phase (f) from the dispersed and therefore solid phase (d).

The term  $\rho_d$  will remain constant since the density of the single particle of colloid does not vary

with the T, while the  $\rho_f$  will feel a variation due to the temperature difference. Applying the Boussinesq approximation (3.9), the mixture's density is expressed as:

$$\rho_{mix} = \rho_{T_0,f} (1 - \alpha (T - T_0))(1 - \varphi_d) + \rho_p(\varphi_d)$$
(3.28)

where  $\rho_{0,f}$  represent the density of the fluid at the reference  $T_0$  and  $\rho_p$  is the density of the single particle of magnetite. Assuming that the density varies linearly with temperature and concentration, we express it with a Taylor polynomial stopped at the first order: we can write that:

$$\rho_{mix} = \rho_0 + \frac{\partial \rho}{\partial T} \bigg|_{T_0} (T - T_0) + \frac{\partial \rho}{\partial \varphi} \bigg|_{\varphi_0} (\varphi - \varphi_0)$$
(3.29)

Considering the equation (3.28) let's evaluate the two derivatives that appear in the development of taylor

$$\frac{\partial \rho}{\partial T}\Big|_{T_0} = -\alpha \rho_{T_0,f} (1 - \varphi_0)$$

$$\frac{\partial \rho}{\partial \varphi}\Big|_{\varphi_0} = -\rho_{T_0,f} + \rho_p$$
(3.30)

at this point we can write:

$$\rho_{mix} - \rho_0 = \Delta \rho = -\alpha \rho_{T_0,f} (1 - \varphi_0) (T - T_0) + (-\rho_{T_0,f} + \rho_p) (\varphi - \varphi_0)$$
(3.31)

considering the concentration  $\varphi_0 \ll 1$ , the term  $(1 - \varphi_0)$  is approximately equal to 1. By rewriting it we get:

$$\Delta \rho = -\alpha (T - T_0) + (\xi - 1)(\phi - \phi_0)$$
(3.32)

where

$$\xi = \frac{\rho_p}{\rho_{T_0,f}} \tag{3.33}$$

In the equation (3.32) one can recognize the classical Boussinesq contribution plus the contribution due to the concentration variation. Considering that gravity acceleration acts only in the vertical direction, The buoyancy force, will only appear in the Navier-Stokes equation along x-direction and will therefore be:

$$F_{x,buoyancy} = -(\Delta \rho)g \tag{3.34}$$

#### 3.4.2 Magnetic force

Before moving to the formulation of the magnetic force acting on the mixture, we introduce some fundamental aspects of thermomagnetic convection.

In addition to natural convection due to a variation in density following a temperature change, magnetic fluids show a type of passive convection called thermomagnetic convection due to changes in the magnetization of the fluid. [23]

In 1970 Lalas and Carmi [24] studied the effects of a uniform magnetic field gradient on convective instability in magnetic fluids. Their results showed that cooler fluid is more attracted towards higher magnetic field regions than warmer one. The behavior of magnetic fluids, with the presence of floating and magnetic forces, was experimentally studied by Sawada et al. [25] while, from the numerical and computational point of view, the studies were conducted by Snyder et al. [26].

To introduce the essential aspect of thermomagnetic convection we can begin to say that, in the absence of an external magnetic field, a finite volume of magnetic material is made up of areas with magnetic moments of different orientations. The response of a material to a magnetic field is called magnetization M[A/m], and it is a vector quantity which corresponds to the ratio between the net magnetic dipole moment  $m[Am^2]$  and the unit volume dV:

$$M = \frac{\sum_{i=1}^{N} m_i}{dV} \tag{3.35}$$

where N indicates the number of magnetic moments within the finished volume. When the external magnetic field disappears, the magnetization of the volume may disappear or remain permanently as explained in Chapter 2.

The fundamental quantities to summarize all the characteristics of the magnetic field and its interactions with matter are two: the magnetic induction vector B[T] and the intensity vector of the magnetic field H [A/m].

The magnetic induction of a material immersed in a magnetic field H is the sum of the contributions of the induction in the vacuum  $\mu_o H$  and of the magnetization of the material  $\mu_0 M$ 

$$B = \mu_0 (M + H) \tag{3.36}$$

where  $\mu_0 = 4\pi \times 10^{-7} H/m$  is the permeability in the vacuum. It is observed that, for most materials, the magnetization is proportional and parallel to the magnetic field H:

$$M = \chi H \tag{3.37}$$

where  $\chi$  (non-dimensional) represents the magnetic susceptibility of the material and it quantifies the degree of magnetization of the material following the application of the magnetic field (fig.2.6). After this brief parenthesis to define the quantities involved, we now derive the magnetic volume force acting on the control volume ( $F_{magnetic}$ ).

In the presence of external field, the magnetic particles acquire magnetization **M**. While the force expression acting in the external field  $\mathbf{H}_0$  on an infinitesimal dipole is well known and given by the Lorentz force  $\mu_0(\mathbf{M} \cdot \nabla)\mathbf{H}_0$ , the macroscopic averaged expression is not easily to obtain. Based on the thermodynamic principles, Korteweg (1880) and Helmholtz (1882) [13], obtained a first formulation that was subsequently generalized by Cowley and Rosenweig to account for the non linear dependence of the magnetization of ferrofluids [27]

$$f_m = -\nabla \left[ \mu_0 \int_0^H \left( \frac{\partial M v}{\partial v} \right)_{H,T} dH \right] + \mu_0 (\mathbf{M} \cdot \nabla) \mathbf{H}$$
(3.38)

and v is the specific volume. The term  $\mu_0(\mathbf{M} \cdot \nabla)\mathbf{H}$  is suggestive of the Kelvin body force [13] [23] on an isolated body but, here, the local field H appears in place of the applied field  $H_0$ . In (3.38) the product Mv represents the magnetic moment per unit mass of the mixture. This can be written alternatively  $Mv = nv\tilde{m}$  because  $M = n\tilde{m}$ , where n is the density of magnetic colloid particles and  $\tilde{m}$  is the average magnetic moment of the solid particles per volume . In a dilute system,  $\tilde{m}$  depends only on the external field  $H_0$  unless compression changes the magnetization of the solid particle. In a typical hydrocarbon-base ferrofluid, the carrier liquid is about a hundred times as compressible as magnetite, so it will be assumed that magnetostriction of the particle solid is negligible [13].

Accordingly, Mv is independent of v, and the integral term in (3.38) vanishes for a dilute colloid. What remains is the Kelvin force density with  $H = H_0$ :

$$f_m = \mu_0 (\mathbf{M} \cdot \nabla) \mathbf{H} \tag{3.39}$$

The additional terms in (3.38) represent the influence of dipole interactions when the fluid is not dilute.

In our case, the magnetic moment of small magnetic particles suspended in a FF adjusts to the applied field <sup>2</sup> almost immediately [28]; the fluid magnetization  $\mathbf{M}$  and the magnetic field  $\mathbf{H}$  remain collinear. The constitutive equation relating the magnetization and magnetic fields is written as [13] [28]:

$$\mathbf{M} = M(H,T)\frac{\mathbf{H}}{H} \tag{3.40}$$

where  $M = |\mathbf{M}|$  and  $H = |\mathbf{H}|$ .

Applying this replacement at eq.(3.39) we can write that  $\mathbf{M} \cdot \nabla \mathbf{H} = (M/H)\mathbf{H} \cdot \nabla \mathbf{H}$ .

Using the vector identity  $\mathbf{H} \cdot \nabla \mathbf{H} = 1/2\nabla (\mathbf{H} \cdot \mathbf{H}) - \mathbf{H} \times (\nabla \times \mathbf{H})$  with the current-free magnetostatic Ampere's law  $\nabla \times \mathbf{H} = 0$  permits one to express  $\mathbf{M} \cdot \nabla \mathbf{H}$  in term of magnitudes of the field vectors. [13]. Accordingly:

$$f_m = \mu_0 (\mathbf{M} \cdot \nabla) \mathbf{H} = \mu_0 M \nabla H \tag{3.41}$$

In order to close a problem, following what is written by Suslov (2008) [28], a magnetic equation of state is required: which is assumed to be in the simplest linear form valid for small temperature and field variations within the layer

$$M = M_* + \chi \Delta H - K \Delta T$$
  

$$\Delta H = H - H_*$$
  

$$\Delta T = T - T_*$$
(3.42)

 $<sup>^2 \</sup>mathrm{we}$  have an experimental setup featuring DC magnetic field generators (permanent magnets)

 $H_*$  and  $M_* = \chi_* H_*$  are the magnitude of the magnetic field and the magnetization at the location with temperature  $T_*$  (i.e in the mid-plane of the layer).

 $\chi = \partial M / \partial H|_{(H_*,T_*)}$  is the differential magnetic susceptibility and  $K = -\partial M / \partial T|_{(H_*,T_*)}$  is the pyromagnetic coefficient.

For a magnetically saturated FF, following what is said in [29], the coefficient K is calculated by the relationship:

$$K = \alpha M_s \tag{3.43}$$

and, using our parameter, this term is  $K \approx 26.3 [Am^{-1}K^{-1}]$ . It is convenient to redefine pressure p entering in the mixture momentum equation so that it includes both a hydrostatic and a potential of Kelvin force [30]. In order to do this, equation

$$\mu_0 M \nabla H = \mu_0 [M_* + \chi \Delta H - K \Delta T] \nabla H = \mu_0 \nabla [M_* H + \frac{1}{2} \chi \Delta H^2] - \mu_0 K \Delta T \nabla H$$
(3.44)

If the temperature sensitivity of the magnetization is linearised using a pyromagnetic coefficient K, the Kelvin body force lead to a force proportional to the pyromagnetic coefficient, the temperature change and the magnetic field gradient [23]: in fact it will demonstrated by [31] that only the non-potential component

$$F_{magnetic} = -\mu_0 K \Delta T \nabla H \tag{3.45}$$

of Kelvin force can lead to a destabilization of a static mechanical equilibrium: this term is the volumetric force acting on our control volume.

The modified pressure now is:

(3.39) is used to write:

$$P = p - \mu_0 [M_* H + \frac{1}{2} \chi \Delta H^2]$$
(3.46)

As a further confirmation of what was obtained above, the equation of the global momentum is definitively written as:

$$\rho\left(\frac{D\mathbf{v}}{Dt}\right) = -\nabla P + \mu \nabla^2 \mathbf{v} + F_{buoyancy} - \varphi \mu_0 K \Delta T \nabla H \tag{3.47}$$

is the same obtained in [32].

#### 3.5Volume fraction equation for particles

Following the mixture model, once we get the mixture continuity and momentum equation, we get the volume fraction equations for the secondary phases. We start from the conservation of mass of dispersed phase:

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v_d}) = 0 \tag{3.48}$$
where  $\rho_d \in \mathbf{v_d}$  are the density and the velocity of the dispersed phase respectively. Regarding the dispersed phase velocity, we can write:

$$\mathbf{v_d} = \mathbf{v} + \mathbf{v}_{slip} \tag{3.49}$$

where  $\mathbf{v}_{slip}$  is the relative velocity between fluid and disperse phase. We can also write:

$$\rho_d = \varphi_p \rho_p \tag{3.50}$$

where  $\rho_p$  is the constant density of the single solid particle, while  $\varphi_p$  is the volumetric concentration of the particles.

Replacing eq.(3.49) and eq.(3.50) inside eq.(3.48):

$$\rho_p \left[ \frac{\partial \varphi_p}{\partial t} + \nabla \cdot (\varphi_p (\mathbf{v} + \mathbf{v}_{slip})) \right] = 0$$
(3.51)

and then:

$$\left[\frac{\partial \varphi_p}{\partial t} + \nabla \cdot (\varphi_p \mathbf{v})\right] = -\nabla \cdot (\varphi_p \mathbf{v}_{slip})$$
(3.52)

As can be seen in this case, the continuity equation for the single dispersed phase turns out to be different from zero. The right-hand side term represents the mass flow of solid particles within the control volume.

The main trouble in this multiphase flow problem lies precisely in determining the term  $J_{tot}$  which makes the equation (3.52) different from zero. We will derive the algebraic expressions for the relative velocities ( $\mathbf{v}_{slip}$ ) considering the forces acting on a single particle. Let's start from:

$$m_p \frac{d\mathbf{v_d}}{dt} = \sum F \tag{3.53}$$

The first mathematical formulation for the motion of particles immersed in a turbulent fluid is due to Basset, Boussinesq and Oseen (in the literature we refer to the BBO equation). The equation is based on the assumption that all forces acting on the particle can be considered as the sum of five distinct contributions: volume forces, Stokes' term, the pressure gradient, the added mass and the Basset's term.

The added mass is that term which takes into account the mass of fluid surrounding the solid particle. If I have to accelerate a spherical particle, the necessary force will be slightly higher because I have to take into account the inertia of the fluid that surrounds it. Considering the small size of our particle, this term is absolutely negligible. Besides the additional force induced by the added mass, when a particle accelerates, it creates additional vorticity which is another source of drag: this effect is taken into account in Basset's term. [33]

In the first mathematical formulation it is assumed that the particles, considered spherical, are subjected to the action of gravity in a still fluid and furthermore, the motion field is at low Reynolds numbers, so that the forces due to the surrounding fluid can be calculated using the Stokes formulation for non-stationary flows. The BBO model was implemented by Tchen [34], accounting for the effect of a non-stationary and non-uniform flow, and by Corrsin and Lumley (1956) [35], whose contribution is mainly related to elimination of some inconsistencies of Tchen's model (1947).

Starting from the studies of Corrsin and Lumley, Maxey and Riley (1983) [36] have provided a mathematical modeling of the motion of particles in a non-stationary and non-uniform flow. Among the hypotheses that characterize this formulation it is highlighted that the Reynolds number of the particles must be very small.

The Maxey and Riley equation for the motion of a rigid particle therefore takes the form:

$$m_p \frac{dV_i}{dt} = (m_p - m_f)g + m_f \frac{DV_i}{Dt} - \frac{1}{2}m_f \left[\frac{dV_i}{dt} + \frac{du_i}{dt}\right] - 6\pi R\mu(V_i - u_i) - f_{basset}$$
(3.54)

where  $m_p$  is the mass of the particle, R is the radius,  $V_i$  is the i-th component of the Lagrangian velocity of the particle,  $u_i$  is the i-th component of the Eulerian velocity of the interpolated flow on the position of the particle,  $m_f$  is the mass of the volume of fluid occupied by the particle, d/dt is the time derivative following the motion of the sphere, D/Dt is the time derivative following the motion of the fluid.

The Maxey and Riley equation contains five different terms: the first is the buoyancy term; the second represents the contribution due to the pressure gradient and due to viscosity in the case of undisturbed fluid, i.e. it characterizes the effect of inertia inside a flow not disturbed by the movement of the whole fluid particle which moves at the speed  $V_i$  (pressure gradient); the third term represents the contribution of the added mass, explained above. The fourth term is the drag force and is due to the disturbance produced by the presence of the particle in the flow (Stokes drag). The last one is the Basset term, explained earlier.

The number that turns out to be decisive in a treatment of this type is the Stokes number. The Stokes number (Stk), named after George Gabriel Stokes, is a dimensionless number that characterizes the behavior of particles suspended in a fluid flow. The Stokes number is defined as the ratio of the characteristic time of a particle (or droplet) to a characteristic time of the flow field.

$$Stk = \frac{t_0 u_0}{l_0}$$
 (3.55)

where  $t_0$  is the relaxation time of the particle (the time constant in the exponential decay of the particle velocity due to drag),  $u_0$  is the fluid velocity of the flow well away from the obstacle and  $l_0$  is the characteristic dimension of the obstacle (typically its diameter). A particle with a low Stokes number follows fluid streamlines (perfect advection), while a particle with a large Stokes number is dominated by its inertia and it continues along its initial trajectory. In the case of Stokes flow, which is when the particle (or droplet) Reynolds number is low enough that the particle drag coefficient is inversely proportional to the Reynolds number itself, the characteristic time of the particle can be defined as:

$$t_0 = \frac{2\rho_d(R_p)^2}{9\mu_f} \tag{3.56}$$

where  $\rho_d$  is the particle density,  $R_p$  is the particle radius and  $\mu_f$  is the viscosity of the fluid. In experimental fluid dynamics, the Stokes number is a measure of flow tracer fidelity. For acceptable tracing accuracy, the particle response time should be faster than the smallest time scale of the flow. Smaller Stokes numbers represent better tracing accuracy; for Stk >> 1, particles will detach from a flow especially where the flow decelerates abruptly. For Stk << 1, particles follow fluid streamlines closely. If Stk << 0.1, tracing accuracy errors are below 1 per cent.

Number	Value
Reynolds	$\approx 220$
Stokes	$\approx 8 \times 10^{-12}$

Table 3.1: Estimation of the Reynolds number and the Stokes number

In our case, we can say that the inertia of the dispersed particles is so low that it allows the latter to accommodate the movement of the fluid almost to perfection. This assumption allows us to say that

$$\sum F = 0 \tag{3.57}$$

Considering also that  $m_f$  is proportional to  $R^3$ , indeed the term of pressure gradient and added mass can be neglected. The equation (3.54) is reduced to just the Stokes resistance and the buoyancy terms.

$$(m_p - m_f)g - 6\pi R\mu(V_i - u_i) = 0 \tag{3.58}$$

In addition to the forces just mentioned, others act on the single particle: one is due to the temperature gradient and one is due to the magnetic field gradient. I can therefore write that:

$$(V_i - u_i) = v_{slip} = \frac{1}{6\pi R\mu} \Big[ (m_p - m_f)g + f_{tp} + f_{mp} + f_{brown} \Big]$$
(3.59)

where  $f_{tp}$  is the thermophoretic force due to thermal gradient between the walls,  $f_{mp}$  is the magnetophoretic force due to magnetic field generated by permanent magnet outside the reactor and  $f_{brown}$  is the brownian force.

The velocity  $v_{slip}$  is the relative velocity of a single particle with respect to the flow: it is therefore necessary to make a summation between the velocities of the individual particles and mediate them.

$$\mathbf{v}_{slip} = \frac{1}{n} \sum_{i=1}^{n} v_{slip} \tag{3.60}$$

For simplicity we consider that all the solid particles n suffer exactly the same forces with the same intensity: to make a summation on n particles and mediate is equivalent to considering the forces on a single particle.

For simplicity of exposition, we continue with the discussion to reach the final equation by acquiring the forces in question, even if these will be described in the following chapters. The relative speed then becomes:

$$\mathbf{v}_{slip} = \left[\frac{(m_p - m_f)g}{6\pi R\mu} + \frac{f_{tp}}{6\pi R\mu} + \frac{f_{mp}}{6\pi R\mu} + \frac{f_{br}}{6\pi R\mu}\right]$$
(3.61)

Once we had calculate those forces and we had obtain the relative speed  $\mathbf{v}_{slip}$ , we can write:

$$\left[\frac{\partial \varphi_p}{\partial t} + \nabla \cdot (\varphi_p \mathbf{v})\right] = -\nabla \cdot (\varphi_p \mathbf{v}_{slip})$$
(3.62)

$$\left[\frac{\partial\varphi_p}{\partial t} + \nabla\cdot(\varphi_p\mathbf{v})\right] = -\nabla\cdot\left[\varphi_p\frac{(m_p - m_f)g}{6\pi R\mu} + \varphi_p\frac{f_{tp}}{6\pi R\mu} + \varphi_p\frac{f_{mp}}{6\pi R\mu} + \varphi_p\frac{f_{br}}{6\pi R\mu}\right]$$
(3.63)

explaining the various forces  $(f_{tp}, f_{mp}, f_{br})$  we finally get:

$$\left[\frac{\partial\varphi_p}{\partial t} + \nabla\cdot(\varphi_p\mathbf{v})\right] = \frac{(m_p - m_f)g}{6\pi R\mu}\nabla\varphi_p + S_t D\nabla\cdot(\varphi_p\nabla T) - Q\nabla\cdot(\varphi_p\nabla H) + D\nabla^2\varphi_p \quad (3.64)$$

#### 3.5.1 Brownian motion

If the size of a particle suspended in a fluid is very small (less than a micron), its motion is affected by the discrete nature of molecular motion, exhibiting a random motion due to collisions of molecules with the particle as shown in figure 3.5. This is called Brownian motion which occurs in both gases and liquids and the amplitude of the fluctuating motion being smaller in a liquid. If the particle spatial concentration is not uniform, the particles migrate toward the region of smaller concentration due to Brownian motion



Figure 3.5: One-dimensional diffusion from a line source [37]

In order to evaluate the mass flow due to Brownian motion, it is necessary to refer to a constitutive relation that describes the molecular diffusion process. This relationship is known as Fick's first law and should be considered as a constitutive axiom.

The following axioms are formulated:

• Axiom 1: the mass flow of solute is a function of the mass concentration gradient. We can therefore write that

$$f_{br} = f(\nabla \varphi_p) \tag{3.65}$$

- Axiom 2 2: the diffusion process does not have preferential directions (isotropy)
- Axiom 3: The characteristics of the diffusion process do not explicitly depend on the position (homogeneity)

• Axiom 4: the link f is linear

The four previous axioms allow us to determine the structure of the bond f in a completely deductive way; we can say that:

$$f_{br} = -D\nabla\varphi_p \tag{3.66}$$

with D molecular diffusivity which, for axiom 3, does not depend on the position. As for the negative sign, it derives from experimental observations for which the solute flow always occurs naturally in the direction of the descending concentrations. Albert Einstein obtained a relation between the macroscopic diffusion constant D and the atomic properties of matter. The relation is:

$$D = \frac{k_b T}{6\pi\mu R} \tag{3.67}$$

where  $k_b$  is the Boltzman constant, T and  $\mu$  are the temperature and the dynamic viscosity of the fluid and finally R is the radius of the particle.

