1. Introduction

The global transition toward sustainable energy systems has positioned hydrogen as a critical energy vector for achieving carbon neutrality and addressing climate change challenges, with hydrogen refuelling infrastructure representing a cornerstone of the emerging hydrogen economy [1]. As the world grapples with the urgent need to move away from carbon-intensive energy sources, hydrogen emerges as a particularly promising alternative due to its high energy content, zero greenhouse gas emissions during use, and potential for production from renewable sources [2]. The hydrogen infrastructure encompasses various stages including production, distribution, storage, and dispensing, with refuelling station storage technology representing one of the most critical components that must be optimized for widespread hydrogen adoption[3].

Hydrogen refuelling stations serve as the vital link between hydrogen production facilities and end-user applications, requiring sophisticated storage systems capable of maintaining large quantities of hydrogen at high pressures while ensuring safe and efficient dispensing operations [4]. The storage tanks at refuelling stations must accommodate significantly larger volumes compared to vehicle tanks, typically ranging from several hundred to thousands of litters, and must be capable of rapid charging and discharging cycles to maintain station availability and throughput [5]. These infrastructure storage systems face unique challenges related to thermal management, pressure control, and operational efficiency that differ substantially from vehicle-mounted storage applications [6].

The development of efficient and safe hydrogen refuelling station storage systems is crucial for achieving the performance requirements necessary for commercial viability of hydrogen infrastructure, including adequate storage capacity, rapid replenishment capabilities, high dispensing rates, and long-term durability under continuous operation [7]. Unlike vehicle applications where weight and volume constraints dominate design considerations, refuelling station storage systems must prioritize operational reliability, maintenance accessibility, and cost-effectiveness over extended service periods [8].

The hydrogen refuelling industry has witnessed significant progress in infrastructure development, with major energy companies and government initiatives investing in comprehensive refuelling networks to support the growing hydrogen vehicle market [9]. Modern refuelling stations typically employ multi-stage storage systems with high pressure tanks operating at 35 to 87.5 MPa, intermediate pressure storage for cascade filling operations, and sophisticated control systems to manage the complex thermodynamic processes involved in hydrogen dispensing [10]. The Toyota Mirai and other commercial fuel cell vehicles have demonstrated the practical feasibility of hydrogen-powered transportation, creating demand for reliable refuelling infrastructure that can match the convenience and speed of conventional fuel stations[11].

Type IV hydrogen storage tanks have emerged as the preferred solution for refuelling station applications due to their high volumetric density, lightweight properties relative to steel alternatives, and excellent fatigue resistance under cyclic loading conditions [12]. These tanks, characterized by polymer liners fully wrapped in carbon fibber composites, must withstand high pressures while maintaining structural integrity throughout numerous charging and discharging cycles that occur during normal station operations [13]. The charging process of station storage tanks presents particular challenges, as rapid hydrogen injection from delivery trucks or pipeline systems can lead to significant temperature increases within the tanks, potentially affecting storage capacity, causing thermal stress in tank materials, and raising safety concerns [14], [15].

Understanding the thermodynamic processes occurring during hydrogen refuelling station tank charging is essential for optimising infrastructure design, ensuring safe operation, and maximising station efficiency and availability [15]. The charging process involves complex heat and mass transfer phenomena, with temperature and pressure evolution governed by fundamental thermodynamic principles that must be carefully managed to prevent equipment damage and ensure operational safety [16]. For inherently safer operation of refuelling station storage systems, gas temperature and pressure inside the tanks must not exceed established safety limits, typically 85°C and 1.25 times the nominal working pressure, respectively, according to established safety standards[17]. Numerical simulation has become an indispensable tool for analysing hydrogen refuelling station storage tank charging processes, enabling infrastructure designers and operators to investigate various operating conditions, optimise charging protocols, and predict system performance without the need for extensive experimental testing on full-scale systems [18]. Computational approaches range from detailed computational fluid dynamics simulations that capture complex flow patterns and heat transfer mechanisms to simplified thermodynamic models that focus on overall system behaviour and can be implemented in real-time control systems [19]. The choice of simulation approach depends on the specific objectives of the analysis, available computational resources, and required level of detail for infrastructure design and operation[20] .

The mathematical modelling of hydrogen refuelling station tank charging typically involves solving coupled differential equations representing conservation of mass and energy within the storage vessel, accounting for the unique operating conditions and constraints of infrastructure applications [21]. For simplified analysis suitable for control system implementation and preliminary design studies, ideal gas assumptions are often employed, particularly when the focus is on understanding fundamental thermodynamic behaviour rather than detailed spatial flow phenomena [22]. The adiabatic assumption, where heat transfer to the surroundings is neglected during rapid charging operations, provides a conservative estimate of temperature rise and is commonly used in safety assessments and worst-case scenario evaluations for station design [23].

