

**Computational Fluid Dynamics Modelling Applied to Urban
Drainage: The Case Study of the Monsanto-Santa Apolónia
Tunnel Inlet Structure, in Lisbon**

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I declare that this document is an original work of my own authorship and that it fulfils
all the requirements of the Code of Conduct and Good Practices of the
Universidade de Lisboa.

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Abstract

Drainage systems are crucial for managing wastewater and rainwater in urban areas and face challenges like urban sprawl, climate change, and aging infrastructure. The conventional methods employed to analyse the performance of drainage systems are inherently limited in their capacity to address the full complexity of these systems. Computational Fluid Dynamics (CFD) emerges as a promising tool by enabling 3D simulation of free-surface flows, incorporating turbulence phenomena.

To create a methodology for developing a CFD model for turbulent free-surface flow, key parameters (mesh discretization, turbulence models, geometry constraints, boundary conditions, convergence criteria, scale-related assessments) were systematized in an optimized flowchart by applying it to the inlet infrastructure to the Monsanto-Santa Apolónia tunnel of Lisbon's Drainage Master Plan, employing the commercial software Flow3D.

The study demonstrates that CFD simulations of free surface turbulent flows, employing a model development with increasingly refined and different mesh formulations and a validation mechanism, based on traditional hydraulic modelling, literature or real data collection, can produce strong results when employing a convergence criterion based on mass balance, with simulation times compatible with decision-making in civil engineering. It was also evidenced that reduced scale CFD models can offer faster convergence and accurate results of velocity fields, water heights or general flow behaviour. However, phenomena like hydraulic jumps can suffer from scale effects, due to the predominance of the viscosity. Finally, the study proves the CFD capabilities to implement Digital Twins in context of design, operation and maintenance, then offering numerous advantages for management utilities.

Keywords: Urban Drainage; Computational Fluid Dynamics (CFD); Flow3D; Hydraulic Modelling; Lisbon Drainage master plan (PGDL)

Resumo

Os sistemas de drenagem são cruciais na gestão das águas residuais e pluviais nas zonas urbanas e enfrentam desafios como a expansão urbana, as alterações climáticas e o envelhecimento das infraestruturas e os métodos convencionais revelam-se limitados na capacidade de abordar a complexidade destes sistemas. A Dinâmica de Fluidos Computacional (CFD) surge como uma ferramenta promissora ao permitir a simulação 3D de escoamentos de superfície livre, incorporando fenómenos de turbulência.

Com o objetivo de criar uma metodologia para o desenvolvimento de um modelo CFD para escoamentos turbulentos em superfície livre, os parâmetros chave (discretização da malha, modelos de turbulência, restrições geométricas, condições de fronteira, critérios de convergência, relações de escala) foram sistematizados num fluxograma, otimizado pela aplicação à obra de entrada do Túnel Monsanto-Santa Apolónia do Plano Geral de Drenagem de Lisboa, utilizando o software comercial Flow3D.

O estudo demonstra que os modelos CFD para estes escoamentos, desenvolvidos com testes de refinamento e formulações de malha, aliado à validação do modelo através de modelação hidráulica tradicional ou na literatura, produz resultados precisos, quando aplicado um critério de convergência baseado no balanço de massa, verificando-se tempos de simulação compatíveis com a tomada de decisões em engenharia civil. Foi ainda evidenciado que os modelos CFD em escala reduzida oferecerem uma convergência mais rápida mantendo resultados precisos dos campos de velocidade, alturas de água e comportamento geral do escoamento. No entanto, fenómenos como ressaltos hidráulicos podem sofrer efeitos de escala, devido à predominância da viscosidade. Finalmente, o estudo demonstra as capacidades do CFD para implementar Gémeos Digitais aquando do dimensionamento, operação e manutenção, oferecendo numerosas vantagens para os serviços de gestão.

Palavras-chave: Drenagem Urbana; Dinâmica de Fluidos Computacional (CFD); Flow3D; Modelação Hidráulica; Plano Geral de Drenagem de Lisboa (PGDL)

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List of Abbreviations

3D - Three Dimensional

APA - Portuguese Water Authority

ERSAR - Regulator of Water and Wastewater Services

WTP - Water Treatment Plants

WWTP - Wastewater Treatment Plant

CSO - Combined Sewer Overflow

DT - Digital Twins

UWWTD - Union's Urban Wastewater Treatment Directive

IAS - Appropriate Solutions

PENSAARP2030 - Strategic Plan for Water Supply and Wastewater and Stormwater Management for the period 2021-2030

RASARP2023 - Annual Report on Water and Waste Services in Portugal of 2023

SUDS - Sustainable Urban Drainage Systems

CFD - Computational Fluid Dynamics

LNEC - National Laboratory of Civil Engineering

CAD - Computer Aided Design

FDM - Finite Difference Method

FEM - Finite Element Method

FVM - Finite Volume Method

RANS - Reynolds-Averaged Navier-Stokes

LES - Large Eddy Simulation

RSM - Reynolds Stress Models

EVM - Eddy Viscosity Models

GUI - Graphical User Interface

FAVOR™ - Fractional Area Volume Obstacle Representation

VOF - Volume of Fluid method

CFL- Courant-Friedrichs-Lewy Condition

PGDL - Lisbon's Drainage Master Plan

TMSA - Monsanto-Santa Apolónia Tunnel

AdTA - Águas do Tejo Atlântico

List of Symbols

u - Velocity Vector (u, v, w)

V - Characteristic Velocity

ρ - Fluid Density (mass per unit volume)

∇ - Differential Operator

σ_t - Fluid's Internal Resistance to Deformation

μ - Fluid's Viscosity

φ - Dissipation Function due to the mechanical energy that is converted into heat

p - Pressure

k - Turbulent Kinetic Energy

μ_t - Eddy Viscosity

ϵ - Turbulent Dissipation Rate

ω - Specific Rate of Dissipation of Kinetic Energy

m - Reduced Model Scale

p - Prototype Scale

F_{ext} - External Forces

K - Heat Conductivity

A_x - Fractional Area Normal to the x -Direction

$F(x, y, z, t)$ - Volume of Fluid function

V_F - Fractional Volumes

I - Internal Energy

q - Turbulence Quantities for Energy

D - Dissipation

Fr - Froude Number

h - Water Depth

Re - Reynolds Number

$^{\circ}\text{C}$ - Degrees Celsius

List of Software

Flow3D®	CFD Simulation software by Flow Science, Inc. version 11.2
FlowSight™	Post processing software by Flow Science, Inc. version 11.2

1 Introduction

1.1 Context and Motivation

Urban drainage systems face many challenges, such as climate change, urban growth and infrastructure deterioration [1] [2]. To address these issues, the network of structures conveying rainwater and wastewater has evolved beyond the traditional pipe network [3]. Cities have started to implement innovative solutions to address the issue of floods and ensure environmental compliance.

The design of complex hydraulic structures is often supported by the construction of physical models to assess flow behaviour, generally occurring under turbulent regimes [5]. Recently, the use of computational models by applying Computational Fluid Dynamic (CFD), has been a complement to the analysis of such flow behaviours, often in the so-called grey infrastructures. These models solve the fundamental equations of fluid dynamics, thereby enabling the prediction of flow characteristics and system performance, providing space to explore an optimal design solution [6].

In this master's dissertation, the software Flow3D was used to simulate the inlet structure of the Monsanto–Santa Apolónia drainage tunnel (TMSA), part of Lisbon's Drainage Master Plan (PGDL). The motivation of this work is to apply advance design tools to study the most important step made in Lisbon urban drainage towards resilience and environmental safety, while European Union makes advances towards urban drainage management.

The challenges faced arise due to the representation of complex geometries, requiring different discretization, applying boundary conditions that match real conditions, and efficient time-consuming discretization of the domain. To validate the process, previously performed experimental tests were used to directly compare results and flow behaviours and then, a prototype/model scale relationship was established through Froude's Similarity Law, to analyse possible scale effects.

1.2 Objectives and Structure

The main objective of this thesis is to produce a key methodology for the development of a CFD model of a free surface turbulent flow, which was supported by a study case analysis of the inlet structure of the TMSA. The methodology involves the comparison of traditional model scale experimental results with model scale numerical results in the validation phase. This is followed by a numerical comparison at model and prototype scale to draw conclusions about possible scale effects and the trade-off between the performance of the two scales.

To achieve this, three secondary objectives are established:

1. Conduct a sensitivity analysis on key parameters (mesh definition, boundary conditions, and others) to understand their influence on simulation results and computational performance, aiming to propose the most suitable approach.

2. Simulate different operational scenarios (frequent rainfall events, design floods, exceptional conditions) to compare computational results at the model scale with experimental results at model scale.

3. Compare both numerical results at the reduced model and prototype scale to analyse possible scale effects and computational trade-off.

This dissertation is organized into seven chapters:

Chapter 1 presents the context, motivation, objectives, and structure of the work.

Chapter 2 provides the background and evolution of urban drainage systems, including the Portuguese context and the challenges faced today.

Chapter 3 introduces the theoretical foundation of CFD, with a focus on the numerical modelling approach and capabilities of Flow3D.

Chapter 4 details the general methodology.

Chapter 5 describes the development of the case study numerical model, including geometry, mesh settings, boundary conditions, turbulence modelling, and the validation process.

Chapter 6 presents and discusses the results of the CFD simulations for different scenarios, including results comparisons.

Chapter 7 has final considerations and recommendations for future work.

2 Urban Drainage

2.1 The rise of drainage systems

2.1.1 General overview

The necessity for drainage systems arises from the interaction between human activities that create wastewater, the natural water cycle, and the need to control the impacts of this wastewater on the well-being of human life and the environment. This chapter examines the genesis and subsequent development of urban drainage systems, with a particular focus on the ways in which early human civilisations initially managed water and waste.

The Mesopotamians, particularly in Assyria and Babylonia around 4000 B.C., were among the first to develop advanced drainage and sanitation systems. Cities like Babylon featured clay drainage pipes in streets and homes, driven by cultural values of cleanliness. These innovations laid the foundation for modern urban infrastructure [7].

The Romans further advanced drainage systems, with the Cloaca Maxima, one of the worlds earliest sewage systems in Rome by 600 B.C. Its primary functions were to drain marshy areas, also connecting public baths and latrines, and served to carry away excess water after rainfall, transporting it to the Tiber River, reducing the spread of diseases. After the Roman Empire's fall, sanitation regressed in Europe until the 19th century, when cities like Paris and London began to slowly reintroduce drainage innovations [7].



Figure 1 - Cloaca Maxima of Rome [8]

In the 17th century, it was believed that parasites thrived in the body due to "poorly controlled transpiration," and hygiene practices were basic, with more emphasis on changing clothes than bathing. However, by the century's end, cleanliness began to be more valued, with prominent figures praising personal hygiene, marking a shift towards greater appreciation for cleanliness and setting the stage for future advancements in hygiene practices [2].

In the 19th century, there were numerous instances of cholera occurring in various locations across Europe. These outbreaks were associated with European colonization. London's outdated drainage system caused significant public health issues due to rapid urbanization. The "Great Stink" of 1858 highlighted the problem, leading to Joseph Bazalgette designing a new sewer system. His innovative intercepting sewers reduced Thames pollution and health hazards, demonstrating the transformative impact of well-designed infrastructure [7].

Paris underwent a significant sanitation improvement during the 19th century. A new covered sewer network was designed to handle wastewater, featuring large tunnels for easy maintenance. Over time, the engineering perception of these sewers evolved, and the concept of self-cleaning was introduced. Consequently, the minimum velocity criterion was first established in London in the 1840's [2].

2.1.2 Portuguese perspective

Urban sanitation in Lisbon became a concern from the late 15th century to modernize the city and prevent plagues. King João II, in 1486, recommended large street drains, and by 1552, King João III hired workers to clean the streets. King João V stressed cleanliness during an epidemic in 1723, but public spaces remained unclean despite these efforts [9].

After the 1755 earthquake, Sebastião José de Carvalho e Melo (Marquis of Pombal) began reconstructing Lisbon with Enlightenment and hygienist principles, aiming for a clean and orderly city. The hygienist ideas, emphasizing clean air and public health, influenced urban interventions, shaped by preventive medical discourses from the 1720s. The Pombaline buildings introduced a waste and sewage collection system to prevent waste from being thrown into the streets, improving cleanliness [9].

In the late 19th century, public water and sanitation policies emerged with the recognition of the link between diseases and poor water systems, leading to legislation in 1899–1901. However, financial and political challenges constrained the progress, and by the 1970s only 17% of the population was connected to a wastewater system, with significant regional disparities. Despite challenges, political investment after 1974 expanded access to water and sanitation, with significant progress following Portugal's 1986 integration into the European Economic Community [10].

Thus, approximately three decades ago, the Portuguese government initiated a comprehensive reform of the country's water and wastewater sector with the objective of expanding coverage and improving the quality of service provided. Nowadays, APA (Portuguese Water Authority) establishes policies and management tools to facilitate the realization of these objectives, in collaboration with other entities such as ERSAR (Regulator of Water and Wastewater Services), in work since 1998 [10].

Over the past three decades, there has been a notable enhancement in the quality of services, with 96% of the population having physical access to a safe water supply network and 87% to wastewater network, by 2023. These indexes are known as network coverage [11].

The high costs of conventional drainage solutions in rural and low-density urban areas, such as those found in Portugal, are a major obstacle to achieving the goals related to wastewater services [2].

However, in the current days, the index of network coverage does not fully reflect the sector situation, and drainage systems are confronted with a multiplicity of challenges, thus demonstrating a potential for further development in terms of its quality and resilience. This issue will be further examined in the subsequent section.

2.2 Urban drainage characterization

There are different sources of wastewater and its interaction with stormwater in drainage systems. Water is collected from natural sources and treated at water treatment plants (WTP) before being made available for human consumption. However, the use of this water for various human activities, including commercial, domestic and industrial activities, results in the generation of wastewater (also known as sewage, and the transport system the sewer system) [2]. For the purpose of this work, and considering the interaction between all sources of effluents, wastewater will often be referred as the mixture or combination of both domestic wastewater and non-domestic wastewater and urban runoff due to precipitation.

Wastewater must be drained through an appropriate drainage system and subsequently treated in a wastewater treatment plant (WWTP) to ensure its safe disposal. The objective of the wastewater treatment plant (WWTP) is to increase the quality of the wastewater to a secure standard for the human life and environment, given that the treated wastewater is released into the surrounding environment, such as watercourses [2]. The treatment process results in the formation of a semi-solid sludge, which requires chemical and biological stabilization. The ultimate potential use of the sludge is for agricultural fertilization, energy production or, most commonly, incineration, a process that might present a detrimental impact on the environment if not properly executed [2].

In addition to wastewater, stormwater (also referred to as rainwater and urban runoff) when intercepted with drainage devices in human settlements (due to the impermeabilization of the city areas), can be conveyed directly to the natural receiving environment. This type of eluent often has a low pollutant content. However, it can also require adequate treatment, as will be discussed subsequently, to ensure the preservation of the receiving water body quality. The urban drainage network is comprised of all devices and infrastructure that are responsible for the collection and conveyance of wastewater and stormwater until it reaches the WWTP and the receiving environment [12]. This illustrated in Figure 2.

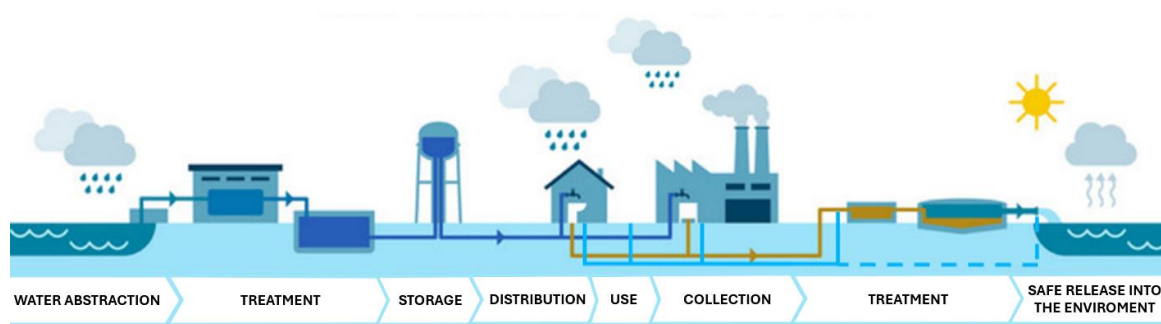


Figure 2 - Urban drainage network adapted from [13]

2.2.1 Types of drainage systems

Usually, drainage systems are classified into four types, depending on the origin of the water they discharge [2]:

a) **Separative**, consisting of two separate networks of pipes, one for domestic, commercial and industrial wastewater and the other for rainwater drainage;



Figure 3 - Separative urban drainage system [14]

b) **Combined**, consisting of a single network where both wastewater and rainwater are admitted together. When too much water enters the pipes the system overflows into waterbodies, in an event called a combined sewer overflow (CSO). Since most drainage systems are still combined, drainage systems are often referred entirely as the sewer system;



Figure 4 - Combined urban drainage system [15]

c) **Mixed**, consisting of a combination of the two previous types, where part of the collecting network functions as a combined system and the rest as a separative system;

d) **Partially separate**, where the connection of rainwater from interior courtyards to the domestic wastewater collector is permitted under exceptional conditions.

The advantages of combined systems include cost savings, a simpler construction than two separate pipes and the ability to treat part of the stormwater flows that may have a higher pollutant concentration. The disadvantages of combined systems include the occurrence of CSO, the exceeding of WWTP

capacity, and the subsequent mixture of stormwater and domestic wastewater that cannot be treated. This can result in pollution and contamination issues when discharged into receiving waters. Furthermore, it is challenging to maintain adequate hydraulic conditions in combined sewers during dry weather periods due to the potential for sedimentation of suspended solids, the risk of hydrogen sulphide odour formation, and the corrosion of sewer materials [2].

2.2.2 System components

As previously stated, wastewater can be divided into three principal effluents: domestic (derived from basic human activities and exhibiting a high organic content), industrial (originating from production processes and often rich in chemical pollutants), and stormwater (originating from surface runoff and varying in pollutant content depending on the precipitation event). It is therefore evident that a multifaceted drainage system is essential for the effective conveyance of wastewater from a variety of sources and so, it is necessary to employ different devices to overcoming any constraints on the network. The most common devices are explained in the following paragraphs.

The pipe network, the main component in urban drainage, is comprised by straight pipes separated by manholes whose main function is to provide access to the network for rehabilitation, maintenance and inspection [2]. Allied to this main sewer network, at households, shops, schools and industrial facilities, lateral pipes convey the effluent to the main pipes that will transport the wastewater to the WWTP. Rainwater at buildings is intercepted with gutters and other devices and at streets by gullies to convey the stormwater to the drainage system [12].

In addition to these principal components, there are other special components that are frequently employed to overcome or avoid hydraulic constraints in the context of wastewater transportation. These include pumping stations (also known as elevation devices), which are utilised when gravitational drainage (the preferred method) is not economically or technically viable. Inverted siphons are also employed to overcome obstacles when free surface flow is not technically or economically feasible and this may include instances where flow must be carried under a road or watercourse, but they present problems related with low velocity that can lead sediment deposition [2].

Ultimately, the construction of tunnels is economically viable in instances where topographical and geological conditions permit. In such cases, the excavation of trenches is unnecessary, and the diameter of the resulting tunnel is typically larger than that of a standard sewer pipe [2].



Figure 5 - Tunnel example in Singapore drainage system [16]

In the context of design, there is a significant corpus of detailed design considerations based on legislation for variables such as the account of the design inflow in the network, maximum and minimum diameters, velocities and slopes, placement of the sewers, manholes and more, which contribute to the multifaceted nature of these projects. In addition to those constraints, consideration must also be given to the built environment in which the project is to be implemented. This requires on-site visits to collect information and to study the impact that the works will have on the urban environment in question [2].

2.3 Urban drainage framework

Trends in urban drainage reflect the necessity for the development of innovative solutions to address emerging issues and anticipate future complexities. This chapter examines the current challenges in urban drainage, the most relevant legislation or regulations, and presents an overview for urban drainage infrastructures design, including hydrodynamic modelling and asset management.

2.3.1 Current challenges

In the past decades, urban drainage has been confronted with a variety of new challenges. In recent decades climate change has become a major issue, by imposing changes in the frequency, intensity, and distribution of precipitation events. Regions that were previously characterized by predictable rainfall patterns are now experiencing more irregular and extreme weather conditions and traditionally arid areas are facing unexpected heavy rainfall, which is challenging existing water management strategies. Urban areas are particularly vulnerable to these changes, with the frequency and intensity of precipitation events exceeding the design capacities of urban drainage systems, originating floods [1].

The occurrence of floods in coastal cities and those situated on river deltas will be also influenced by climate change, which will be manifested in several ways which include rising sea levels, affecting the performance of existing infrastructure and the design of future works [17]

The discharge of urban stormwater runoff carries a suite of pollutants, including suspended solids, nutrients, trace metals, and organic micropollutants, which have the potential to significantly contaminate natural waters. The phenomenon of urbanization serves to intensify this issue, as it gives rise to an increase in both the number of pollution sources and the volume of runoff [18].

Thus, combined with inadequate performance of combined drainage systems, the discharge of untreated wastewater and stormwater into the environment is frequent, which has an adverse effect on water quality and pollution in receiving bodies.

Drainage systems are also experiencing deterioration and collapse due to several factors, including conditions that accelerate corrosion, economic and environmental unsustainability, insufficient infrastructure capacity and aging infrastructure. This phenomenon is particularly evident in densely populated urban areas, where, in addition to the issues previously outlined, the increasing impermeabilization and unplanned land use have resulted in a notable rise in peak flow rates. The recognition of these challenges has led to a shift in the analysis and design of urban drainage systems.

The necessity to address these new difficulties requires the application of innovative approaches that extend the traditional engineering techniques [2].

2.3.2 Urban Wastewater Treatment Directive

To address these challenges, the European Union's Urban Wastewater Treatment Directive (UWWTD), that has been in effect for over 30 years, was revised in 2024 and has recently been approved.

This new directive introduces stricter technical requirements across multiple fronts, and sets targets well defined, leaving no doubts about the future steps. A short overview of the recently introduced directive[19] is first necessary to gain insight into the trajectory of the drainage systems:

- It limits the use of Individual and Appropriate Solutions (IAS) to exceptional cases or in areas with a certain limit of inhabitants, giving relevance to centralized treatments via collecting systems as physical setups intended for the collection, conveyance, and transmission of wastewater to treatment plants or discharge points, designed and managed to meet environmental and safety standards.
- When it comes to treatments obligations, there's a stricter approach to implement at least secondary treatment, with new obligations to tertiary and encouragement to quaternary treatments to address eutrophication and micropollutants and a producer responsibility: Producers are responsible for contributing financially to cover costs related to waste management, based on the hazardousness and quantity of substances in their products. These are especially to promote water reuse and safeguard ecosystems.
- Urban areas must implement wastewater management plans that include dynamic flow analyses, discharge monitoring, and measures to limit stormwater overflow, reduce microplastic pollution, and prevent unpolluted rainwater from entering the system. These plans should focus on optimizing and better managing existing infrastructure to minimize untreated runoff, increase system capacity, and prioritize preventive blue and green solutions that promote natural water retention or rainwater harvesting.
- The directive sets targets for total energy neutrality in treatment facilities until 2045. Specifically, Member States must ensure that the total annual energy consumption of urban wastewater treatment plants does not exceed the amount of renewable energy produced by or for these plants, with treating loads of 10.000 population equivalent in terms of pollution load.
- Member States should include measures in their integrated urban wastewater management plans to limit the pollution from storm water overflows to no more than 2% of the annual collected urban wastewater load under dry weather conditions. These measures should also address the pollutant capacity of the urban runoff, especially during first rains after dry periods, which often carry higher pollutant loads.
- The directive explicitly states the importance of ensuring access to sanitation for all, emphasizing that every person should have access to safe and adequate sanitation services, in line with the human right to water and sanitation and mandates transparency in reporting on wastewater management data.