#### 3.5.2 Thermophoresis

In presence of a temperature gradient, a colloidal particle experiences a directional motion: this motion is known as Thermophoresis.

The first to discover this phenomenon was German Ludwig [38] but, in 1879, Charles Soret described this effect in detail, formulated equations and finally wrote a paper on the subject.[39] In his experiment Soret observed that a salt solution contained in a tube with two ends at different temperatures did not remain uniform in composition: the salt was more concentrated near the cold end than near the hot one of the tube. He concluded that a flux of salt was generated by a temperature gradient resulting, in a steady-state conditions, in a concentration gradient and nowadays, the name "Soret effect" is usually attributed to mass separation indiced by temperature gradients.

Experimental evidence have shown that the thermophoretic velocity is insensitive to particle size, opposed to dielectrophoresis or magnetophoresis, where the velocity scales with the square of the particle radius [40]. It has also been observed that thermophoresis combined with convection can be used as a focusing technique to achieve strong accumulation of DNA [41] indicating that in the formation of life this process could have played a fundamental role [42].

Practical application of thermophoresis are numerous, for example, it could be a promising technique for the fractionation [43] or accumulation[44] of biomolecules. Another less known effect of colloidal thermophoresis is the induced fluid flow. The thermophoretic force exerted on the colloid is not an external driving force but the results of the interaction of the colloid with the solvent which is inhomogeneous due to the temperature gradient.

The thermal motion of the colloid is mainly driven by local hydrodynamic stresses in the surrounding liquid, confined in a region close to the particle surface; in fact, numerous experiments have shown that the amplitude of thermophoretic effect is independent by particle general bulk or surface physical properties, such as its size, material density, thermal conductivity, or total surface charge, but it seems to be related to the detailed microscopic nature of the particle/solvent interface.

Because of this thermophoresis is much harder to understand than other field-driven transport effect such as electrophoresis.



Figure 3.6: Schematic depiction of hydrodynamic stresses caused by a temperature gradient. The gradient in excess pressure induced a thermo-osmotic flow close to the colloidal surface(grey lines). In response, the colloid moves in the opposite direction(big red arrow) [45]

Now let's try to define a formula that expresses the strength of thermophoresis that acts on a single particle.

To begin we consider the Fokker-Planck equations proposed by Von Kampen [46] to describe the flow of particles in diluted systems.

$$J = \rho_p b \mathbf{f} - b \nabla [\rho_p k_b T] \tag{3.68}$$

where **b** is the colloid mobility and it is linked to the self-diffusion coefficient by the Einstein relation.

$$D = k_b T b \tag{3.69}$$

The force  $\mathbf{f}$ , in presence of a temperature gradient, will be the thermophoretic force  $f_{tp}$  exerted on the colloid by a surrounding solvent. We can rewrite the equation (3.68) by adding and subtracting the term  $k_b T \nabla b$ 

$$J = \rho_p \mathbf{v}_d - \nabla[\rho_c D] \tag{3.70}$$

The term  $\mathbf{v}_d$  is the drift velocity besides being proportional to the driving force, it has an additional contribution due to the inhomogeneities of the mobility

$$\mathbf{v}_d = b\mathbf{f} + k_b T \nabla b \tag{3.71}$$

Yang and Ripoll [47], by computer simulations, have proven the validity of this framework in the presence of temperature gradient. In the case of dilute suspension, we can compare the equation

(3.70) with the classical thermodiffusion phenomenological equation for the particle flux <sup>3</sup> and we obtain:

$$\mathbf{v}_d = -D_t \nabla T - \alpha_T D \nabla T + \nabla D \tag{3.72}$$

where  $\alpha_T$  is the thermal expansion coefficient at constant pressure of the solvent. Following the widely believed opinion [48] [40] [49] we approximate (3.72) as

$$\mathbf{v}_d \cong -D_T \nabla T \tag{3.73}$$

and with  $\mathbf{v}_d = b f_{tp}$  we obtain the thermophoretic force

$$f_{tp} = -S_t k_b T \nabla T \tag{3.74}$$

 $S_t$  is called Soret coefficient.

The experimental results have shown that the Soret coefficient depends strongly on the average temperature of the system; moreover it was found that, for all the concentrations examined, (even very low concentrations), the dependence of temperature remained strong [50]. This indicates that the Soret effect exists if the average distance between the colloids is much greater than their size or range of inter-particle interactions. For low temperatures the colloids have a negative Soret coefficient and accumulate in the warm side of the system. By increasing the temperature the situation is reversed and the Soret coefficient is positive, except at very high concentrations [48]. Figure 3.7 shows the temperature dependence of the Soret coefficient for dilute colloid suspension with different particle sizes.

The first empirical formulation that establishes a relationship between the temperature and the Soret coefficient, was proposed by [52] and it is:

$$S_t(T) = S_t^{\infty} \left[ 1 - exp\left(\frac{T^* - T}{T_0}\right) \right]$$
(3.75)

Soret coefficient is negative for small temperatures and that there is a temperature  $T^*$  for which the Soret coefficient changes its sign. The equation also reflects that  $S_t$  saturates at large temperatures given by  $S_t^{\infty}$ .  $T_0$  takes into account that, for some substances, the temperature dependence is stronger than in others [48].

Nevertheless, it can be said that the Soret coefficient strongly varies with the size of the colloidal particles (in experiments with highly diluted solutions), which is another indication of the relevance of the single colloid properties.

Following what has been said in [54] there is no universal technique to measure the Soret coefficient of a binary mixture. Among the measurement techniques each one has its own advantages and

Subject of the study was also the variation of the Soret coefficient with different size of the colloids. In this case, the experimental results obtained show both a linear dependence (Braibanti at al [51]) and a quadratic dependence (Duhr and Braun [53]): the reason for this variation is still subject to debate.

<sup>&</sup>lt;sup>3</sup>Phenomenologically thermodiffusion of a multi-component mixture is described by two opposing mass fluxes that cancel each other in a stationary state. One flux stems from the temperature gradient and the other flux from the resulting concentration gradient  $J = -D\nabla c - cD_t\nabla T$  [48]



Figure 3.7: Experimental results for dilute colloidal suspensions for the dependence of the Soret coefficient on the temperature for different particle sizes. Figure from [51]

disadvantages, depending on the situations examined in the laboratory.

It is not in the interest of this thesis to describe the different techniques and for this reason we refer to [54] but, for our present case, the choice of the value to be used for the Soret coefficient, it is based on general considerations.

We have observed which hypotheses could be comparable to our case and we used the appropriate coefficient.

In absolute value an order of magnitude for usual organic mixtures or aqueous solution is  $|S_t| \approx 10^{-3} - 10^{-2} K^{-1}$ .

#### 3.5.3 Magnetophoresis

Since a magnetic ferrofluids consist of a stable colloidal dispersion of a solid ferromagnetic, it is natural that, in addition to the Brownian diffusion and thermophoresis already mentioned above, there will be a magnetophoresis process. Fluid motion in ferrofluid does not require gravity to started in a non-uniformly heated fluid. It can be controlled by varying the applied external magnetic field [56] [57] [58].

Therefore so-induced convection is considered to be an important alternative to gravitational convection in heat exchange systems where natural convection cannot arise due to the lack of gravity (orbital stations)[59].

The particle in a colloidal ferrofluid, each with its embedded magnetic moment, are analogous to the molecules of a paramagnetic gas. In the absence of an applied field, the particles are randomly oriented and the fluid has no net magnetization. In the presence of the external field the magnetic particles acquire magnetization **M**.

However, for ordinary field strengths the tendency of the dipole moments to align with the applied field is partially overcome by thermal agitation. As the field magnitude is increased, the particles become more and more aligned with the field direction; at very high field strengths the particles may be completely aligned and the magnetization achieves its saturation value. In our system the magnetization **M** is assumed to be co-directed with the internal magnetic field; as discussed, for example, in Odenbach (2004)[60] and references therein this is true if the magnetic particle size does not exceed  $d_p \approx 13nm$ .

In this case the ratio of the Brownian particle magnetization relaxation time  $\tau_b = (4\pi (d_p)^3 \nu)/(k_b T)$ , to viscous time  $\tau_v = (\rho (d_p)^2)/\nu$  characterizing the macroflow development is  $\tau_b/\tau_v \approx 10^{-5}$ . Thus it is safe to assume that the orientation of the magnetic moments of individual particles and thus of the fluid magnetization follows the direction of a local magnetic field. When the intensity of magnetic field is non-linearly distributed in a magnetic fluid, magnetic particles are concentrated in those regions, where the magnetic field intensity is larger. Accordingly, the fluid magnetization increases in these regions.

The presence of a ferromagnetic fluid can distort an external magnetic filed if magnetic interaction (dipole-dipole) takes place, but this is negligible for small particle concentration (less than 10%)[?]. Now we proceed to point out the general expression for the magnetic force acting on a general magnetized body.

To begin consider a small cylindrical volume of magnetically polarized substance with geometric axis d aligned with the magnetization vector  $\mathbf{M}$ .



Figure 3.8: Development of the gradient-field force and the magnetic torque on a small element of magnetically polarized substance.[13]

The material is affected by an external magnetic field  $\mathbf{H}_{0}$  and, at the ends of the volume, two poles appear with density  $\rho_{s} = \mu_{0}M$  and opposite sign.

The applied field  $\mathbf{H}_0$  may be taken to be the force on a unit pole, and hence the force esperienced by the volume is:

$$-\mathbf{H}_{\mathbf{0}}\rho_{s}a_{d} + (\mathbf{H}_{\mathbf{0}} + \delta\mathbf{H}_{\mathbf{0}})\rho_{s}a_{d} = \delta\mathbf{H}_{\mathbf{0}}\rho_{s}a_{d}$$
(3.76)

where  $\delta \mathbf{H}_0$  is the change in  $\mathbf{H}_0$  along the direction of d. Thus  $\delta \mathbf{H}_0 = (d \cdot \nabla) \mathbf{H}_0$  and the Kelvin force per unit volume is given by

$$\mu_0(\mathbf{M}\cdot\nabla)\mathbf{H_0}\tag{3.77}$$

to obtain the force acting on a particle it is necessary to consider the volume V of the particle: thus the force becomes:

$$F = \mu_0 V_p (\mathbf{M} \cdot \nabla) \mathbf{H_0} \tag{3.78}$$

Note that for "soft" magnetic materials  $\mathbf{M}$  is parallel to  $\mathbf{H}_0$ ; in this way the force is reduced to

$$f_{mp} = \mu_0 M_d V_p \nabla H_0 \tag{3.79}$$

# **3.6** Mixture energy equation

In addition to the equations obtained so far, a temperature equation is needed. Using the Boussinesq approximation, we suppose that the fluid has a constant heat capacity per unit volume,  $\rho C_p$ ; then  $\rho C_p DT/Dt$  is equal to the rate of heating per unit volume of a fluid particle. The choice of  $C_p$ , the specific heat at constant pressure, is physically sensible, since the pressure is not free to respond directly to the heating process. This heating is brought about by transfer of heat from neighboring fluid particles by thermal conduction. The corresponding terms in the thermal equation are analogous respectively to the viscous term in the dynamical equation. The conductive heat flux is:

$$\mathbf{Y} = -k\nabla T \tag{3.80}$$

where k is the thermal conductivity of the fluid. Thus

$$\rho C_p \frac{DT}{Dt} = -\nabla \cdot \mathbf{Y} \tag{3.81}$$

Taking k to be costant, the equation above can be rewritten as:

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \kappa \nabla^2 T \tag{3.82}$$

where  $\kappa = k/\rho C_p$  is known as the thermal diffusivity or sometimes as the termometric conductivity. The term  $\mathbf{v} \cdot \nabla T$  rappresent the transport of heat by the motion and is called advection term. The equation just obtained and equation (3.10) (3.24), without considering the external magnetic forces, constitute the basis equation of convection in the Boussinesq approximation. They are one vector and two scalar equations for the one vector and two scalar variables  $\mathbf{v}$ , p and  $\Delta T$ .

# 3.7 Dimensional analysis

The estimation of the relative importance of different terms in the balance equations (3.83) can be carried out by the dimensional analysis.

First we rewrite for completeness the system of equations that will be adimensionalized:

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho \left(\frac{D\mathbf{v}}{Dt}\right) = -\nabla P + \mu \nabla^2 \mathbf{v} + \alpha (T - T_0)g - (\xi - 1)(\varphi - \varphi_0)g - \varphi \mu_0 K \Delta T \nabla H_0$$

$$\frac{D\varphi}{Dt} = \frac{(m_p - m_f)g}{6\pi R\mu} \nabla \varphi + S_t D \nabla \cdot (\varphi \nabla T) - Q \nabla \cdot (\varphi \nabla H) + D \nabla^2 \varphi$$

$$\frac{DT}{Dt} = \kappa \nabla^2 T$$
(3.83)

The equations in this form, with the introduction of non-dimensional groups or parameters, have a considerable importance as they facilitate both the correct experimental similarity and the accuracy of the numerical solutions.

We define the following dimensionless sizes  $()^*$ , indicating with  $()_{ref}$  the reference values, which will be chosen later on the basis of the physical characteristics of the problem under examination.

$$\begin{aligned} x^*, y^*, z^* &= \frac{x, y, z}{L_{ref}} \\ u^*, v^*, w^* &= \frac{u, v, w}{U_{ref}} \\ t^* &= \frac{t}{t_{rif}} \\ P^* &= \frac{P}{P_{rif}} \\ T^* &= 2\frac{T - T_0}{\Delta T_{ref}} \\ \varphi^* &= \frac{\varphi - \varphi_{ref}}{\varphi_{ref}} \\ H^* &= \frac{H}{H_{ref}} \end{aligned}$$
(3.84)

Now let's see how to choose the reference values considering the physical characteristics. From a geometric point of view, the reference length will be half of the channel opening ie:

$$L_{ref} = 0.01m$$
 (3.85)

In the absence of external force, the term that actually contributes to the change in global momentum is buoyancy, which will be used to derive the  $U_{ref}$ 

$$\rho \frac{U}{t} \approx \rho \frac{U^2}{L} \approx \Delta \rho g \tag{3.86}$$

from here revenue that:

$$U_{ref} = \sqrt{\frac{\Delta\rho}{g}\rho L_{ref}} = \sqrt{\alpha\Delta T_{ref}L_{ref}g}$$
(3.87)

and represents the velocity generated by convective motions. Once the key terms of the adimensionalizations have been clarified, the others are easily deduced:

$$t_{ref} = \frac{L_{ref}}{U_{ref}} \tag{3.88}$$

As for the  $p_{rif}$  it is better to write it as:

$$p_{ref} = \rho U_{ref}^2 \tag{3.89}$$

The table below shows the main unimensionalization factors and their values: By applying what

Parameter	Value
$L_{ref}$	0.01 m
$U_{ref}$	0.022  m/s
$H_{ref}$	$1 \times 10^6 A/m$
$\varphi_{ref}$	$1.92 \times 10^{-3}$
$\Delta T_{ref}$	10 K

Table 3.2: reference quantities and associated values

has just been written and isolating for each equation the time-dependent term we get:

$$\nabla \cdot \mathbf{v}^* = 0$$

$$\begin{aligned} \frac{\partial \mathbf{v}^*}{\partial t^*} + \nabla \cdot (\mathbf{v}^* \mathbf{v}^*) &= -\nabla P^* + \frac{1}{\sqrt{Gr}} \nabla^2 \mathbf{v}^* + \frac{1}{2} T^* - \frac{(\xi - 1)\varphi_0}{\Theta} \varphi^* - C_M (1 + \varphi^*) T^* \nabla H^* \\ \frac{\partial \varphi^*}{\partial t^*} + \nabla \cdot (\varphi^* \mathbf{v}^*) &= C_{grav} \nabla \varphi^* + \frac{S_{t(ref)}}{Sc\sqrt{Gr}} \nabla \cdot ((1 + \varphi^*) \nabla T^*) - C_{Mphi} \nabla \cdot ((1 + \varphi^*) \nabla H^*) + \frac{1}{Sc\sqrt{Gr}} \nabla^2 \varphi^* \\ \frac{\partial T^*}{\partial t^*} + \nabla \cdot (T^* \mathbf{v}^*) &= \frac{1}{Pr\sqrt{Gr}} \nabla^2 T^* \end{aligned}$$

$$(3.90)$$

In the table below we write the term that are fundamental in the definition of the dimensionless parameters

	Parameter	Value
$k_b$	Boltzman's costant	$1.38 \times 10^{-23} \text{ J/K}$
$T_0$	T in the middle at the start	313.15 K
α	Coefficient of thermal expansion	$5 \times 10^{-4} \ 1/\mathrm{K}$
$\mu_0$	Magnetic permeability in vacuum	$4\pi \times 10^{-7} \text{ H/m}$
g	gravity acceleration	9.81 $m/s^2$
K	pyromagnetic Coefficient	26.3A/mK
$M_s$	saturation magnetization of FF	$5.25 \times 10^4 A/m$
$M_p$	saturation magnetization of particle	$4.12 \times 10^5 A/m$
$\rho_{mix}$	fluid density	$1 \times 10^3 kg/m^3$
$\rho_p$	single particle density	$5.2 \times 10^3 kg/m^3$
$\mu_{mix}$	dynamic viscosity of fluid	$8 \times 10^{-3} kg/ms$
ν	cinematic viscosity of fluid	$9.86 \times 10^{-7} m^2/s$
k	thermal diffusivity of fluid	$1.39 \times 10^{-7} m^2/s$
$\varphi_0$	concentrazione media iniziale	$1.92 \times 10^{-3}$

Table 3.3: Fundamental parameters of the flow

We can now define the characteristic number that take places in the equations above

## • Gr= $(g\alpha\Delta T_{ref}L_{ref}^3)/\nu^2$

For a given fluid, the Grashof number is a non-dimensional parameter used in the correlation of heat and mass transfer due to thermally induced natural convection at a solid surface immersed in a fluid: it contains information of a mechanical nature only.

The significance of the Grashof number is that it represents the ratio between the buoyancy force due to spatial variation in fluid density caused by temperature differences (numerator) to the restraining force due to the viscosity of the fluid (denominator). Once the motion is started, to understand if the motion is laminar or turbulent (in natural convection) the Grashof number is evaluated; if  $Gr > 10^9$  the motion is laminar, if instead  $Gr < 10^9$  the motion is turbulent.

#### • $Pr = \nu/k$

This non-dimensional parameter, called the Prandtl number, is a property of the fluid, and represent the ratio of two diffusivity: the diffusivity of momentum and vorticity  $\nu$  and the diffusivity of heat k.

The momentum diffusivity, or as it is normally called, kinematic viscosity, tells us the materials resistance to shear-flows (different layers of the flow travel with different velocities due to e.g. different speeds of adjacent walls) in relation to density. Small values of the Prandtl number,  $Pr \ll 1$ , means that the thermal diffusivity dominates. Whereas with large values,  $Pr \gg 1$ , the momentum diffusivity dominates the behavior. For example, the typical value for liquid mercury, which is about 0.025, indicates that the heat conduction is more significant compared to convection, so thermal diffusivity is dominant. When Pr is small, it means that the heat diffuses quickly compared to the velocity.

• Sc= $\nu$ /D

The Schmidt number is defined as the ratio of momentum diffusivity (kinematic viscosity) and mass diffusivity, and is used to characterize fluid flows in which there are simultaneous momentum and mass diffusion convection processes. The Schmidt number describes the mass momentum transfer. It physically relates the relative thickness of the hydrodynamic layer and mass-transfer boundary layer. The Schmidt number corresponds to the Prandtl number in heat transfer. A Schmidt number of unity indicates that momentum and mass transfer by diffusion are comparable, and velocity and concentration boundary layers almost coincide with each other. Mass diffusivity or diffusion coefficient is a proportionality constant between the molar flux due to molecular diffusion and the gradient in the concentration of the species (or the driving force for diffusion). Mass diffusion in liquids grows with temperature, roughly inversely proportional viscosity-variation with temperature, so that the Schmidt number, quickly decreases with temperature.

- $\boldsymbol{\xi} = \boldsymbol{\rho}_{\mathbf{p}} / \boldsymbol{\rho}_{\mathbf{T}_{0},\mathbf{f}}$ ratio between the density of the single solid particle of magnetite and the mixture in which it is immersed.
- $\Theta = \alpha \Delta T_{ref}$
- $C_M = \varphi_0 \mu_0 K H_{ref} / 2 \rho \alpha g L_{ref}$
- $\mathbf{C}_{\mathbf{grav}} = \frac{\mathbf{Gr}^{0.5}\mathbf{Stk}}{\Theta} \left(1 \frac{1}{\xi}\right)$
- $\mathbf{S}_{\mathbf{t}(\mathbf{ref})} = \mathbf{S}_{\mathbf{t}}(\Delta \mathbf{T}_{\mathbf{ref}})/2$ parameter that takes into account the Soret coefficient.
- $\mathbf{Q} = \mu_0 \mathbf{M}_p \mathbf{V}_p / 6\pi \mathbf{R} \mu$
- $C_{Mphi} = QH_{ref}/U_{ref}L_{ref}$

#### • $Pe = Gr^{0.5}Pr$

The Pclet number may be interpreted as a measure of the relative importance of advection and conduction of heat. When Pe is small, the flow is having negligible effect on the temperature distribution. At high Pe, conduction can be important in thermal boundary layers.

• Re=Pe/Pr

The Reynolds number is a dimensionless parameter whose physical meaning is the ratio between the inertia forces and the viscous forces that originate within a moving fluid. Low Reynolds numbers ( $Re \leq 1000$ ) are characteristic of motions in which the viscous aspect prevails, for example in machine lubrication whereas, conversely, high Reynolds numbers ( $Re \geq 2000$ ) characterize motions at high speed in which the viscous forces are totally negligible with respect to those of inertia.

## • Ra=GrPr

The Rayleigh number is closely related to Grashof number and both numbers are used to decribe natural convection (Gr) and heat transfer by natural convection (Ra). The Rayleigh number is used to express heat transfer in natural convection. The magnitude of the Rayleigh number is a good indication as to whether the natural convection boundary layer is laminar or turbulent.

The table below shows the values of the coefficients derived from the standardization, in order to make it clearer what the weight of the individual terms is.

Parameter	Value
Gr	$5.04 \times 10^4$
Pr	7.12
Ra	$3.58  imes 10^5$
$\operatorname{Sc}$	$1.72 \times 10^5$
D	$5.73 \times 10^{-12}$
Pe	$1.5983 \times 10^4$
ξ	5.196
Θ	0.005
$C_M$	0.647
$C_{grav}$	$1.09 \times 10^{-4}$
$S_{t(ref)}$	0.015
Q	$3.6 \times 10^{-16}$
$C_{Mphi}$	$1.62 \times 10^{-6}$

Table 3.4: Non-dimensional numbers that make up the coefficients of the equations

# 3.8 Simulation and Magnetic field

In this section we will describe how we calculated the magnetic field acting within the domain and what are the parameters and approximations adopted for fluid dynamics simulations. Following [28] a set of Maxwell equations describing the magnetic field in the absence of induction current is introduced

$$\nabla \times \mathbf{H} = 0 \tag{3.91}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{3.92}$$

From the equation above it follows that  $\mathbf{B}$  in analogous to the velocity vector of an incompressible fluid. The amount of the fluid entering an arbitrary volume equals the amount flowing out; also the lines of  $\mathbf{B}$  cannot terminate but must form closed loops or extend indefinitely far.

The vector **B** is known as the magentic induction and we can say that  $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) \simeq \mu_0 \mathbf{H}$  if

the field due to ferrofluid is neglected.

From eq.(3.92) we can say that  $\mathbf{H} = \nabla \varphi$ , where  $\varphi$  is the magnetic potential: replacing in eq.(3.91) we obtain:

$$\nabla^2 \varphi = 0 \tag{3.93}$$

or harmonic potential. We must resolve in the domain with appropriate boundary conditions for the magnets. The potential due to a magnet of moment  $\mathbf{M}$  placed in the origin (solution of the Laplace equation in three dimensions) is <sup>4</sup>

$$\varphi(\tilde{\mathbf{x}}) = \frac{1}{4\pi} \frac{\mathbf{M} \cdot \tilde{\mathbf{x}}}{|\tilde{\mathbf{x}}|^3}$$
(3.94)

so, if we admit we have a moment density  $\mathbf{m}$  per unit of volume inside the magnet, we have the solution, out of the magnet

$$\varphi(\tilde{\mathbf{x}}) = \frac{1}{4\pi} \int_{V_m} \frac{\mathbf{m}(\tilde{\mathbf{y}}) \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{y}})}{|\tilde{\mathbf{x}} - \tilde{\mathbf{y}}|^3} \mathrm{d}\tilde{\mathbf{y}}$$
(3.95)

(i.e the sum of the potentials of the dipoles of intensity  $\mathbf{m}(\tilde{\mathbf{y}})$  placed in the points  $\tilde{\mathbf{y}}$  inside the magnet. The integral extends on the volume  $V_m$  occupied by the magnet).

We will admit that the magnetization of the magnets is uniform in the volume inside the magnets, for now it is sufficient that  $\mathbf{m}$  is normal to the walls, ie in the direction y. Let us assume that the magnets extend unlimited in the x- direction and that  $\mathbf{m}$  is in the y- direction and uniform inside the magnet, so we evaluate the resulting (two-dimensional) potential that will only be a function of y and  $z(A_m \text{ is the section of volume } V_m \text{ in the plane y,z})$ :

$$\begin{aligned} \varphi(\tilde{\mathbf{x}}) &= \frac{1}{4\pi} \int_{A_m} \int_{-\infty}^{\infty} \frac{\mathbf{m}(\tilde{\mathbf{y}}) \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{y}})}{|\tilde{\mathbf{x}} - \tilde{\mathbf{y}}|^3} \mathrm{d}\tilde{y}_z \mathrm{d}\tilde{y}_x \mathrm{d}\tilde{y}_y \\ &= \frac{1}{4\pi} \int_{A_m} \int_{-\infty}^{\infty} \frac{m_y(\tilde{x}_y - \tilde{y}_y)}{\left[(\tilde{x}_x - \tilde{y}_x)^2 + (\tilde{x}_y - \tilde{y}_y)^2 + (\tilde{x}_z - \tilde{y}_z)^2\right]^{3/2}} \mathrm{d}\tilde{y}_z \mathrm{d}\tilde{y}_x \mathrm{d}\tilde{y}_y \end{aligned}$$

We execute the integral first with respect to  $\tilde{y}_x$ : with the substitution  $\tilde{y}_x = \xi \left[ (\tilde{x}_y - \tilde{y}_y)^2 + (\tilde{x}_z - \tilde{y}_z)^2 \right]^{1/2}$  we have

$$\begin{split} \int_{-\infty}^{\infty} \frac{m_y(\tilde{x}_y - \tilde{y}_y)}{\left[(\tilde{x}_y - \tilde{y}_y)^2 + (\tilde{x}_z - \tilde{y}_z)^2\right]^{3/2}} \mathrm{d}\tilde{y}_z &= \frac{m_y(\tilde{x}_y - \tilde{y}_y)}{(\tilde{x}_y - \tilde{y}_y)^2 + (\tilde{x}_z - \tilde{y}_z)^2} \int_{-\infty}^{\infty} \frac{1}{\left[1 + \xi^2\right]^{3/2}} \mathrm{d}\tilde{y}_z \\ &= 2 \frac{m_y(\tilde{x}_y - \tilde{y}_y)}{(\tilde{x}_y - \tilde{y}_y)^2 + (\tilde{x}_z - \tilde{y}_z)^2} \end{split}$$

<sup>&</sup>lt;sup>4</sup>If the dipole is not at the origin but at a point  $\tilde{\mathbf{y}}$ , then just replace  $\tilde{\mathbf{x}}$  with  $\tilde{\mathbf{x}} - \tilde{\mathbf{y}}$ .



Figure 3.9: Domain scheme (section in the horizontal plane (y, z) showing the position of the magnets. In the domain extension in the direction three pairs of magnets are shown, corresponding to the choice of N\_magn equal to 3. Note that all the lengths are dimensionless with the half-height of the channel (half the distance between the two plates).

so that

$$\varphi(\tilde{\mathbf{x}}) = \frac{1}{2\pi} \int_{A_m} \frac{m_y(\tilde{x}_y - \tilde{y}_y)}{(\tilde{x}_y - \tilde{y}_y)^2 + (\tilde{x}_z - \tilde{y}_z)^2} \mathrm{d}\tilde{y}_y \mathrm{d}\tilde{y}_z$$

The integral must therefore be extended to the section of the magnetic plate (a rectangle). If we admit that the magnetic plate is very thin (compared to the other dimensions), then we can admit that it can be approximated with a plate without thickness parallel to the walls of the channel, or  $m_y(\tilde{x}_y, \tilde{x}_z) = \tilde{m}_y \delta(\tilde{x}_y - \tilde{x}_{yp})$ , where  $\tilde{x}_{yp}$  is the position of the plate, in y direction (normal to the walls), which will extend along z from a and b ( $z \in (a, b)$ );  $\tilde{m}_y$  it is the magnetization per unit of length, supposedly uniform, of the magnet. In this case the integral becomes.

$$\varphi(\mathbf{x}) = \frac{\tilde{m}_y}{2\pi} \int_a^b \frac{\tilde{x}_y - \tilde{x}_{yp}}{(\tilde{y}_y - \tilde{x}_{yp})^2 + (\tilde{y}_z - \tilde{x}_z)^2} \mathrm{d}\tilde{y}_z \tag{3.96}$$

We can then calculate the magnetic field, which has components

$$H_{y} = \frac{\partial \varphi}{\partial y} = -\frac{\tilde{m}_{2}}{2\pi} \int_{a}^{b} \frac{(\tilde{x}_{z} - \tilde{y}_{z})^{2} - (\tilde{x}_{y} - \tilde{x}_{yp})^{2}}{\left[(\tilde{x}_{z} - \tilde{y}_{z})^{2} + (\tilde{x}_{y} - \tilde{x}_{yp}^{2}\right]^{2}} \mathrm{d}\tilde{y}_{z}$$
(3.97)

$$H_{z} = \frac{\partial \varphi}{\partial z} = +\frac{\tilde{m}_{2}}{2\pi} \int_{a}^{b} \frac{2(\tilde{x}_{z} - \tilde{y}_{z})(\tilde{x}_{y} - \tilde{x}_{yp})}{\left[(\tilde{x}_{z} - \tilde{y}_{z})^{2} + (\tilde{x}_{y} - \tilde{x}_{yp}^{2}\right]^{2}} \mathrm{d}\tilde{y}_{z}$$
(3.98)

I can then calculate the module and the gradient of the module, H, which I need in the equations.



Figure 3.10: Visualization of the magnetic field module, its component and of its derivatives. Parameters:  $L_z = 2$  (domain long  $2\pi$  in the direction z,  $f_z = 0.4$  (40% domain covered by magnets),  $y_m = 0.4$  (distance of magnetic plates from walls.) The grid has 257 unequal points in the direction y and 128 points equally spaced in the direction z.

We now define the settings and the simplifications adopted to simulate computationally what happens inside the reactor.

Considering the arrangement of the magnets and the Peltier cells on the walls, we can say that a single configuration repeat itself along the entire perimeter of the reactor. The fluid dynamic simulations will therefore concern a single block, and the flow that will be obtained from the CFD simulations can be considered periodic along the whole toroidal axis of the device.

Since it is difficult to simulate the effect of Peltier cells for the only area in which they are arranged, we consider the whole wall as a warm or cold one; in this way we create the thermal gradient that acts inside the fluid. As for the magnets, they are placed at a fixed distance from the wall, and this is necessary to consider the real thickness of the latter.

As far as the vertical axis is concerned, the simulations neglect the upper and lower walls of the device as the flow passing through the block is considered to be completely developed, ie not affected by the presence of those walls. In the figure 3.11 one of the simulated configurations is shown



Figure 3.11: 3D Visualization of computational domain with axis of reference. The red wall have a temperature equal to  $T_0 + \Delta T/2$  while blue wall represent the temperature  $T_0 - \Delta T/2$ . The magnets are represented by gray blocks whose magnetic field is perpendicular to the surface attached at the walls.

# Chapter 4

# Discretization

# 4.1 Introduction

First of all, it is necessary to clarify what is meant by the word "discretization": in essence, to discretize a closed-form mathematical expression, like a differential equation, characterized by an infinite continuum of values throughout the domain, means approximating it to its equivalent algebraic expression which supplies values only in a finite number of discrete points or volumes in the domain. The set of these nodes takes the name of mesh or computational domain while the set of nodes that are involved from time to time writing an algebraic equation that approximates the derivatives for each node is called a stencil.

The computational code for numerical integration used to discretize the Navier-Stokes equations rely on Passoni's paper.

In [63] the system of nonlinear partial differential equations is discretized thanks to a mixed method of spectral-finite difference in which two different numerical techniques are adopted to obtain a fast and accurate computational code.

A mixed approach like the one developed in this thesis work has been used for different flow configurations and different problems: for example in [63] such computational schemes are applied to the case of channel flow. With respect to the channel flow problem, purely spectral techniques were used in [64] using a Fourier-Chebyshev computational algorithm; progress over time is guaranteed through a semi-implicit scheme. A fully spectral Fourier-Chebishev method was also used in [65] to analyze the linear and nonlinear stability of the Poiseuille air flows and the Couette plane. Very important is the result obtained by [66] where it was shown that, with half the grid points in space, spectral methods reached an accuracy comparable to that of finite difference schemes.

A spectral-finite differences scheme for the Navier-Stokes equations in the plane channel was developed in [67]: in space, Fourier decomposition is used in homogeneous directions and finite differences in the orthogonal direction with respect to solid walls; as regards progress over time, a semi-implicit third-order Runge-Kutta scheme was used.

In general, there are a large number of publications in the literature that develop the theme of solving the Navier-Stokes equations applied to the case of channel flow and based on fully spectral, fully finished and spectral-finite hybrid algorithms.

Before discretizing the governing equations obtained in the previous chapter, we observe how a model equation can be discretized with a spectral method: the results obtained for this equation will then be reported in the present case.

# 4.2 Spectral method

"Spectral methods" is a general name to indicate the spatial discretization methods that are based on an expansion of the solution as coefficients for the test functions. These test functions generally have global support on the domain and the spatial derivatives are defined in terms of derivatives of these functions. The name of the method derives from the fact that the coefficients related to the test functions can be seen as a spectrum of the solution.

Because of the global nature of the test functions, spectral methods are usually global methods, that is, the value of a derivative at a given point in space depends on the solution in all other points in space and not just on neighboring grid points.[71].

A graphical distinction between traditional approximations and spectral ones is provided in figure 4.1.



Figure 4.1: Comparison of finite difference (left) and Legendre spectral (right) differentiation. The solid curves represent the exact solution, and the dashed curves are their numerical approximations. The solid lines are the exact tangents at z = 0, and the dashed lines the approximate tangents. The error in slope is noted, as is the number of intervals N. [68]

In this figure a second-order (central) finite-difference approximation is compared with a Legendre spectral collocation approximation.

The finite difference approximation estimates the derivative from the parabola which interpolates the function at the point in question, and at the two adjacent grid-points: different grid points, therefore, use different parabolas. The spectral approximation, on the other hand, uses all the available information about the function. If there are N + 1 grid-points, then the interpolating polynomial, from which the derivative is extracted, has degree N, and the same polynomial is used for all the grid-points.[68]

For few numbers of grid-points, the accuracy of two methods results are comparable. However, as N increases, the accuracy of the spectral approximation increases dramatically (its error decays exponentially).

By virtue of the foregoing, spectral methods have a very high order of convergence, i.e the error decreases exponentially by increasing the points of the calculation grid  $(\alpha(L/N)^N)$  [69].

Furthermore, the dispersion and diffusion properties of the derivative operator are better than the finite difference methods. This can be easily seen considering that the spectral methods usually give the exact derivative of a function, the only error that is committed is due to the truncation to a finite set of functions / test coefficients. The cons of these methods is that they are geometrically less flexible than lower order methods and they are usually more complicated to implement. Furthermore, the spectral representation of the solution is difficult to combine with problems involving strong gradients, such as problems involving shock and discontinuity.

A wider application of spectral methods found difficulties due to: 1) poor resolution of discontinuous solutions; 2) inefficient implementation of implicit methods; and 3) drastic geometric constraints. All these barriers were gradually reduced in the 1980s, in particular the last two: as a result, the applicability and appeal of spectral methods for computational fluid dynamics has broadened considerably [68].

Considering mainly elliptic / parabolic problems with simple geometries, spectral methods are very adequate and efficient discretization schemes: in fact, these methods were among the first to be used in practical flow simulations.

Spectral methods may be viewed as an extreme development of the class of discretization schemes known as the method of weighted residuals (MWR).

The basic idea is to assume that the unknown function u(x,t) can be approximated by a sum of N + 1 "trial" functions  $\phi_k(x)$ 

$$u(x,t) \approx u^N(x,t) = \sum_{k=0}^N a_k(t)\phi_k(x)$$
 (4.1)

This assumption leads us from a problem of infinite dimension (we need infinite information to specify u(x,t) in every point of the domain), to one in which a finite number of information will suffice, which are the  $a_k(t)$  coefficients of the expansion truncated of our function u(x,t). When the series above is substituted into the equation

$$Lu(x,t) = f(x,t) \tag{4.2}$$

we obtain the "residual function" defined as:

$$R(x; a_0, a_1, \dots a_N) = Lu^N - f$$
(4.3)

The function (4.3) is equal to zero when we consider the exact solution and, to determine the

coefficients  $a_k$ , it is necessary that the residual function, multiply with N+1 test functions and integrated over the domain, is equal to zero.

$$\int_D w_j(x) \cdot R(x,t) dx = 0 \qquad \qquad \forall j = 0, ..., N$$
(4.4)

This means that the residual R is required to be orthogonal to all test functions (weights)  $w_j$ . This is the reason why the method is called method of weighted residual. The choice of test and trial functions is the main discriminating factor to distinguish the various spectral methods that can be implemented: let's now proceed to generalize the possibilities of choice and then dwell more in detail on the choices used for our code.

## 4.2.1 Test function

The choice of test functions allow us to distinguish between the three most commonly used spectral schemes, namely, the Galerkin, collocation, and tau versions.

• Galerkin method The first serious application of spectral methods to PDE's- that of Silberman (1954) for meteorological modeling- was a Galerkin method [69]. The Galerkin approach is perhaps the most aesthetically pleasant of the methods of weighted residuals since the test functions are the same as the trial

$$w_j = \phi_j \qquad \qquad \forall j = 0, ..., N \tag{4.5}$$

• Collocation method In the collocation approach a set of N+1 points is chosen in the domain on which the residual R is required to vanish. The test functions become

$$w_j = \delta(x - x_j) \qquad \qquad \forall j = 0, ..., N \tag{4.6}$$

with  $\delta$  being the Dirac delta function. This approach requires the differential equation to be satisfied exactly at the collocation points.

• Tau method Spectral tau methods are similar to Galerkin methods in the way the differential equation is enforced. It may be viewed as a special case of the so-called Petrov-Galerkin method. However, none of the test functions need to satisfy the boundary conditions. Hence, a supplementary set of equations is used to apply the boundary conditions [69].

For the computational code implemented in our thesis work, we have used the Galerkin method, therefore, the focus of the discussion moves on the choice of trial function: this choice will be explained below.

## 4.2.2 Trial function

The choice of trial functions is one of the characteristics that distinguishes spectral methods from finite element ones for example. The functions adopted for spectral methods are global and infinitely differentiable, indicating with what they are defined, and in general different from zero, on the whole computational domain. In the case of finite element methods instead, the domain is divided into small elements and a trial function is specified in each element. The trial functions are therefore of a local nature and are optimal when it is necessary to manage complex geometries.

There are many possible choices, in particular trigonometric (Fourier) functions, Chebyshev and Legendre polynomials, but also lower-order Lagrange polynomials with local support (finite element method) or b-splines. However, we focus on the groups of functions adopted in this work: the Fourier modes.

#### • Fourier Series

The Fourier series are particularly indicated for the discretization of the peridic functions u(x) = u(x+L); considering a periodic domain with periodicity L, defined the fundamental wave number  $\alpha = 2\pi/L$ , the Fourier functions are:

$$u^{N}(x) = \sum_{|k| < \mathbf{K}} c_{k} e^{ik\alpha x} = \sum_{|k| < \mathbf{K}} c_{k} \Phi_{k}$$

$$(4.7)$$

Note that the summation limits are sometimes denoted as  $|k| \leq N/2$  with  $N = 2\mathbf{K}$ . Additionally, a Fourier-transformed quantity  $c_k$  is often denoted by  $\hat{u}_k$ . The N+1 coefficients  $c_k$  are the complex Fourier coefficients for the Fourier mode  $\Phi_k(x)$ . When we consider a smooth function, a Fourier series based on it converges rapidly with increasing N, since the magnitude of the coefficients |ck| decreases exponentially. This behaviour is called spectral convergence [71]



Figure 4.2: Fourier functions  $\Phi_k(x) = e^{i\alpha kx}$  for k = 0, ..., 3 with  $\alpha = 2\pi/L = 1$  [71].

The transformation from the space of the discrete representation of  $u_N$  (physical space)to the space of the Fourier components  $c_k$  (spectral space)is called the (forward) discrete Fourier transform  $F(u_N)$ . Correspondigly, the reverse transform is the inverse Fourier transform  $F^{-1}(c_k)$ . A practical and efficient way to compute this is via the fast Fourier transform (FFT) (Cooley ande Tukey 1965 going back to an idea by Carl Friedrich Gauss 1805), thereby reducing the computational effort from  $O(N^2)$  to O(Nlog(N)) [71]. Considering what is stated in the description of both the test and the trial functions, the method used in our calculation code is the Fourier-Galerkin spectral method where the imposed boundary conditions satisfy the periodicity. As an example, it will be discretized with the Fourier-Galerkin Spectral Method, a simple evolutionary equation in one dimension; the results will then be applied, with corrections to the equation system obtained in Chapter 3.

Then the finite difference methods will be described, used for spatial discretization along the non-periodic component, and an explicit fourth-order Runge-Kutta method used instead for temporal discretion.

#### 4.2.3 An example of Fourier-Galerkin method

Consider a non linear (partial) differential equation, e.g. the Burgers equation (Johannes Martinus Burgers 1895-1981).