- Collecting systems must comply with the design, operation and maintenance to ensure consistent performance during typical local weather conditions, in accordance with Directive (EU) 2022/2557, which classifies such systems as critical entities that must be safeguarded against diverse threats to public health and the environment.

Each member state of the European Union is responsible for adapting European directives to its laws and administrative structures within their respective national frameworks. This requires the adoption of new laws and regulations to ensure compliance with the directive's requirements. Following this, the European directive becomes part of the national law of the member state, and it is then the responsibility of the national authorities. The European Commission oversees and evaluates the implementation of directives, issuing periodic reports on their impact and implementation.

Considering the reviewed literature and the recent UWWTD, the most problematic urban drainage factors are identified in Table 1. It is noteworthy that even those member states that have demonstrated positive performance in this sector may still encounter new pivotal challenges to meet the future and current standards.

Table 1 - Urban Drainage Challenges

Climate change		Unplanned land use		Lack of Asset Management	
Intensification of precipitation	Sea level rise	New/More Pollutants	Increasing impervious surface	Infrastructure deterioration	Insufficient infrastructure capacity

2.3.3 National Framework

To address Portugal's legal framework for urban drainage and pluvial runoff disposal is primarily governed by the Water Law (*Decreto Lei N° 226-A/2007*) and the General Regulation for Public and Building Water and Wastewater Systems (*Decreto Regulamentar No. 23/95*). The Water Law establishes that the use of water resources and treats stormwater runoff as a potentially harmful discharge that must be managed through planning, environmental assessment, and regulatory control, especially in urban areas where impermeable surfaces increase the risk of pollution and flooding. *Decreto Lei N° 23/95* provides the core technical and operational rules for designing, building, and maintaining public and private drainage systems. It distinguishes between wastewater and stormwater networks, defines requirements for separate and combined systems, and sets obligations for both public utilities and property owners, making it the most specific regulation for urban drainage infrastructure.

Complementary to these, *Decreto-Lei N° 77/2021* updates national rules for urban wastewater treatment, adjusting them to environmental sensitivities by requiring stricter treatment in sensitive zones. *Portaria N° 188/2021* supports this by officially identifying those sensitive and less sensitive zones, influencing how and where drainage systems must meet higher environmental standards. While these last two focus more on treatment, they indirectly affect how urban runoff is collected and managed.

In Portugal, the ministry responsible for the environment, in collaboration with the Portuguese Parliament, has the direct political responsibility of creating new national legislation that transposes European directives alongside with APA, that plays a pivotal role in the implementation and assurance of conformity with European environmental standards. In parallel, ERSAR serves as an autonomous regulatory entity, overseeing the adherence of water and wastewater management service providers to established regulatory standards, ensuring the integrity of their operations within the defined legal framework.

In addition, other agencies engaged in the fields of environmental protection, water management, and wastewater utilities and energy are also involved in the development of the PENSAARP2030, which stands for Strategic Plan for Water Supply and Wastewater and Stormwater Management for the period 2021-2030 [20].

PENSAARP2030 serves as a guiding instrument for policies and investments related to the urban water cycle and its integration with other relevant sectoral policies. This plan builds upon the achievements of three preceding programs, which have been continuously refined over time to address the sector's current challenges within the context of the country, the European Union and the main international entities, for example United Nations. The present edition reflects the growing significance attributed to wastewater drainage systems that extend beyond the conventional network coverage and households' connection to the network [21].

Given the above, it could be argued that once PENSAARP 2030 was established and approved at the end of 2023 in conformity with the former UWWTD, the Portuguese plan will be no longer entirely aligned with the new UWWTD. Consequently, stakeholders must consider this discrepancy in their decision-making processes for the foreseeable future until an update is made.

Despite these considerations, PENSAARP2030 [21] establishes a list of the most critical measures that must be taken to achieve the most important goals by the year 2030:

- Improving infrastructure asset management, improving cadastral and operational knowledge of infrastructure and rehabilitate infrastructure
- Operational improvement, modernization and automation/digitization of services
- Improving the quality of wastewater discharged
- Reducing undue inflows into wastewater and rainwater systems
- Accountability of industrial wastewater discharges into public systems
- Strengthening the safety and resilience of systems
- Improving the energy efficiency of systems
- Adapting services to climate change
- Strengthening the commitment of the various political bodies, service regulators, state-owned management utilities and municipal

- Improving the mechanism for managing European funds for financing and investment decisions by entities
- Improving the economic and financial performance of management utilities

This list matches some of the most critical indexes related with drainage systems highlighted in RASARP2023, (Annual Report on Water and Waste Services in Portugal of 2023) [11] elaborated by ERSAR:

- In 2023, Portugal's public wastewater network experienced 10,2 floods per 100 km in the bulk system, far from the satisfactory target of zero annual floods;
- In 2022, only 0,4% of the pipelines over 10 years old were rehabilitated in the bulk system and 0,2% in the retail system, existing 47772 km of pipeline over 10 years old, a figure that worsened since 2018. These values reflect the low management since only 2% of pipeline over 10 years old was inspected in the last 5 years;
- Structural collapses in collectors showed some improvement but still happening 1,1 structural collapses per 100 km in 2022 in the retail system. Lisbon had 3,2 collapses per 100 km, higher than northern urban areas, with 0,1 but below the national average for central urban areas with 3,7;
- In 2022, almost any water was reused, with important attention to areas with extreme water scarcity as they reused 0% of treated wastewater, despite growing concerns about water reuse;
- Emergency and storm discharge control is poor, with less than 30% of direct discharges to the receiving environment that are monitored, for both bulk and retail system, far below the value of a satisfactory index at 80%. In Lisbon, this index is only 2%.

In conclusion, while numerous indicators for sustainable urban drainage demonstrate negative trends, those associated with the new rigorous European standards tend to exhibit superior performance. This emphasizes the need for establishing new transparent and objective goals in conformity with the new European directive. To this end, the legal framework and the objectives of PENSARP2030 are expected to be updated in order to align with the future requirements. The following chapter will explore the engineering solutions that have the capability to meet these evolving goals.

2.3.4 Current engineering practices

To achieve sustainability and resilience, investment in infrastructure is essential, focusing on both rehabilitating existing systems and building new ones in smaller communities. In these areas, eco-friendly infrastructure can be designed from scratch, while in cities, adapting existing infrastructure is key. Sustainable urban drainage requires a range of stormwater management techniques, such as tank sewers, tunnels, separate runoff systems, and managing combined sewer overflows. To promote efficient drainage systems a review of the engineering practices has been made [3]:

Storage Tanks: also known as retention tanks, are underground structures designed to capture and temporarily store excess stormwater during heavy rainfall events. Allied to the drainage pipes, they help

to increase the system capacity by reducing the overload, and so, avoiding the flood. After the rain event, the stored water is released and special attention must be made to anaerobic conditions during storage.

Drainage Tunnels: drainage tunnels are underground structures that serve as conduits to transport large volumes of stormwater from urban areas to suitable discharge points, such as rivers or treatment plants. They act as efficient drainage pathways to divert water and so improve the network capacity in densely populated urban areas thus, prevent flooding in urban areas.

Promote Separative Systems: separative systems direct stormwater and sewage to separate drainage networks, keeping them apart throughout the collection and treatment process, facilitating an effective treatment of both flows and prevents CSO thus, water pollution by emergency discharges.

Modernize Combined Sewer Overflows: CSO are essential safety valves in combined sewer systems. When there is excessive flow in a sewer during heavy rainfall, that would exceed downstream capacity, CSO divert and discharge the excess flow to less damaging locations. Modern CSO are equipped with screens to prevent large solids from passing through to the discharge point. However, frequent operation indicates underlying issues in the system.

In addition to the conventional solutions previously discussed, a considerable number of innovative techniques have emerged in recent times regarding urban drainage practices and their contribution to sustainability. These are collectively known in Europe as Sustainable Urban Drainage Systems (SUDS) and are based on the sustainable management of surface water through the replication of natural drainage processes. To facilitate a more comprehensive understanding of these systems, the examples listed by Zhou [4] were classified into three principal categories based on their impact on water runoff and rainfall interaction:

Source Control Measures: These aim to manage and attenuate water runoff at its origin. Examples include local infiltration systems like impervious pavements, and green roofs. These measures help reduce peak flow and improve water quality during heavy rainfall;

On-Site Control Measures: These focus on mitigating flood hazards directly at the site. Techniques include individual asset protection and topographic modifications to reduce the susceptibility to flooding. The practical examples are Detention basins and Retention ponds;

Downstream Measures: These enhance the water quality treatment with bodies that use sedimentation and filtration to provide treatment of surface water runoff, for example wetlands.

The scarcity of data on the performance of different SUDS presents a significant challenge in assessing their effectiveness and developing clear guidelines. For instance, determining the extent to which the hazard can be reduced is a major issue in this regard. A significant challenge associated with SUDS is their spatial requirements for effective water retention and infiltration, which can be a limitation in densely populated urban areas. Moreover, there is frequently a lack of confidence among decision-makers regarding the long-term benefits of these systems [22].

Nevertheless, integrating SUDS with traditional drainage systems can be crucial to enhance the overall resilience and sustainability of drainage systems in areas with less space constraints or in locations where these are not possible to implement [22].

2.3.5 Modelling as a tool

In view of the concepts presented in the preceding chapter, it becomes evident that the complexity of urban drainage systems is considerable, due to the presence of ageing networks that are hard and costly to maintain, most of the times insufficiently or inadequately mapped, with low response capacity to emerging challenges. It is imperative that new projects not only navigate these challenges but also gain a profound understanding of the existing infrastructure, ensuring effective hydraulic interaction between the existing network and future developments. This reflects the necessity to comprehend these complex structures, which extends beyond the conventional design.

The inherent complexity of drainage systems gives rise to complex flows interactions and flow prediction becomes a challenge and models play a major role to overcome this. A model is either a scale model (a physically reduced but representative version of a system) or a mathematical model (using equations, variables, and parameters to describe system behaviour, such as fluid dynamics simulations) [5].

Hydraulic modelling has transitioned from one-dimensional Fortran-based 'black box' programs in the 1960s to today's three-dimensional software. With the significant improvement of computer speed two-dimensional modelling is well established and nowadays almost all modelling software's have this capability, at the same time they provide fast results [23]. These techniques have enabled the prediction of the flow behaviour by computing their physical nature, with their usage in civil engineering becoming increasingly common and accessible.

This master thesis will explore numerical modelling, with a particular focus on Computational Fluid Dynamics (CFD), a powerful tool to analyse the behaviour of fluids.

CFD involves the numerical simulation of fluid flow within a defined domain, which is achieved by dividing the problem into discrete cells. The governing partial differential equations of mass, momentum and energy conservation are solved in each cell, alongside boundary conditions and other physical phenomena. CFD has the capability to compute several flow properties in three-dimensional (3D) domains, with transient flows [23].

As tool to hydraulic infrastructure design, CFD has already been employed in the field of urban drainage with focus on CSOs, storage and attenuation systems, stormwater sediment interceptors, and sewerage conveyance structures [6].

Previous studies confirmed that CFD simulations provided a high-fidelity model of complex flow behaviour during urban flooding, accurately predicting flood propagation and turbulence patterns [24]. Besides this, CFD has been shown to enable detailed prediction of hydrodynamic behaviour and

sediment capture in drainage units, and has proved to be effective in designing efficient structures and reducing the need for physical prototyping through accurate simulation [25]. Another study has demonstrated the capabilities of CFD to predict flow depths and pressure heads, noting challenges in converging results in complex regions [26]. The reviewed studies range from a variety of analyses, either at reduced or real scale (prototype scale). In addition to these two analysis options, combinations were identified with the validation method, such as using field data [25] or laboratory experimental tests for validation [26].

With the papers analysed, keywords can be already identified regarding CFD usage, such as accurately predict and assessing the hydraulic performance, reducing the need for extensive experimental tests.

This master thesis differs from those analysis once the infrastructure performance has already been analysed and evaluated in previous experimental model tests. The performed CFD implementation has the goal to provide the implemented methodology based on a case study, at the same time that results are evaluated in terms of the simulation trade-off analysis at both scales to compare either scale effects or computational trade-off.

2.3.6 Digital Twins for asset management

Technologies play a significant role in the field of engineering, yet they serve different purposes and possess different capabilities. Digital twins (DT) are frequently considered to be a dynamic, real-time digital replica of a physical asset. This comprises not only a virtual model, but also a connection to the real-world environment via sensors to reflect the current physical state. Nevertheless, the definition of DT remains ambiguous and is subject to variation across different scientific disciplines [27].

Glaessgen and Stargel stipulated a broad definition in the context of aerospace engineering defining DT as “(...) an integrated Multiphysics, multiscale, probabilistic simulation of an as-built system that uses the best available physical models, sensor updates, (...), etc., to mirror the life of its corresponding flying twin.” [28]

In the field of civil engineering, the role of DT can be distinguished in two different phases, the design phase and after the design phase when the infrastructure is built. In the first phase, it is suggested that DT can be used to predict solicitations to the future built environment and after that, promote a deeper and high quality integrated three-dimensional design through a simulation-based analysis [29].

In the domain of civil engineering, the ability to anticipate responses to occurrences is advantageous, as it facilitates the testing of various scenarios prior to implementing design or operational measures. This has been applied to the scenario of pipe filling procedure with air release valves. The DT linked calibrated CFD results with collected real-time experimental data. Both CFD and experimental outputs were treated and optimised with trained artificial intelligence. This provided actionable insights that enabled the establishment of a predictive system for the purpose of enhancing the safety and efficiency of pipeline filling operations [30].

With this being said, CFD simulations can be directly linked to hydraulic engineering to establish a DT. By anticipating possible scenarios and through CFD simulations, compatible decision making can be performed, overcoming the real-time barrier with the time that those CFD simulations can take, representing an important management asset for hydraulic infrastructures. The evolution is seen towards machine learning and artificial intelligence to provide optimized models and improved calibration of the DT [31].

3 Numerical Models - Computational Fluid Dynamics

3.1 Overview

This chapter is an introduction to the field of Computational Fluid Dynamics (CFD) as it pertains to the analysis of fluid flow within the context of complex hydraulic structures. Furthermore, this chapter will examine the specific capabilities and limitations of Flow3D, a commercial software developed by *FlowScience, Inc.*

CFD synthesises principles from fluid mechanics, mathematics and computer science to model the movement and interaction of fluids with surfaces. In practice, CFD software divides the domain in which the fluid can move into discrete elements, which are combined to form a mesh (grid). Subsequently, the software performs calculations at each cell to predict the behaviour of the fluid under specific conditions, such as varying temperatures, pressures, or velocities, in order to provide a comprehensive and accurate representation of the fluid's behaviour.

CFD is a valuable tool for simulating fluid flows as it helps reducing lead times and costs in design and production. It also allows for the modelling of complex flow problems that analytical methods cannot. Modern hardware and associated declining costs have made CFD tools more increasingly available to the academic and technical communities [32].

CFD software users can use a commercial or open-source software package. Commercial software is more user-friendly and includes user support. Open-source software allows users to make changes directly but requires a deeper understanding [23].

3.2 General software environment

CFD code packages are made up of three main parts: preprocessor, solver, and post-processor. In the pre-processing stage, the system's geometry, physical conditions, computational mesh, and computational domain are defined. The solver uses numerical techniques to solve the involved transport equations (namely the mass and momentum - Navier-Stokes - equations) and calculates a wide range of flow properties. The post-processor allows to present a high volume of results data in 3D and many other graphical or tabular layouts, allowing for project design interpretation [33]. The interrelationship between the various phases of the majority of CFD software is illustrated in Figure 6, in the next page.

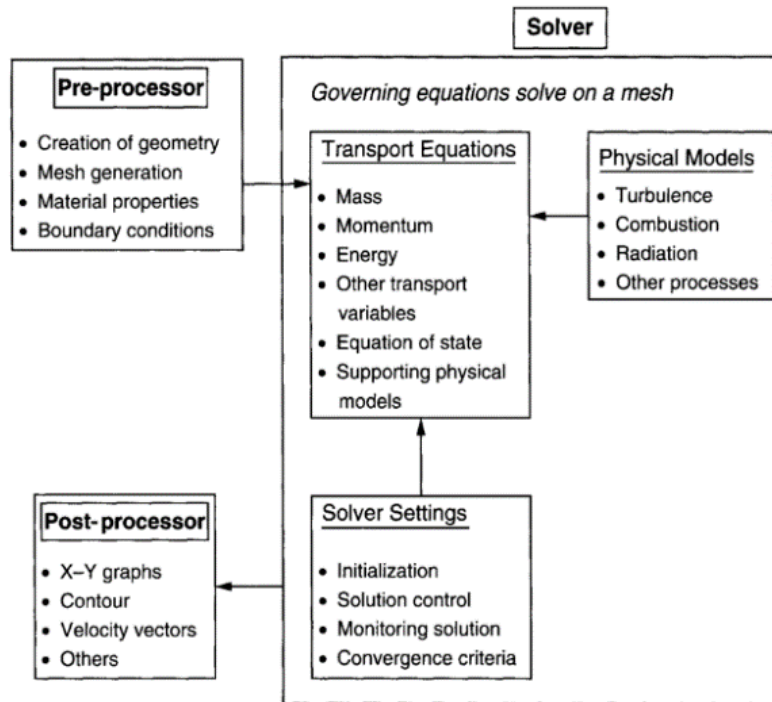


Figure 6 - CFD approach [32]

3.2.1 Pre-processor

The pre-processor stage comprises the definition of the model geometry, the creation of a computational mesh, and the specification of the fluid properties, the boundary conditions, and the physical phenomena to be considered.

3.2.1.1 Geometry

The initial step is defining the problem geometry, which can be done with computer aided design (CAD) software. However, software can have requirements regarding the geometry, so it is often necessary to modify it to overcome those. Discrepancies in the imported geometry can lead to less accurate solutions due to gaps that misled the calculations [23].

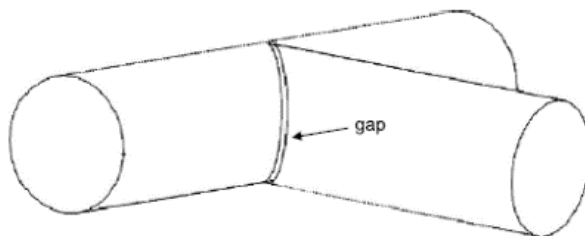


Figure 7 - Example of a geometry error, with non-coincident edges [23]

3.2.1.2 Computational Mesh

The subsequent stage is the generation of the mesh, as the process of a CFD simulation requires the subdivision of the domain into smaller subdomains, frequently referred to cells. This is a critical and frequently challenging aspect of CFD modelling, as the process demands an optimised subdivision. Mesh adaptations are a common occurrence during the course of simulation trials given that this step is often perceived as being particularly challenging and so, this process should be seen as an interactive and dynamic step [33].

The method of using infinitesimal fluid elements is fundamental to deriving the governing equations for fluid flow, thus enabling the creation of an accurate and efficient model of the entire flow field. By considering a small differential volume within the flow field, the fundamental physical principles are applied directly to this element, thereby leading to the formulation of partial differential equations. These infinitesimal elements are treated as continuous, despite their size, thus enabling the application of calculus to describe changes in flow properties, such as velocity and pressure, at every cell within in the domain.

The mesh can be cartesian, entire set of discrete cells are aligned along the orthogonal axis, or non-cartesian that by itself can be structured or non-structured if elements are arranged in a randomly. The term structured denotes that positions of the nodes of a face can be stored in two-dimensional arrays and their neighbours are consequently also well defined. The most common 3D solids used for cells are tetrahedra, pyramids, wedges and hexahedra [23].

3.2.1.3 Boundary Conditions

Once the computational domain has been defined, the subsequent step is to set the boundary conditions within the domain. These conditions will subsequently be employed to solve the governing equations. This involves the definition of the actual conditions observed in the system at the inlet, outlet, and other sections of the domain relevant to the problem. This ensures that the model is not subject to unrealistic conditions and are essential so that the partial differential equations describing the flow can be solved unambiguously. The material and fluid properties, and others that are independent to the flow behaviour are also imputed in the model, including viscosity, heat transmission coefficient, surface roughness, and others [32].

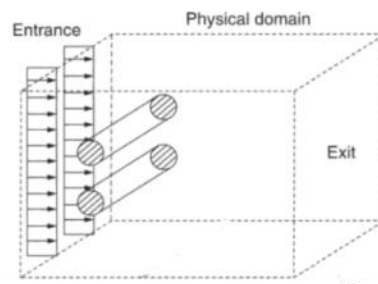


Figure 8 - Illustrative example of fluid passing around two cylinders adapted from [32]

3.2.2 Solver

One of the most challenging aspects CFD is the complexity involved in its numerical foundations. The objective of a CFD solver is to numerically solve the governing equations of fluid dynamics across the entire computational domain, typically for each time step (simulation advance by small increment in time). These equations are usually expressed in their partial differential form, as this formulation allows for the representation and resolution of local flow quantities [32].

The use of a higher level of resolution allows for a more accurate representation of physical phenomena. This, in turn, leads to the formulation of the problem with cells in a mesh using methods that define the calculated flow variables at discrete points, known as nodes. These nodes are related to the cells and are employed for numerical operations [32].

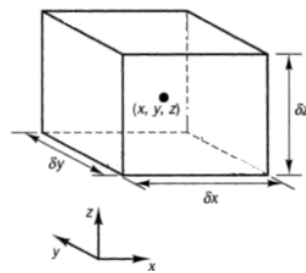


Figure 9 - Example of a Tri-dimensional fluid element/cell and its node

To obtain approximate solutions to partial differential equations that govern fluid flow, CFD solvers typically employ one of three primary numerical methods: the Finite Difference Method (FDM), the Finite Element Method (FEM), and the Finite Volume Method (FVM). Each method has its own set of advantages and disadvantages in terms of accuracy, computational cost and ease of implementation. A common characteristic among these methods is that they discretise the computational domain and represent the continuous fluid behaviour by approximating the values of flow variables — such as velocity, pressure, and temperature — at a finite set of nodes or control points. This discretisation forms the basis of a numerical solution to a continuum problem [33].

The FDM employs Taylor series to approximate derivatives by finite differences, facilitating straightforward integration with equidistant structured meshes. In contrast, the FEM is a more complex approach, using basis functions (which may be polynomial-like in nature but are not derived from a Taylor series) to approximate the solution of the differential equation across each cell. Furthermore, FVM offers greater flexibility in decomposing the solution domain. It begins by applying the integral form of the conservation laws (such as conservation of mass, momentum, and energy) across the boundaries of the controlled volumes followed by the conversion of volume integrals into surface integrals with the divergence theorem, allowing to handle fluxes across boundaries [34] as illustrated in Figure 10, in the next page.

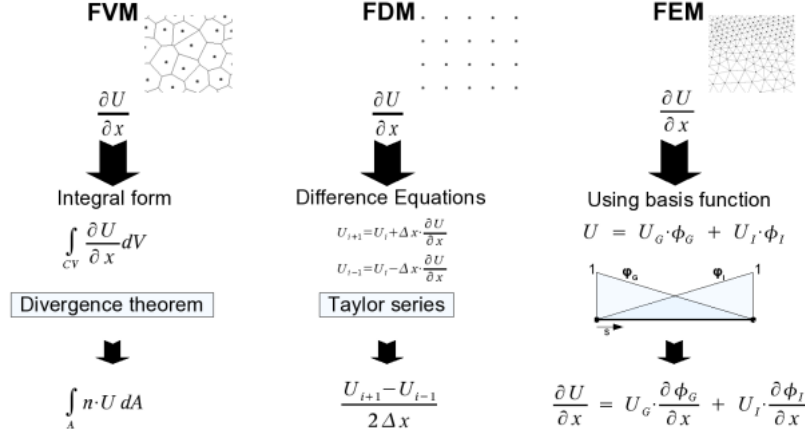


Figure 10 - General overview of the numerical methods and their essentials differences adapted from [34]

One of the key advantages of FVM is its capacity to inherently preserve conservation laws, making it ideal for complex engineering, including shock waves and high Reynolds number flows. FVM struggles to accurately define higher-order derivatives and achieve higher accuracy beyond the second order [32].