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \qquad \qquad 0 \le x < 2\pi \qquad (4.8)$$

with periodic boundary conditions on a domain  $L = 2\pi$ . Due to the periodicity, it is convenient to use a Fourier-Galerkin scheme for the spatial discretisation. The approximation for the solution is

$$u^{N}(x,t) = \sum_{k=-N/2}^{N/2-1} \hat{u}_{k}(t)\phi_{k}(x) = \sum_{k=-N/2}^{N/2-1} \hat{u}_{k}e^{ikx}$$
(4.9)

Replacing  $u^N$  in (4.8), we notice that the fundamental unknowns now are the coefficients  $\hat{u}_k(t)$  for k = -N/2, ..., N/2 - 1, and we have obtained the residual function.

$$\frac{\partial u^N}{\partial t} + u^N \frac{\partial u^N}{\partial x} = \nu \frac{\partial^2 u^N}{\partial x^2} \tag{4.10}$$

To make sure that the residual function is equal to zero, it is necessary multiply it with the test function and integrate over the domain:

$$\int_{0}^{2\pi} \left( \frac{\partial u^{N}}{\partial t} + u^{N} \frac{\partial u^{N}}{\partial x} - \nu \frac{\partial^{2} u^{N}}{\partial x^{2}} \right) e^{-ikx} dx = 0$$
(4.11)

Due to the orthogonality property of the test and trial functions [70], we obtain a set of ODEs for the  $\hat{u}_k$ 

$$\frac{\partial \hat{u}_k}{\partial t} + \left(\widehat{u^N \frac{\partial u^N}{\partial x}}\right)_k + k^2 \nu \hat{u}_k = 0 \qquad \forall k = -N/2, ..., N/2 - 1 \qquad (4.12)$$

where

$$\left(\widehat{u^N \frac{\partial u^N}{\partial x}}\right)_k = \frac{1}{2\pi} \int_0^{2\pi} u^N \frac{\partial u^N}{\partial x} e^{-ikx} dx$$
(4.13)

To complete the discretization of the eq. 4.12, the advection term, written just above, remains to

be treated. This term is a particular case of the general quadratic nonlinear term

$$\widehat{(uv)}_{k} = \frac{1}{2\pi} \int_{0}^{2\pi} uv e^{-ikx} dx$$
(4.14)

where u and v denote generic trigonometric polynomials of degree  $\leq N/2.[70]$ 

Their expansion is similar to eq.4.9: when these are inserted into the equation just above, and the orthogonality property is invoked, we obtain the expression:

$$\widehat{(uv)}_k = \sum_{p+q=k} \hat{u}_p \hat{v}_q \tag{4.15}$$

This is a convolution sum. Therefore, the Fourier-Galerkin approximation to the Burgers equation is:

$$\frac{\partial \hat{u}}{\partial t} + \sum_{\substack{p+q=k\\p,q=-N/2,...,N/2-1}}^{\infty} \hat{u}_p i q \hat{u}_q = -k^2 \nu \hat{u}_k \qquad \forall k = -N/2,...,N/2 - 1$$
(4.16)

The complex summation of the second term requires  $O(N^2)$  operations, which makes this evaluation sum the most expensive part of the calculator. There is a simpler and more efficient way to calculate this sum. The most important approach to do this is via Fourier transforms leading to an order  $O(Nlog_2N)$  for the same operation, which is significantly less than  $O(N^2)$  for large N. We consider a general one-dimension convolution sum of the form

$$\sum_{\substack{p+q=k\\p,q=-N/2,...,N/2-1}}^{\infty} \hat{u}_p i q \hat{v}_q \tag{4.17}$$

in order to illustrate the basic approach to calculate it.

The basic approach is to transform  $\hat{u}_p$  and  $\hat{v}_q$  to physical space, to perform a pointwise multiplication, and then to transform the result back to Fourier space [68]. We introduce the discrete transform

$$U_j = \sum_{k=-N/2}^{N/2-1} \hat{u}_k e^{ikx_j} \qquad \forall j = 0, 1, ..., N-1$$
(4.18)

$$V_j = \sum_{k=-N/2}^{N/2-1} \hat{v}_k e^{ikx_j} \qquad \forall j = 0, 1, ..., N-1$$
(4.19)

and we define the physical space product

$$W_j = U_j V_j \tag{4.20}$$

and its discrete Fourier transform

$$\hat{W}_k = \frac{1}{N} \sum_{j=0}^{N-1} W_j e^{-ikx_j} \qquad \forall k = -N/2, ..., N/2 - 1$$
(4.21)

Using the discrete orthogonality relation, we obtain:

$$\hat{W}_k = \sum_{\substack{p+q=k\\p,q=-N/2,\dots,N/2-1}}^{\infty} \hat{u}_p \hat{v}_q + \sum_{\substack{p+q=k\pm N\\p,q=-N/2,\dots,N/2-1}}^{\infty} \hat{u}_p \hat{v}_q$$
(4.22)

Such an evaluation of the spectral convolution in physical space is usually termed pseudo-spectral evaluation of the nonlinear terms. The first term on the right-hand side is the desired result; the second one is called aliasing error.[68]

The convolution sum in the pseudospectral method is evaluated at the cost of 3 FFT's and N multiplications. The total operation count is  $(15/2)Nlog_2N$  multiplications.[70]

Everything that has been observed for a simple equation like that of Burgers, is used in the same way in the case of the equations 3.25 described in the previous chapter.

When dealing with a discrete representation of continuous data, the frequency content beyond the critical frequency (Nyquist) is generally misinterpreted. We are talking about "aliasing" when critical frequencies are erroneously attributed to lower frequencies within the range taken into consideration. [73]



Figure 4.3: A sine-wave function sampled at a lower frequency than Nyquist has the same samples of a lower-frequency sine wave (aliasing)

This example shows that high frequencies in the original signal, seen at an insufficient sampling step, are presented as low frequencies in the reconstructed signal. If a signal, such as an image, is sampled at an insufficient frequency, then, after reconstructing the latter from such samples, high-frequency components of the original signal appear as low-frequency components in the reconstructed one at starting from these inadequate samples. This is the typical example of aliasing.

The Nyqvist theorem said that one needs more than two grid-points per wavelength in order to represent a solution on a numerical grid: in other words, the wavenumber k must be in the range

$$-k_{x,Nyqvist} < k < k_{x,Nyqvist} \tag{4.23}$$

where

$$k_{x,Nyqvist} = \pi/\Delta x \qquad \Delta x = L_x/N_x \qquad (4.24)$$

 $k_{x,Nyqvist}$  is the Nyqvist wavenumber,  $L_x$  is the domain size, and  $N_x$  the number of grid-points. According to the sampling theorem, if we sample under the Nyquist frequency, the sampled values we get for the maximum frequency component are the same as we would have obtained by sampling the signal at a lower frequency, as shown in fig 4.3.

There are some possibilities to remove (or at least reduce) these errors. One popular variant is the so-called 3/2-rule: the original grid in physical space is refined by a factor M = 3/2N in every direction, and the nonlinear multiplications are then performed on this finer grid. Afterwards, the results product in transformed to spectral space, cutting away the wavenumbers with |k| > N/2. The operation count for this transform method, considered the necessary grid expansion, is  $(45/4)Nlog_2(3/2)N$  [70]. Another choice, computationally less expensive, is represented by the 2/3-rule: in this thesis work, following what was explained by Passoni et al [63], we opted for this last algorithm to eliminate aliasing error.

With this rule, the aliasing effect is eliminated by keeping only frequency components corresponding to wavenumbers less than 2/3 of the Nyqvist wavenumber, in each dimension i.e. components corresponding to  $|k_x|(2/3)N_{x,Nyqvist}$ , and  $|k_y|(2/3)N_{y,Nyqvist}$  are deleted from the solution. This is illustrated in the figure 4.4 where, wave components corresponding to  $|k_x| > 8/3$  and  $|k_y| > 8/3$  should be removed from the solution. [74]



Figure 4.4: The 2/3-rule dealiasing scheme [74]

As explained above, it is carried out in the code by the **dealiasing** subroutine

# 4.3 Finite difference method

In the case of finite differences, we discretize our domain (usually limited) through a succession of computational nodes. With such discretization, a generic function is "approximated" by the values that it assumes at the nodes themselves.

Through the use of numerical formulas deriving from the combination of appropriate developments in Taylor's series, it is possible to approximate the differential operators to obtain a linear system, whose unknowns are the nodal values of the function. This finite set will approximate our unknown function.

As explained in [63] a finite-centered differences scheme was used, to the second order of accuracy. Most common finite-difference representation of derivatives ar based on Taylor's series expansions. Consider a continuous function of x, namely f(x), with all derivatives defined in x. Thanks to a Taylor series expansion about point x, the value of  $f(x + \Delta x)$  can be found:

$$f(x + \Delta x) = f(x) + \frac{\partial f}{\partial x} \Delta x + \frac{\partial^2 f}{\partial x^2} \frac{\Delta x^2}{2} + \dots + \frac{\partial^n f}{\partial x^n} \frac{\Delta x^n}{n!} + \dots$$
(4.25)



Figure 4.5: Illustration of behavior of the first three terms in a taylor series [21]

The significance of eq. (4.25) is explained on the fig. 4.5.

Observing the right-hand side of equation (4.25), we see that the first term, f(x), is not a good approximation for  $f(x + \Delta x)$ , unless, the function f(x) is a horizontal line between points 1 and 2. To obtain an even better estimate of f in  $x + \Delta x$ , in addiction to the second term, the third is necessary and it approximately accounts for the curvature between points 1 and 2. In general, greater accuracy implies inclusion of additional higher-order terms. Indeed, to have an exact representation of  $f(x + \Delta x)$ , eq.(4.25) should include an infinite number of terms on the right-hand side [21]. Solving the (4.25) for  $\partial f/\partial x$  we obtain:

$$\frac{\partial f}{\partial x} = \frac{f(x + \Delta x) - f(x)}{\Delta x} - \frac{\partial^2 f}{\partial x^2} \frac{\Delta x}{2} - \frac{\partial^3 f}{\partial x^3} \frac{\Delta x^2}{6} + \dots$$
(4.26)

The first term is a finite-difference rappresentation of the partial derivative.

The remaining terms on the right side constitute the truncation error; this term measure the accuracy of the approximation and determine the rate at which the error decrease as the grid is refined. In equation (4.26), the lowest-order term in the truncation error involves  $\Delta x$  to the first

power; hence, the expression (4.26) is called first order accurate. We can more formally write:

$$\frac{\partial f}{\partial x} = \frac{f(x + \Delta x) - f(x)}{\Delta x} + O(\Delta x) \tag{4.27}$$

Observing the equation (4.27) we can see that expression uses information only to the right of grid point x; as a result, the finite difference in eq (4.27) is called *forward difference*. Writing a Taylor series expansion for  $f(x - \Delta x)$ , expanded about f(x), and solving for  $\partial f/\partial x$ , we obtain:

$$\frac{\partial f}{\partial x} = \frac{f(x) - f(x - \Delta x)}{\Delta x} + O(\Delta x) \tag{4.28}$$

As highlighted above the finite difference in eq (4.28) is called *backward difference* and also in this case, the error involves  $\Delta x$  to the first power: the expression (4.28) is called *first-order backward difference*.

As said previuosly, we have a *second-order finite difference* scheme: the way to construct this scheme is simple. In the case of a non-uniform grid, the second-order centered scheme is written as the weighted average of the two backward and forward derivatives and the weight is proportional to the inverse of the considered interval. Referring to the figure below I can write that:



Figure 4.6: example of an non-uniform grid

$$\left(\frac{\partial f}{\partial x}\right)_{i} = \frac{1}{x_{i+1} - x_{i-1}} \left(\frac{f_{i+1} - f_{i}}{x_{i+1} - x_{i}} (x_{i} - x_{i-1}) + \frac{f_{i} - f_{i-1}}{x_{i} - x_{i-1}} (x_{i+1} - x_{i})\right)$$
(4.29)

We now write the discretization with finite differences for the second derivative that will appear within the diffusive terms. Once you have written Taylor's development for  $f(x_{i+1})$  e per  $f(x_{i-1})$ we proceed adding the terms and isolating  $(\partial^2 f/\partial x^2)_i$ .

For non-uniform grids, we can use a backward difference to eliminate the first derivative, and after sobstitution and some algebra, we get:

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i = \frac{f_{i+1}\Delta x_{i-1} - f_i(\Delta x_{i-1} + \Delta x_i) + f_{i-1}\Delta x_i}{\frac{1}{2}\Delta x_{i-1}\Delta x_i(\Delta x_{i-1} + \Delta x_i)}$$
(4.30)

Since the steepest gradients are located near the walls, it is necessary to use a non-uniform grid: the streching laws for the grid points along y is introduced for completeness [63].

$$y_{str} = Py + (1 - P) \left( 1 - \frac{\tanh[Q(1 - y)]}{\tanh Q} \right)$$
(4.31)

P and Q are two parameters characterizing the distribution (in our code P = 1.7, Q = 1.9). The partial derivatives along y are calculated accordingly.

# 4.4 Runge-Kutta Method

In mathematical analysis a differential equation is an equation that links an unknown function to its derivatives: if all derivatives are computed with respect to a single independent variable, the equation is an ordinary differential equation (ODE). When derivatives are present with respect to several independent variables, we will have instead a differential equation to the partial derivatives (PDE). A differential equation will have order n, if n is the maximum order of the derivatives that appear in it.

Most ODE problems encountered in practice cannot be solved analytically or the solution cannot be expressed in a form that can easily be calculated; numerical techniques are therefore necessary for the resolution of an ODE.

The first numerical resolution technique dates back to Newton, for the study of the motion of a comet, and, although it is very simple and intuitive, is not generally used in scientific computing for two main reasons. Firstly, the truncation error per step associated with this method is far larger than those associated with other, more advanced, methods. Secondly, Euler's method is too prone to numerical instabilities; it has such a large truncation error per step because in evolving the solution from  $x_n$  to  $x_{n+1}$  it evaluates derivatives at the beginning of the interval: the method is, therefore, very asymmetric with respect to the beginning and the end of the interval.

The methods most commonly employed to integrate ODE's were first developed by the German mathematicians C.D.T. Runge and M.W. Kutta in the latter half of the nineteenth century. We can construct a more symmetric integration method by making an Euler-like trial step to

the midpoint of the interval, and then using the values at the midpoint to make the real step to across the interval. A method like this is generally known as a second-order Runge-Kutta method because the symmetrization cancels out the first-order error.

Euler's method can be thought of as a first-order Runge-Kutta method. There is no need to stop at a second-order method. By using two trial steps per interval, it is possible to cancel out both the first and second-order error terms, and, thereby, construct a third-order Runge-Kutta method. Likewise, three trial steps per interval yield a fourth-order method, and so on. Note that, in general, an *n*th-order Runge-Kutta method requires *n* evaluations of this function per step. It can easily be appreciated that as *n* is increased a point is quickly reached beyond which any benefits associated with the increased accuracy of a higher order method are more than offset by the computational cost involved in the necessary additional evaluation of f(x, y) per step.

In the most general form an RK method can be written as a linear combination in the following way:

$$y_{n+1} = y_n + \Delta t F(t_n, y_n, h; f)$$
(4.32)



Figure 4.7: Representation of the point estimated by the Euler method and how it differs from the true solution. The error committed decreases with step h

where  $n \geq 0$  and F is the increment function written this way:

$$F(t_n, y_n, h; f) = \sum_{i=1}^{s} b_i K_i$$

$$K_i = f(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ik} K_j)$$

$$i = 1, 2, ..., s$$
(4.33)

s indicates the number of stages of the method. The coefficienti  $a_{ij}$ ,  $b_{ij}$  and  $c_{ij}$  completely characterize a RK method and are generally collected in the so-called Tableau of Butcher

## Figure 4.8: (Tableau di Butcher)

being  $A = (a_{ij}) \in \mathbb{R}^{sxs}$ ,  $b = (b_1, ..., b_s)^T \in \mathbb{R}^s$  and  $c = (c_1, ..., c_s)^T \in \mathbb{R}^s$ . We will also assume that the following relationship applies:

$$c_i = \sum_{j=1}^{s} aij$$

$$i = 1, \dots, s$$

$$66$$

$$(4.34)$$

For a four-stage scheme (s = 4) like the one used in our code, the equation (4.32), can be explained as:

$$y_{n+1} = y_n + \Delta t (b_1 K_1 + b_2 K_2 + b_3 K_3 + b_4 K_4)$$
(4.35)

where

$$K_{1} = F(t_{n} + c_{1}\Delta t, y_{n})$$

$$K_{2} = F(t_{n} + c_{2}\Delta t, y_{n} + \Delta t(a_{21}K_{1}))$$

$$K_{3} = F(t_{n} + c_{3}\Delta t, y_{n} + \Delta t(a_{31}K_{1} + a_{32}K_{2}))$$

$$K_{4} = F(t_{n} + c_{4}\Delta t, y_{n} + \Delta t(a_{41}K_{1} + a_{42}K_{2} + a_{43}K_{3}))$$
(4.36)

The choice of the parameters a, b and c is not random, but they are chosen so that the accuracy of the scheme is of the fourth order  $E(\Delta t) \approx O((\Delta t)^5)$ .

If the coefficients  $a_{ij}$  in A are null for  $j \ge 0$ , with i = 1, 2, ..., s, then every  $K_i$  can be explicitly calculated as a function of only i - 1 coefficients  $K_i, ..., K_{i-1}$  already previously calculated. For this reason, in this case, the scheme is called explicit. Otherwise, the RK scheme is implicit and the calculation of  $K_i$  requires the resolution of a nonlinear system of size s.

The main disadvantage of the Runge-Kutta scheme compared to that of Euler is the fact that in the first case we need to calculate the function F(t; y) a certain number of times for each step  $\Delta t$ . If F(t; y) is a complicated function this calculation leads to an obvious slowing of numerical calculation time. The obvious advantage is an increase in calculation accuracy.

All Runge-Kutta schemes are convergent, in the sense that the error  $E(\Delta t) \rightarrow 0$  in the limit  $\Delta t \rightarrow 0$ , however also the Runge-Kutta scheme is subject to instability if values are used too time steps.

The coefficients assume the following values:

$$s = 4$$

$$a_{21} = \frac{1}{2}$$

$$a_{31} = 0 \quad a_{32} = \frac{1}{2}$$

$$a_{41} = 0 \quad a_{42} = 0 \quad a_{43} = 1$$

$$b_1 = \frac{1}{6} \quad b_2 = \frac{1}{3} \quad b_3 = \frac{1}{3} \quad b_4 = \frac{1}{6}$$

$$c_1 = 0 \quad c_2 = \frac{1}{2} \quad c_3 = \frac{1}{2} \quad c_4 = 1$$

$$(4.37)$$

Therefore, in order to evaluate the equation 4.35, our code acts in this way:

- I compute as first thing  $K_1$  using "RHS" subroutine
- I compute  $y = y_n + 0.5\Delta t K_1$

- I update the output variable with the *Proiezione* subroutine
- I compute  $K_2$  using "RHS" subroutine with updated values
- I compute  $y_* = y_n + 0.5\Delta t K_2$  and i update the output variable with the *Proiezione* subroutine
- I execute the same steps for te calculation of  $K_3$  and  $K_4$
- calculate the value at the next step  $y_{n+1} = y_n + \Delta t (b_1 K_1 + b_2 K_2 + b_3 K_3 + b_4 K_4)$  and update with the "Projectione" subroutine.



Figure 4.9: Geometric visualization of the behavior of a RK4 scheme

From a numerical point of view, the solution of a differential equation with partial derivatives is affected by two types of error: the discretization error, given by the difference between the analytical solution and the exact solution, and the rounding error, which represent the numeric error introduced after a series of repetitive calculations in which a computer constantly rounds in numbers.

Another property of a numerical scheme is consistency: a numerical system is said to be consistent if its discrete operators (with finite differences) converge towards continuous operators (with derivatives) of a PDE for  $\Delta t, \Delta x \to 0$ .

For explicit Runge-Kutta methods the parameters must satisfy the following condition

$$\sum_{i=1}^{s} a_i = 1 \tag{4.38}$$

and this condition guarantees the consistency of this methods.

There is stability if "the noise" (given by initial conditions, rounding errors, ...) does not increase, while there is convergence if the solution of a numerical scheme converges towards the real solution of a PDE for  $\Delta t, \Delta x \to 0$ .

The Lax equivalence theorem establishes the condition for convergence: given a problem that satisfies the condition of consistency, stability is the necessary and sufficient condition for convergence.

To maintain stability, we can refer to the Courant-Friedrichs-Lewy condition (CFL condition)

$$C = c \frac{\Delta t}{\Delta x} \le 1 \tag{4.39}$$

Where "C" is called the Courant number, and the constant "c" depends on the equation to be solved.

Keep in mind that not all  $\Delta t$  values are to be considered good: how to establish for which values of h a numerical method is stable for a given problem? To establish it, just apply the one-step method to the test problem  $y' = \lambda y$  i.e. with  $f(t, y) = \lambda y$  and we bring ourselves back to an expression of the type

$$y_{n+1} = F(\Delta t\lambda)y_n \tag{4.40}$$

where, for a Runge-Kutta methods we obtain:

$$F(\Delta t\lambda) = 1 + \Delta t\lambda + \frac{1}{2}(\Delta t\lambda)^2 + \dots + \frac{1}{s!}(\Delta\lambda)^s$$
(4.41)

The stability region is the set in the complex plane such that:

$$R_a = [\Delta t \lambda \in \mathbb{C} : |F(\Delta t \lambda)| < 1]$$
(4.42)

To solve the problem, it is necessary to choose  $\Delta t$  small enough to ensure that  $\Delta t \lambda$  is in the stability region, otherwise the sequence of approximations produced in many steps will be unbounded. We interpret this as unstable behaviour.

In our simulation we have  $(\Delta x)_{max} = L_x/N_x = 2\pi/128$  and  $\Delta t = 4 \times 10^{-4}$ .

The real part of the graphics above measures the speed to zero, the imaginary part measures the oscillations, and the stability plot shows you how well a method can handle the combinations. For a nonlinear problem, you will have stability if you always have that the "instantaneous speed and oscillations",  $\lambda$ , are within the stability region [77].

When we have a very large  $\lambda$ , either complex or real, our problem is stiff: another way is to say if our highest eigenvalue is "large" and our smallest eigenvalue is "small", since this separation causes many numerical problems. In that case, we can see from the stability plots that most explicit methods will require a very small timesteps (h) in order to be stable.

# 4.5 **Projection Method**

Through the assumption of  $\rho_{mix} = cost$  the energy equation has been completely decoupled from the analysis. The implication here is that the continuity and momentum equations are all that are necessary to solve for the velocity and pressure fields in an incompressible flow, and that if a given problem involves heat transfer, and hence temperature gradient exist in the flow, the temperature field can be obtained directly from the energy equations after the velocity and pressure fields are obtained.

In incompressible flow problems, as observed by the system (3.25), there is no equation where a main variable appears directly linked to pressure; this leads to the affirmation that in incompressible fluids, pressure is the variable that assumes the values necessary to "force" respect for the continuity equation. The differential pressure equation, obtained starting from the equations of



Figure 4.10: stability regions for some Runge-Kutta methods up to order 4

motion and continuity, is called the Poisson equation for pressure. In our code, the scheme for the solution of the incompressible Navier-Stokes equations is the so-called projection method due to Chorin [78]. At each substep of the Runge-Kutta procedure:

- We compute an intermediate velocity field **v**<sup>\*</sup>.
  - In this first step, the contribution of pressure is neglected and does not appear in the RHS subroutine. After this, the velocity field will not be zero divergent and therefore the continuity equation will not be satisfied. In order to have zero divergence the contribution of the pressure must be added to the intermediate velocity

$$\mathbf{v} = \mathbf{v}^* - \nabla P \tag{4.43}$$

• In a second step, we compute a correction of the intermediate velocity field via the pressure Poisson equation which leads to a divergence free velocity field.

$$\nabla^2 P = \nabla \cdot \mathbf{v}^* \tag{4.44}$$
### 4.6 Code Implementation

Summing up when written so far, the method used for the discretization of the equations 3.90, is a spectral-finite difference scheme: in space, Fourier decomposition is used in x and z-direction, and finite difference is used to discretize the equation along the y-axis perpendicular to the walls. An explicit 4th order Runge-Kutta scheme was used to obtain progress over time. For the sake of clarity we now outline the basic steps to implement the equations (3.90).

Starting from the mixture momentum equation:

$$\frac{\partial \mathbf{v}^*}{\partial t^*} + \nabla \cdot (\mathbf{v}^* \mathbf{v}^*) = -\nabla P^* + \frac{1}{\sqrt{Gr}} \nabla^2 \mathbf{v}^* + \frac{1}{2} T^* - \frac{(\xi - 1)\varphi_0}{\Theta} \varphi^* - C_M (1 + \varphi^*) T^* \nabla H^* \quad (4.45)$$

- We bring everything to a second member by isolating the term  $\partial \mathbf{v}^* / \partial t^*$
- In the subroutine **conv** we calculate the convective term of the equation and the term of magnetic force

$$\mathbf{A} = -\nabla \cdot (\mathbf{v}^* \mathbf{v}^*) \tag{4.46}$$

$$\mathbf{F} = -C_M (1 + \varphi^*) T^* \nabla H^* \tag{4.47}$$

• In the subroutine RHS recall what was obtained above and add the diffusive term. When the mixture momentum equation is calculated for the x-axis, the contributions of the terms due to the buoyancy force will be also added.

$$\mathbf{A} \leftarrow \mathbf{A} + \mathbf{F} + \frac{1}{\sqrt{Gr}} \nabla^2 \mathbf{v}^* + \frac{1}{2} T^* - \frac{(\xi - 1)\varphi_0}{\Theta} \varphi^*$$
(4.48)

• We then proceed with the time discretization and the insertion of the pressure contribution as explained in the previous section.

For the mixture energy equation we proceed in a similar way

$$\frac{\partial T^*}{\partial t^*} + \nabla \cdot (T^* \mathbf{v}^*) = \frac{1}{Pr\sqrt{Gr}} \nabla^2 T^*$$
(4.49)

• we isolate the term  $\partial T^* / \partial t^*$ 

• In the subroutine **conv** we calculate the term

$$\mathbf{A}_T = -\nabla(T^* \mathbf{v}^*) \tag{4.50}$$

 $\bullet\,$  In the subroutine RHS we add a diffusion term

$$\mathbf{A}_T \leftarrow \mathbf{A}_T + \frac{1}{Pr\sqrt{Gr}} \nabla^2 T^* \tag{4.51}$$

• We proceed with the discretization in time with the method explained in the previous section

All that remains is to observe how we proceed to implement the equation of the volume fraction of the dispersed phase

$$\frac{\partial \varphi^*}{\partial t^*} + \nabla \cdot (\varphi^* \mathbf{v}^*) = C_{grav} \nabla \varphi^* + \frac{S_{t(ref)}}{Sc\sqrt{Gr}} \nabla \cdot ((1+\varphi^*)\nabla T^*) - C_{Mphi} \nabla \cdot ((1+\varphi^*)\nabla H^*) + \frac{1}{Sc\sqrt{Gr}} \nabla^2 \varphi^*$$
(4.52)

• We isolate the time-dependent term

$$\frac{\partial \varphi^*}{\partial t^*} = -\nabla \cdot \left[ \varphi^* \mathbf{v}^* - \frac{S_{t(ref)}}{Sc\sqrt{Gr}} ((1+\varphi^*)\nabla T^*) + C_{Mphi} ((1+\varphi^*)\nabla H^*) \right] + C_{grav} \nabla \varphi^* + \frac{1}{Sc\sqrt{Gr}} \nabla^2 \varphi^*$$
(4.53)

• In the subroutine **conv** we calculate all the terms that appear in the square bracket:

$$\mathbf{f} = \varphi^* \mathbf{v}^* - \frac{S_{t(ref)}}{Sc\sqrt{Gr}} ((1+\varphi^*)\nabla T^*) + C_{Mphi} ((1+\varphi^*)\nabla H^*)$$
(4.54)

$$\mathbf{A}_{\varphi} = -\nabla \cdot \mathbf{f} \tag{4.55}$$

• In the subroutine RHS we add the diffusion term and the buoyancy term:

$$\mathbf{A}_{\varphi} \leftarrow \mathbf{A}_{\varphi} + C_{grav} \nabla \varphi^* + \frac{1}{Sc\sqrt{Gr}} \nabla^2 \varphi^*$$
(4.56)

• We proceed with the discretization in time with the method explained in the previous section.

The equation of the volumetric concentration of particles, unlike the equations for velocity and temperature, is also solved on the walls, because we do not know the value of  $\varphi$  on the walls, but the boundary conditions concern its derivatives, as explained in next chapter.

## 4.7 Boundary and initial conditions

The no-slip/no-penetration conditions require that all velocity components vanish at solid walls and the assumption of a thermodynamic equilibrium requires that the fluid temperature at the walls be equal to the wall temperature.

Referring to the figure, by discretizing the size of the channel along the y-axis with Ny points, the side walls are found at nodes 1 and Ny. Therefore, imposing wall conditions means canceling the velocities u, v, w in those points of the domain, ie:

$$u(:,1,:) = u(:,Ny,:) = 0$$
  

$$v(:,1,:) = v(:,Ny,:) = 0$$
  

$$w(:,1,:) = w(:,Ny,:) = 0$$
  
(4.57)

Considering the adimensionalizations made previously, the conditions to be imposed on the wall with regard to the Temperetura are easily obtained, ie:

$$T(:,1,:) = -1$$
  

$$T(:,Ny,:) = 1$$
(4.58)

As written, it is clear that the wall in position 1 is the cold wall, vice versa in Ny the warm wall is positioned.

All of this is implemented in the code by the subroutine condcont.

Regarding the boundary conditions to be considered for the particle concentration conservation equation, the x and z directions do not cause problems because they only impose the periodicity of  $\varphi$ . The boundary conditions in the direction y must guarantee that there is no flow of particles across the border (For clarity of exposition, the abbreviations indicating the dimensionless coefficients preceding each term are substituted for the real parameters in the equation). This happens if you have on the wall

$$\varphi \mathbf{v} \cdot \mathbf{n} = \left(\frac{1}{Sc\sqrt{Gr}} \nabla \varphi - C_{Mphi}(1+\varphi) \nabla H + \frac{S_{t(ref)}}{Sc\sqrt{Gr}}(1+\varphi) \nabla T\right) \cdot \mathbf{n}$$
(4.59)

But velocity on the walls is zero, so one has

$$\left(\frac{1}{Sc\sqrt{Gr}}\nabla\varphi - C_{Mphi}(1+\varphi)\nabla H + \frac{S_{t(ref)}}{Sc\sqrt{Gr}}(1+\varphi)\nabla T\right) \cdot \mathbf{n} = 0$$

that is

$$\frac{\partial \varphi}{\partial y} = Sc\sqrt{Gr} \left( C_{Mphi} (1+\varphi) \partial_y H \right) - Sc\sqrt{Gr} \left( \frac{S_{t(ref)}}{Sc\sqrt{Gr}} (1+\varphi) \partial_y T \right)$$

Taking the Fourier transform in the direction x and z we have

$$\frac{\partial \hat{\varphi}}{\partial y} = C_{Mphi} Sc \sqrt{Gr} (\widehat{1 + \varphi}) \partial_y H - Sc \sqrt{Gr} \left(\frac{S_{t(ref)}}{Sc \sqrt{Gr}}\right) (\widehat{1 + \varphi}) \partial_y T$$

We have to calculate the product transform between  $1 + \varphi$  and  $\partial_y H$  and also between  $1 + \varphi$  and  $\partial_y T$ , and this product should be made on the wall and just to apply the boundary conditions. The Fourier transforms are only in x and z and are actually calculated plane by plane at y constant. It is therefore sufficient to operate the anti-transform of  $\hat{\varphi}$  only on the two walls at y = -1 and y = 1 (indices j = 1 and  $j = N_y$ ) and run the product. Therefore two additional subroutines have been created:

- atrasf3\_parete(uT,uR1,uR2): takes a 3D field as an input in Fourier space and outputs the anti-transforms in the physical space.
- atrasf2\_parete(uR,uT): performs the transformation of a plan.

If we discretize the derivative at the points of the wall  $(1,...,N_y)$  we get

$$\frac{\hat{\varphi}_2 - \hat{\varphi}_0}{y_2 - y_0} = Sc\sqrt{Gr} \left[ C_{Mphi} \left[ (1 + \widehat{\varphi})\partial_y H \right]_1 - \left( \frac{S_{t(ref)}}{Sc\sqrt{Gr}} \right) \left[ (1 + \widehat{\varphi})\partial_y T \right]_1 \right]$$
(4.60)

$$\frac{\hat{\varphi}_{N_y+1} - \hat{\varphi}_{N_y-1}}{y_{N_y+1} - y_{N_y-1}} = Sc\sqrt{Gr} \left[ C_{Mphi} \left[ (1+\widehat{\varphi})\partial_y H \right]_{N_y} - \left( \frac{S_{t(ref)}}{Sc\sqrt{Gr}} \right) \left[ (1+\widehat{\varphi})\partial_y T \right]_{N_y} \right]$$
(4.61)

from which we find the "extra domain" points  $(0, ..., N_{y+1})$  that are useful for having the wall derivatives (which are used to solve the equation):

$$\hat{\varphi}_{0} = \hat{\varphi}_{2} - Sc\sqrt{Gr} \left[ C_{Mphi} \left[ (1+\varphi)\partial_{y}H \right]_{1} - \left( \frac{S_{t(ref)}}{Sc\sqrt{Gr}} \right) \left[ (1+\varphi)\partial_{y}T \right]_{1} \right] (y_{2} - y_{0})$$

$$(4.62)$$

$$\hat{\varphi}_{N_y+1} = \hat{\varphi}_{N_y-1} + Sc\sqrt{Gr} \left[ C_{Mphi} \left[ (1+\varphi)\overline{\partial}_y H \right]_{N_y} - \left( \frac{S_{t(ref)}}{Sc\sqrt{Gr}} \right) \left[ (1+\varphi)\overline{\partial}_y T \right]_{N_y} \right] (y_{N_y+1} - y_{N_y-1})$$

$$(4.63)$$

The subroutine, condcont are implemented as

- I call the subroutine atrasf3\_parete to get the values of φ in the physical space on the wall: atrasf3\_parete (phi,phif1,phif2)
- I call the subroutine atrasf3canale to get the values of T in the physical space in 3D (not only on the walls): atrasf3canale (T,Tf)
- I call the subtoutine der\_y to calculate the long y derivative of the 3D matrix of T in physical space: der\_y (Tf,dTfy)
- I calculate the product of  $\varphi$  in the lower wall with the magnetic field and with the gradient of T (put in the variable **prod** through a double for loop, to be sure to consider only the indices corresponding to the walls also in the 3D matrix of T)

- anti-transform the product and determine the value of  $\hat{\varphi}_0$
- I repeat the last two points for the upper wall.

# Chapter 5

# Results

We now proceed to the analysis of the results obtained from the CFD simulations: we will describe and comment five different configurations, where the magnetic field, within the considered domain, be the thing that will mainly vary. The different cases, therefore, consist of a different geometric arrangement of the magnets that interface to the walls.

The configurations tested reflect some of the simplest conditions to be experimentally simulated in the laboratory.

# 5.1 Basic configuration



Figure 5.1: 3D visualization of the calculation domain and reference axes in the basic configuration. The red wall is the one at  $T_0 + \Delta T/2$  while the blue wall is at  $T_0 - \Delta T/2$ . The magnets are represented by the gray blocks whose magnetic field, perpendicular to the walls, penetrates into the calculation domain .



Figure 5.2: Domain scheme seen from above (section in the horizontal plane (y, z) showing the position of the magnets.) Parameters:  $L_z = 2$  (domain  $2\pi$  long in direction z,  $f_z = 0.4$  (40% of the domain covered by the magnets),  $y_m = 0.4$  (distance of the magnetic plates from the walls.) The grid has 257 unevenly spaced points in the y-direction and 128 evenly spaced points in the z-direction.

The position of the magnets shown in fig 5.1 and in fig 5.2 creates a magnetic field shown in fig. 5.3.



Figure 5.3: Visualization of the main figures of the magnetic field, with reference to the configuration of the base case.

Looking at the first image, we can see that the modulus of H is maximum where the edges of the magnets are located ( $z \approx 1.2$  and  $z \approx 5$ ) and, consequently, the whole area in front of the edges, even if the magnetic field drops in intensity, is characterized by higher values of H than the rest of the cavity.

The area in front of the body of the magnets, instead,  $(0 < z < 1.2, 5 < z < 2\pi)$  is characterized by lower values starting from the walls; moving towards the center of the domain (y = 0) the magnetic field decreases its intensity up to H=0. These points with null values of H are due to the field lines coming out of the magnets: they will have only vertical component, equal in form, but opposite in sign. The other area where H is null, it is located in the exact center of the computation domain (y = 0 and  $z = \pi$ ). In general, the whole central part of the cavity shows very low H values up to the point of being canceled; this could be explained by the progressive thinning of the field lines up to their total absence at that point, in fact both  $H_z$  and  $H_y$  are zero. With reference to the variation of the H module along the z-axis, starting from z = 0 and moving on along z-direction, we observe how |H| increases in intensity, and, once the maximum peak is reached, it decreases up to the center of the wall  $(z = \pi)$  where it settles at constant values. This trend is showed by the graph  $\partial H/\partial z$ , where the increasing-modulus zone has values of  $\partial H/\partial z > 0$ . Where the peak is located, we have  $\partial H/\partial z = 0$ , as well as where the module of H remains almost constant. Where the modulus of H is decreasing, we observe a blue zone in the graph of  $\partial H/\partial z = 0$  (1.2  $\leq z \leq \pi$ ). This behavior is repeated symmetrically starting from  $z = \pi$ up to the end of the domain.

We can observe how |H| varies along the y-axis: starting from the center of the domain (y = 0), values are gradually intensified as we move towards the walls, with peaks at the edges. Also this trend is highlighted in the graph  $\partial H/\partial y$ : the central zone for example has very low values of  $\partial H/\partial y$  because |H| does not register any relevant variation.

The graphs of  $H_z$  and  $H_y$  highlight how the field lines develop within the domain: in particular, we can see how, for what concerns  $H_z$ , both for left and right magnets, the lines are oriented towards the center of the domain, because they need to close on themselves and this can only happen in the center of the domain where no source is present. For what concerns  $H_y$  in the area in front of the magnets, the vertical component of the magnetic field is always outgoing from the latter and points towards the axis of symmetry (y = 0). Moving beyond the edges, the vertical component changes direction and the field lines are oriented towards the walls of the calculation domain.

We now proceed with the visualization of the results representing the configuration obtained after the transient phase of the system, that is after approximately 10 seconds of simulation.



5 - Results

Figure 5.4: Visualization of  $T^*, \varphi$  and  $u^*$  after 10 seconds. The plane considered is the yz plane positioned halfway up the domain perpendicular to the magnets arranged in the basic configuration.

The figure 5.4 show how the  $T^*$ ,  $\varphi^*$  and  $u^*$  behave once the system transient phase has passed. It is immediately observed that the  $T^*$  is transported by convection and diffusion within the calculation domain: in particular, the areas with major  $T^*$  are located at the extremes of the area under examination, or in front of the magnets placed on the warm wall. The other area that sees an increase of  $T^*$ , compared to the starting configuration, is placed exactly in the middle in correspondence with to the internal edges of the magnets positioned at y = 1. In front of the internal edges of the magnets placed on the cold wall (y = -1), there's a zone which is developed instead at  $T^*$  lower than the starting configuration.

The third image in figure 5.4 shows the velocity component  $u^*$ . The velocity in question is the

one that develops along the vertical x-axis of the system, therefore it is subject only to buoyancy forces, since the gradient of H along the x-axis is zero: the magnetic force does not act in this direction. The clear similarity between the behavior described above for the  $T^*$  and the one observed for the speed  $u^*$  is immediately evident. The zones where the  $T^*$  turns out to be higher are zones where the flow density is smaller, so it is there that the ascending modes of the flow are localized  $(u^* > 0)$ . On the opposite side, zones at minor  $T^*$  imply a greater density and, therefore, the flow moves in the direction of negative x  $(u^* < 0)$ . In the momentum equation that calculates this velocity component, the concentration of particles is also at stake: where we have a higher concentration. In our case, however, the  $\varphi^*$  turns out to be quite uniform and above all too small to be able to heavily influence the flow along the x-axis. The velocity is higher than in all other directions and this suggests that this type of motion is predominant inside the cavity, but it is not the only one.



Figure 5.5: Visualization of  $v^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the base configuration



Figure 5.6: Visualization of  $w^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the base configuration

The figures 5.5 and 5.6 show the velocity components  $v^*$  and  $w^*$  which act on a plane perpendicular to the walls.

Looking at these velocities, we note that the central area of the cavity between -0.5 < y < 0.7 is characterized practically only by the component  $v^*$  that moves the flow between the two walls: the velocity in z-direction instead develops mainly close to the walls.

Analyzing what happens at the center of the examined yz plane, we observe that a blue zone is generated where the velocities have negative values, and this indicates that the flow generated is in the direction of the cold wall at y = -1. The values found in this point are comparable, in module, to the velocity observed in the two adjacent red zones, where the flow has opposite direction and, therefore, it is pushed towards the warm wall (y = 1). This trend can partially be justified by observing the momentum equation that calculates the  $v^*$ . The terms due to buoyancy are no longer at stake, but the magnetic force must be taken into account  $F_y = -C_M(1+\varphi^*)T^*\partial H^*/\partial y$ whose contribution is dominant in the equation.

Combining the signs of the  $T^*$  and of  $\partial H/\partial y$  we obtain the verse where the  $F_y$  acts, and such verse is exactly the same that is found in the velocity  $v^*$ .

The flow that moves from the central zone to the wall (y = -1) must necessarily skirt it, and, in fact, the only component of velocity needed is in the z-direction, while the  $v^*$  has values very close to zero. The descending flow will, therefore, go to the right (red zone) and to the left (blue zone) with practically identical speeds in form and opposite in sign. To decide why the red zone at  $w^*$ positive is in localized in z = 4, rather than in z = 2, we had to calculate the magnetic force term  $F_z = -C_M(1 + \varphi^*)T^*\partial H^*/\partial z$ . In both areas the  $T^*$  is less than zero, so the  $F_z$  changes sign due to the fact that  $\partial H^*/\partial z$  has the opposite sign. After skirting the wall, the flow meets the area where the internal edges of the magnets are located: the values of  $\partial H/\partial y$  are greater than in the center of the domain and, combined with a negative  $T^*$ , generate a positive  $F_y$  which pushes the flow towards the warm wall (y = 1). Once it reaches the upper wall, as happened previously, the incoming flow will be diverted according to the configuration assumed by the magnetic field and will develop the flow with  $v^*$  negative at the center of the channel and at the ends of the domain. Overall, within the cavity, are established 4 different vortices that occupy the entire available width. The two innermost are located for  $1.5 \leq z \leq 3.1$  and for  $3.1 \leq z \leq 5$ , while the two outer vortices are positioned for  $0 \leq z \leq 1.5$  and for  $5 \leq z \leq 6.2$ . We proceed now with the analysis of the  $\Phi$  magnetic flux calculated on different planes. A first analysis involves the calculation of the flux  $\Phi_{xy}$  on different planes perpendicular to the z -axis, while in a second analysis the calculated flux is  $\Phi_{xz}$  for planes perpendicular to the y -axis. Following what is written in chapter 1:

$$\Phi_{xy} = \int_{A} (1+\varphi) * w * H_z \quad dxdy \tag{5.1}$$

$$\Phi_{xz} = \int_{A} (1+\varphi) * v * H_y \quad dxdz \tag{5.2}$$

Where A is the surface of the plane. All values are considered in the form.