During the processing phase, these methods approximate calculations linearly or with second order (or higher) schemes that use more complex interpolations. This accuracy order is directly related to how well the processor can estimate the partially differential equations in the discrete mesh. Nevertheless, FVM flexibility and robustness make it a widely used CFD method in cases where first-order accuracy is sufficient [32] such as in turbulent free surface flows.

3.2.2.1 Governing Equations

The three governing equations of fluid dynamics embedded in the solver to calculate the flow variables along time are well studied and their presentation has many variations. According to the formulations by Henk [33] and Jiyuan [32] a pragmatic approach to these partial differential equations has been done and enumerated below, accompanied by a summary description of their variables:

- Mass conservation equation (Continuity equation of mass conservation, continuity equation or mass continuity equation):

$$\left\{ \begin{array}{l} \text{rate of increase of} \\ \text{mass of fluid in the cell} \end{array} \right\} = \left\{ \begin{array}{l} \text{net rate of flow of} \\ \text{mass in the cell} \end{array} \right\}$$

$$\frac{\partial \rho}{\partial t} = -\rho \nabla \cdot \mathbf{u} \quad \text{Eq.(1)}$$

Where all the fluid properties are function of time and space. The variable $\mathbf{u}$ denotes the velocity vector (u, v, w) in x, y , and z respectively and ρ the fluid density (mass per unit volume), this also applies to the following equations. When dealing with an incompressible fluid, as water, the density ρ is constant and so Eq.(1) becomes:

$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad \text{Eq.(2)}$$

- Momentum conservation equations (also expressed by Newton's second Law or Navier Stokes equation):

$$\left\{ \begin{array}{c} \text{rate of change of} \\ \text{momentum of} \\ \text{the fluid in the cell} \end{array} \right\} = \left\{ \begin{array}{c} \text{net rate of momentum} \\ \text{added to the} \\ \text{fluid in the cell} \end{array} \right\} + \left\{ \begin{array}{c} \text{net external forces} \\ \text{acting on the} \\ \text{fluid in the cell} \end{array} \right\}$$

The middle term of this balance represents the contribution of pressure gradients acting across an infinitesimal fluid element, which serve to accelerate or decelerate the fluid. It also includes viscous forces arising from the fluid's internal resistance to deformation, represented by the normal stress, σ_i , and viscosity, μ . Finally, it accounts for diffusive effects, involving second-order derivatives of the velocity field, which stem from the fluid's viscosity. The right term is related with external forces, F_{ext} , such as gravity in the z direction, centrifugal forces, or electromagnetic forces:

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \mathbf{p} + \mu \nabla^2 \mathbf{u} + \nabla \sigma + \mathbf{F}_{ext} \quad \text{Eq.(3)}$$

- Energy conservation equation (known as first law of thermodynamics)

$$\left\{ \begin{array}{c} \text{rate of change of} \\ \text{energy in the fluid in the cell} \end{array} \right\} = \left\{ \begin{array}{c} \text{net rate of heat added} \\ \text{to the fluid in the cell} \end{array} \right\} + \left\{ \begin{array}{c} \text{net rate of work done} \\ \text{on the fluid in the cell} \end{array} \right\}$$

$$\rho \frac{DE}{Dt} = \frac{\partial}{\partial x} \left[K \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[K \frac{\partial T}{\partial y} \right] + \frac{\partial}{\partial z} \left[K \frac{\partial T}{\partial z} \right] - \nabla \cdot (\mathbf{u} \cdot \mathbf{p}) + \varphi \quad \text{Eq.(4)}$$

Where K represents the heat conductivity and the effects due to the viscous stresses are represented by the dissipation function φ and are due to the mechanical energy that is converted into heat [33].

3.2.2.2 Additional Physical Processes Modelled

In addition to the governing equations of fluid dynamics, many CFD problems require the numerical modelling of additional physical processes. Common examples include heat transfer, solid transportation, cavitation, electro-mechanic formulations and others. Since this work aims at simulating the flow field in a hydraulic structure, the most relevant additional physical phenomenon to be considered is turbulence, as most flow scenarios encountered will be turbulent.

Turbulence is as a chaotic and irregular fluid motion typically associated with high Reynolds numbers, where inertial forces prevail over viscous forces. It is characterized by the formation of eddies and vortices of various scales, which interact through an energy cascade from large to small structures. This dynamic increases the transfer rates of momentum, heat, and mass, leading to highly complex flow patterns [35].

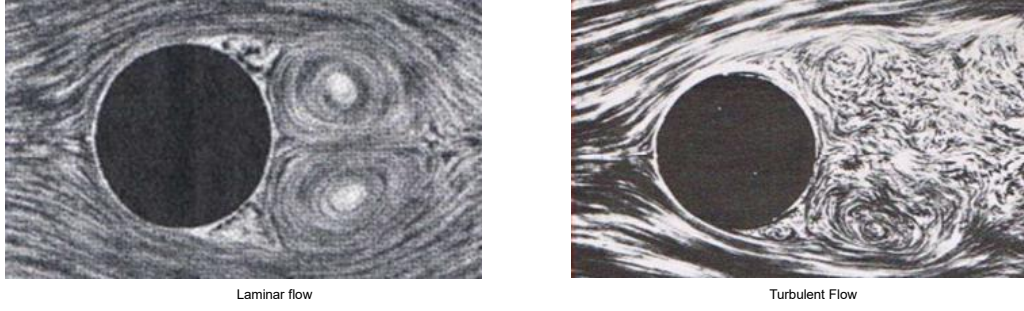


Figure 11 - Laminar and Turbulent flow [35]

To analyse turbulent flows, a process known as Reynolds decomposition can be applied, where each flow variable is expressed as the sum of a time-averaged (mean) component and a fluctuating component. When these decomposed variables are substituted into the Navier–Stokes equations and averaged over time, the resulting equations — known as the Reynolds-Averaged Navier–Stokes (RANS) equations — describe the behaviour of the mean flow, while accounting for the effects of turbulence through additional terms representing the averaged influence of the fluctuations [36].

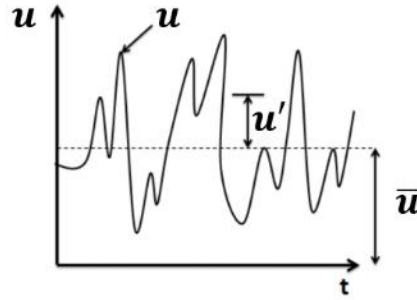


Figure 12 - Reynolds decomposition of a turbulent flow, adapted from [36]

Applying Reynolds decomposition, each instantaneous velocity component (e.g., in the x-direction, u) is expressed as the sum of a time-averaged (mean) value and a fluctuating component, u' :

$$u = \bar{u} + u' \quad \text{Eq.(5)}$$

RANS equations differ from the original Navier–Stokes equations by the presence of an additional term, the Reynolds stress tensor, which accounts for the effects of turbulence/fluctuating component.

Because the Reynolds stresses introduce more unknowns than available equations, they require turbulence models to close the system. Several modelling approaches exist — such as Eddy Viscosity Models (EVM) and Reynolds stress models (RSM) — each with varying implications for accuracy, computational cost, and mesh requirements. The choice of turbulence model directly influences the quality of the numerical results, particularly in complex geometries or highly anisotropic flows, and may require adjustments in mesh refinement and solver settings. This is typically achieved by introducing the turbulent viscosity, μ_t and the transport equations for the turbulent kinetic energy, k . RSM solves additional transport equations for each component of the Reynolds stress tensor, making them more

computationally intensive. EVMs, on the other hand, are based on the Boussinesq hypothesis, which assumes turbulent flows behave similarly to Newtonian fluids [23].

In EVMs, the turbulence viscosity, μ_t , is computed algebraically solved by relating the Reynolds stresses to the mean velocity gradients. by one-equation models or two-equation models, such as, $k - \epsilon$ model and $k - \omega$ model. This can be achieved through one-equation models, where μ_t is computed as function of k or through two-equation models that also solve a second equation for either the dissipation rate of turbulent kinetic energy, ϵ , or the specific dissipation rate, ω . Common two-equation models include the $k-\epsilon$ and $k-\omega$ formulations [35].

The following text provides an overview of the six commonly used turbulence modes, based on Ideen [32], including their numerical formulations, strengths, weaknesses, and the typical application domains.

Zero-Equation Models: Does not solve transport equations; they rely on empirical correlations to estimate turbulent viscosity, typically using a mixing length approach.

- Extremely fast and robust; suitable for preliminary and fully developed simple flows, such as in laminar-to-turbulent transition scenarios.
- Poor accuracy in predicting turbulence effects, especially in complex flows where detailed turbulence prediction is needed.

One-Equation Models: Solve a single transport equation, k , or a related variable.

- Computationally efficient and suitable for simple flow configurations..
- Less accurate than two equation models, especially in complex geometries or flows with significant anisotropy.

Standard $k-\epsilon$ Model: Employs the Boussinesq hypothesis, which relates the Reynolds stresses to the mean velocity gradients through the turbulence viscosity concept. It solves two transport equations: one for k and another for ϵ . The model assumes isotropic turbulence, which simplifies the representation of turbulent flows. It is based on empirical observations and has been extensively validated across various engineering applications.

- It is computationally efficient and relatively easy to implement. The model provides reasonable predictions for a wide range of engineering applications, particularly in external flows. Best suited for fully developed turbulent flows, particularly in pipe flows
- The model struggles with flows that exhibit strong curvature, separation, or low Reynolds numbers. It also fails to capture the anisotropic nature of turbulence, leading to inaccuracies in certain flow conditions.

RNG k - ϵ Model: Modifies the standard k - ϵ model by incorporating additional terms derived from statistical mechanics. This model includes a more sophisticated treatment of μ_t and includes modifications to ϵ equation.

- It provides improved predictions for flows with significant curvature, separation, swirling motions, such as in mixing tanks and around obstacles, compared to the standard k - ϵ model. The model is also capable of capturing the effects of rotation and other complex flow features.
- The increased complexity leads to higher computational costs. Additionally, it may still struggle with low Reynolds number flows and requires careful calibration.

k – ω Model: Solves two transport equations: one for k and another for ω . The k – ω model is advantageous in low Reynolds number flows.

- Effective in capturing the behaviour of turbulence near walls, boundary layers and flows involving separation. The model is effective in capturing the effects of turbulence in complex geometries and can handle adverse pressure gradients effectively.
- The k – ω model can over-predict turbulence in regions with strong acceleration and may require a fine mesh near walls for accurate results.

Reynolds Stress Model (RSM): Solves transport equations for each component of the Reynolds stress tensor, allowing for a more detailed representation of turbulence.

- Provides a detailed and accurate representation of turbulent flows, especially in complex geometries, swirling flows, flow separation, rotation and flows with strong shear, such as in turbomachinery and mixing processes. Suitable for a wide range of applications. This model accounts for anisotropic turbulence and captures the directional effects of turbulence more accurately than EVM.
- High computational cost due to the need to solve multiple equations. The model requires careful calibration and validation to ensure accurate predictions.

An alternative to RANS for turbulence modelling is Large Eddy Simulation (LES). LES explicitly resolves the large, energy-containing turbulent structures, while the effects of the smaller scales — typically responsible for dissipation — are accounted for through subgrid-scale (SGS) models. This approach reduces reliance on empirical turbulence modelling, thereby offering higher accuracy in capturing the dynamics of unsteady and anisotropic turbulent flows. However, the increased fidelity comes at the cost of significantly greater computational demands, particularly for complex geometries or high Reynolds number flows. As a result, LES is typically employed in applications where detailed flow predictions are essential, such as in aerodynamic design, combustion modelling, and others [23].

A schematical representation of the main types of turbulence models addressed above is summarized in Figure 13 in the next page.

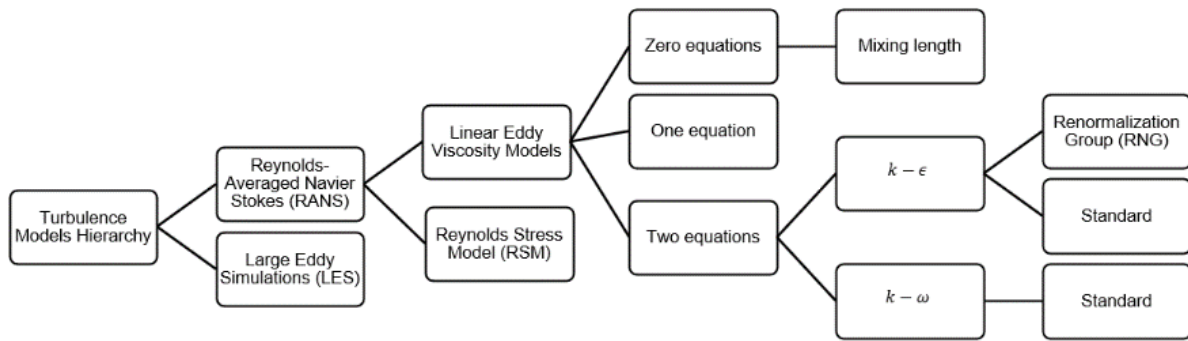


Figure 13 - Described turbulence models

In the context of the common solver settings, the initial conditions of the simulations can be defined. If the initial conditions are close to the actual steady-state solution, the simulation process will converge at a faster rate. However, if the initial conditions are unrealistic, the simulation may take longer or result in instability [32].

3.2.3 Post Processor

Post-processing of CFD results entails the visualization and interpretation of the results to gain insight into the behaviour of parameters across the domain. This facilitates the detection of potential inaccuracies or unsatisfactory outcomes, enabling adjustments by revisiting earlier steps. Some CFD software provides a comprehensive range of plots for this data, since text files to 3D plots [33].

Comparing the numerically obtained results with corresponding experimentally obtained is essential for verifying the accuracy and reduce discrepancies. Besides this, it is recommended that users divide complex simulations into smaller, more manageable components, beginning with a basic model and gradually introducing complexity. The accuracy of the model can be validated using analytical solutions [33] such as, Manning's equation for uniform regimes in open flows to estimate water depth or velocity, critical depth estimation in parallel with Froude number calculation, and other literature formulations.

3.3 Flow3D environment

The following review on Flow3D software is based on the available user manual [37] which provides essential guidance for setting up CFD simulations using this software. It outlines the key steps and procedures involved in building and running simulations with the Flow3D environment.

Flow3D is a commercial software program that employs a graphical user interface (GUI). Its numerical methods are less flexible for user manipulation than those of freeware, although the GUI has a more intuitive aspect. As with other CFD software, Flow3D employs the FVM to solve the governing equations of fluid dynamics.

For setting the geometry of the problem, users can use the Flow3D primitive shapes within the GUI, such as spheres, cylinders, cones, ellipsoids and toroids. Most design packages can convert solid

models into a format used for stereolithography known as the stereolithography format (STL), imported to the domain in the GUI and the combination of both methods can be used to define the problems geometry.

In terms of the mesh, Flow3D subdivides the flow domain into a cartesian grid, which can be uniform or non-uniform by varying cell size along specific coordinate directions (x , y or z) of the domain.

As said before, cells store information in certain locations, known as nodes, in Flow3D fluid velocities and pressures are located at staggered mesh locations as shown for a typical cell in Figure 14: u and fractional area A_x at the centres of cell-faces normal to the x -direction, v and A_y at the centres of cell-faces normal to the y -direction, and w and A_z at the centres of cell-faces normal to the z -direction. Pressures (p), fluid fractions (F), fractional volumes (V_F), densities (ρ), internal energy (I), turbulence quantities for energy (q), dissipation (D), and viscosity (ν) are at cell centres.

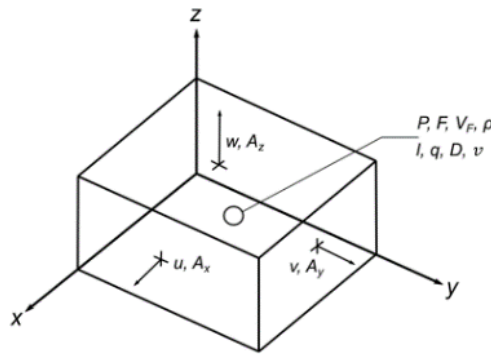


Figure 14 - Location of variables in a rectangular Flow3D cell, adapted from [37]

Flow3D can operate in various modes, depending on the assumptions applied to the general fluid equations. These include configurations for incompressible or compressible flow as well as for tracking multiple fluids. For incompressible assumption, the fluid density and energy may be assumed constant and do not need to be computed. Besides the delineation of the fluid intrinsic properties, other physical phenomenon like heat transfer, turbulence, particle transport, and others, can be defined by the user.

3.3.1 Mesh Generation

In flow Flow3D there are several ways to combine mesh blocks, a single block for simple flows or multi-block for more complex ones. The single block approach may be insufficient for complex flows where the mesh refinement may not align with the required resolution. This could result in longer simulation times or an inability to accurately reproduce the flow or the geometry.

To address this, the user can apply multiple blocks of mesh to the domain. Other type of mesh is the “nested-block”, which is situated within another mesh block. This results in an improvement in resolution in specific areas. These last two examples must adhere to specific computational requirements, for example mesh planes must be fully coincident, Figure 15, or a maximum cell ratio between adjacent

blocks and nested block, to avoid abrupt reduction in cell size that can result in numerical instability and errors.

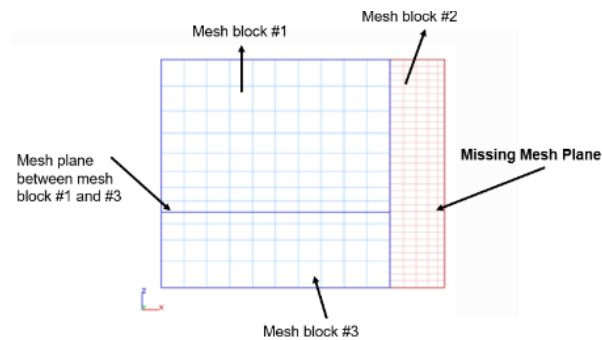


Figure 15 - Coincident Mesh Planes

In Flow3D, the mesh size (total amount of cells in the domain) can be defined in two distinct ways, and both are a mathematical consequence of the geometric position of each mesh plane, that limits the three-dimensional position of the cube/paralepidid shape. The first way is a mesh size as a consequence of setting a certain cell size and the second is a user-defined total amount of cells in the mesh that results in a certain cell size.

3.3.2 Fractional Area Volume Obstacle Representation

In Flow3D the equations are formulated with area and volume porosity functions and this formulation, called Fractional Area Volume Obstacle Representation (FAVOR™) and, so, zero-volume porosity regions are used to define obstacles. Porosity functions introduce simplifications in the specification of free surface and wall boundary conditions inside the mesh. With FAVOR™ method, the geometry is embedded in the mesh by the preprocessor which computes the fractional areas of the mesh cells open to flow, alongside with the volume fraction open to flow.

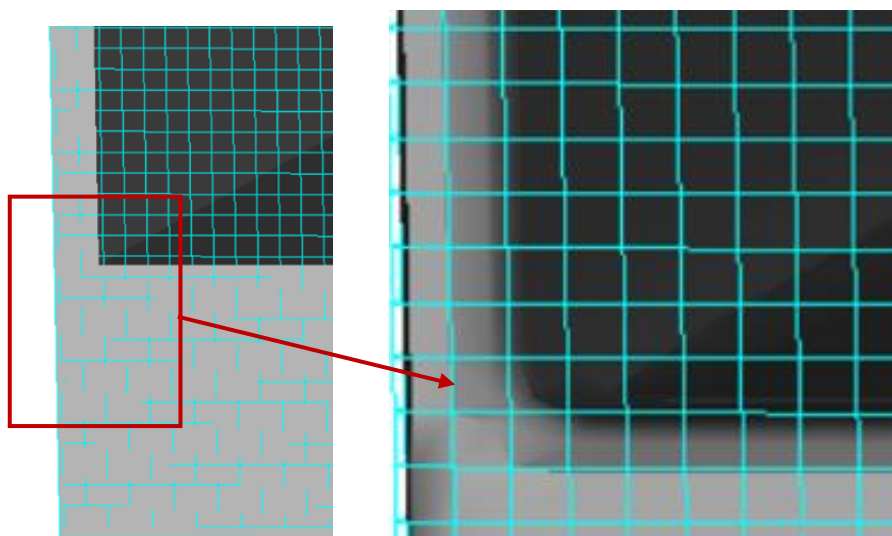


Figure 16 - Example of FAVOR™ method result in a perfect corner

With this method, the final shape of the obstacle can depend on the mesh specified by the user. A mesh with smaller cells will better reproduce the geometry, but this increases the numerical effort and so, a balanced and good mesh choice should be made, and for complex geometry and taking advantage of the mesh generation tools in Flow3D is crucial to achieve this balance.

3.3.3 Volume of Fluid method

In one-fluid simulations using Flow3D, free surfaces are common but difficult to model due to discontinuities in flow parameters like density, velocity, and pressure. Flow3D simplifies this by neglecting the inertia of the gas next to the liquid, replacing the gas volume with an empty, massless static space. This reduces computational effort, as the gas movement is usually insignificant compared to the liquid's heavier flow, and so, the model does not capture air entrainment or turbulence effects from air injection or momentum exchange between air and water. The free surface acts as an external boundary for the liquid, and accurate boundary conditions are key to capturing its dynamics.

To model this, Flow3D utilizes the Volume of Fluid (VOF) method. This method consists of three key components: defining the VOF function, $F(x, y, z, t)$, solving the VOF transport equation, and setting boundary conditions at the free surface.

For a single fluid, F represents the fraction of volume occupied by the fluid within a cell, and F value is defined to be equal to 1 in the fluid and 0 outside fluid, i.e. in the void, for single fluid simulations. Over a control volume, the value of F will be within the segment $[0.0, 1.0]$, as shown in the following image. With this, the volume of fluid in a cell is given by the fluid fraction times the cell volume.

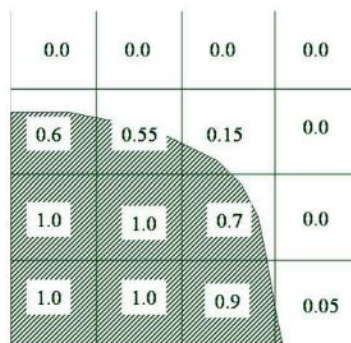


Figure 17 - Typical values of VOF function near the free surface [25]

The transport equation of F uses a type of Donor-Acceptor flux approximation, the cells will lose and gain volume according to the velocity in the cell face. For example, the x -direction if u is positive, the upstream or left cell is the donor and the downstream or right cell the acceptor.

In Flow3D there are different methods to track fluid interfaces, each suited for a certain type of flow problem: a sharp interface and a diffuse interface. In a single fluid free surface problem, it is recommended to simulate it as a sharp interface, thus will use the above described VOF method.

4 Methodology

4.1 General Overview

This chapter delineates the methodology to be employed in a numerical analysis of a free surface flow with CFD. The analysis comprises the numerical model formulation followed by the convergence observation and lastly, theoretical aspects when extrapolating numerical simulation results at reduce scale (e.g. the one considered in a physical model) to the prototype scale to evaluate possible scale effects.

4.2 Numerical Model Set-up

The numerical formulation comprises the main aspect in view with the employed software, Flow3D, to reach an optimal trade-off between the elapsed time to produce results and the quality of those results.

To sustain the definition of the critical decisions during the development of the numerical formulation, the software particularities that will directly affect the performance must be known previously. With the literature revision made on the previous chapter and for a free surface flow, the following aspects are identified as critical decision barriers:

- Correct geometry definition;
- Adequate boundary conditions;
- A suitable mesh definition allowing mesh independent results;
- Proper turbulence model for the problem being modelled;
- Appropriate set-up enabling numerical convergence.