### |Øxy|basic configuration

Figure 5.7: Magnetic field flow trend  $|\Phi_{xy}|$  calculated on different planes with time variation

Once past the transient, or after about 10 seconds of simulation, we realize how the planes placed in z = 0.8 z = 1.6 z = 4.8 and z = 5.6 are the ones characterized by values of the average magnetic field flux that are clearly higher than the other planes located more centrally in the calculation domain. Referring to the figure 5.6 we note that the planes placed in correspondence of the major velocity values  $w^*$ , are those which show a minor average flow; this happens because regardless of the values visible from the plots, the strong symmetry means that there is as much outgoing as it is incoming, which brings the average on the plane to be much smaller than in other parts. The planes that see a greater flow are those placed in very asymmetrical areas in relation to the y-axis, where the velocity  $w^*$  in one direction is not balanced by an equal speed in the opposite direction, which is clearly visible for z = 0.8 z = 5.6.

Also contributing to the flow calculation is the component in z-direction of the magnetic field, or  $H_z$ . From the figure 5.3 it is also possible to observe this aspect: the planes that show a greater

average flow pass through areas where the magnetic field has higher values than the remaining floors taken in the central area of the domain.

We proceed now with the analysis of the magnetic field flow perpendicular to the different xz planes considered.



|Øxz| basic configuration

Figure 5.8: Magnetic field flow trend  $|\Phi_{xz}|$  calculated on different planes with time variation

With the planes placed perpendicular to the y-axis, we can observe two positions that show an higher average magnetic field flow than all those considered: this happens for y = 0.4 and y = 0.7. The principle is the same as what is written for the xy plans. A greater flow is observed where it is positioned at the turn of an imbalance between the directions of the velocities  $v^*$  perpendicular to the planes.

From fig. 5.5 we notice in fact how the plane placed at y = 0.7 manages to incorporate the upper part of the red zone at a speed of  $v^*$  positive, without being traversed by velocities  $v^*$  that are too negative (the zones blue are not touched by the plane). Although the plane is surely crossed by negative speeds, these have values too low to be able to balance positive speeds. Also it is important to keep in mind the configuration of the magnetic field component  $H_y$ .

Any plan considered for y < -0.7 is characterized by very small rates  $v^*$  and, consequently, sees a similarly small magnetic field flow, although the component  $H_y$  has considerable value in that area.

The behavior of the plane at y = 0.4 is interesting. This plan crosses all the areas of the domain characterized by high positive and negative velocities  $v^*$  and we would expect that such velocities, counterbalancing each other, would cancel the medium magnetic field flow: this does not happen because the velocity directions, combining with  $H_y$ , generate a flow  $|\Phi_{xz}|$  which turns out to be positive for most of the considered plane; that's why z=0.4 turns out to be an area to be taken into account. In this analysis, a plan with y = 0 was not inserted because  $H_y$  is zero.

# 5.2 Configuration 1



Figure 5.9: 3D visualization of the calculation domain and reference axes in the first configuration. The red wall is the one at  $T_0 + \Delta T/2$  while the blue wall is at  $T_0 - \Delta T/2$ . The magnets are represented by the gray blocks whose magnetic field, perpendicular to the walls, penetrates into the calculation domain.



Figure 5.10: Domain scheme seen from above (section in the horizontal plane (y, z) showing the position of the magnets.) Parameters:  $L_z = 2$  (domain  $2\pi$  long in direction z,  $f_z = 0.4$  (40% of the domain covered by the magnets),  $y_m = 0.4$  (distance of the magnetic plates from the walls.) The grid has 257 unevenly spaced points in the y-direction and 128 evenly spaced points in the z-direction.

Placing the magnets with the geometry highlighted in figure 5.9 and figure 5.10, generates a

magnetic field inside the channel shown in figure 5.11.



Figure 5.11: Visualization of the main figures of the magnetic field, with reference to the configuration of the first case.

As already observed for the previous case, |H| is at its maximum on the part of the wall where the edges of the magnets interface, while this value is slightly lower in those areas that interface with the magnets' body. The regions where H = 0 are on the central axis of the domain (y = 0), where a magnet ends and the next one begins. The area placed in front of the magnets, on the other hand, does not show any points with null values, but H is maintained with a decreasing trend as one moves away from them. Observing the variation of the H along the z-axis, in correspondence of the walls and starting from z = 0, there is an increasing trend  $(\partial H/\partial z > 0)$ up to the maximum of H where it is recorded the minimum of  $\partial H/\partial z$ . After that, we observe a decrease of the magnetic field value correspondent to a negative z-direction gradient (blue). Once in the middle of the domain, we have an area where H remains constant and in fact  $\partial H/\partial z$  is approximately equal to zero. The situation is mirrored considering the second part of the domain  $(\pi < z < 2\pi)$ . No longer concentrated on the walls, but in the central area of the cavity, starting from the left, H first decreases until it reaches zero, and then grows again to settle at a constant value up to half of the domain: for  $\pi < z < 2\pi$  the behavior is symmetrical to what just described. The graph of  $\partial H/\partial z$  precisely mirrors this trend: the first blue zone starting from the left is the first zone with decreasing magnetic field, the null value point is indicated at the point where the blue and red zone meet a (y = 0), after that the growth of H in the z-direction is highlighted by the red zone followed by a central part with null values (H=cost).

Focusing, instead, on the variation of H in the y-direction, starting from y = 0, we observe a general growth of his the value as we approach the walls: this reflects what is visible in the graph of  $\partial H/\partial y$  with higher values of gradients at the edges of the magnets.

By looking at the individual components it is possible to deduce how the field lines behave: for example, the alternation in the direction of  $H_z$  that is found in the lower magnet (y = -1) is caused by the necessity of the field lines to close on themselves and this can happen only if they are outside the magnet. Talking about the component  $H_y$ , the area that corresponds to the central magnet positioned in y = -1, shows values that are greater than zero; this is because the vertical component of the field lines, coming out of the magnet, and finding no obstacle in front of them, develop along the entire width of the channel up to the opposite wall. Near the edges of the upper magnets, the vertical field lines of the latter are added to those coming from below, leading to higher values than the ones in the central zone of the channel. The same as what has been explained so far occurs for the vertical field lines coming out of the upper magnets. We now proceed with the display of the results representing the configuration obtained after the system transient phase, that is after approximately 10 seconds of simulation.



Figure 5.12: Visualization of  $T^*, \varphi$  and  $u^*$  after 10 seconds. The plane considered is the yz plane positioned halfway up the domain perpendicular to the magnets arranged in the first configuration.

The figure 5.12 shows how the  $T^*$ ,  $\varphi^*$  and  $u^*$  behave once that the system transient phase is over. Looking at the convection and diffusion transport of the  $T^*$ , we can observe two main zones where there is an increase of the  $T^*$  respect to the initial condition, and these zones propagate within the corresponding calculation domain of the inner edges of the magnets placed on the hot wall (y = 1). Instead, there is a decrease of  $T^*$  from the starting configuration near to the body of the single magnet placed on the cold wall and at the sides of the domain. The third image of figure 5.12 shows indeed how the velocity component  $u^*$  behave. The velocity in question is the one which develops along the vertical x- axis of the system, therefore it is subject only to buoyancy forces: the magnetic force does not act in this direction. Also in this case it is clearly, as in the previous one, the correlation that exists between the trend of  $T^*$  and of  $u^*$ . In the presence of higher  $T^*$ , the flow density tends to decrease and therefore is transported upwards with speed  $u^*$  positive (red zones). Conversely, a lower  $T^*$  implies a higher mixture density which causes the moving of the flow in the direction of negative x (blue zones). Combining these two trends, the convective motion that sets up parallel to the magnets is evident: in front of the central magnet, positioned on the cold wall, an entire flow descent area will be observed, as will be seen in front of the upper magnets. The areas where the flow passed by the cavity in the x-positive direction are instead positioned where the edges of the magnets interface. Bearing in mind the qdm equation calculated for  $u^*$ , even the  $\varphi^*$  would contribute to generating vertical convective motions: where the particle concentration is higher, the flow tends to be heavier and, therefore, to sink more easily than in other parts of the domain. In all cases in analysis, including this one, the concentration of particles is still too small to let that the  $T^*$  can influence alone the motion in the x-direction.



Figure 5.13: Visualization of  $v^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the first configuration.

The figures 5.13 and 5.14 show the velocity components  $v^*$  and  $w^*$  acting on a plane perpendicular to the walls. Combining the  $v^*$  and  $w^*$  components, we can see a series of convective motion along the entire width of the cavity. Starting to analyze the only component of  $v^*$  of the velocity, we immediately notice how the motions along the direction y occupy almost all the thickness of the cavity extending for  $-0.6 \le y \le 0.7$ . In front of the central magnet, at around  $z \approx 3$ , the flow is pushed towards the warm wall with a positive speed  $v^*$ , to then be transported again towards the cold wall at the two blue areas at  $v^*$  negative located in  $z \approx 1.5$  and  $z \approx 4.8$ . The reason why the velocity between the walls has this trend has to be found in the momentum equation that calculates the  $v^*$ . The terms, due to floating, are no longer at stake, but the magnetic force must be taken into account  $F_y = -C_M(1 + \varphi^*)T^*\partial H^*/\partial y$  whose contribution is dominant in the equation. Where a positive  $F_y$  works, We will have a positive  $v^*$  rate and vice versa: by combining the  $T^*$  and  $\partial H/\partial y$  signs, the sign characterizing the magnetic force will indicate the direction in which the fluid motion is expected. Once the flow reaches the walls, the  $v^*$  is reduced and we mainly observe the action of the component  $w^*$  which will make the flow deviate respectively



Figure 5.14: Visualization of  $w^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the first configuration.

towards the positive z (red zone) and towards the negative z (blue zone). The reason why the flow moves towards in a positive z-direction rather than in a negative one, is also justified in this case by the magnetic force  $F_z$  calculated as  $F_z = -C_M(1 + \varphi^*)T^*\partial H^*/\partial z$  and acting in this direction. If you look at any point in the domain, taking the sign of  $T^*$  and  $\partial H^*/\partial z$  we will immediately notice that a positive  $F_z$  will match a red zone to  $w^*$  major of zero and vice versa. Combining the speeds just described, 4 different convective vortices that occupy the calculation domain can be found. The two most external vortices are localized for  $0 \le z \le 1.6$  and for  $4.8 \le z \le 2\pi$  and considering the values of the speeds in play, they are surely the two strongest motions detectable in the plan. The other two vortices, slightly weaker in intensity, are positioned more centrally and are placed for  $1.6 \le z \le \pi$  and for  $\pi \le z \le 4.8$ .

We proceed now with the analysis of the  $\Phi$  magnetic flux calculated on different planes. A first analysis involves the calculation of the flux  $\Phi_{xy}$  on different planes perpendicular to the z -axis, while in a second analysis the calculated flux is  $\Phi_{xz}$  for planes perpendicular to the y -axis. Following what is written in chapter 1:

$$\Phi_{xy} = \int_{A} (1+\varphi) * w * H_z \quad dxdy$$
(5.3)

$$\Phi_{xz} = \int_{A} (1+\varphi) * v * H_y \quad dxdz \tag{5.4}$$

Where A is the surface of the plane. All values are considered in the form.



|Øxy|configuration1

Figure 5.15: Magnetic field flow trend  $|\Phi_{xy}|$  calculated on different planes with time.

Analyzing different planes perpendicular to the z- axis, only those located in z = 0.8 and z = 5.6 show values of the average magnetic field flux that are clearly higher than the others.

Referring to the figure 5.14 we notice how the planes crossed by a greater medium magnetic field flow are placed at points where the perpendicular velocity component, incoming or outgoing, is not counterbalanced by an equally strong speed, but of opposite sign. Furthermore, we must also consider the component in the z- direction of the magnetic field H: positioning a plane where  $H_z$ is large can offset a not very high  $w^*$  and vice versa. The best of the selected plans combine both solutions as they cross both  $w^*$  and  $H_z$  relevant zones. On the other hand, the plane at z = 3.2not only traverses a zone where velocity  $w^*$  is almost nothing, but where the component  $H_z$  is also zero.

In general, having in mind how the magnetic field is combined, the planes where the speed is mostly incoming or outgoing are those to consider optimal regardless of the value assumed by the latter.



We proceed now with the analysis of the magnetic field flow perpendicular to the different xz planes considered.

Figure 5.16: Magnetic field flow trend  $|\Phi_{xz}|$  calculated on different planes with time.

Once the transient has elapsed, we observe how the plans to show a medium magnetic field flux are greater than those placed at y = 0, y = 0.4 and y = 0.7. The basic principle is the same as written for the xy plans. A greater flow is observed where it is positioned at the turn of an imbalance between the directions of the velocities  $v^*$  perpendicular to the planes.

From figure 5.13 we note, in fact, how the plane placed at y = 0.7 succeeds in capturing the two outer zones at positive speed  $v^*$ , but passes over the blue zones at negative speeds without considering them. The  $v^*$  that passes through this plane is therefore all positive. The factor that prevents us from having an even higher flow is unfortunately the component  $H_y$  of the magnetic field that presents a different sign moving on the plane under examination. As for y = 0 and y = 0.4, although the speeds are both incoming and outgoing along the whole domain, such a high flow can only be explained by observing the values of these perpendicular speeds: the  $v^*$  negative are so much higher than the positive ones and this can cause that the average flow in modulus is high.

# 5.3 Configuration 2- whole magnet

Figure 5.17: 3D visualization of the calculation domain and reference axes in the second configuration (whole magnet). The red wall is the one at  $T_0 + \Delta T/2$  while the blue wall is at  $T_0 - \Delta T/2$ . The magnets are represented by the gray blocks whose magnetic field, perpendicular to the walls, penetrates into the calculation domain .



Figure 5.18: Domain scheme seen from above (section in the horizontal plane (y, z) showing the position of the magnets.) Parameters:  $L_z = 2$  (domain  $2\pi$  long in the direction z),  $f_z = 0.4$  (40% of the domain covered by the magnets for y = -1),  $f_z = 0.8$  (80% of the domain covered by the magnets for y = 1),  $y_m = 0.4$  (distance of the plates magnetic from the walls). The grid has 257 unevenly spaced points in the y-direction and 128 evenly spaced points in the z-direction.



Figure 5.19: Visualization of the main figures of the magnetic field, with reference to the configuration of the second case with whole magnet.

An arrangement such as this one means that the space between the magnets facing the upper wall is very small, and therefore the field leaving the edges necessarily suffers the presence of the field lines generated by the adjacent magnet. This means that the peak of H is located slightly off-center to the empty space left. For the lower magnet, however, the peaks are located exactly on the edges, with a progressive decline of intensity as it converges towards the center of the latter. There are 3 different zones where H = 0 and in general all these points are located beyond the centerline of the domain: this is probably due to the fact that the upper magnets, being so close, generate field lines that contrast with each other and therefore their strength decreases, to the advantage of the lower magnet whose magnetic field is free to develop without interference. Let's comment the trend of H along the z -axis: starting from the left, while at the center we observe a progressive decrease up to the first point with zero value, on the walls there is a progressive increase in H which will then lead to the peaks described above. In the central part, after having reached the first point with zero value, there is a growth again, followed by another decrease of H which will lead to the second point with zero value. This decrease in H also involves the walls of the domain as we move from the peaks to areas with lower values.

The description is symmetrical starting from  $z = \pi$  until the end of the domain and is displayed in the graph of  $\partial H/\partial z$ . The first decrease, which leads to the first minimum point of H is found in the first blue zone on the left; after which the consecutive increase and decrease of H are highlighted by the red zone (positive gradient) and the blue zone (negative gradient). In general, few points are found where H remains constant, in fact zero gradient areas are only at the ends of the domain mainly.

The graph of  $\partial H/\partial y$  shows how H varies by moving along the y-axis: starting from the areas where the null values are located, the magnetic field increases by moving towards the walls, with intensity peaks located in the edges. In this case, most of the cavity is affected by gradients directed towards the lower wall (blue).

Let's now look at the graph of  $H_z$ : on the upper wall we can count 4 different changes of direction of the horizontal component and each peak corresponds to a corner of a magnet. The first one encountered from the left highlights the end of the first magnet, whose outgoing field lines, having to close in the adjacent empty space, are directed towards the positive z (red). The second peak indicates the beginning of the upper central magnet, whose outgoing field lines, are oriented in the negative direction of the z (blue) given their need to close again through the only available gap. Proceeding to the right, the horizontal component decays, since mainly central lines with vertical components start from the central part of the magnet. The above is reflected exactly for the other part of the domain. Inside the cavity a horizontal component of H is observed practically very close to zero where there are no magnets (lower left), whereas, the blue zone located at *zat2* is due to the two central magnets, whose field lines coming out of those edges have a concordant sign and therefore create this area with values slightly above zero. The central part has zero  $H_z$  because the field lines are mostly vertical. The same reasoning applies to the next part of the domain.

The vertical component of the magnetic field is easier to read: as it exits from the external magnets, the component is directed downwards and without encountering obstacles it occupies the entire cavity (blue); in the corners the sign inversion is localized where from negative becomes positive going to increase the value of  $H_y$  located in the gaps between the magnets. As for the central magnets we can say that from the lower one, the field lines are outgoing and directed upwards (red) until they meet the outgoing lines from the opposite magnet (blue), cancelling each other.



We now proceed with the display of the results representing the configuration obtained after the transient phase of the system, ie after about 10 seconds of simulation.

Figure 5.20: Visualization of  $T^*, \varphi$  and  $u^*$  after 10 seconds. The plane considered is the yz plane positioned halfway up the domain perpendicular to the magnets arranged in the second configuration whit the whole magnet.

The figure 5.20 shows the behavior of  $T^*$ ,  $\varphi^*$  and  $u^*$  after about 10 seconds from the starting of the simulation. In particular, the first image shows how the  $T^*$  is transported by convection and diffusion within the calculation domain. Higher temperature zones are developed starting from the innermost edges of the upper magnets and from the whole central magnet which extends to the center of the cavity. In opposition to this movement, in front of the edges of the single magnet placed in y = -1 and at the edges of the domain, areas will be generated where the  $T^*$  is lower

than the initial condition. Let us now analyze the component  $u^*$  of the velocity which develops along the axis x parallel to the walls and is visible in the third image of figure 5.20. In the momentum equation that calculates this component, buoyancy terms are the dominant ones, and these terms involve both the  $T^*$  and the concentration  $\varphi^*$ . The term that involves concentration does not play a fundamental role, since the particles dispersed in these first simulations are very few and tend to concentrate on the cold wall: in this area I therefore expect a heavier and descending fluid with a negative velocity  $u^*$ . As was for the other two cases previously described, there is a clear similarity between the temperature and  $u^*$  configurations since, where the temperature is higher, the density of the mixture is lower and therefore the flow will tend to be pushed upward inside the cavity. Most of the y-positive domain is therefore affected by a movement in the direction of positive x that is established in three specific areas: frontally to the smaller magnet and in correspondence with the internal edges of the magnets. By contrast, most of the y < 0 reactor area will see the flow move in the negative x-direction since the lower  $T^*$  makes the flow density higher and the higher particle concentration contributes to establish a downward flow of the flow. Combining the two effects we can say that the flow will be characterized by a rising motion in an area in front of the central magnet and the inner edges of the side magnets. The flow will complete its convection motion by descending into the two areas located between the upper magnets and above all at the ends of the domain.



Figure 5.21: Visualization of  $v^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the second configuration with whole magnet.

Figures 5.21 and 5.22 show the velocity components  $v^*$  and  $w^*$  that develop on a plane perpendicular to the walls of the cavity. The convective motions that develop on the plane seem to be attracted to the wall that has more magnets (y = 1), thus bringing the lower half of the cavity practically without any significant motion. To understand the flow movements that are established in the cavity, we first observe the component  $v^*$  of speed, responsible for the movement of the flow between one wall and the other. Where the central magnets are located, that is, in  $z \approx 3$ , the  $v^*$  negative (blue zone), move in flow towards the cold wall as it happens in other two areas that are identified for  $z \approx 1$  and for  $z \approx 5.2$  and these areas coincide with the inner edges of the larger magnets placed on the warm wall. The two areas with positive velocities  $v^*$ , where the flow is transported to the warm wall, are observed for  $z \approx 2$  and for  $z \approx 4$  and are areas adjacent to the magnets placed centrally. This trend is explained by observing the momentum equation that calculates the component under examination: the contribution that determines a positive rather than a negative speed is the magnetic volume force acting in the y- direction, i.e.



Figure 5.22: Visualization of  $w^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the second configuration with the whole magnet.

 $F_y = -C_M(1 + \varphi^*)T^*\partial H^*/\partial y$ . Looking at any point in the plane, and combining the signs of the  $T^*$  and of  $\partial H/\partial y$  at that point, we get the sign of the magnetic force, which directly affects the  $v^*$ : where there is a positive  $F_y$ , the flow will be pushed towards the hot wall and vice versa. Looking at the component  $w^*$  of the velocity we can have a clearer idea of the overall motion that takes place on the plane: the most intense translational motions in the z- direction are established mainly close to the warm wall. Throughout the remainder of the domain, velocities in the z- direction are much smaller but equally fundamental in generating the different convection motions that appear. The sign of these speeds is also in this case attributable to the magnetic force acting in the z- direction, ie  $F_z = -C_M(1 + \varphi^*)T^*\partial H^*/\partial z$ . For example, looking at fig 5.22, and considering the red zone in  $z \approx 5$  we notice that the  $T^*$  at that point is positive, but the value of  $\partial H/\partial z$  is negative. This combination leads to a positive  $F_z$  which pushes the flow to the right, and in fact the speed  $w^*$  at that point is directed to the right. This example can be traced back to the entire range of motion found on the plane.