The geometry construction of a complex infrastructure is aided through the use of CAD and small geometry errors, not perceptible in the CAD software resolution, can lead to incorrect flow propagation. This can occur when mesh resolution can identify those errors and compute the volume as open to fluid by the FAVOR™ method. This leads to losing part of the flow, a problem only identified later in the simulation.

Besides the iterative process to build an optimal simulation trade-off, if different scenarios are also to be simulated, thus resulting in different hydraulic solicitations, improvements can be achieved after those trial runs identify weaknesses that can compromise the model accuracy and numerical efficiency or accuracy.

The approach to reach an optimal simulation has an iterative development, due to the interconnectivity of these aspects in the simulation performance that will influence the validation towards an optimal definition of the numerical model. Due to this interconnectivity that results in an iterative process, a synthetic flowchart for the numerical set-up methodology of a CFD model is proposed in Figure 18.

The flowchart comprises 3 main stages: The construction of the model, its validation, and the execution of the simulation (simulations runs).

The model construction is finished after the initial four steps have been completed, thereby after a positive response to the first question of whether the boundary conditions reflect the expected behaviour, referred as boundary conditions validation, the first stage of validation. The model validation is completed when convergence is achieved. This is done by testing several mesh and turbulence models to optimize the computational efforts and guarantee mesh independent results, while the observed flow behaviour and results are compared with experimental data, bibliography or field data, to better identify incongruencies. The last stage is to perform the desired experiences and collect data, making the correct adaptations for different scenarios, with a focus on exploiting the insights gained from preceding work.

The flowchart starts with this first iteration, the main goal is to guarantee that the boundary conditions are imposing a correct flow propagation according with the expected, and the advice given in the user manual [37] is to stipulate boundary conditions with physical formulation using stagnation pressure, hydraulic head or velocity.

With the boundary conditions reproducing the expected behaviour comparing with experimental results or literature formulations, the following iterations are focused on the optimization of the mesh, in terms of well integration of the geometry (avoidance of geometry gaps due high cell size), optimization of computational times and mesh independent results.

Following this, other turbulence models should be studied in order to analyse the trade-off between computationally efficiency and accuracy, as discussed in section 3.2.2.2.

To collect data, measuring points and flux control surfaces should be considered in specific locations of the domain and post-processing enables users to have a three-dimensional view of the flow facilitating a fast understanding of the boundary conditions, localize areas where the flux separation may require more refinement or even areas requiring improved reproduction of the actual geometry. The debugging file must also be consulted, where user is alerted with errors and possible improvements in certain locations of the domain, in a more detailed way than the in the GUI.

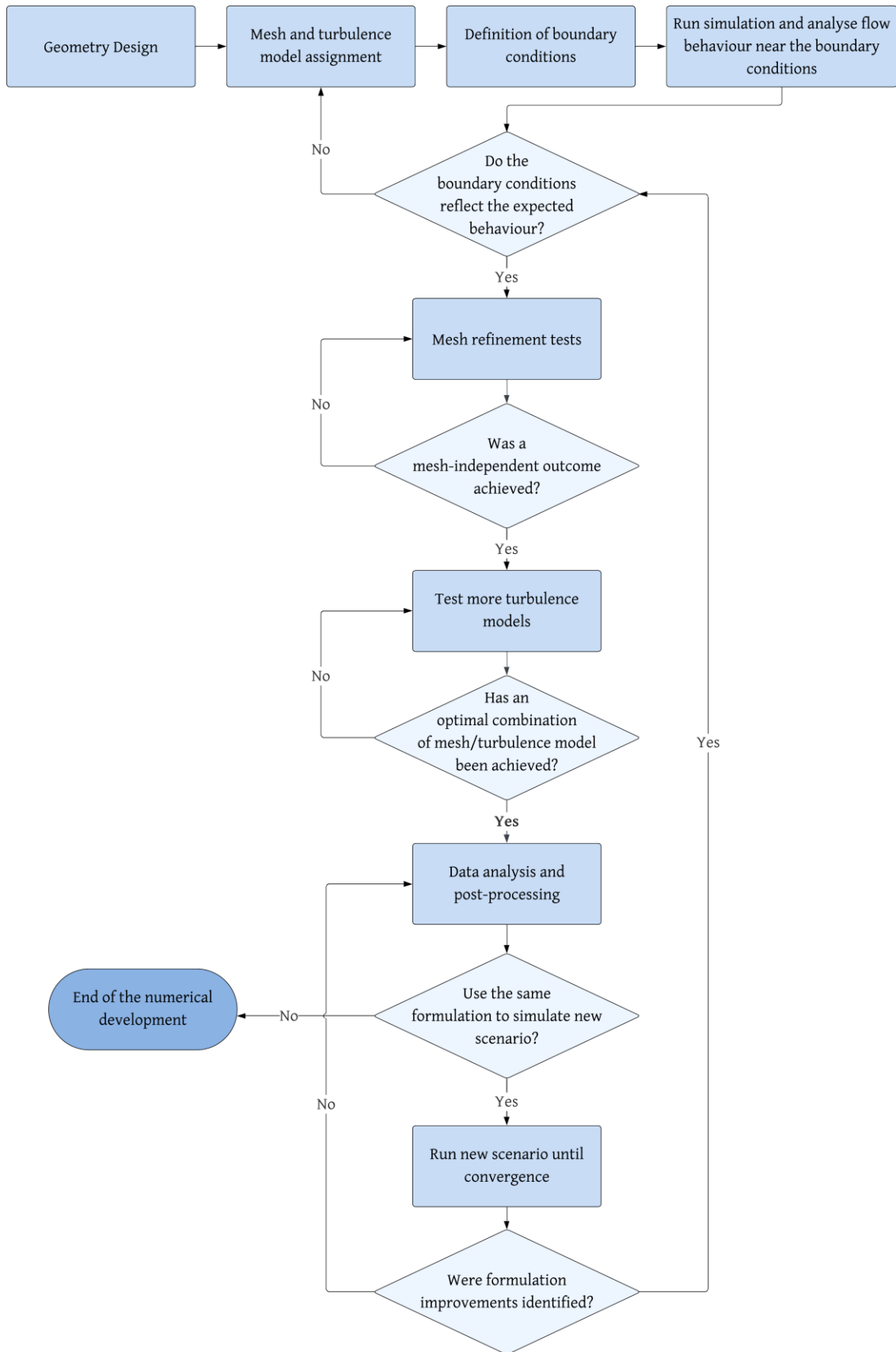


Figure 18 - Flowchart for the Numerical Formulation of the Free Surface Flow

4.3 Convergence Monitoring

To collect the results obtained in each simulation, two main aspects can be used, control sections designed with a known theoretical hydraulic behaviour capable of being calculated, or towards traditional experimental results. Both of these options are related with results comparison and so, results from the simulation must be collected.

Convergence is said to have been achieved when the iterative process doesn't change the governing equations solution from one iteration (internal computational loop within a time step to numerically solve the discretized equations) to the next, and the discretised equations are satisfied to a certain level of accuracy. In the last one, residuals are the metric used to quantify how close the numerical solution is to truly satisfy the governing equations [33].

Concluding, convergency is achieved when: residuals reach steady values, when key physical values stop changing and lastly when mass/energy balances is satisfied. The main aspects of no-convergence are poor mesh quality, incorrect boundary conditions, overly large time steps and turbulence modelling issues [33].

Flow3D monitors residuals of key variables including velocity components, pressure and VOF. Convergence is considered achieved when these residuals fall below predefined tolerance levels, which by default are set to 1×10^{-3} for velocity and pressure, and 1×10^{-4} for VOF [37].

Additionally, residuals must stabilize, showing no significant changes over successive iterations. Beyond residuals, the software also checks global mass conservation, requiring the mass error to remain below 1%. History Probes can be set up to track specific physical quantities like water height to ensure they reach a steady state, further confirming convergence [37].

Related to convergence tracking, Flow3D dynamically adjusts the time step based on the Courant-Friedrichs-Lewy (CFL) condition to maintain numerical stability. This condition limits how big the time step can be in order to obey a certain CFL value: if the time step is too large, the simulation "misses" important fluid motion, causing errors and divergence and so, the CFL condition forces the time step to reduce, ensuring that the fluid does not move more than one computational cell in a single time step. To do so, CFL condition, described in Eq.(6), is less than 1 in cells where advection is treated explicitly [37].

$$CFL = \frac{v \times \Delta t}{\Delta x} \quad \text{Eq. (6)}$$

Where, V is the characteristic velocity of the fluid (m/s), Δt is the time step (s) and Δx is the spatial step size (i.e., cell size in the direction x of the flow).

Related with the time step, if residuals increase abruptly, indicating potential instability, the software reduces the time step and conversely, if the solution remains stable, it increases the time step to improve computational efficiency [33].

4.4 Scale Effects Evaluation

In hydraulic modelling, scale effects refer to the discrepancies that arise when reduced scale model tests (conducted at reduced scales, mentioned as reduced model) fail to perfectly replicate real-world prototype conditions (mentioned as prototype), based on the non-dimensional Froude number expressed in Eq.(7) [38].

$$Fr = \frac{V}{\sqrt{gL}} = \left(\text{inertial force} / \text{gravity force} \right)^{0.5} \quad \text{Eq.(7)}$$

In this context, Froude's similarity law is the fundamental principle governing the comparison to take place, as it is a common practice when simulating free surface flows.

This similarity law provides the physical foundation for how the model replicates the behaviour of the flow in the prototype, thereby setting the relationships between the results obtained in the reduced model (m) and the corresponding ones in the prototype (p) conditions.

Froude's similarity law states that, in flows affected only by gravity and inertia forces, in two systems with boundaries geometrically similar, if the ratio between the gravitational and inertial forces (Froude number) is the same on both systems, there is a dynamic similarity based on their linear geometric relationship (L_m/L_p) also referred as geometric scale ($1/n$) [39].

$$\frac{L_m}{L_p} = \frac{1}{n} \quad \text{Eq.(8)}$$

The model and prototype relationship based on Froude's similarity law is shown below, as well with the adopted geometric scale:

$$Fr_m = Fr_p \Leftrightarrow \frac{V_m}{\sqrt{gL_m}} = \frac{V_p}{\sqrt{gL_p}} \Leftrightarrow \frac{V_m}{V_p} = \sqrt{\frac{L_m}{L_p}} \Leftrightarrow \frac{V_m}{V_p} = \sqrt{\frac{1}{n}} \quad \text{Eq.(9)}$$

The geometric scale results in the following relationship with the geometric scale:

$$V_m = V_p \times \left(\frac{1}{n} \right)^{0.5} \text{ as the velocity relationship} \quad \text{Eq.(10)}$$

$$A_m = A_p \times \left(\frac{1}{n} \right)^2 \text{ as the area relationship} \quad \text{Eq.(11)}$$

$$Q_m = Q_p \times \left(\frac{1}{n} \right)^{2.5} \text{ as the flow relationship once } Q = A \times V \quad \text{Eq.(12)}$$

$$t_m = t_p \times \left(\frac{1}{n} \right)^{0.5} \text{ as the time relationship} \quad \text{Eq.(13)}$$

Once the effect of the viscosity forces of the fluid is disregarded in Fr , the transposed results will inevitably lack full similarity, once both systems deal with the same fluid (same viscosity, μ) although, viscosity forces have more impact in the model much smaller water depths (h). With this, the model internal flow turbulence, represented by the Reynolds number (Re) is underestimated, leading to so called scale effects. This limits the dynamic similitude between the model and prototype and a way to assure that scale effects don't have a pronounced influence is limiting the validity of Froude similarity law as a function of the values of Re and so, the higher the Re , the lesser the scale effects, once it reflects the minimization underestimations of this impact. [38].

The limit value of Re in order to consider Froude Similarity Law is considered at 10^4 which corresponds to the transition zone of laminar to turbulent flow [40].

$$Re = \frac{Vh}{\mu} \geq 10^4 \quad \text{Eq.(14)}$$

The following chapter will present the application of these steps to the case study, which will also be introduced.

5 Case Study Numerical Development

5.1 Case study Overview

Lisbon faces significant challenges related to urban flooding, especially in the low-lying and densely populated urban areas where this phenomenon has been intensified by increasing urbanization, more impervious areas and extreme rainfall events, which have become more frequent due to climate change. Urban flooding often occurs during periods of intense rainfall, causing major disruptions such as human losses, material damage, disruption of mobility and negative economic and social impacts. The Lisbon's Drainage Master Plan (PGDL) aims to alleviate this problem by improving the existing drainage system.

This work considers a case study within the Alcântara drainage basin, Lisbon's major catchment basin, and, more specifically, the new inlet infrastructure to the new tunnel TMSA, one of the major infrastructures foreseen in the new PGDL. This new drainage infrastructure alone will serve directly 500,000 habitants [41] and it is designed to intercept the wastewater to an inlet structure localized in Campolide and then, divert the water flows from critical flooding areas, near river zones and low-lying zones throughout TMSA, until the discharge point localized in Santa Apolónia, adjacent to the Tagus River. This will be done by combining a series of hydraulic and environmental concepts, including a pre-treatment mechanism at the inlet infrastructure ranging from a well to capture large solids, an anti-pollution basin, wastewater screens and a tunnel, to divert the pre-treated flood flows from the existing downstream network, conveying them directly to the Tagus River. The locations of both the inlet structure and the tunnel are shown in Figure 19 [41]

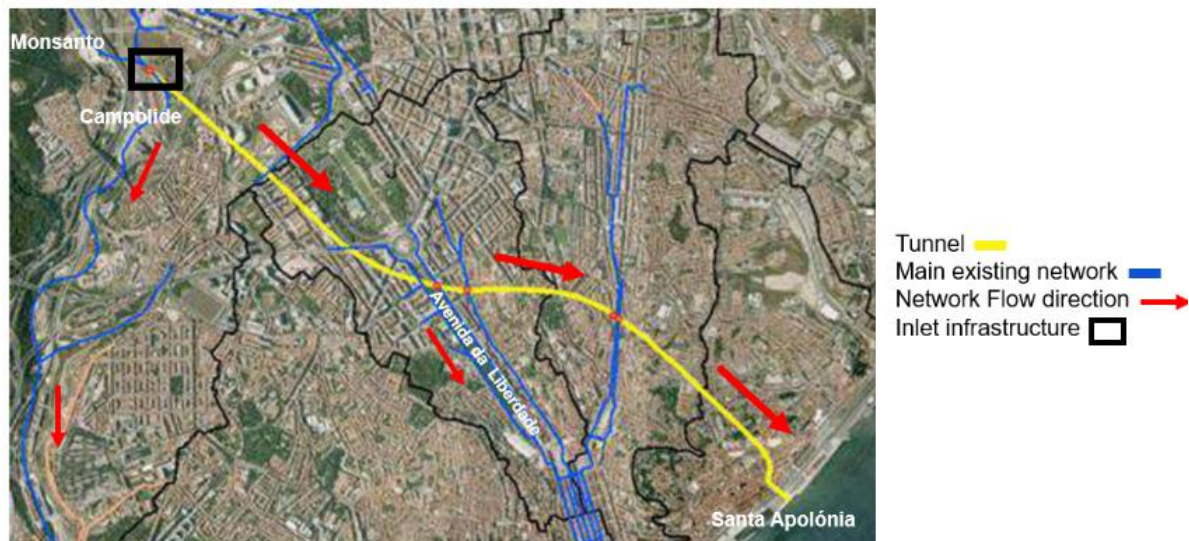


Figure 19 – Localization of the inlet structure and tunnel adapted from [42]

This new inlet structure represents a series of complex hydraulic features as it incorporates the management of dry weather flows, mostly domestic, frequent stormwater flows and peak stormwater flows that cause urban flooding in the current drainage system, during the wet period.

The design considered three crucial parameters, related to climate change and land use, which are, respectively: the increase in the intensity of heavy rainfall, the rise in the water level of the Tagus River and finally, the increase in the impervious areas due urban expansion [42].

The detailed concept of the inlet structure and the tunnel is described below, and a code of colours for each component in Figure 20 was made to identify each component.

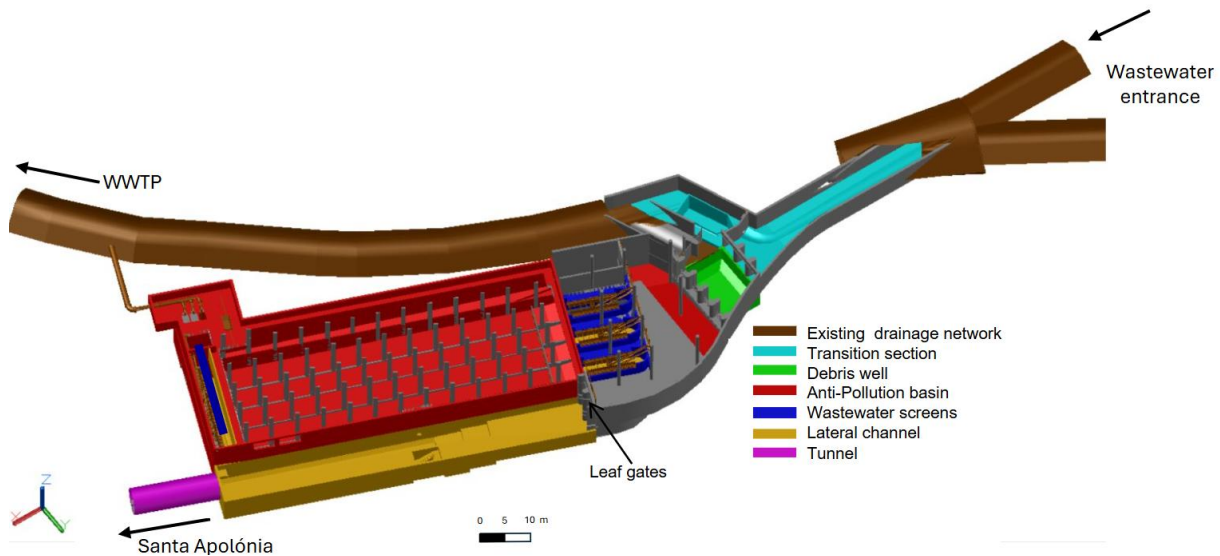


Figure 20 - Inlet Structure of the TMSA adapted from [41]

Transition section: This section carries the dry weather flows from the existing network to the Alcântara WWTP.

Debris well: Located after the transition section, the debris well retains larger debris/solids and protects downstream equipment's like the stormwater screens, gates and structural columns.

Anti-Pollution Basin: The anti-pollution basin enables the retention and pre-treatment (sedimentation) of the combined affluent and first flush volumes, ensuring that most rainfall events are managed effectively once these volumes, with the highest pollutant load, are retained in the anti-pollution basin and latter pumped and conveyed to the WWTP. During a rain event, after the basin has reached its capacity, the overflow is conveyed through the side channel into the tunnel, being, however, subject to a pre-treatment process by the stormwater screens installed downstream the anti-pollution basin.

Stormwater screens: The stormwater screens are used for the more frequent storms, involving discharges up to 43 m³/s, to pre-treat the flow before it is channelled into the tunnel and conveyed straight to the Tagus River. The screens are used to filter suspended solids/waste to improve the quality of the floodwaters discharged into the river.

Side Channel: The side channel conducts the wastewater treated by the screens to the tunnel. The flow exceeding the screens' capacity is directly discharged to the side channel without any treatment, being the discharge/water level in the stormwater screens' chamber controlled by means of two automatic leaf gates placed in the transition between this chamber and the side channel.

Tunnel: The tunnel initiates at the downstream section of the inlet structure and crosses the existing network at three strategic points of the city, diverting additional flows from other critical areas of downtown Lisbon. The tunnel has a total extent of nearly 5 km, a diameter of 5.5 m and a slope between 0.5 and 0.7%.

In summary, the inlet structure of the tunnel will facilitate the conveyance of the drainage effluent to a series of pre-treatment schemes, with due consideration given to the hydraulic flow and the associated pollutant load. In instances where the flow is sufficiently diluted, it is conveyed almost directly to the river, given that the wastewater sieves have reached their maximum capacity, but without larger debris since they are retained in the debris well and first flush pollution effects are managed by the anti-pollution basin. The tunnel subsequently diverts the flow to the Tagus River, capturing some additional flows at three locations along its development (Liberdade Avenue, Santa Marta Street and Almirante Reis Avenue). This infrastructure will considerably reduce the risk of flooding in low-lying areas of Lisbon and minimize direct overflow discharges to the Tagus River without any treatment, in alignment with the new UWWTD.

Having this into account, the flow has the following main operation modes, due to its hydraulic constraints:

- Up to 6.6 m³/s, flow is returned to the existing Caneiro de Alcântara tunnel, to reach the WWTP.
- Additional affluence up to 7 m³/s is conveyed to the stormwater anti-pollution basin;
- The following 36 m³/s of affluence is screened by the main chamber wastewater screens (for frequent rain events). In this operation mode the discharge gates are closed to ensure the screen's operation and discharge;
- When the flow exceeds the pre-treatment design capacity (~50 m³/s), up to the design flood of 120 m³/s for the return period of 100 years, an automatic system allows controlling of the water level in the main chamber by automatic operation of the two leaf gates, the exceeding discharge being directly conveyed to the side channel.

As the inlet structure represents several technical challenges, AdTA (Águas do Tejo Atlântico, the company responsible for the management and operation of the multi-municipal wastewater sanitation system in Lisbon and the West zone) requested LNEC to undertake a physical model study, to verify and the performance of the new tunnel inlet structure. Therefore, a 1:30 scale model was built reproducing all main features of the inlet structure, as shown in Figure 22, except the stormwater anti-pollution basin as its role in terms of flood discharge capacity is not relevant (since its role being linked to water quality), and several tests were conducted by LNEC. The results obtained in these experiences at the reduced physical model will be used as the source of the information to validate the numerical model since they represent a deep understanding of the infrastructure.

5.2 Approach Definition

In this work, the validation of the numerical model will be based on previously performed experimental tests on a physical reduced model and, to do so, the numerical model was firstly built considering the geometrical dimensions of those experiences, at a reduced scale, so that the results to be compared do not suffer from scale effects (this scale will be mentioned as “Reduced Model”, M labelled scenarios in Table 2.). Having this in mind, the validated numerical principles were then extrapolated for real-world dimensions (this scale will be mentioned as “Prototype”, P labelled scenarios in Table 2.). The results will be compared and analysed in terms of the numerical performance of both prototype and reduced model scale, to assess possible scale effects. The simulations presented in this master thesis were performed on a workstation equipped with 16 processing cores, 32 threads, and 32 GB of RAM, running a 64-bit server operating system.

The performed scenarios based on experimental tests ranged a variety of operating modes, but from those the following three were selected based on their relevance to the hydraulic performance of the inlet structure:

- **Frequent operational scenarios:** characterised by discharge at the wastewater screens corresponding to return periods of less than one year;
- **Design flood scenarios:** no control is imposed by the two leaf gates (fully open), with water flowing freely to the side channel, and assuming the discharge associated to the project return period of 100 years (design flood);
- **Exceptional design flood scenarios (ME100 and PE100):** overtopping of the two closed leaf gates as a result of malfunction of the gate manoeuvring system and the project return period of 100 years design flood.

To synthesize, the numerical studies associated to the case study were carried out as much as possible considering the flow chart described in chapter 4 and sketched in Figure 18, both for the cases with geometrical dimensions of the physical model and the prototype. The performed approach is elucidated in Figure 21, where the process at light blue is treated in this chapter and the remaining, in grey, is discussed in the results sections.

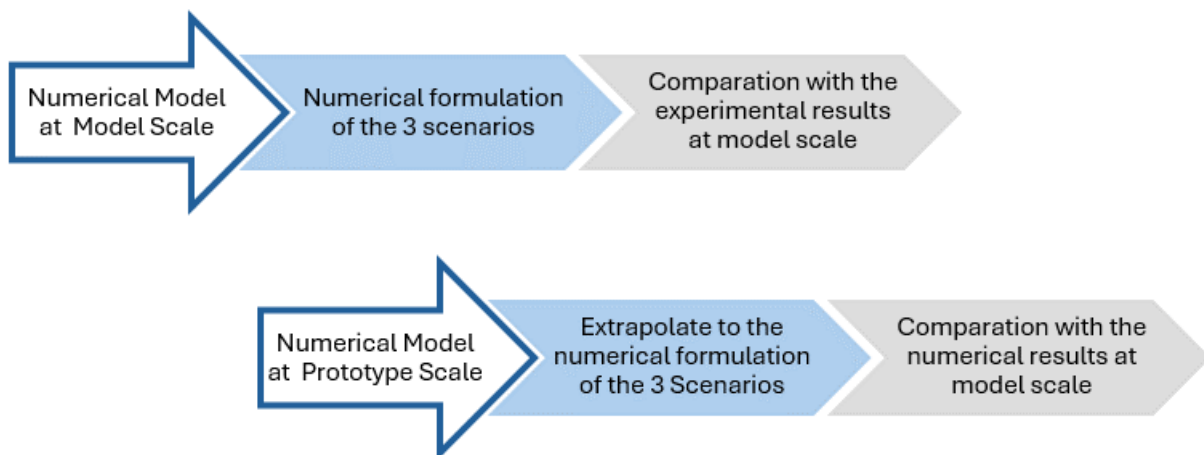


Figure 21 - Approach of the numerical analysis for the case study

Finally, with both combination of scales and operating modes six scenarios were considered, as summarized in Table 2.

Table 2 - Scenarios Overview

Scenario	Return Period (years)	Description	Q (m ³ /s)
M100	100	Model Scale, Design Scenario	120
ME100	100	Model Scale, Exceptional Scenario	120
M1	1	Model Scale, Frequent flood	36
P100	100	Prototype Scale, Design Scenario	120
PE100	100	Prototype Scale, Exceptional Scenario	120
P1	1	Prototype Scale, Frequent flood	36

Based on the observations made by LNEC the main aspects to be analysed are:

- Water head at the weir crests of the wastewater screens, to verify that the maximum emergency value of 0.87 m set by the manufacturer was not reached, and observe the maximum operational water head of 0.55 m;
- Flow field behaviour and water head around the wastewater screens, at the leaf gates, tunnel entrance and other locations that showcase design constraints;
- Free surface flow inside the tunnel for all the scenarios;
- Hydraulic jump location in the side channel.

5.3 Model Scale Development

5.3.1 General Settings

To initiate the flowchart described in Figure 18, the M100 scenario was used. In a first glance, in the beginning of the problem formulation, user is presented with general simple definitions such as the simulation finish time, which is the time window of flow we want to simulate. For the flow options, one fluid and incompressible fluid was selected, since it will be dealing only with water, which is also the fluid to be inputted from the available library as water at 20 °C. For instance, the advection of the VOF as 'one fluid, free surface', as the most suited for this single fluid problem, since this represents how the software will apply the algorithm for the VOF transport equation and the 'first other' solution for the moment advection has been deemed sufficient for addressing this particular type of problem [37].

In the subsequent sections, all the dimensions (e.g. cell size or hydraulic outputs) are presented at the prototype scale to provide more clarity. Thus, although it was considered in some scenarios the geometrical dimensions of the physical scale model, these were transformed to the prototype corresponding dimensions using Froude's similarity law.

5.3.2 Geometry Definition

In the experimental setting, the physical model replicated essential zones and features of the inlet structure, which were considered relevant for evaluating the structure performance and design. With this, there were some structure elements that LNEC excluded in the experiences, since they were not considered to be a hydraulic constraint, and others in the numerical model. These simplifications are listed below:

- Anti-pollution basin designed to have a well-controlled flow through a regulating valve, it was considered not to be a hydraulic problem, thus, not representing a need to study its performance;
- Connection to the existing downstream drainage tunnel that links to the WWTP was not represented in the numerical model, differing from the experimental set-up;
- The downstream wastewater screens were not considered in the in the numerical model, only the weirs that regulate de flow into them having been reproduced;
- The structural columns around the well and wastewater screens were also discarded in the context of the numerical model.

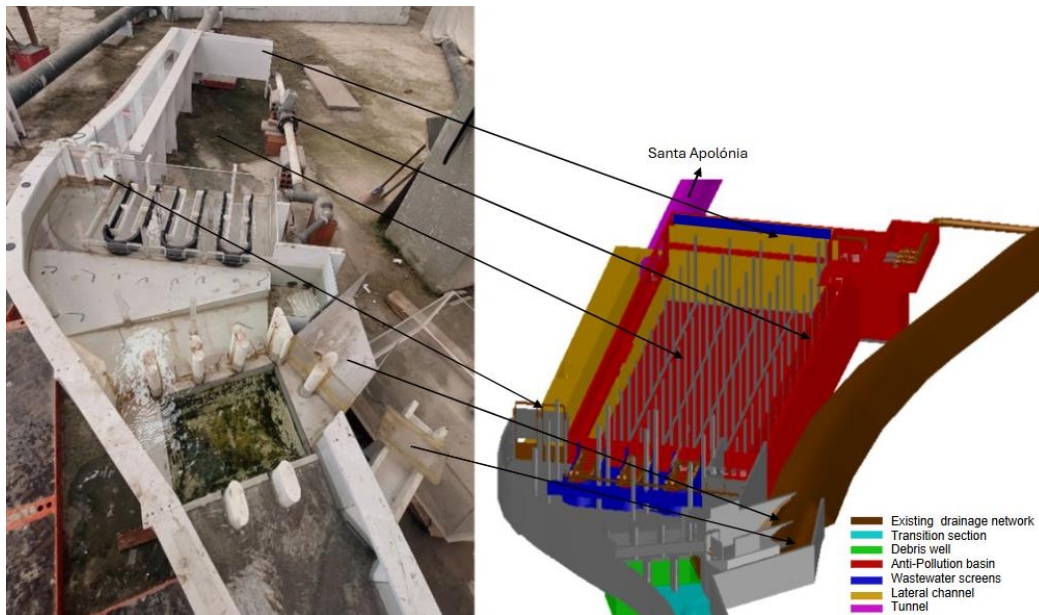


Figure 22 - Numerical Model geometry simplifications [43]

At this stage, it is imperative to take in mind the conditions imposed on the geometry construction. Since the mesh is defined as a parallelepiped, with the boundary conditions in each face, by employing the FAVOR™ method any extraneous regions will be excluded from the calculation domain, the problem geometry has to follow up this formulation, resulting in the geometry seen in Figure 23.

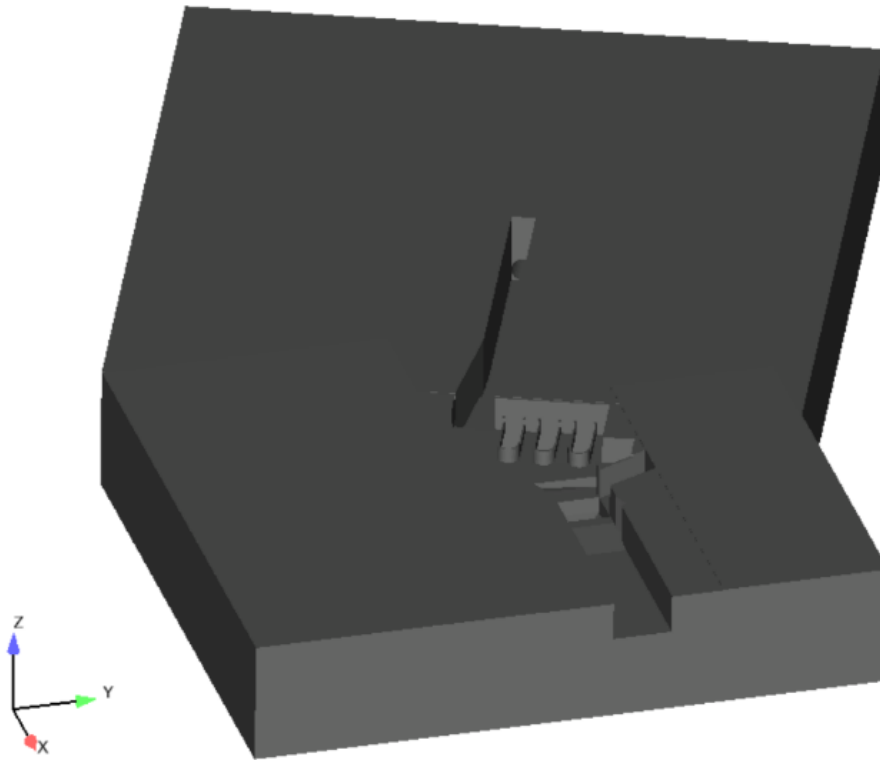


Figure 23 - Geometry formulation for the numerical simulations

5.3.3 Mesh and Cells

Following this, the mesh placement and size of the orthogonal cells in each direction, that compose the mesh was done. The increasing of the total amount of cells represents longer elapsed time to calculate the same simulation time. In the other hand, bigger cells may compromise the simulation stability, reducing its time step which directly increases the elapsed time taken for the same simulation time. Therefore, three options of mesh formulation were meticulously devised for testing:

- (1) Single mesh block comprising cells that are comparatively large in relation to the thickness of specific obstacles, with 20 cm. This was the first approach given its propensity to produce results rapidly, due the low amount of cells as direct result;
- (2) Single and more refined mesh block with cell size of 10 cm;
- (3) Multiple mesh blocks, strategically placed and nested mesh block to more refinement without unnecessary cell refinement, with cells ranging from 20 to 5 cm.

5.3.4 Turbulence Model

The subsequent stage involves delineating the appropriate physical models. As previously stated, in addition to the fundamental laws of fluid dynamics, certain water flows require the simulation of additional physical phenomena such as sediment transport, heat transfer, or turbulence. In this case study, the accurate representation of turbulence is a critical aspect of the numerical analysis.

As outlined in 3.2.2.2 section, various turbulence models are available to simulate the effects of fluctuating velocity fields on the mean flow. Flow3D provides several formulations, each suited to different flow regimes and computational goals. From the research conducted, it was determined that the RNG (Renormalization Group) model, the $k - \varepsilon$, and the $k - \omega$ models were the most appropriate candidates for this application. Among them, the RNG model was selected as the starting point for this analysis due to its enhanced capacity to model swirling and rapidly strained flows, which are characteristic of complex hydraulic structures. The RNG model improves upon the standard $k - \varepsilon$ formulation by incorporating a differential formulation for the turbulent viscosity and additional terms in the ε equation that account for non-linear strain effects.

Simpler turbulence models, such as the Prandtl mixing length or one-equation turbulent energy models, were excluded from consideration due to their limited applicability in capturing anisotropic and transient features of turbulent flow, particularly in regions of flow separation and reattachment, predicted to occur in the case study. Conversely, while more sophisticated models like Large Eddy Simulation (LES) offer increased fidelity, they were deemed as computationally excessive for the scope and resolution of this study.

5.3.5 Boundary Conditions

To proceed with the formulation, the boundary conditions must be defined. These conditions essentially delineate the points between which the propagation of the flow is calculated by the governing equations and the other physical models. These conditions are delineated on each of the six faces of each mesh block.

Flow3D offers a range of options, some of which are particularly pertinent to the intended purpose of their use. For instance, the "Inflow" boundary condition is specifically designed to simulate the entry of flow into the specified boundary. This was designated as the inlet boundary condition at the most upstream face of the mesh.

Another option is the "Wall" function, which serves to determine a barrier to the flow on a certain mesh face. Given the geometry input in the system the use of the "Wall" function becomes redundant, but still as it is the most adequate it was used for the bottom and lateral faces of the mesh, in view with the geometry inputted, as in Figure 23.

The upper face of the mesh is equivalent to atmospheric pressure, as it represents the open space under the ceiling of the structure. To conduct that, the "Pressure" boundary condition was used, which allows the definition of water columns, stagnation pressure and percentage of fluid. Flow3D manual [37]. provides guidance on the use of this boundary condition to simulate a free surface by setting the stagnation pressure to zero.

At the most downstream face of the mesh, the flow is supposed to be exiting the system under certain assumed/known conditions. To simulate the flow exiting, the "Outflow" boundary condition was utilised, which is a predefined setting within Flow3D and has been observed to conduct what it implies, in other case studies. Although the software advises defining the boundary conditions on a physical basis, as was done for the free surface, the "Outflow" boundary condition was applied to simulate the flow exiting the system.

The boundary conditions at the mesh faces as well as the limits of the single mesh block as in mesh (!1), in light blue lines, can be observed in the following Figure 24.

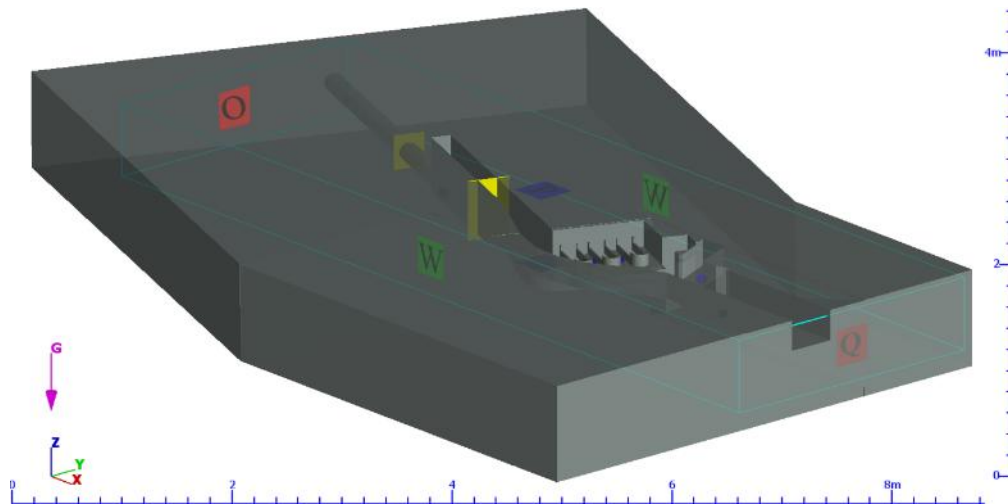


Figure 24 - Boundary conditions of the first simulation of M100, with mesh (1)

5.3.6 Validation Process

As outlined in the proposed flowchart, the validation process starts with the validation of the boundary conditions and finishes with the validation of a mesh definition and turbulence model. Through the first scenario tested, M100 scenario, relevant observations were performed regarding the validation of the boundary conditions.

It was demonstrated by the simulation that, during M100, the flow representation was inadequate due to the defined boundary conditions. This is equivalent to a negative response to the flowchart's initial question. This was due to the physical phenomena imposed by the "outflow" boundary condition, differing from the experimental observations and from the design information of the tunnel. This occurrence can be observed two distinct instants in Figure 25 and Figure 26. The tunnel starts to perform with full section with the flow rate decreasing inside the tunnel (observed through a flux surface inside the tunnel). At certain time of the simulation, the tunnel loses entirely the capacity to transport the flow out of the domain, filling the numerical domain with water, by occurring backflow.

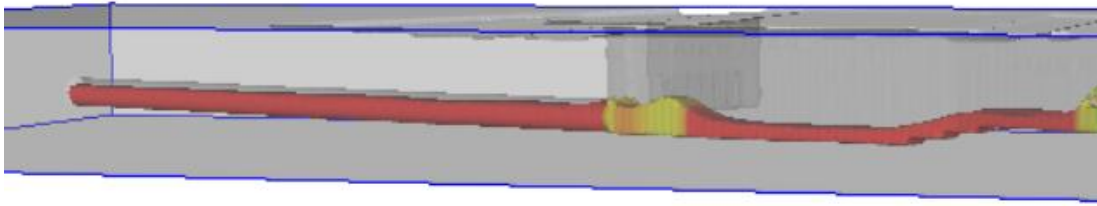


Figure 25 - Tunnel before the backflow at the simulation time of 25 seconds

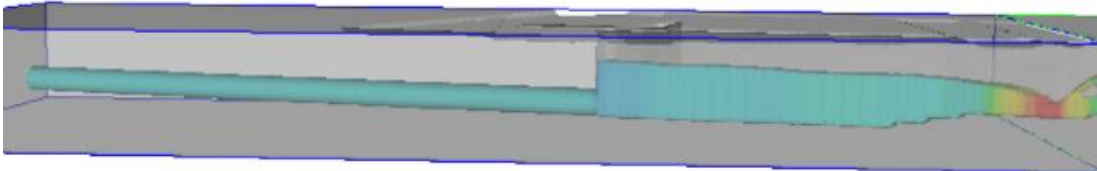


Figure 26 - Tunnel during backflow at the simulation time of 50 seconds

The downstream boundary condition was then altered to a self-determined physical condition, and this was achieved by simulating atmospheric pressure at the tunnel outlet. By observing the results, it was concluded that changing to this new boundary condition, the flow representation was adequate and generally in line with the physical modelling observed flow pattern, and so, the boundary conditions were considered validated.

Following the next stages in the validation process, different meshes were implemented to ensure mesh independent results. It was observed that the single mesh block considering only one rather coarse cell size (mesh formulation number (1)) didn't lead to an adequate detailing of some key areas of the hydraulic structure. Therefore, a local refinement was first implemented leading to cell formulation number (2), further perfected by considering a "nested mesh block" for mesh formulation number (3), which enabled a better representation of all relevant structural details. These successive improvements can be observed in Figure 27 regarding the zone of the weirs equipped with the wastewater screens.

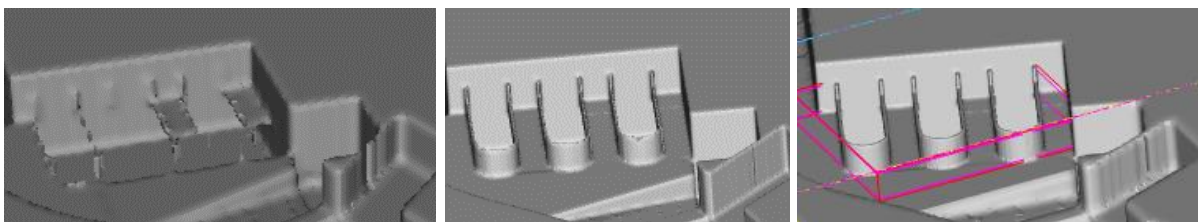


Figure 27 - Details of the wastewater screens with different mesh formulation and cells size from (1), (2) to (3) respectively

During these tests, besides the elapsed time observed, the results observed did not showcase significant variations from one mesh formulation to another, and so, the results were concluded to be mesh independent. The decision made on which mesh formulation, (2) or (3), to use was done concerning the elapsed time that each option took to reach mass balance.

At this phase of the studies, it was identified that M100 scenario reached the stop criteria regarding mass balance approximately upon 35 seconds of simulation and to evaluate each mesh performance, the elapsed time that each mesh took to perform this time of simulation, and the total amount of cells were the factors to conclude about the optimal mesh. The results are shown in the following Table 3.

Table 3 - Mesh (1), (2) and (3) evaluation

Mesh Definition	Total amount of cells	Elapsed time until mass balance
(1)	0.175×10^6	10 days
(2)	1.3×10^6	8 days
(3)	0.991×10^6	2 days

These results showcase how geometry errors of less refined cells can lead to non-converging situations and so, more computational effort but also, how a localized refinement allows improvement of the trade-off between mesh size and computational effort.

Considering the above, the nested block mesh (3) was chosen as the most suitable mesh formulation from the ones developed in setting up the numerical model, since it allows an adequate level of detail in the most important areas, engaging locally a high number of small size cells, and also leads to the optimization of computational times that are not excessive considering the problem being analysed.

With the mesh defined, the turbulence model's performance was studied regarding the turbulence models RNG, $k - \varepsilon$ and $k - \omega$. Results evidenced that both these turbulence models are able to translate the flow adequately, the hydraulic jump location and the observed behaviour near obstacles being similar for both turbulence models. The elapsed time in the RNG model was similar to the $k - \omega$, 2 days, and the $k - \varepsilon$ model required 3 days.

Once $k - \omega$ represented a smoother stability limit evolution and larger time steps than RNG (observed through the plot in the GUI), the $k - \omega$ model was finally selected for further simulations. It is also important to note that the $k - \varepsilon$ did not represent a more stable simulation, requiring more time step adjustments and lower time steps, as it is evidenced in Figure 28 and Figure 29, leading to larger simulation times, as observed, when compared to the other turbulence models.

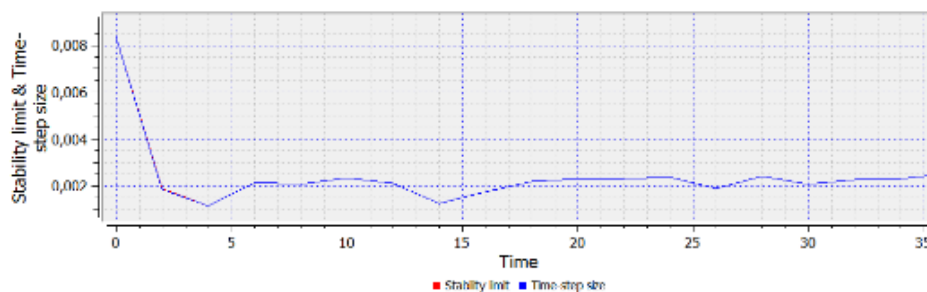


Figure 28 - Turbulence model $k - \omega$ stability limit and time-step size of M100 with mesh (3)

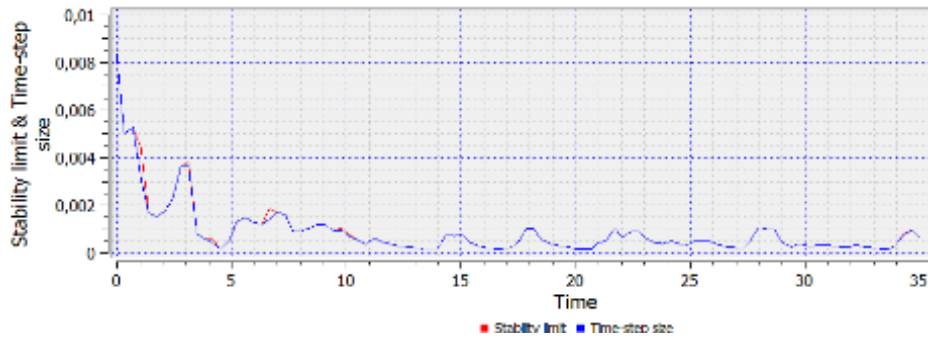


Figure 29 - Turbulence model $k-\varepsilon$ stability limit and time-step size of M100 with mesh (3)

Once a model set-up for scenario M100 was perfected and led to an adequate flow modelling (boundary conditions, mesh definition and $k-\omega$ turbulence model) scenarios ME100 and M1 were then launched based on the same model set-up, besides the inflow.

During the simulation of ME100, the simulation was not completed due to the need to reduce the time-step to a value below the minimum accepted, set by the software. By consulting the debugging file of this simulation, numerical instabilities were identified near the wastewater screens, due to the CFL condition of flow stability and so, the software automatically decreased the time step to meet CFL condition reaching lower values than the admitted.

To address this problem, the unstable behaviour was firstly attributed to inadequacy of the mesh resolution of mesh (3), so an additional refinement was considered leading to what was labelled as mesh (4). This mesh was defined considering six coplanar mesh blocks, as well as the elimination the nested block previously considered for mesh (3). In mesh (4), cells' size increase in the direction of the wastewater screens, reproducing similar refinement in the wastewater screens, in a more continuous pattern in the vicinity of these, as in Figure 30. The total amount of cells of mesh number (4) duplicated compared to mesh number (3) but the simulation proceeded without computational problems and without producing a significant increase of the elapsed time compared to M100 and so, this formulation was then used for the M1 scenario, also offering a well-balanced simulation.