At this point the motions that develop perpendicularly to the magnets are clearer. Starting from the center of the domain the first two vortices that are observed go from  $2 \le z \le \pi$  and from  $\pi \le z \le 4.3$ , while adjacent to these first two, they develop as many for  $1.2 \le z \le 2$  and  $4.3 \le z \le 5.5$ . All 4 vortices are mainly confined to the half of a cavity that interfaces with the warm wall.

We proceed now with the analysis of the  $\Phi$  magnetic flux calculated on different planes. A first analysis involves the calculation of the flux  $\Phi_{xy}$  on different planes perpendicular to the z- axis, while in a second analysis the calculated flux is  $\Phi_{xz}$  for planes perpendicular to the y -axis. Following what is written in chapter 1:

$$\Phi_{xy} = \int_{A} (1+\varphi) * w * H_z \quad dxdy \tag{5.5}$$

$$\Phi_{xz} = \int_{A} (1+\varphi) * v * H_y \quad dxdz \tag{5.6}$$

Where A is the surface of the plane. All values are considered in the form.



Figure 5.23: Magnetic field flow trend  $|\Phi_{xy}|$  calculated on different planes with time.

Let us now analyze how much the magnetic field flux is valid on different xy planes taken at different positions along the z- axis. As they have been calculated, we must pay attention to the velocity component perpendicular to the plane itself, ie the  $w^*$  but we must also consider the zdirection component of the magnetic field: the right compromise between these two quantities defines the optimal plane through which we observe the greatest flow  $\Phi_{xy}$ . For example, among the plans examined, those placed at z = 1.6, z = 2.4, z = 4 z = 4.8 are certainly a good choice. Looking at the figure 5.22 it is possible to observe how the velocities  $w^*$  that cross them are practically the most important ones inside the domain, and to this we add that the magnetic field in the z- direction assumes values close to the maximum ones found. Furthermore, as noted above, not only are the planes crossing zones at  $w^*$  high, but the incoming or outgoing speed is not counterbalanced at any other point crossed by these planes.

All the other planes are located in areas of the domain where, due to the low perpendicular speed

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value, they are not very suitable for obtaining an important magnetic field flow.

Figure 5.24: Magnetic field flow trend  $|\Phi_{xz}|$  calculated on different planes with time.

Exactly as done before, let's now analyze how much the magnetic field flux is valid on different planes xz taken in different positions along the y- axis. The optimal plan for observing a flow  $Phi_{xz}$  considerable is the one that combines, in the best possible way, both the values of the magnetic field and of the velocity component, perpendicular to it, ie  $H_y$  and  $v^*$ . Consequently, placing oneself in a plane where I have strong perpendicular velocities can be unproductive if  $H_{\mu}$  is very low and vice versa. Moreover, as already stated above, it is necessary that the speed perpendicular to the plane, however strong it may be, must not be counterbalanced by a velocity of similar intensity but of opposite sign. For an xz plan this is the main difficulty, to be able to consider only an incoming or outgoing part of the speeds without incorporating the entire convective motion. With the exception of only one clearly worse plan, y = -0.9, all the others, register a flow of magnetic field in the same order of magnitude; among these, the plans at y = 0.7and at y = 0.4 are slightly better. Looking at figure 5.21, the aforementioned foreground laps exclusively the upper zone of the  $v^*$  positive flow, and sees speeds entering perpendicular to it whose value is not completely counterbalanced by as many speeds. As for the plane at y = 0.4 it is true that it crosses an area where positive and negative speeds are counterbalanced, but this does not happen for the central zone at  $v^* < 0$ , this can explain the value of the maximum of the magnetic field flow detected.

# 5.4 Configuration 2- half magnet



Figure 5.25: 3D visualization of the calculation domain and reference axes in the second configuration (half magnet). The red wall is the one at  $T_0 + \Delta T/2$  while the blue wall is at  $T_0 - \Delta T/2$ . The magnets are represented by the gray blocks whose magnetic field, perpendicular to the walls, penetrates into the calculation domain.



Figure 5.26: Domain scheme (section in the horizontal plane (y, z) showing the position of the magnets.) Parameters:  $L_z = 2$  (domain  $2\pi$  long in the direction z),  $f_z = 0.4$  (40% of the domain covered by the magnets for y = -1),  $f_z = 0.6$  (60% of the domain covered by the magnets for y = 1),  $y_m = 0.4$  (distance of the plates magnetic from the walls). The grid has 257 unevenly spaced points in the y-direction and 128 evenly spaced points in the z-direction.



Figure 5.27: Visualization of the main figures of the magnetic field, with reference to the configuration of the case 2 with a half magnet.

Placing the magnets with the geometry highlighted in fig. 5.25 and fig. 5.26, the magnetic field that is created inside the channel is shown in fig. 5.27.

We now analyze a variation of previous configuration (figure 5.26), where the central magnet, placed on the upper wall, is half that the one used previously; the resulting magnetic field and its components are shown in fig.5.27.

We immediately observe how the free space between a magnet and the other is doubled compared to the last configuration, and this allows us to observe more clearly the H's peaks which do not contrast as previously. This means that the upper wall has a larger area with values of H that tend to be higher if compared with the previous case. The stop points are always 3, but this time the central one is slightly lowered towards the centerline of the channel.

Let's observe the H's trend along the z-axis: starting from the left, while at the center we observe a progressive decrease up to the first point with zero value, on the walls there is a progressive increase of of H which will then lead to the peaks described before. In the central part, after having reached the first point with zero value, it's visible a growth again, but this will be followed by an another decrease of H which will lead to the second point with zero value. This decrease in H will also involve the walls of the domain as we move from the peaks to areas with lower values. The description is symmetrical starting from  $z = \pi$  until the end of the domain and is well displayed in the graph of  $\partial H/\partial z$ . The first decrease, which leads to the first minimum point of H, is found in the first blue zone on the left; after which the consecutive increase and decrease of H are highlighted by the red zone (positive gradient) and the blue zone (negative gradient).

The graph of  $\partial H/\partial y$  shows how the H varies by moving along the y-axis: starting from the areas where the null values are located, the magnetic field is increasing by moving towards the walls, with localized intensity peaks in the corners. In this case, most of the cavity is affected by gradients directed towards the lower wall (blue). The upper left and right zones instead of having  $\partial H/\partial y \approx 0$  because of the field lines coming out of the side magnets will have an intensity that varies a little compared to what happens in the rest of the domain.

Let's now look at the graph of  $H_z$ : on the upper wall we can distinguish 4 different changes of direction of the horizontal component and each peak corresponds to a corner of a magnet. The first one encountered from the left highlights the end of the first magnet, whose outgoing field lines, having to close in the adjacent empty space, are directed towards the positive z (red). The second peak indicates the beginning of the upper central magnet, whose outgoing field lines, this time will be oriented in the negative direction of the z (blue) given their need to close again through the only gap available. Moving to the right, the horizontal component is decayed, since mainly central lines with vertical components start from the central part of the magnet. The above is reflected exactly in the other part of the domain. Inside the cavity a horizontal component of H is observed practically very close to zero where there are no magnets (lower left), whereas, the blue zone located at  $z \approx 2$  is due to the two central magnets, whose field lines coming out of those edges have a concordant sign and therefore create this area with values slightly above zero. The central part has  $H_z$  null because the field lines are mostly vertical. The same reasoning applies to the next part of the domain. The vertical component of the magnetic field is easier to read: as it exits from the external magnets, the component is directed downwards and without encountering obstacles it occupies the entire cavity (blue); in the corners the sign inversion is localized which from negative passes to positive going to increase the value of  $H_{y}$  located in the gaps between the magnets. As for the central magnets we can say that from the lower one the field lines are outgoing and directed upwards (red) until they meet the outgoing lines from the opposite magnet (blue) going to cancel each other.



We now proceed with the display of the results representing the configuration obtained after the system's transient phase, that is after about 10 seconds of simulation.

Figure 5.28: Visualization of  $T^*, \varphi$  and  $u^*$  after 10 seconds. The plane considered is the yz plane positioned halfway up the domain perpendicular to the magnets arranged in the second configuration with half magnet.

The figure 5.28 shows the behavior of  $T^*$ ,  $\varphi^*$  and  $u^*$  after about 10 seconds from the start of the simulation. In particular, the first image shows how the  $T^*$  is transported by convection and diffusion within the calculation domain. From the innermost edges of the upper magnets and from the whole central magnet there are areas of higher temperature that reach over half of the cavity. By virtue of this movement, in front of the single magnet's edge and at the ends of the domain, there will be generated areas where  $T^*$  is lower than the initial condition.

Let's now analyze the component  $u^*$  of the velocity which develops along the axis x parallel to the walls and is visible in the third image of figure ??. In the momentum equation that calculates this component, in fact, the buoyancy terms are the absolutely dominant ones, and these terms involve both  $T^*$  and concentration  $\varphi^*$ . The term that involves  $\varphi^*$ , however, will influence in a less decisive way, since the particles dispersed in these first simulations are very few and tend to concentrate on the cold wall: in this area we expect an heavier and therefore descending fluid with negative velocity  $u^*$ . There is a clear similarity between the configurations of temperature and of  $u^*$  since, where the temperature is higher, the density of the mixture is lower and, therefore, the flow will tend to be pushed towards the high inside the cavity. Most of the domain at y > 0is, therefore, affected by a motion in direction of positive x that is established in three very specific areas: in front of the smallest magnet and in correspondence with the internal edges of the placed magnets. By contrast, most of the y < 0 reactor area will see the flow moving in the negative x-quirection since the lower  $T^*$  makes the flow density higher and the higher particle concentration contributes to establish a downward flow of the flow. Combining the two effects we can say that the flow will be characterized by a rising motion in an area in front of the central magnet and the inner edges of the side magnets. The flow will complete its convection movement by descending into the two areas located between the upper magnets and above all at the ends of the domain.



Figure 5.29: Visualization of  $v^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the second configuration with half magnet.


Figure 5.30: Visualization of  $v^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the second configuration with half magnet.

The figures 5.29 and 5.30 show the velocity's components  $v^*$  and  $w^*$  that develop on a plane perpendicular to the walls of the reactor. The first thing that we notice is that, as happened in the previous case, the wall that has the most magnets (y = 1) seems to attract towards itself the convective motions developed on the plane, leaving the lower half of the domain practically without any significant motion. To understand well the motions that are established in the cavity, we start by observing the velocity's component  $v^*$ , responsible for the flow's movement between one wall and the another. Where the smaller magnet has its center, that is, in  $(z \approx 3)$ , the  $v^*$ negative (blue zone) move in flow towards the cold wall as it happens in two other areas that are identified for  $z \approx 1.4$  and for  $z \approx 5$  and these zones coincide with the inner edges of the larger magnets placed in y = 1. The two zones with positive velocities, where the flow is transported towards the warm wall, are observed for  $z \approx 2.3$  and for  $z \approx 4$  and they are adjacent to the small magnet placed centrally. On the domain's side, there are also two other areas characterized by  $v^*$  positive but having lower values than the other described motions. This configuration is explained by looking at the qdm equation that calculates the component under examination: the contribution that determines a positive velocity rather than a negative one is the magnetic volume force acting in the y-direction, ie  $F_y = -C_M(1+\varphi^*)T^*\partial H^*/\partial y$ . Looking at any point in the plane and combining the signs of the  $T^*$  and of  $\partial H/\partial y$  at that point, we get the sign of the magnetic force, which directly affects the  $v^*$ : where there is a positive  $F_y$ , the flow will be pushed towards the warm wall and vice versa.

To get a complete overview of what is happening it is also necessary to observe the velocity's component  $w^*$ : the most intense translational motions in the z-direction are established mainly close to the warm wall, while weaker motions, always in the z-direction are found in the lower half of the cavity. The sign of these velocities is also attributable to the magnetic force acting in the z- direction, ie  $F_z = -C_M(1 + \varphi^*)T^*\partial H^*/\partial z$ . For example, looking at figure 5.30, and considering the blue zone in  $z \approx 1.8$  we see that the  $T^*$  at that point is positive as well as the value of  $\partial H/\partial z$ . This combination leads to a negative  $F_z$  that pushes the flow to the left and, in fact, the speed  $w^*$  at that point, is direct poured left. This example can be traced back to the entire range of motion found on the plane.

At this point the motions that develop perpendicularly to the magnets are clearer. Starting from the center of the domain the first two vortices that are observed go from  $2.3 \le z \le \pi$  and from  $\pi \le z \le 4.1$  and develop for  $0.8 \le y \le 0$ . Laterally to these first two, the same number is developed for  $1.2 \le z \le 2.3$  and for  $4.1 \le z \le 5$ , but they occupy a space in direction y slightly larger. The last two vortices are visible at the sides of the domain for  $z \approx 0$  and  $z \approx 6.2$ . These last two, although weaker, occupy a portion of a higher cavity than the others described before, in fact they are both located for -0.5 < y < -0.7.

We proceed now with the analysis of the  $\Phi$  magnetic field flow calculated on different planes. A first analysis involves the calculation of the flow  $\Phi_{xy}$  on different planes perpendicular to the z-axis, while in a second analysis the calculated flow is  $\Phi_{xz}$  for planes perpendicular to the y-axis. Following what is written in chapter 1:

$$\Phi_{xy} = \int_{A} (1+\varphi) * w * H_z \tag{5.7}$$

$$\Phi_{xz} = \int_{A} (1+\varphi) * v * H_y \tag{5.8}$$

Where A is the surface of the plane. All values are considered in the form.



Figure 5.31: Magnetic field flow trend  $|\Phi_{xy}|$  calculated on different planes with time.

Let's now analyze how much the magnetic field flux is valid on different xy planes taken at different positions along the z- axis. As they have been calculated, both the velocity component perpendicular to the plane itself, or the  $w^*$ , is fundamental, but also the z- direction component of the magnetic field has to be considered: the right compromise between these two quantities defines the optimal plane through which we observe the greatest flow  $\Phi_{xy}$ . For example, among the plane examined, the one placed at z = 3.2 is certainly not a good choice, not for the speeds that cross it, but because  $H_z$  is practically zero. Another factor to keep in mind is the following: it is not enough just to consider a plane where the perpendicular speeds are maximum, but it is necessary that the incoming or outgoing  $w^*$  are not counterbalanced by an equally strong speed,

but of opposite sign. By virtue of what has been written, once the transition is over, the highest values are found for the planes placed z = 1.6 and z = 4.8.



|Øxz| configuration 2- half magnet

Figure 5.32: Magnetic field flow trend  $|\Phi_{xz}|$  calculated on different planes with time.

Exactly as done before, let's now analyze how much the magnetic field flux is valid on different planes xz taken in different positions along the y-axis. The optimal plan for observing a considerable flow  $\Phi_{xz}$  is the one that combines, in the best possible way, both the values of the magnetic field and of the velocity component, perpendicular to it, ie  $H_y$  and  $v^*$ . Consequently, placing oneself in a plane where I have strong perpendicular speeds can be unproductive if  $H_y$  is very low and vice versa. Moreover, as mentioned above, it is necessary that the speed perpendicular to the plane, however strong it may be, must not be counterbalanced by a velocity of similar intensity of opposite sign. For an xz plan the main difficulty is to being able to consider only an incoming or outgoing part of the speeds without incorporating the entire convective motion. Looking at the graph what said becomes much clearer: a plane placed at y = 0.4 cuts all the convective motions described in fig 5.29, balancing incoming and outgoing velocities from it. The plan placed at y = 0.7, always bearing in mind the figure 5.29, manages to touch only the upper part of the zones to  $v^*$  positive, so the speeds are not counterbalanced: in addition of that, the component  $H_y$  has values very close to the maximum ones found, which leads that position to be the best for the calculation of  $\Phi_{xz}$ .

## 5.5 Configuration 3



Figure 5.33: 3D visualization of the calculation domain and reference axes in the third configuration. The red wall is the one at  $T_0 + \Delta T/2$  while the blue wall is at  $T_0 - \Delta T/2$ . The magnets are represented by the gray blocks whose magnetic field, perpendicular to the walls, penetrates into the calculation domain.



Figure 5.34: Domain scheme seen from above (section in the horizontal plane (y, z) showing the position of the magnets.) Parameters:  $L_z = 2$  (domain  $2\pi$  long in direction z,  $f_z = 0.4$  (40% of the domain covered by the magnets),  $y_m = 0.4$  (distance of the magnetic plates from the walls). The grid has 257 unevenly spaced points in the y-direction and 128 evenly spaced points in the z-direction.



Figure 5.35: Visualization of the main figures of the magnetic field, with reference to the configuration of the third case.

With this configuration, 4 different stopping points are observed: the two central units are localized by y = 0 for z corresponding to the internal edges of the magnets, while stopping points in the ends of the domain are higher than the central ones and they are where there is no presence of magnets either in the upper or lower wall. The form of H is higher in the area immediately in front of the magnets, but in this case, since these are smaller than in the previous ones, the H's peak is not only on the edges but seems to extend over their entire length. It is also noted that the central area in front of the lower magnet has slightly higher H values than the rest of the domain.

Observing  $H_z$ , the edges of the magnets are immediately captured; from their left end the horizontal field lines have a negative component (blue): this is because they need to close but this cannot happen to their right due to the presence of the magnet body. Opposite speech for the field lines coming out of the corners to the right. The components are always maximum at the ends of the magnets. For  $H_y$ , in the area in front of the lower magnet there is a positive component (red) because the field lines coming out of the entire cavity up to the opposite wall. The same behavior applies to the area in front of the upper magnets, where the vertical component of the field lines occupies the entire region in question, up to the lower wall: the direction, however, is negative in this case (blue). The two areas at the top left and top right corresponds, instead, to the part of the domain not covered by magnets: in this case, we observe a positive component of  $H_y$  because in that area the closing of the field lines coming out from the magnets occurs which will necessarily be facing upwards.

Observing the trend of H we can deduce the behavior of  $\partial H/\partial z$ . Starting from the left, although in z = 0 very different values are found depending on the position y, moving towards the center of the cavity, shows an increase in the values of H or we have a first zone at  $\partial H/\partial z > 0$  (red). Continuing to the right, to reach the second point with a null value of H it is necessary that the values of the magnetic field start to decrease, and this is highlighted by the blue zone at  $\partial H/\partial z < 0$ . In the middle of the channel, that is in  $z = \pi$ , we observe a zone with constant and higher H values than before, this means that the gradient of H, in z-direction, is positive again (red zone). The central area at H = cost translates to a  $\partial H/\partial z = 0$  (white zone) at the center of the cavity.

Dwelling on the walls located at  $y \pm 1$ , each alternation of positive (red) and negative (blue) gradients correspond to the edge of a magnet: starting from the outside there is an increase of H up to the first edge to the left (gradient positive ie red) after which decrease along the body of the magnet (negative gradient ie blue) and again an increase (positive gradient) leading to the second peak, located on the right edge. This behavior is repeated for all the magnets in question and, in general, the trend of H and its gradient along z is repeated symmetrically for the part of domain between  $\pi$  and  $2\pi$ .

The last graph shows  $\partial H/\partial y$  and, as in the previous cases, the principle that the vertical component is greater near the magnets is valid: therefore the gradients, starting from y = 0 will intensify as you move towards the upper and lower walls with the peaks located on the edges of magnets.

We now proceed with the display of the results representing the configuration obtained after the transient phase of the system, ie after about 10 seconds of simulation.



Figure 5.36: Visualization of  $T^*, \varphi$  and  $u^*$  after 10 seconds. The plane considered is the yz plane positioned halfway up the domain perpendicular to the magnets arranged in the third configuration.

Figure 5.36 shows the behavior of  $T^*$ ,  $\varphi^*$  and  $u^*$  after about 10 seconds from the start of simulation. The first image represents how the  $T^*$  is transported within the calculation domain by convection and by diffusion. The highest  $T^*$  zones are established at all the edges of the magnets placed on the warm wall and occupy about half of the domain. This development, on the other hand, leads to zones where the  $T^*$  becomes lower than the initial condition, and this

happens at the single magnet positioned on the cold wall. Analyzing, instead, the third image of figure 5.36, we observe how the component behaves in the x-direction of speed. From the momentum equation for  $u^*$ , we deduce that the buoyancy terms are the main responsible of this motion: in these terms are involved both the  $T^*$  and the concentration  $\varphi^*$  each with a different weight in the equation. Between the two, the  $\varphi$  provides the smallest contribution since the concentration of particles is still minimal in our simulations. The second image, however, shows how the particles tend to accumulate on the cold wall: this implies that surely that area will be affected by this presence and will be characterized by an average heavier flow than the rest of the cavity, therefore, this will tend to be pushed downwards into negative x-direction. So, considering the reduced effect of concentration, the speed component  $u^*$  will be mainly influenced by the  $T^*$ , in fact, its behavior reflects what happens to the  $T^*$ . Where higher temperatures are observed, are created areas in which the flow, being warmer and therefore of lower density, will tend to rise in the positive x-direction  $(u^* > 0)$ . Where the temperature is lower, the flow will be denser and therefore, a downward motion will be generated. At this point the convective motions developed along the x-axis and above all it, interact with each other as no one is isolated from the others, but each speed column feeds the counterpart adjacent to it.



Figure 5.37: Visualization of  $v^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the third configuration.

Figures 5.37 and 5.38 show the velocity components  $v^*$  and  $w^*$  on a plane yz perpendicular to the magnets.

Considering the figure 5.37, we immediately observe how in correspondence of the central magnet positioned at y = -1 a very large zone is created at  $v^*$  positive, which carries the flow towards the warm wall. The areas where the flow is transported towards the hot wall are also located at the upper magnets, but they occupy a smaller portion of the domain compared to the central area. Interspersed with these areas of  $v^*$  positive, there are different areas where, instead, the negative speed carries the flow towards the cold wall. This trend is justified observing the momentum equation that calculates the component under examination: the contribution that determines a positive speed rather than a negative one is the magnetic volume force acting in the y- direction, ie  $F_y = -C_M(1 + \varphi^*)T^*\partial H^*/\partial y$ . Looking at any point in the plane and combining the signs of the  $T^*$  and  $\partial H/\partial y$  at that point, we get the sign of the magnetic force, which directly affects the  $v^*$ : where there is a positive  $F_y$ , the flow will be pushed towards the warm wall and vice versa. To get a complete overview of what is happening it is also necessary to observe the velocity's



Figure 5.38: Visualization of  $w^*$  on a yz plane placed a  $x = \pi$ , perpendicular to the walls, after the simulation has completed the transient, or about 10 seconds later. The image refers to the third configuration.

component  $w^*$  shown in the figure 5.38: the most intense translational motions in the z-direction are established mainly close to the warm wall and in correspondence of the edges of the single magnet set at y = -1. Weaker motions but always in the z- direction are found in the lower half of the cavity for  $0 < z \leq 1.5$  and for  $5 \leq z \leq 2\pi$ . The sign of these speeds is, also in this case, attributable to the magnetic force acting in the z-direction, ie  $F_z = -C_M(1 + \varphi^*)T^*\partial H^*/\partial z$ . For example, looking at figure 5.38, and considering the blue zone placed in  $z \approx 4$ , we observe how the  $T^*$  at that point is negative as well as the value of  $\partial H/\partial z$ . This combination leads to a negative  $F_z$  which pushes the flow to the left and, in fact, the speed  $w^*$  at that point is directed to the left. This example can be traced back to the entire range of motion found on the plane. At this point, the motions that develop perpendicularly to the magnets are clearer. Starting from the center of the domain, the first two vortices observed go from  $1.8 \leq z \leq \pi$  and from  $\pi \leq z \leq 4.5$  and develop over the entire width of the cavity. Laterally to these first two, the same number is developed for each side, that is, for  $0 \leq z \leq 1$ , for  $1 \leq z \leq 2$ , and symmetrically to these, but occupy a space in the smaller y-direction, in fact they are mainly in the part at y > 0. We proceed now with the analysis of the  $\Phi$  magnetic field flow calculated on different planes. A first analysis involves the calculation of the flow  $\Phi_{xy}$  on different planes perpendicular to the z-axis, while in a second analysis, the calculated flow is  $\Phi_{xz}$  for planes perpendicular to the y-axis. Following what is written in chapter 1:

$$\Phi_{xy} = \int_{A} (1+\varphi) * w * H_z \tag{5.9}$$

$$\Phi_{xz} = \int_{A} (1+\varphi) * v * H_y \tag{5.10}$$

Where A is the surface of the plane. All values are considered in the form.



|Øxy|configuration 3

Figure 5.39: Magnetic field flow trend  $|\Phi_{xy}|$  calculated on different planes with time.

Let's now analyze how much the magnetic field flux is valid on different xy planes taken at different positions along the z-axis. As they have been calculated, we must pay attention to the velocity component perpendicular to the plane itself, ie the  $w^*$ , but we must also consider the z-direction component of the magnetic field: the right compromise between these two quantities defines the optimal plane where we observe the greatest flow  $\Phi_{xy}$ . For example, among the plans examined, that placed at z = 3.2 is certainly not a good choice. In fact, looking at the figure 5.38 we can see that the velocities  $w^*$  that run through it are practically null, just as  $H_z$ that results about zero. Choosing the optimal plane it is not enough to consider one where the perpendicular speeds are maximum, but it is necessary that the incoming or outgoing  $w^*$  are not counterbalanced by an equally strong speed, but of opposite sign. This is what has been found in all the cases before this, but now something slightly different happens. Once the transient has elapsed, the highest values are found for planes placed at z = 4 and z = 2.4, but if we look at fig. 5.38, both cut exactly two areas where the positive and negative speeds seem to counterbalance each other but, nevertheless, provide the maximum value. This happens because where the  $v^*$  are positive are multiplied by a positive  $H_z$  and then give a  $\Phi_{xy} > 0$ , but where they are negative, being multiplied by a negative  $H_z$ , provide a flow  $\Phi_{xy}$  positive which is added to the previous one.



Figure 5.40: Magnetic field flow trend  $|\Phi_{xz}|$  calculated on different planes with time.

Exactly as done before, let's now analyze how much the magnetic field flux is valid on different planes xz taken along the y-axis. The optimal plan for observing a flow  $\Phi_{xz}$  considerable is the one that combines, in the best possible way, magnetic field and the velocity component's value, perpendicular to it, ie  $H_y$  and  $v^*$ . Consequently, placing oneself in a plane where I have strong perpendicular speeds can be unproductive if  $H_y$  is very low and vice versa. Moreover, as already stated above, it is necessary that the speed perpendicular to the plane, however strong it may be, must not be counterbalanced by a velocity of similar intensity but of opposite sign. For an xz plan the main difficulty is to be able to consider only an incoming or outgoing part of the speeds without incorporating the entire convective motion. With this configuration it is possible to obtain different planes whose magnetic field flux in module is considerable; in particular the plane at y = -0.4, observing figure 5.5, laps exclusively the central zone of the flow at  $v^*$  positive, and sees velocity entering perpendicular to it whose value is not counterbalanced by as many ones. What said above is valid both for the plane placed at y = -0.7 and for the plane at y = 0.7even though the latter has lower values than the previous ones. Unlike the previous cases, none of the plans considered possess values that are clearly lower than the others, indeed, although with smaller values, they all settle on the same order of magnitude.

## Chapter 6 Conclusion

The problem of global warming requires innovative solutions to be stemmed and industries are challenged to improve their production processes and reduce emissions into the atmosphere. In this context, a possible solution provides the use of waste heat recovery system (WHR). Among all WHR systems, the "CERES" is an energy harvesting system based on a FF and his prototype, the DOUGHNUT, was the subject of study in this thesis work. This system, by means of a FF enclosed within a thin shell, is able to exchange only electromagnetic or thermal energy with the external environment. After having written a mathematical model that takes into account all the forces acting on the mixture inside the reactor, the equations have been discretized using a spectral-finite difference method; as regards progress over time, an explicit fourth-order Runge-Kutta scheme was used. Once the simulations have shown how the speeds develop within the computational domain, it is possible to draw conclusions about which arrangement of the magnets, among those selected, leads to a better result. To obtain considerable speeds on a plane perpendicular to the walls, the magnetic force acting in the system must be as high as possible: the gradient of the magnetic field, combined with Temperature values, provide the direction in which the flow is pushed to the inner part of the cavity. The more I can get high speeds, the higher the magnetic field flux values I will record on an arbitrary considered plane. Once this aspect has been optimized, knowing the flow behavior is fundamental for choosing the plans to consider. Analyzing the various cases under examination, all have several points in common:

- Velocity asymmetry: the best plane is the one where the velocity component perpendicular to it is not counterbalanced by an other speed in the opposite direction. A first improvement hypothesis could therefore involve this aspect. Ideally we would consider a reduced portion of the plan in such a way as to collect only the component in one verse rather than another; since this hypothesis is difficult to implement, a further development could be to consider a plane that sees both positive and negative speeds, but to ensure that one of the two is clearly higher than the other.
- Magnetic field: the magnetic field perpendicular to the considered plane is included in the flow calculation and we can deduce that higher values would significantly contribute to obtain higher flows.

Extrapolating the best plans from those chosen and comparing all the cases analyzed, we obtain the trends shown in the figures 6.1 and 6.2.

6-Conclusion



Figure 6.1: Best magnetic field flow trend  $|\Phi_{xz}|$  evaluated for the different cases.



|Øxz| Comparison

Figure 6.2: Best magnetic field flow trend  $|\Phi_{xz}|$  evaluated for the different cases.

Among the various configurations under consideration they all present merits and defects, but in all of them it is observed that the planes perpendicular to the z -axis provide higher flow values than a plane perpendicular to the y- axis.

The optimal xy planes for the third configuration provide absolutely the highest values of  $|\Phi_{xy}|$ among those studied, followed by the second configuration with the half magnet, followed by the first configuration, to provide the planes with  $|\Phi_{xy}|$  high. The second configuration with the entire magnet instead stands out as it provides as many as four possible positions to obtain the magnetic field flow, but the maximum value reached is lower than that obtained in the previous cases. The basic configuration, considering the xy plans does not lead to optimal results. Considering instead the xz planes, perpendicular to the y- axis, we immediately realize how we have to deal with flow values that are in any case lower than the xy planes. The optimal plane for the first configuration is the one that returns the highest magnetic field flux value. The other cases all see a very similar value of  $|\Phi_{xz}|$ , with particular attention to the third configuration, where there are 4 different positions to record values of  $|\Phi_{xz}|$  modestly high. Also for this analysis, the basic configuration does not seem to be a good choice.

In conclusion both the third and the first configuration can be considered the best, and both have one thing in common: the magnets are staggered and this can be an indication of any future development of the prototype.



Figure 6.3: CERES reactor 2.0

## Bibliography

- United States Global Change Research Program, Global Climate Change Impacts in the United States, New York, Cambridge University Press, 2009
- [2] https://climate.nasa.gov/causes
- [3] F. Huang, J. Zheng, J. M. Baleynaud and J. Lu, Heat recovery potentials and technologies in industrial zones *Journal of the Energy Institute*, 2016, 90,111.
- [4] M. F. Remeli, L. Kiatbodin, B. Singh, K. Verojporn, A. Date and A. Akbarzadeh, Energy Procedia, 2015, 75, 64565
- [5] M. Papapetrou, G. Kosmadakis, A. Cipollina, U. La Commare, G. Micale, Industrial waste heat: Estimation of the technically available resource in the EU per industrial sector, temperature level and country, *Applied Thermal Engineering*, 2018, 138, 207216
- [6] A.Chiolerio, M.B. Quadrelli, Colloidal Energetic Systems, Energy Technology, 2019
- [7] https://www1.eere.energy.gov
- [8] https://ec.europa.eu/eurostat
- [9] An open letter to the Australian PM on the climate crisis, from 154 scientists 28 Agosto 2016
- [10] H.Jouhara, N. Khordehgah, S. Almahmoud, B.Delpech, A. Chauhan, S.A. Tassou, Waste heat recovery technologies and applications, Institute of Energy Futures, Brunel University London, Thermal Science and Engineering Progress 6 (2018) 268-289
- [11] F. Mattiussi, A Thermomagnetic Energy Harvester, CERES PROJECT, Master thesis, Politecnico di Torino, 2018
- [12] E.Jordan, K. Balmain, Electromagnetic waves and radiating systems, prentice hall, Englewood Cliffs, New Jersey, 1968
- [13] R.E.Rosenweig Ferrohydrodynamics, New York, Cambridge University Press, 1985
- [14] https://ferrofluid.ferrotec.com/technology

- [15] Aleksandra A. Bozhko, Sergey.A. Suslov, Convection in Ferro-Nanofluids: Experiments and Theory, Springer.
- [16] A. Sartori, Metodi di caratterizzazione di nanoparticelle magnetiche per applicazioni di Magneto-Fluido Ipertermia, Master Thesis, Universita' degli studi di Padova, 2012-2013
- [17] G.H. Yeoh, J. Tu, Computational Techniques for multi-phase flow, Oxford, Butterworth-Heinemann, 2010, 1st edition
- [18] http://www.afs.enea.it/fluent/Public/Fluent-Doc/PDF
- [19] D. D'Ambrosio, Computational Fluidi Dynamics, dispense, Politecnico di Torino, 2017-2018
- [20] P.G. Drazin, W.H.Reid Hydrodynamic and Hydromagnetic Stability, London, Oxford university Press, 1961
- [21] J.D. Anderson, Jr., Fundamentals of Aerodynamics, New York, McGraw-Hill, 1991, 2nd Edition.
- [22] D.J.Tritton, Physical fluid dynamics, Workingham, Van Nostrand Reinhold, 1997
- [23] P.S.B. Szabo, W-G. Fruh, The transition from natural convection to thermomagnetic convection of a magnetic fluid in a non-uniform magnetic field, *Journal of Magnetism and Magnetic Materials*, 2017
- [24] D.P.Lalas, S.Carmi , Thermoconvective Stability of Ferrofluids, Physics of Fluids, 14, 1971, 436-438
- [25] T. Sawada, H. Kikura, T. Tanahashi, Visualization of wall temperature distribution caused by natural convection in a cubic enclosure, *International Journal of Applied Electromagnetics* in Materials, 4, 1994, 329335.
- [26] S. M. Snyder, T. Cader, B. A. Finlayson, Finite element model of magnetoconvection of a ferrofluid, *Journal of Magnetism and Magnetic Materials*, 262, 2003, 269279.
- [27] M.D. Cowley, R.E. Rosenweig, The interfacial stability of a ferromagnetic fluid, Journal of Fluid Mechanics, 30 (4), 1967, 671-688
- [28] S.A.Suslov, Thermomagnetic convection in a vertical layer of ferromagnetic fluid, *Physics of Fluids* 20, 2008;
- [29] P.J.Stiles, M. Kagan, Thermoconvective Instability of a horizontal layer of ferrofluid in a strong vertical magnetic field, *Journal of Magnetism and Magnetic Materials*, 85, 1990, 196-198
- [30] S.Odenbach, H.W. Mller, On the microscopic interpretation of the coupling of the symetric velocity gradient to the magnetization relaxation, *Journal of Magnetism and Magnetic Material*, 289, 2005, 242245.

- [31] Md Habibur Rahman, Analysis of thermomagnetic convection in a vertical Layer of magnetic fluid with arbitrary orientation of magnetic field, Ph.D thesis, Swinburne University of Technology, Hawthorn, 2005
- [32] http://faculty.washington.edu/finlayso/ferrofluid/eq.html
- [33] Dr. Chiu Fan Lee, Introduction to Multiphase Flows, Department of Bio engineering Imperial College, London, 2015
- [34] C.M.Tchen, Mean value and correlation problems connected with the motion of small particles suspended in a turbulent fluid, Ph.D thesis, Delft, 1947
- [35] S.Corrsin, J.Lumley, On the equation of motion for a particle in turbulent fluid, Applied Scientific ResearchA 6, 114,1956
- [36] M.R.Maxey, J.J Riley, Equation of motion for a small rigid sphere in a nonuniform flow, *Physics of Fluids* 26, 883, 1983
- [37] C.T.Crowe, J.D.Schwarzkopf, M.Sommerfeld, Y.Tsuji Multiphase Flows with Droplets and particles, New York, CRC Press, 2012, 2nd edition
- [38] G. Ludwig, Diffusion zwischen ungleich erwrmten Orten gleich zusammengesetzter Lsung, Aus der K.K. Hof-und Staatsdruckerei, Akademie der Wissenschaften, 1856
- [39] C.Soret, Sur l'tat d'quilibre que prend au point de vue de sa concentration une dissolution saline primitivement homohne dont deux parties sont portes des tempratures diffrentes, Archives des Sciences Physiques et Naturelles, 2, 1879, 48-61
- [40] R.Piazza, A.Parola, Thermophoresis in colloidal suspensions, Journal of Physics: Condensed Matter, 20, 2008
- [41] D. Braun, A. Libchaber, Trapping of DNA by thermophoretic depletion and convection, *Physical Review Letters* 89, 2002
- [42] P. Baaske, F.M. Weinert, S. Duhr, K.H. Lemke, M.J. Russell, D. Braun, Extreme accumulation of nucleotides in simulated hydrothermal pore systems, *Proceedings of the National Academy of Sciences of the United States of America*, 104, 93469351, 2007
- [43] S.J.Jeon, M.E.Schimpf, A. Nyborg, Compositional effects in the retention of colloids by thermal field-flow fractionation, *Analytical Chemistry* 69 3442-3450, 1997
- [44] S.Duhr, D.Braun, Optothermal Molecule Trapping by Opposing Fluid Flow with Thermophoretic Drift Physical Review Letters 97, 2006
- [45] J. Burelbach, D. Frenkel, I.Pagonabarra, E.Eiser, A unified description of colloidal thermophoresis, *European Physical Journal*, E(2018) 41:7
- [46] N. G. Van Kampen, Diffusion in inhomogeneous media, Journal of Physics and Chemistry of Solids, 49(6):673–677, 1988.

- [47] M. Yang, M. Ripoll, Drift velocity in non-isothermal inhomogeneous systems, The Journal of Chemical Physics 136, 2012
- [48] D.Lusebrink, Colloidal Suspensions in Temperature Gradients with Mesoscopic Simulations Universitat zu Koln, 2011
- [49] A. Wrger, Thermal non-equilibrium transport in colloids, *Reports on Progress in Physics*, 73(12), 2010.
- [50] H. Ning, J. Buitenhuis, J. K. G. Dhont, S. Wiegand. Thermal diffusion behavior of hard-sphere suspensions, *Journal of Chemical Physics*, 125, 2006.
- [51] M. Braibanti, D. Vigolo, R. Piazza. Does thermophoretic mobility depend on particle size?, *Physical Review Letters*, 100, 200
- [52] S. Iacopini, R. Piazza, Thermophoresis in protein solutions, Europhysics Letters, 63:247, 2003
- [53] S. Duhr, D. Braun. Thermophoretic depletion follows Boltzmann distribution, *Physical Review Letters*, 96, 2006.
- [54] J.K.Platten, The Soret effect: A review of recent experimental results, Journal of Applied Mechanics, 73/5, 2006
- [55] M.Yang, M.Ripoll, Thermophoretically indiced flow field around a colloidal particle, Soft Matter, 9, 4661, 2013
- [56] L.Schwab, U. Hildebrandt, K. Stierstadt, Magnetic Benard convection, Journal of Magnetism and Magnetic Materials, 39, 113114, 1983
- [57] C. Tangthieng, B.A. Finlayson, J. Maulbetsch, T.Cader, Heat transfer enhancement in ferrofluids subjected to steady magnetic fields, *Journal of Magnetism and Magnetic Materials* 201, 252255. 1999
- [58] A.A. Bozhko, G.F. Putin, Heat transfer and flow patterns in ferrofluid convection, Magnetohydrodynamics 39, 147169, 2003
- [59] A.A. Bozhko, G.F. Putin, Thermomagnetic convection as a tool for heat and mass transfer control in nanosize materials under microgravity conditions, *Microgravity Science and Technology*, 21, 8993, 2009
- [60] S. Odembach, Recent progress in magnetic fluid research, Journal of Physics: Condensed Matter, 16:32, 2004
- [61] V.G. Bashtovoi, V.K.Polevikov, A.E.Suprun, A.V.Stroots, S.A.Beresnev, Influence of brownian diffusion on the statics of magnetic fluid, *Magnetohydrodynamics*, 43:1, pp 17-25, 2007

- [62] M.S.Krakov, I.V.Nikiforov, Effect of diffusion of magnetic particles on the parameters of the magnetic fluid seal: a numerical simulation, *Magnetohydrodynamics*, 50:1, pp 35-43, 2014
- [63] G.Passoni, G. Alfonsi, M.Galbiati, Analysis of hybrid algorithms for the Navier-Stokes equations with respect to hydrodynamic stability theory, *International Journal for Numerical Methods in Fluids*, 38: 1069-1089, 2002
- [64] J.Kim, P. Moin, R.Moser, Turbulence statistics in fully developed channel flow at low Reynolds number, *Journal of Fluid Mechanics*, 177:133-166, 1987
- [65] SA. Orszag, LC Kells, Transition to turbulence in plane Poiseuille and plane Couette flow, Journal of Fluid Mechanics, 61:64-88, 1980
- [66] JR. Herring, SA. Orszag, RH. Kraichnan, DC. Fox, Decay of two-dimensional homogeneous turbulence, *Journal of Fluid Mechanics* 66:417-444, 1974
- [67] RP. Garg, JH. Ferziger, SG. Monismith, Hybrid spectral finite difference simulations of stratified turbulent flows in distributed memory architectures, *International Journal for Numerical Methods in Fluids*, 24: 1129-1158, 1997
- [68] T.A. Zang, C. L. Streett, H.Y. Bussaini, Spectral methods for CFD, NASA Contractor Report 181803, Marzo 1989
- [69] C.Canuto, A.Quarteroni, M. Yousuff Hussaini, T.A. Zang "Spectral Methods in Fluid Dynamics", Berlin, Springer-Verlag, 1988
- [70] C. Canuto, A. Quarteroni, M. Y. Hussaini, T. A. Zang, Spectral Methods Fundamentals in Single Domains, Berlin, Springer-Verlag,
- [71] P.Schlatter, Spectral Methods Computational Fluid Dynamics lectures notes
- [72] G.S.Patterson, S.A Orszag, Spectral calculation od isotropic turbulence: efficient removal of aliasing interactions, *Physics of Fluids*, 14, 2538-2541, 1971
- [73] M. Uhlmann, The need for de-aliasing in a Chebyshev pseudo-spectral method, March, 2000
- [74] B.Eliasson, Aliasing effects and de-aliasing methods in turbulence simulations, College on Advanced Plasma Physics, Trieste, 2014
- [75] J.P.Body Chebyshev and Fourier Spectral Methods, New York, DOVER Publications, 2000, 2nd edition.
- [76] J.D. Anderson, Jr., "Computational fluid dynamics: the basic with applications, New Delhi, McGraw Hill Education, 1995
- [77] https://scicomp.stackexchange.com/questions/25578/runge-kutta-stability-regions
- [78] A.Chorin, Numerical solution of the Navier-Stokes equations, Mathematics of Computation, 22, p.745, 1968

[79] M. Ishii, T. Hibiki, Thermo-Fluid Dynamics of Two-phase Flow, New York, Springer, 2005