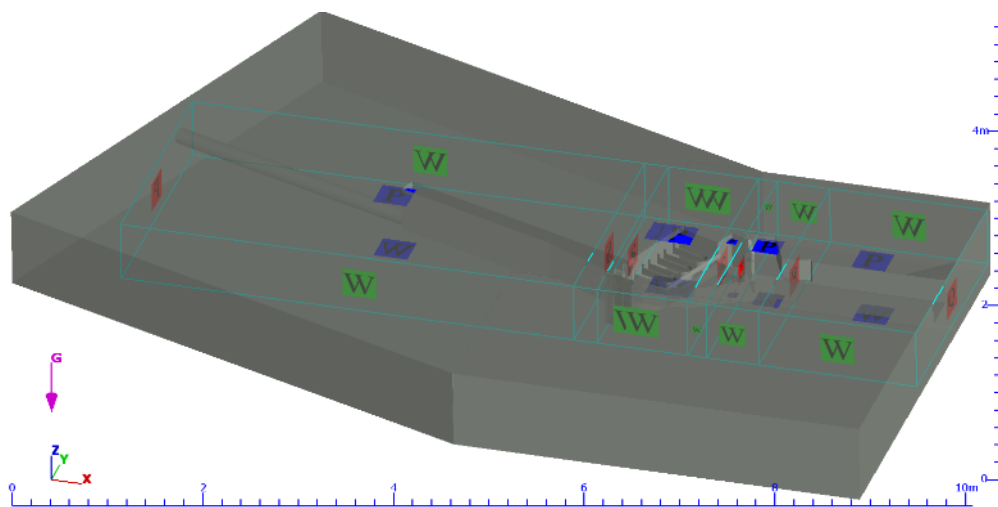


Figure 30 - New mesh formulation, number (4), with 6 coplanar mesh blocks for ME100 and M1

5.4 Prototype Scale Development

A final procedure was considered for the case study analysis, in which the assumptions presented in previous sections were considered, but now for the prototype geometrical dimensions, as already referred in section 5.2. The modifications from the previously tested model geometrical dimensions scenarios are confined solely to comply with Froude similarity law. Such modifications encompass the design flow rate, as the input at the inlet boundary condition and the dimensions of the cells.

Regarding the prototype scale, the first scenario simulated was P100, with mesh formulation like mesh number (3) and $k - \omega$ turbulence model. The simulation revealed the error encountered before: the time step of the calculations dropped below the minimum value allowed by the software.

In an initial attempt to rectify these issues, since in the debugging file revealed that the instability lies within the wastewater screen zones, the cell size was reduced to half the initial size of mesh number (3) but, the simulation error persisted. The debugging file suggested increasing the “CPFK” coefficient. This coefficient is the instrumental numerical formulation in determining the degree of definition in which the calculation of certain cells is discarded, with the objective of avoiding computational divergence when small volumes, for example originated by a splash, that destabilize the flow calculation, and consequently, increase the computational requirements [37].

Despite the adoption of this suggestion, the same computational error persisted. Consequently, it was concluded that the very same mesh formulation number (3) associated with nested mesh blocks, successfully employed for M100, cannot be considered for P100. While the geometrical scale in mesh number (3) has been respected from M100 to P100, this incompatibility can be expected since the fluid (water) in both model and prototype scenarios has the same intrinsic characteristics. Consequently, in the model scale, the fluid exhibits a more viscous behaviour, resulting in enhanced control over the separation of liquid veins and much lower Reynolds numbers for similar hydraulic conditions. Thus, at the prototype scale, it requires much higher discretization/mesh refinement to address fluid advection, thereby avoiding the requirement of such reduced time steps.

The mesh was then improved by adopting fewer singularities and higher refinements, by removing the nested block, including seven adjacent blocks (this will be referred as mesh number (5)), as it was previously done with mesh number (4). This new mesh is shown in Figure 31, and was applied to both P100, P1 and PE100, since those last two are also expected to require this type of mesh definition, since the hypothesis of this need is based on the same explained fluid behaviour at the prototype scale.

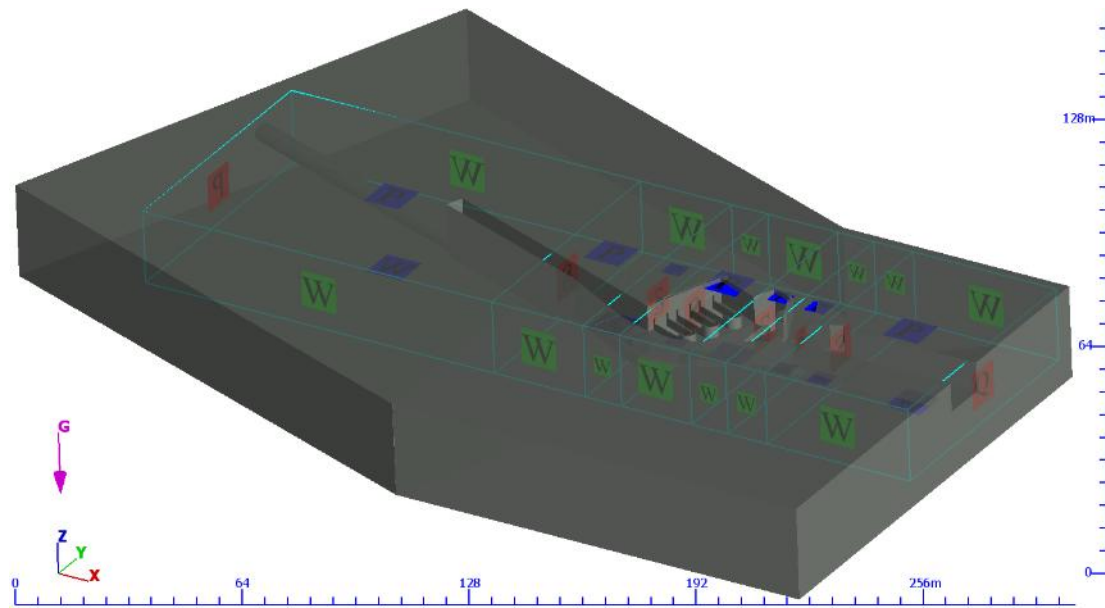


Figure 31 - Mesh formulation number (5) for the scenarios P100, P1 and PE100

Summarizing the content of this chapter regarding the case study, the model is validated for all scenarios by following the flowchart defined in the methodology. Subsequently, an analysis and comparison of the results derived from the prototype and model scale scenarios can be conducted, as presented in detail in the following chapter.

6 Results Presentation and Discussion

6.1 General Overview

In the course of these simulations, although a classical steady-state was not fully attained, a sufficiently stable flow condition was reached — consistent with best practices for free-surface CFD. Due to the natural instabilities of free-surface flows, achieving a true steady state is often impractical. Instead, a *pseudo-steady* condition was established, where the free surface and flow parameters exhibited negligible variation over time. Convergence was considered achieved when the downstream flow matched the inlet flow within a threshold of $\pm 2\%$, and the total volume of fluid in the domain stabilized to a nearly constant level. This approach, alongside with the results observed in the performed experimental tests, ensured that the results were reliable and representative, enabling meaningful interpretation of the simulation outcomes [44].

Having this in mind, the following sections will detail the last procedures represented in grey in Figure 21, comprising the comparison of the results between the numerical results at model scale versus the experimental results performed by LNEC at model scale. Lastly, the comparison between the numerical results at model and prototype scale. All the results are presented at the prototype scale, by employing Froud's similarity law for the model scale results or directly calculated for the prototype scale.

To conduct each simulation analysis in detail, measurement points were placed in the geometry to measure flow heads, free surface elevations, flow rates and many other hydraulic data. This is done by selecting variables to be included in the simulation output file. The measuring points and surfaces allocated to the problem are shown in Figure 32 below.

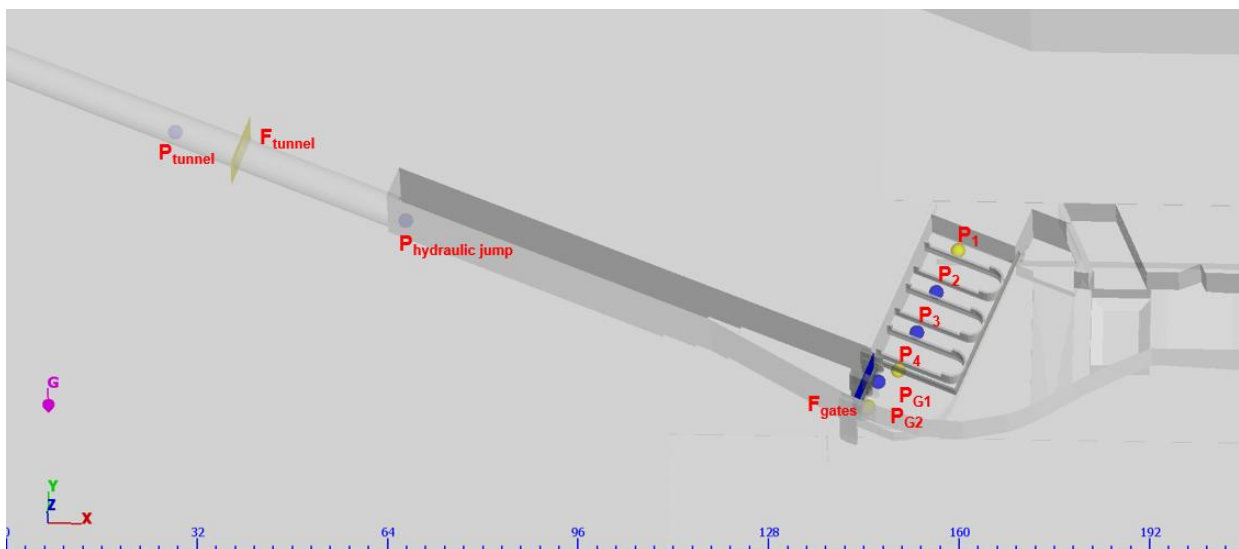


Figure 32 - Measuring points and surfaces defined for the simulations

6.2 Model Scale and Experimental Results Comparison

6.2.1 Design Flood Scenario

The design flood scenario has an input of $120 \text{ m}^3/\text{s}$, and the mass stabilization was observed around 50 seconds of simulation, and the elapsed time of 3 days and 8 hours for a total amount of 9950,520 cells, with a variation threshold of the flux in the tunnel of 1.58%, as illustrated in the following Figure 33 and Figure 34.

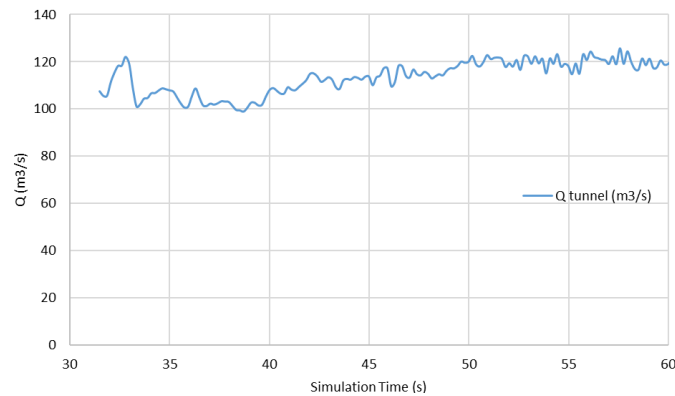


Figure 33 - Flow inside the tunnel for M100

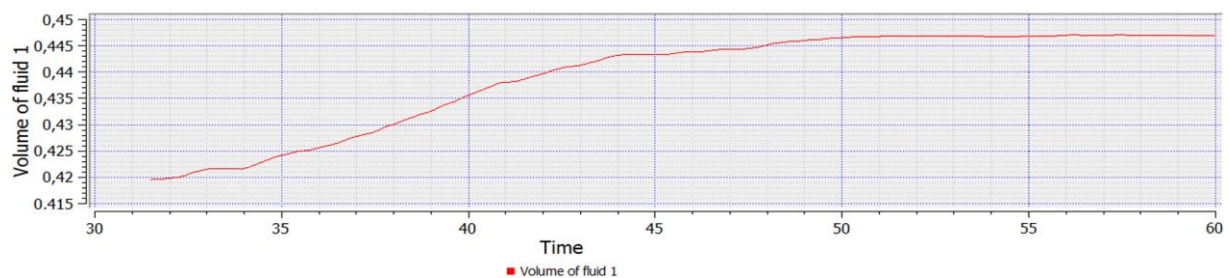


Figure 34 - Volume of fluid 1 in the domain for M100

Table 4 - M100 total amount of cells, stabilization time and elapsed time until stabilization

Total Amount of Cells	Stabilization Time (s)	Elapsed Time Until Stabilization	Variation threshold
990,520	50	3 days and 8 hours	1.58%

Regarding the water head around the screens, in Figure 35, as observed in the experimental results, respected the maximum head of overflow, with lower values near the discharging gates. This elucidates a different hydraulic efficiency of each screen deriving for their respective locations, being less effective the ones closer to the two discharging gates (fully open for this operation scenario).

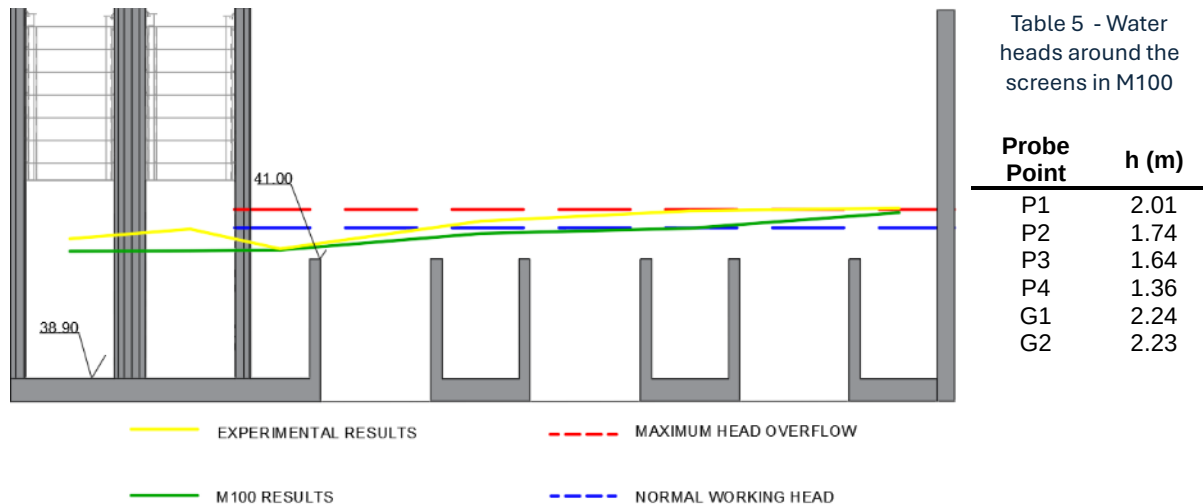


Figure 35 - Comparison of M100 results with experimental results regarding water heads

The velocity field, Figure 36, showed a similar behaviour when it comes to the orientation of the velocity vectors, evidencing that, due to the significant outflow at the leaf gates section, a significant increase of velocity and reduction of flow depth is observed in the wastewater screens near the gate section. Also, the protection beam around the screens, clearly has a positive effect mitigating flow separation in the approach zone of the wastewater screens, improving the flow distribution in that zone.

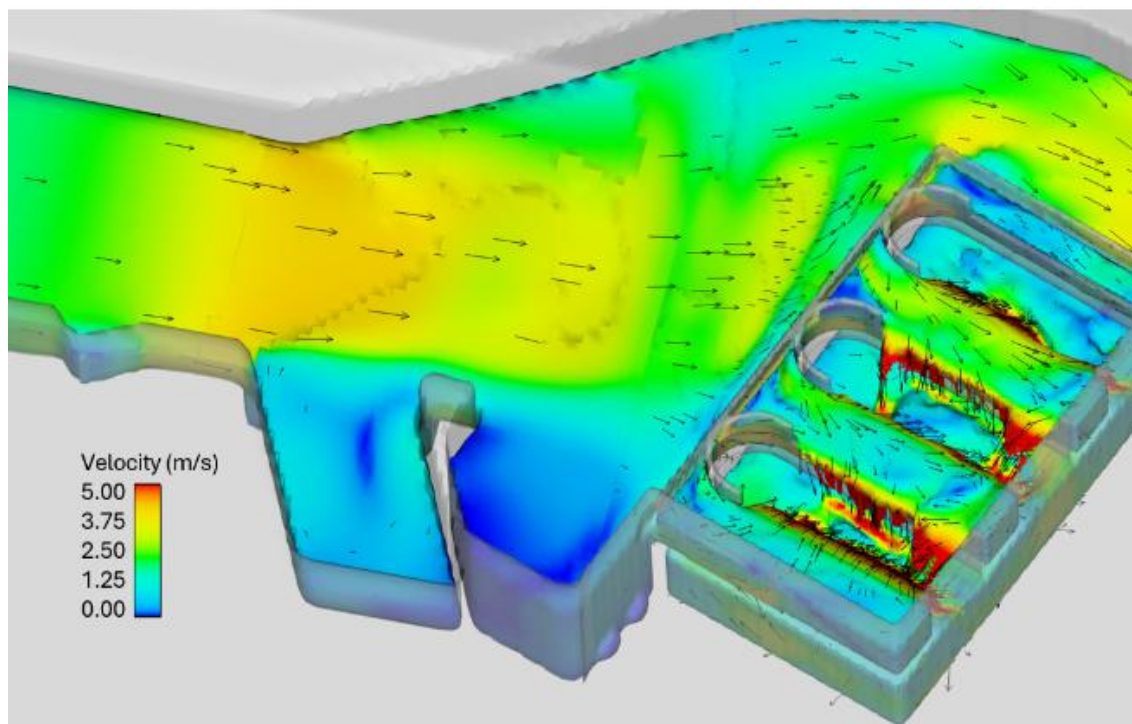


Figure 36 - Velocity field in M100

Regarding the tunnel inlet, Figure 36, a hydraulic jump is identified similar to the one observed in the physical model. The hydraulic jump in the side channel occurs in order to allow critical flow conditions in the upstream section of the tunnel. The flow inside the tunnel proceeds with free surface as intended in the project.

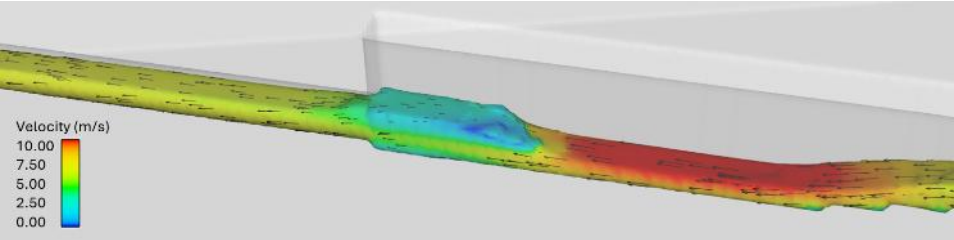


Figure 37 - Velocity field in the tunnel in M100

Table 6 - Water heads in the tunnel in M100

Probe Point	h(m)
Hydraulic jump	5.12
Tunnel	3.60

6.2.2 Exceptional Scenario

The exceptional scenario involves an incoming flow with a discharge of 120 m³/s, and closed control leaf gates (assuming some accidental malfunction). The mass stabilization was observed around 30 seconds of simulation, and the elapsed time of 3 days and 20 hours for a total amount of 2,546,113 cells, with a variation threshold of the discharge in the tunnel of 2.80%, as illustrated in the following Figure 38 and Figure 39.

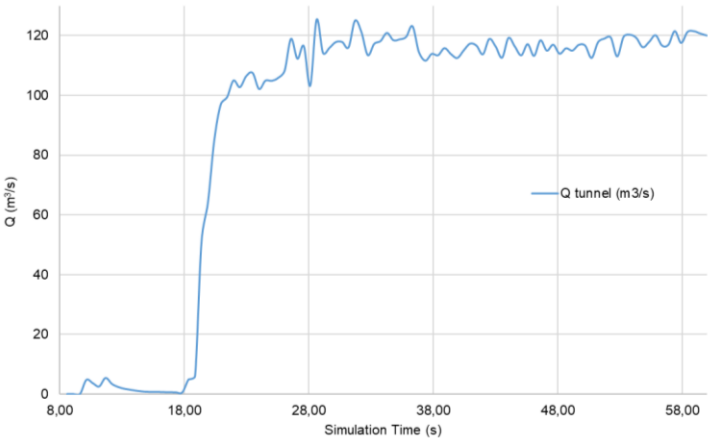


Figure 38 - Flow inside the tunnel for ME100

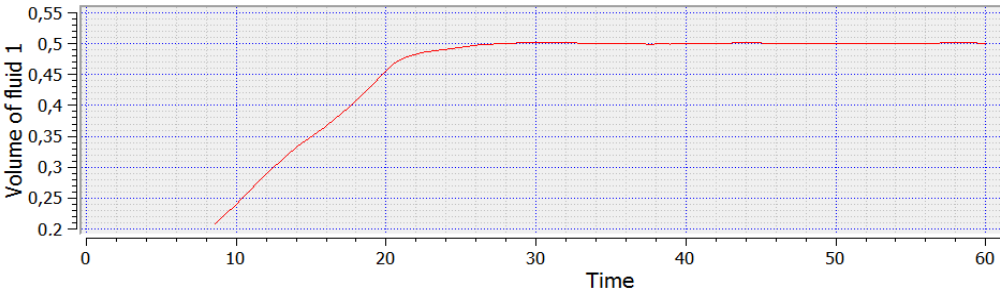


Figure 39 - Volume of fluid 1 in the domain for ME100

Table 7 - ME100 total amount of cells, stabilization time and elapsed time until stabilization

Total Amount of Cells	Stabilization Time (s)	Elapsed Time Until Stabilization	Variation threshold
2,546,113	30	3 days and 20 hours	2.80 %

The water head in the vicinity of the screens, Figure 40, increased, as expected, since the closed gates induce a critical scenario of malfunction, causing an upstream increase of the water head that also affects the wastewater screens. In this unlikely malfunctioning scenario, only in two out of six screens, the maximum overflow head is slightly exceeded. Experimental results were not included in Figure 40 since the experimental tests for this scenario were evaluated considering slightly different geometry settings.

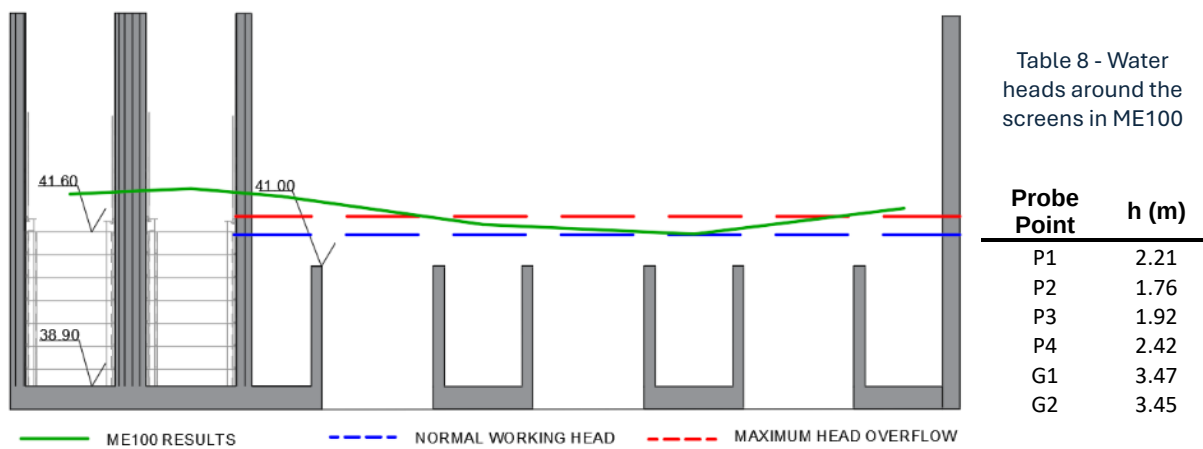


Figure 40 - ME100 results regarding water heads

Figure 41 in the next page showcases the high-water heads around the screens and lower velocities that in the previous scenario. The closed gates are being overflowed as expected from the experimental results.

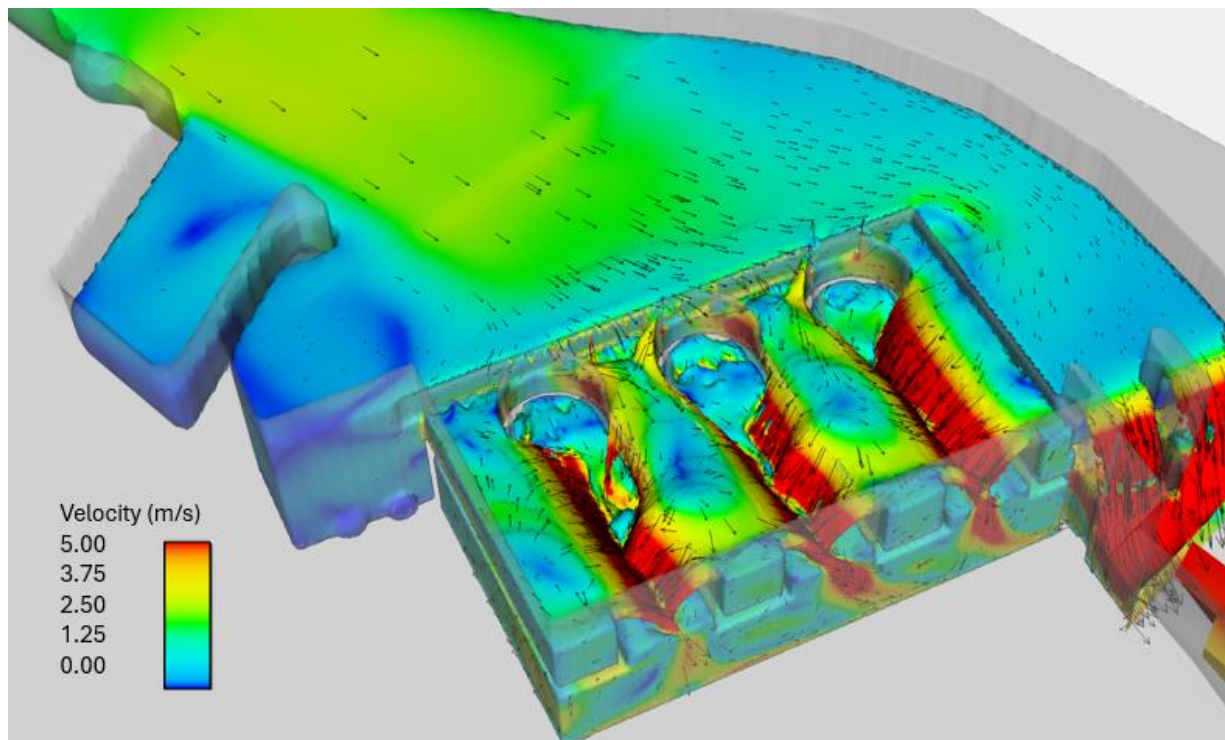


Figure 41 - Velocity field in ME100

As observed in the experimental results and as in the M100 scenario, at the tunnel inlet section, a hydraulic jump is identified, Figure 42, and the flow inside the tunnel proceeds with free surface. Comparing the results of M100 and ME100 a small increase in the tunnel water depth, of 0.07 m is identified as well as an increase of 0.05m in the hydraulic jump height.

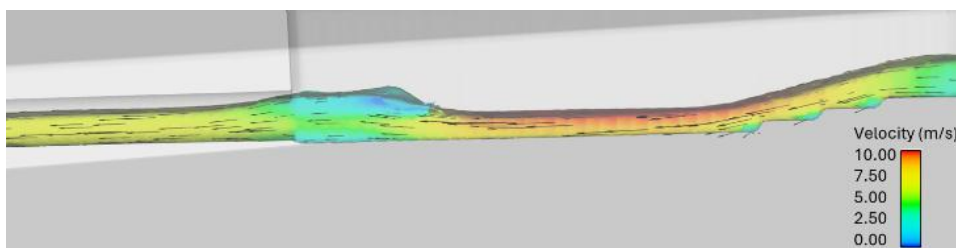


Figure 42 - Velocity field in the tunnel in ME100

Table 9 - Water heads in the tunnel in ME100

Probe Point	h(m)
Hydraulic jump	5.17
Tunnel	3.67

6.2.3 Frequent Scenario

The frequent scenario has an input of 36 m³/s, and the mass stabilization was observed around 55 seconds of simulation, and the elapsed time of 3 days and 3 hours for a total amount of 2,546,113 cells, with a variation threshold of the flux in the tunnel of 1.73%, as illustrated in Figure 42 and Figure 44.

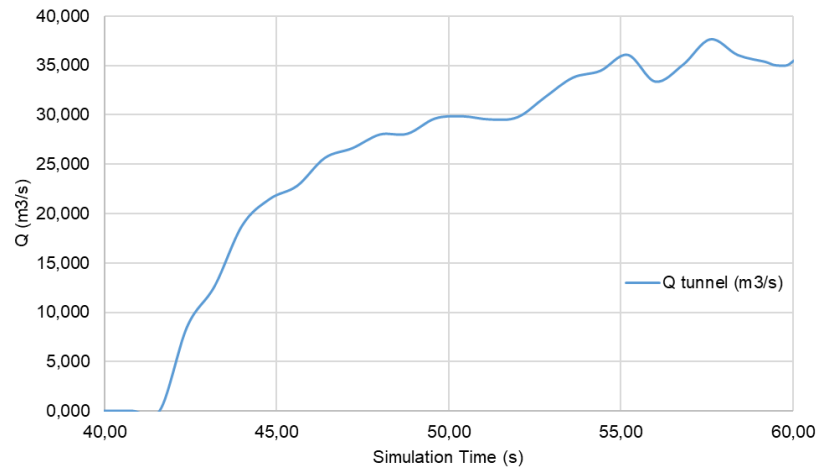


Figure 43 - Flow inside the tunnel for M1

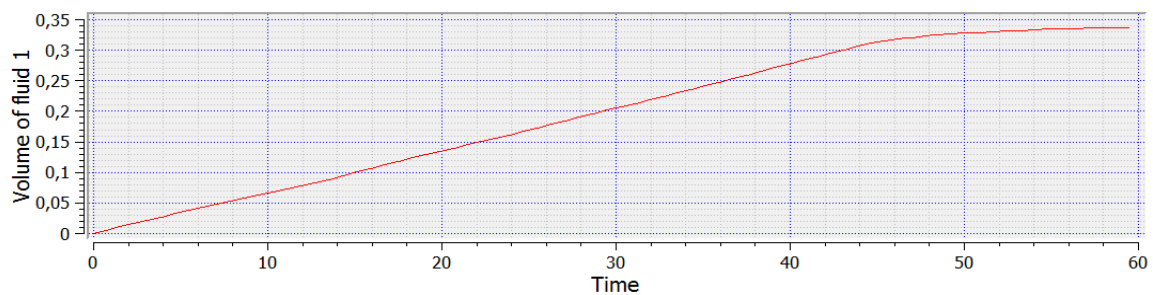


Figure 44 - Volume of fluid 1 in the domain for M1

Table 10 - M1 total amount of cells, stabilization time and elapsed time until stabilization

Total Amount of Cells	Stabilization Time (s)	Elapsed Time Until Stabilization	Variation threshold
2,546,113	55	3 days and 3 hours	1.73%

Regarding the water heads around the screens, Figure 45, as observed in the experimental results, they were under the maximum head of overflow, with similar values in the 6 screens revealing that in the scenario where the screens must work ideally, the expected working flow conditions in both screens are verified. Besides this, lower values than in the experimental results are observed and this can be justified by the simplification made in the wastewater screens geometry since in the experimental tests, a structure was added to better reproduce the screens discharge through the mechanical process that they provide. Near the discharging gates, slightly higher values were registered in the numerical analysis, but the main aspect to be pointed out is that the gates were not overflowed.

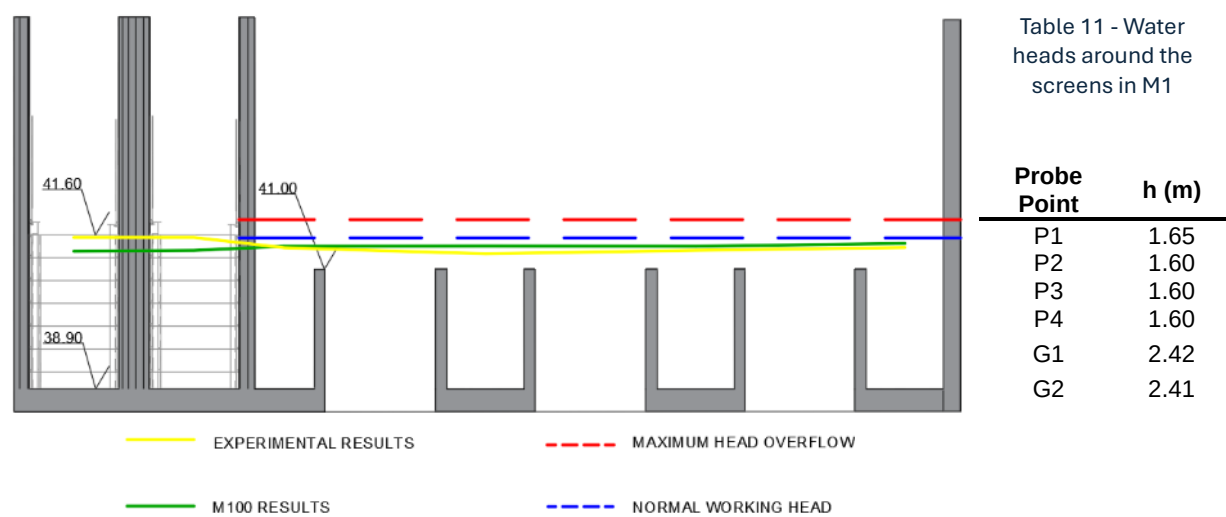


Figure 45 - Comparison of M1 results with experimental results regarding water heads

The velocity field, Figure 46, has similar values comparing with the experimental results, and the direction of the velocity vectors is also similar.

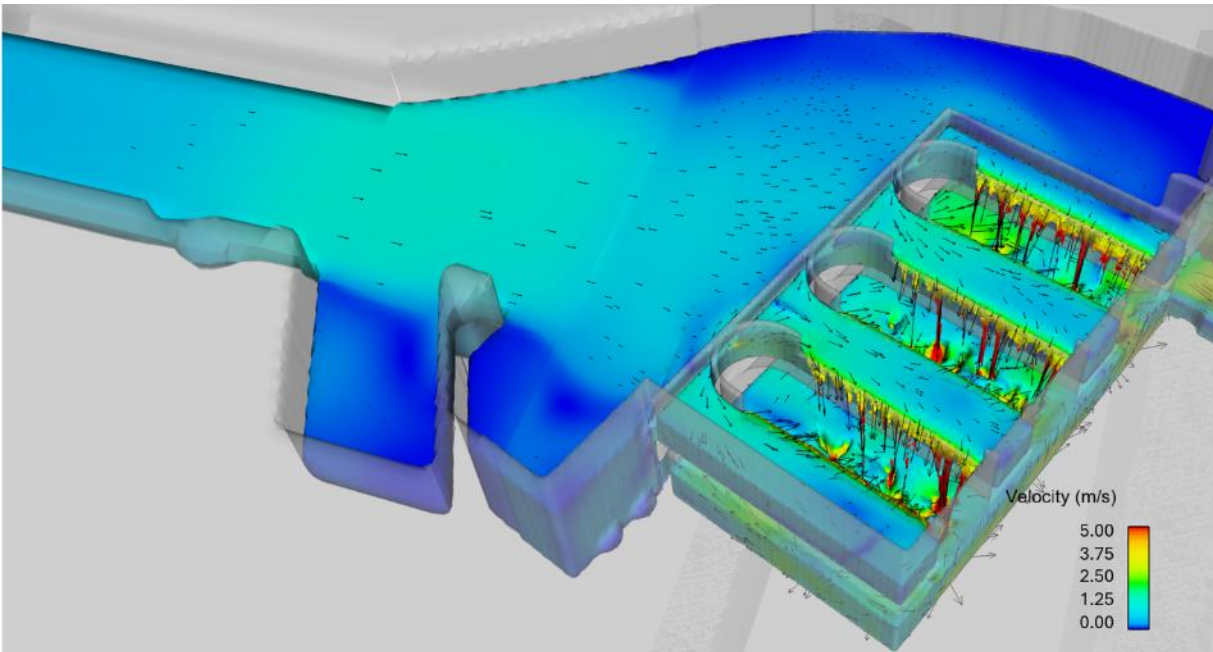


Figure 46 - Velocity field in M1

The tunnel entrance, Figure 47, showcases the expected results, with lower heights, occurring the hydraulic jump, and free surface flow in the tunnel.

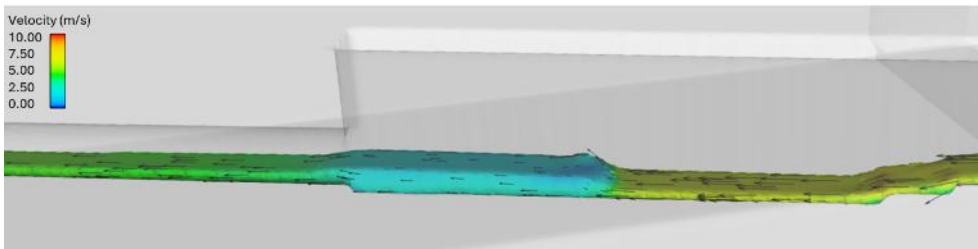


Figure 47 - Velocity field in the tunnel in M1

Table 12 - Water heads in the tunnel in M1

Probe Point	h(m)
Hydraulic jump	2.76
Tunnel	1.88

6.3 Model and Prototype Scale Comparison

6.3.1 Design Flood Scenario

The design flood scenario has an input of 120 m³/s, and the mass stabilization was observed around 240 seconds of simulation, and the elapsed time of 8 days and 20 hours for a total amount of 2,613,418 cells, with a variation threshold of the flux in the tunnel of 1.81%, as illustrated in Figure 48 and Figure 49.

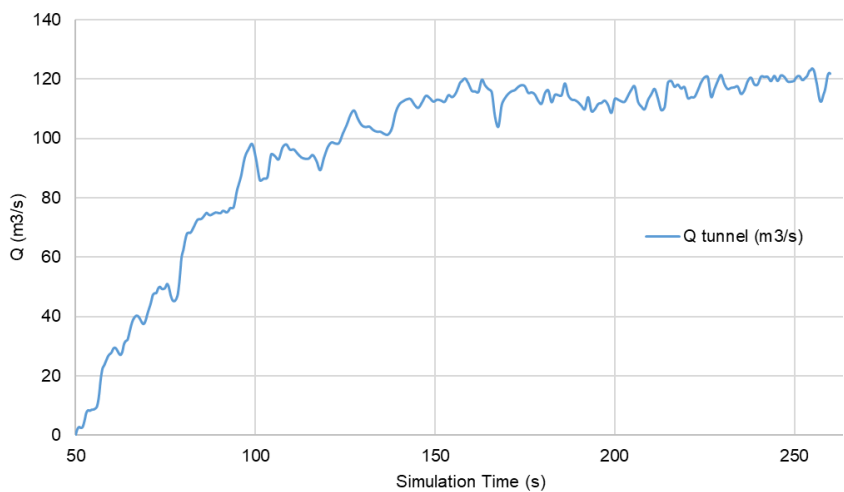


Figure 48 - Flow inside the tunnel for P100

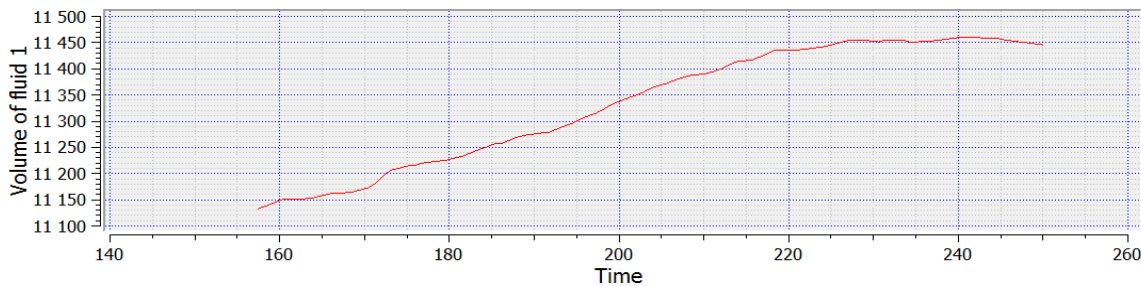


Figure 49 - Volume of fluid 1 in the domain for P100

Table 13 - P100 total amount of cells, stabilization time and elapsed time until stabilization

Total Amount of Cells	Stabilization Time (s)	Elapsed Time Until Stabilization	Variation Threshold
2,613,418	240	8 days and 20 hours	1.81%

Comparing the stabilization time with the one at the model scale, since similar simulation formulation was used, by Froud's Similarity Law, the stabilization time should around 274 seconds of simulation, to reach an equivalent mass balance state. This showcases a difference around 14% lower compared with the observed.

Qualitatively P100 presents a similar behaviour to M100, Figure 50 ,with water heads lower than the maximum head of overflow and lower values as the proximity to the discharging gates increases. Differences are from 0% to 31% compared with the M100. Generally, P100 as accentuated extremes, with P3 and P4 with lower values but P1 and P2 with higher values.

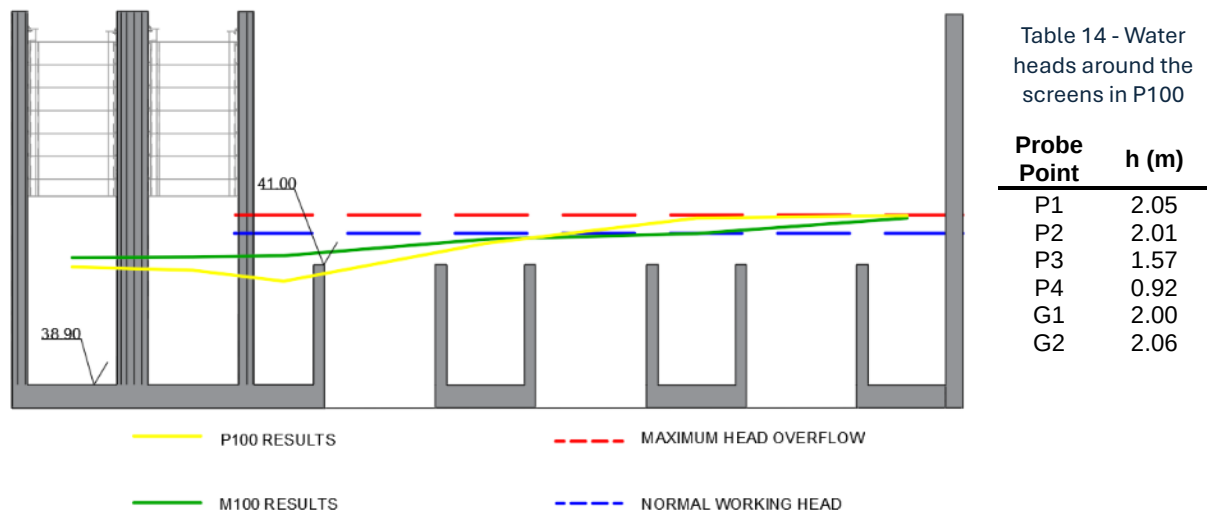


Figure 50 - Comparison of P100 results with experimental results regarding water heads

The velocity field, Figure 51, is quite similar, with visually higher values for P1 near the approach of the discharging gates.

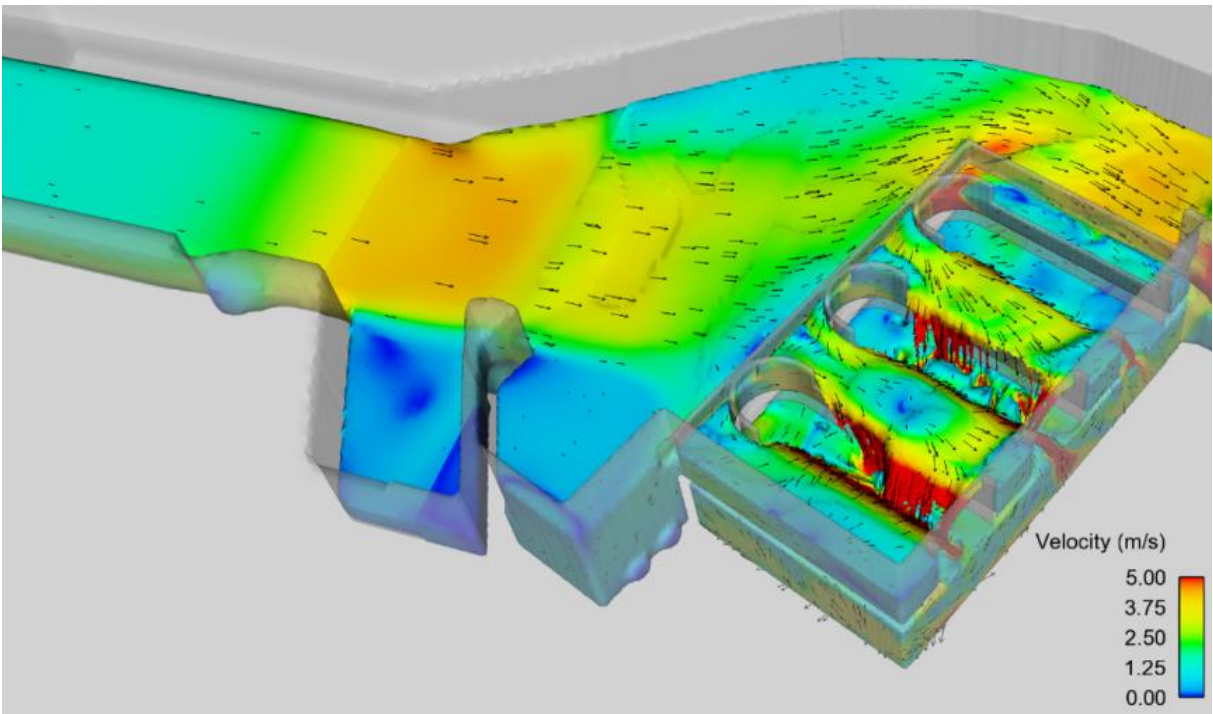


Figure 51 - Velocity field in P100

The hydraulic jump at the tunnel entrance, Figure 52, does not occurs and the flow inside the tunnel proceeds in free surface.

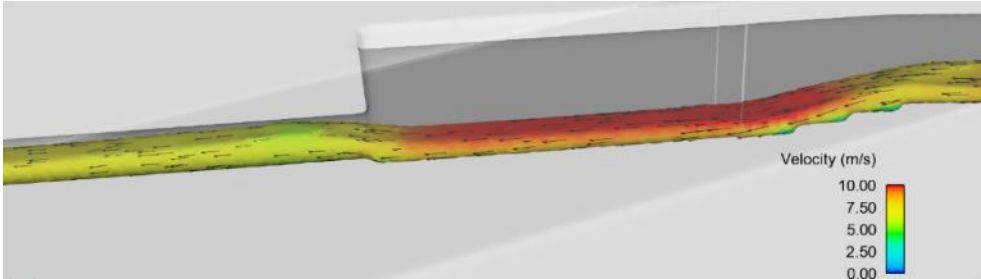


Figure 52 - Velocity field in the tunnel in P100

Table 15 - Water heads in the tunnel in P100

Probe Point	h(m)
Hydraulic jump	3.12
Tunnel	3.77

6.3.2 Frequent Scenario

The frequent scenario has an input of $36 \text{ m}^3/\text{s}$, and the mass stabilization was observed around 300 seconds of simulation, and the elapsed time of 4 days and 10 hours for a total amount of 2,613,418 cells, with a variation threshold of the flux in the tunnel of 1.68%, as illustrated in Figure 53 and Figure 54.

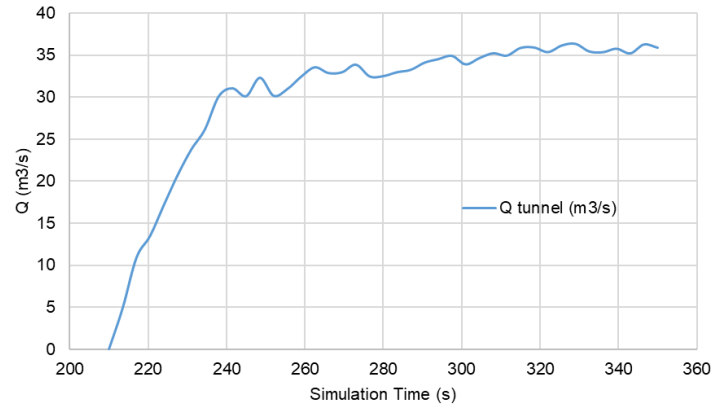


Figure 53 - Flow inside the tunnel for P1

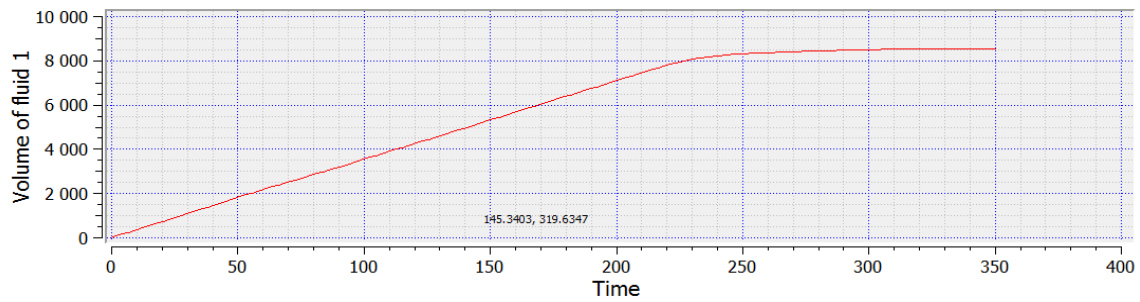


Figure 54 - Volume of fluid 1 in the domain for P1

Table 16 - P1 total amount of cells, stabilization time and elapsed time until stabilization

Total Amount of Cells	Stabilization Time (s)	Elapsed Time Until Stabilization	Variation threshold
2613418	300	4 days and 10 hours	1.68%

Comparing the stabilization time with the one at the model scale, since similar simulation formulation was used, by Froud's Similarity Law, the stabilization time should be around 301 seconds to reach an equivalent mass balance state. This showcases a difference near 0%.

Qualitatively P1 presents a similar behaviour to M1, Figure 55, with water heads lower than the maximum head of overflow. In general, P1 results regarding water heads around wastewater screens shows lower values, with differences of 3-4% when compared to M1, as observed in the following figure and table.



Figure 55 - Comparison of P1 results with experimental results regarding water heads

The velocity field, Figure 56, has similar values comparing with M1, and the direction of the velocity vectors is also similar.

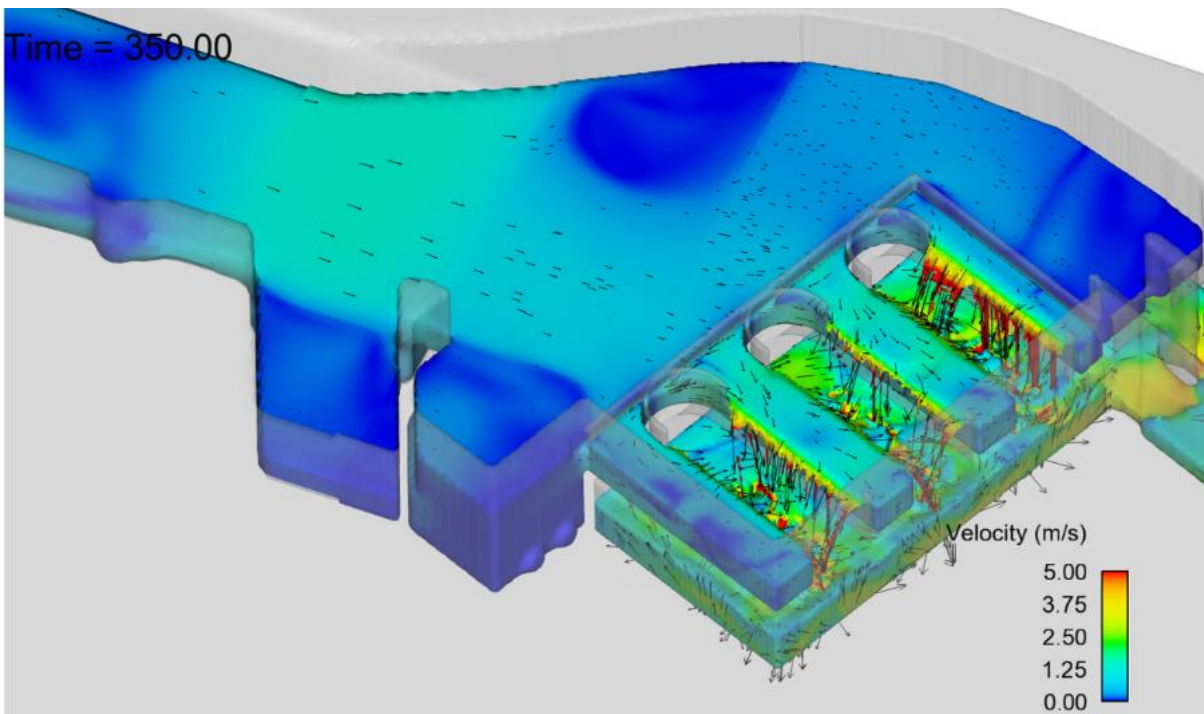


Figure 56 - Velocity field in P1

The hydraulic jump at the tunnel entrance, Figure 57, does not occurs and the flow inside the tunnel proceeds in free surface.

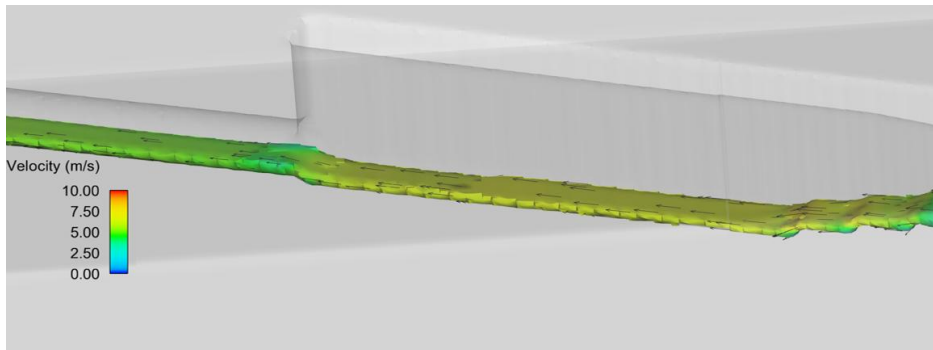


Figure 57 - Velocity field in the tunnel in P1

Table 18 - Water heads in the tunnel in P1

Probe Point	h(m)
Hydraulic jump	1.58
Tunnel	1.71

6.3.3 Exceptional Scenario

The exceptional scenario has an input of 120 m³/s, as the mass stabilization was observed around 220 seconds of simulation, and the elapsed time of 6 days, with a variation threshold of the flux in the tunnel of 2.67% as illustrated in Figure 58 and Figure 59.

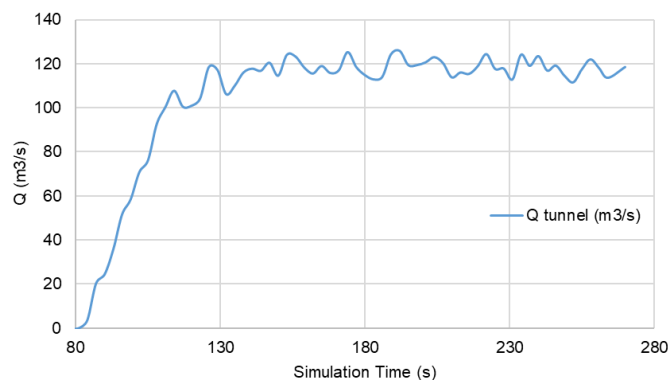


Figure 58 - Flow inside the tunnel for PE100

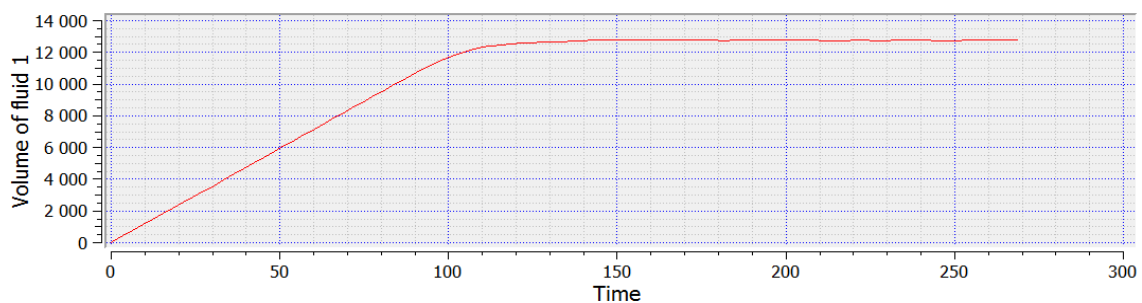


Figure 59 - Volume of fluid 1 in the domain for PE100

Table 19 - PE100 total amount of cells, stabilization time and elapsed time until stabilization

Total Amount of Cells	Stabilization Time (s)	Elapsed Time Until Stabilization	Variation threshold
2613418	220	6 days	2.67%

Comparing the stabilization time with the one at the model scale, since similar simulation formulation was used, by Froud's Similarity Law, the stabilization time should be around 164 seconds to reach an equivalent mass balance state. This showcases a difference around 24% lower compared with the observed.

Qualitatively PE100 presents a similar behaviour to ME100, Figure 60, showing higher water heads in general. In PE100 scenario 4 out of 6 screens reached the maximum head of overflow. The results show differences from 0% to 21%.

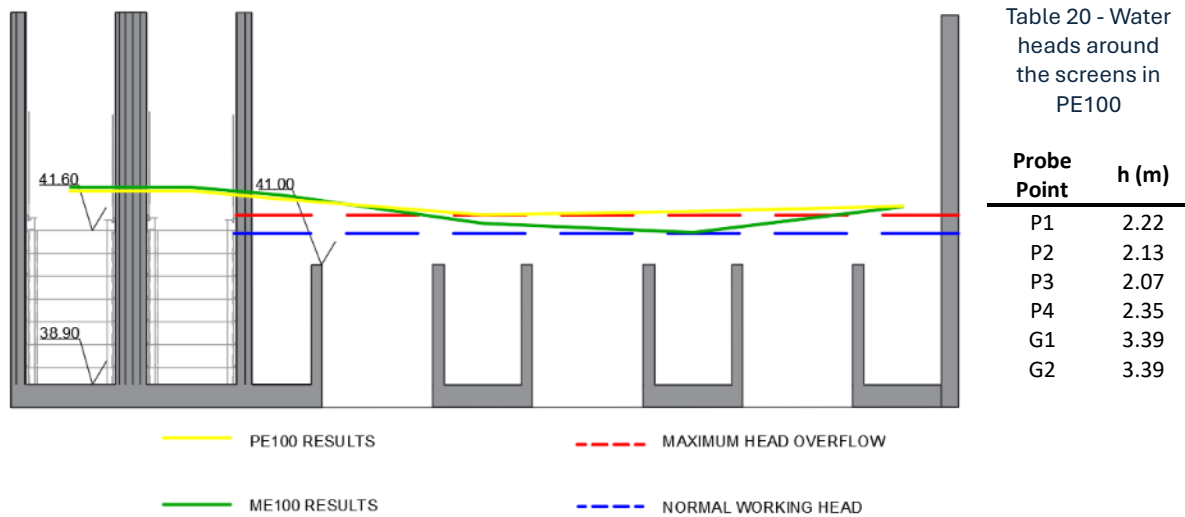


Figure 60 - Comparison of PE100 results with experimental results regarding water heads

The velocity field, Figure 61, has similar values and velocity vectors direction, when compared to ME100.

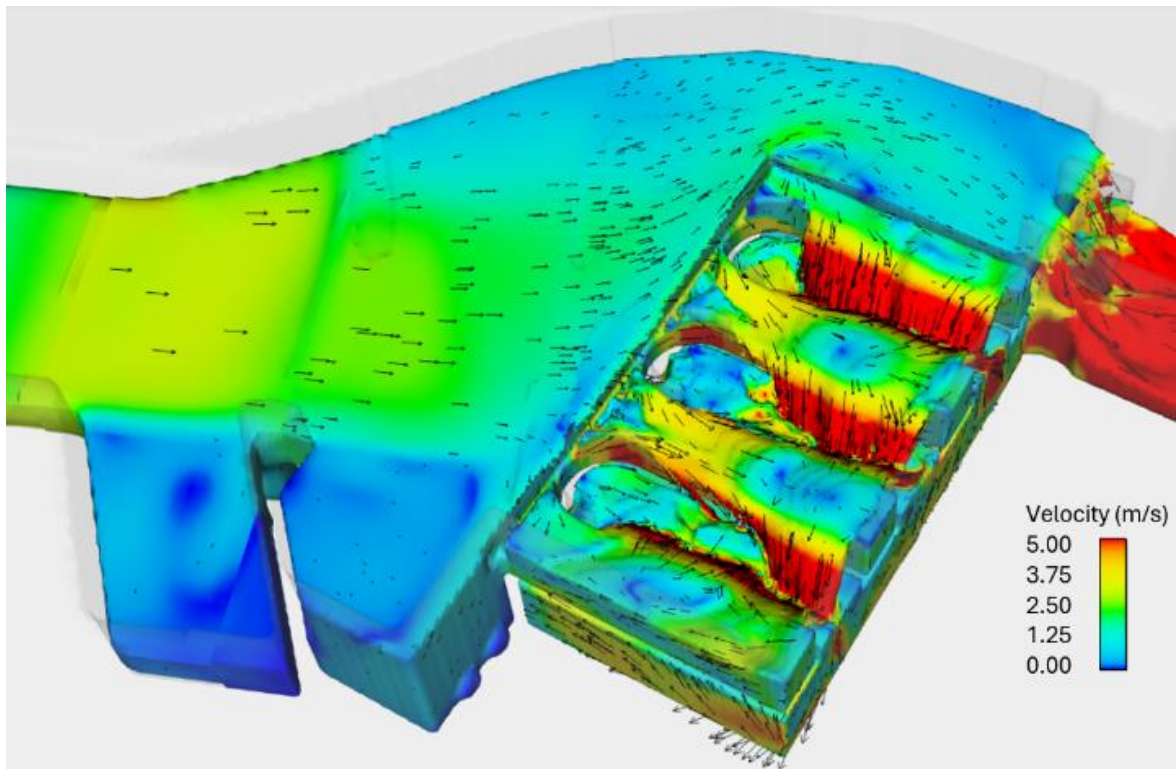


Figure 61 - Velocity field in PE100

The hydraulic jump, Figure 62, at the tunnel entrance does not occurs and the flow inside the tunnel proceeds in free surface.

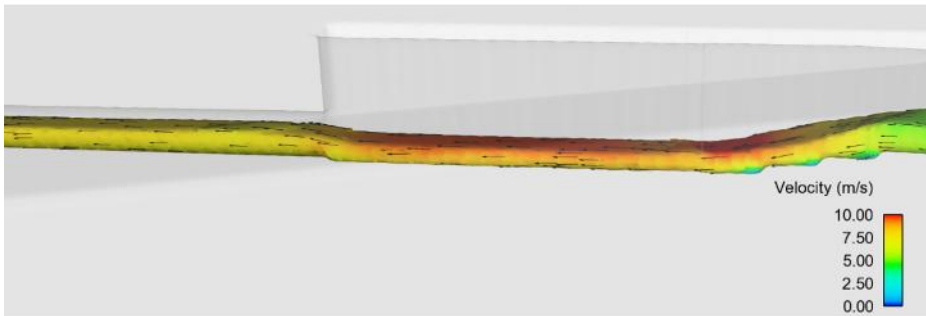


Figure 62 - Velocity field in the tunnel in PE100

Figure 63 - Water heads in the tunnel in PE100

Probe Point	h(m)
Hydraulic jump	2.77
Tunnel	3.40

6.4 Results Summary

At an early stage, the numerical results revealed discrepancies due to the boundary conditions, that resulted in unrealistic backflow, making it clear that reliable information is necessary to accurately identify incorrect formulations, such as experimental data or literature.

During the case study numerical analysis, the most time-consuming processes were found to be mesh optimisation and validation, as well as the geometry 3D construction. Mesh optimisation and validation can be a time-consuming and challenging process, yet when performed correctly, the simulation is more likely to converge and generate results faster.

In general, the model scale results showed similar and expected results when compared to the preformed experimental results, at the same scale, by only showing the exceedance of the maximum head of overflow in the expected exceptional scenario, the leaf gates overtopping in the exceptional scenario and free surface flow inside the tunnel for all the scenarios. By its turn, prototype scale results did not differ from the expected results around the wastewater screens, only showing the exceedance of the maximum head of overflow, leaf gates overtopping in the exceptional scenario and free surface flow inside the tunnel for all the scenarios. However, a notable discrepancy arises: while a hydraulic jump is evident in the model-scale simulation, it is absent in the prototype-scale simulation, despite both being configured with identical boundary conditions, mesh formulations, and same turbulence model.

This difference implies a deeper examination into the potential causes of scale effects and modelling limitations. In reduced scale simulations, maintaining the same fluid viscosity while reducing geometric dimensions and velocities, typically results in lower Re numbers, increasing the relative impact of viscous forces and thus exaggerating hydraulic losses compared to the prototype scale, this is supported by the Moody diagram [39]. These increased losses reduce the specific energy of the flow, potentially altering flow conditions such as the occurrence or characteristics of hydraulic jumps. With this, it is indeed observed at the prototype scale the flow in the lateral channel exhibits higher Reynold values than at the prototype scale. The flow in this case has sufficient specific energy to enter the tunnel without the need of the hydraulic jump.

It is important to emphasize the poorer flexibility that the numerical model at the prototype scale demonstrated in terms of mesh definition. Whilst the initial mesh formulation was found to be capable of producing results for the M100 scenario, it was unsuccessful for the ME100 however, but the same mesh formulation was not sufficient to produce results for any of the prototype scale scenarios. Consequently, a new and optimized mesh formulation was required for those simulations and implementing a mesh with less singularities although with similar cell sizes was key to solve the numerical instability problem.

Throughout the course of the simulations, Re values were found to exceed 10^4 as intended. In the context of turbulence model evaluation, the $k - \omega$, $k - \varepsilon$ and RNG models exhibited comparable capacity in representing the turbulent flow. With this, primary criterion for the turbulence model selection was the elapsed time for mass stabilization, for the exact conditions in both turbulence models, alongside with observations considering the development of the time-step size in time. This is due to the direct

correlation between these parameters and a stable simulation, in terms of its capacity towards convergence. Ultimately, the $k - \omega$ model was selected due to its superior performance in this regard.

Regarding the convergence criteria, these were overall satisfied. Nevertheless, it is recognized that additional improvements could have been made if the computation times had been extended. However, based on the results obtained through the preformed experimental tests, there was already substantial knowledge of the behaviour of flow variables. This facilitated the validation of the models and demonstrated credibility and acceptance of the results, despite the potential for improvement in the convergence criteria adopted.

Following a review of the elapsed times, it was found that the computation of the reduced scaled scenarios necessitated a duration of approximately three days. In contrast, the prototype scale scenarios required between four to eight days, despite the utilisation of a similar mesh configuration, boundary conditions and turbulence model in both scales. This discrepancy is consistent with the reviewed principle that, within the model scale, the behaviour of the fluid with identical viscosity from the prototype scale, will be characterised by the predominance of viscous forces. Consequently, this will result in enhanced control of the separation of liquid veins, which, in computational terms, demands less effort with higher time-steps, that reduce the elapsed times.

Finally, the total amount of cells increased between M100 to more than double to M1 and ME100 delineated how a good mesh balance can be achieved without affecting the numerical elapsed time until stabilization, thus enhancing the necessity to test different mesh formulations to achieve mesh independent results and optimized simulation times.

7 Final Considerations and Future Developments

The new paradigm of the recently revised UWWTD will undoubtedly introduce fresh dynamics into urban drainage systems. To take advantage of this evolution, national targets should harness the momentum of this new context to accelerate the digitalization of systems, which in turn requires an updated cadastral information, as well as knowledge of the condition of the drainage elements that compose it in terms of deterioration. This aligns with the monitoring and cadastral development objectives outlined in the new directive but also in PENSAARP2030.

Alongside with digitalization comes a symbiosis with CFD modelling, aiming to create digital twins—both at the stage of improving the design of new projects and later during operational control and rehabilitation—by using real-time data or, alternatively, as a tool to support decisions on which measures to adopt and what types of optimizations should be applied to existing systems. In this way, system resilience can be strengthened against the diverse new challenges, such as higher pollutant loads, intensified rainfall, loss of capacity in gravity-based systems due to sea level rise and deterioration. This digital approach facilitates and enhances the operational capability of management utilities in decision making.

The methodology presented in this master's thesis provides the necessary tools for the formulation of a CFD numerical model, highlighting the general key aspects involved in the efficient creation of the computational model such as, the mesh optimization, correct boundary conditions definition and how validation relies on either in experimental data, literature or real data collection. The proposed methodology has been designed to align with the commercial software Flow3D, although it should be noted that the key concepts presented in the proposed flowchart are suitable for CFD software in general.

Through the process of validation of the numerical models, traditional experiments carried out by LNEC were used. With the knowledge on the flow behavior given by those results, it was possible to accept that via the proposed methodology, the convergence of the results via mass balance, a simplified convergence method compared to those presented in the existing literature, can produce results with robust levels of confidence for civil engineering applications, enabling informed decisions in the design of this type of structure. This highlights the importance that comparison though control sections well established in literature or experimental data has to strength CFD simulations.

In the conducted scale tests, it is also worth noting the cost–benefit advantages of using reduced scales. These lead to simulations which, due to the more viscous behavior of the fluid and therefore the reduced need for computational detail, can be carried out more quickly and easily. Nevertheless, phenomena such as hydraulic jumps may yield different results when comparing results at the prototype and reduced model scale, due to scale effects in relation to viscous dissipation of energy. Therefore, in cases where this aspect is critical, special attention must be given.

In a more detailed analysis, such as those involving hydraulic jumps, one way to optimize simulation time is to extrapolate results from reduced-scale simulations and then carry out more localized simulations at prototype scale. This can be done by linking boundary conditions to results previously

obtained at the reduced scale, to then preform, for example, multiphase simulations (air and water interaction) or the adoption of more advanced turbulence models, such as LES, that naturally require more computational efforts that may not be practicable in first simulations trials, for example during the validation phase of boundary conditions. In line with this, other more demanding tests such as the study of solid or pollutant transport, that are of significant relevance within the context of urban drainage could be approached in a similar manner or even further investigation into the detailed operation of wastewater screens.

In conclusion, digitalization is the future of all scientific fields, as evidenced by the direction taken by the new UWWTD regarding automation control and increasingly demanding design requirements. In support of this reality, particularly within civil engineering, computational tools are becoming even more accessible, and their implementation ensures a resilient future. With this, it is evident that, by harnessing the potential of these models, hydraulic engineers can leverage CFD to develop Digital Twins to meet design targets and facilitate the construction of resilient, sustainable drainage networks, providing tools to enhance existing infrastructure to prevent hazards and also, leading to improved decision-making by management entities.

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