MATLAB's ordinary differential equation solvers, particularly the ODE45 function based on the Runge-Kutta method, have proven effective for solving the governing equations of hydrogen refuelling station tank charging processes [24]. The ODE45 solver offers a good balance between computational efficiency and accuracy for non-stiff problems, making it suitable for thermodynamic simulations where the governing equations do not exhibit extreme sensitivity to small changes in variables [25]. The availability of built-in error control and adaptive step size selection further enhances the reliability of numerical solutions for infrastructure applications where accuracy and robustness are paramount[26] .

Current research in hydrogen refuelling infrastructure emphasizes the need for improved storage systems, enhanced safety protocols, and robust operational procedures to support hydrogen adoption at scale [1]. The integration of advanced materials, smart monitoring systems, and predictive control algorithms represents key areas of development for next-generation refuelling stations [27]. Composite materials play a central role in the advancement of refuelling station storage technology, requiring comprehensive understanding of their mechanical behaviour under the demanding operating conditions of infrastructure applications[28], [29] . The integration of hydrogen storage and safety concepts remains an active area of research, with interdisciplinary collaboration essential for overcoming existing challenges and facilitating safe and efficient hydrogen infrastructure deployment[28].

The present study addresses the critical need for understanding thermodynamic processes in hydrogen refuelling station storage tank charging through the development and implementation of a numerical simulation model specifically tailored for infrastructure applications. The research focuses on simulating hydrogen charging of rigid storage tanks under ideal gas assumptions with constant mass inflow rate and adiabatic conditions, representing typical operating scenarios encountered in refuelling station operations. The mathematical model incorporates fundamental mass and energy balance equations, solved using MATLAB's ODE45 solver to predict temperature, pressure, and mass evolution during the charging process of station storage systems.

The original contribution of this work lies in the systematic development of a simplified yet physically meaningful simulation framework that can serve as a foundation for refuelling station design, operation optimization, and safety analysis. The study provides insights into the fundamental thermodynamic behaviour of hydrogen refuelling station tank charging processes, offering a computational tool that can be readily adapted for various station configurations, storage capacities, and operating protocols. The simulation results contribute to the understanding of temperature rise mechanisms during rapid tank replenishment and provide guidance for safe operating procedures in refuelling infrastructure.

The practical applications of this research extend to hydrogen refuelling station design, operational protocol development, and safety system optimization. The simulation framework can be used to evaluate different charging strategies, optimize tank replenishment procedures, assess the impact of various parameters on station performance, and develop predictive maintenance protocols. Furthermore, the model serves as a valuable tool for infrastructure planning, enabling assessment of storage requirements, charging system sizing, and operational capacity planning for hydrogen refuelling networks.

This thesis is organized into seven main sections that systematically present the research methodology, results, and conclusions from the perspective of refuelling station infrastructure. Following this introduction, Section 2 provides a comprehensive literature review covering hydrogen storage technologies for infrastructure applications, refuelling station tank charging processes, numerical simulation methods, and composite materials in large-scale hydrogen storage. Section 3 details the mathematical model development and numerical implementation using MATLAB ODE45 for refuelling station applications. Section 4 presents the simulation results and discusses their implications for hydrogen refuelling infrastructure design and operation. Section 5 explores safety and engineering considerations specific to refuelling station storage systems. Section 6 summarizes the key conclusions and suggests directions for future research in hydrogen infrastructure technology. The thesis concludes with a complete reference list and appendices containing simulation code adapted for refuelling station applications.

2. Literature Review

2.1 Hydrogen Storage Technologies for Infrastructure Applications

The development of efficient hydrogen storage technologies for refuelling station infrastructure represents one of the most critical challenges in the advancement of the hydrogen economy. Unlike vehicle applications where weight and volume constraints dominate design considerations, refuelling station storage systems must prioritize operational reliability, high capacity, rapid charging and discharging capabilities, and cost-effectiveness over extended service periods [30]. Hydrogen storage methods for infrastructure applications can be broadly categorised into three main approaches: solid storage, liquid storage, and gaseous storage, each with distinct advantages and limitations that determine their suitability for refuelling station operations [31].

Solid storage systems, involving the storage of hydrogen atoms in the form of simple hydrides or complex hydrides such as borohydrides, alanates, or lithium amides within metallic crystal lattices or carbon nanostructures, offer potential advantages for stationary infrastructure applications [32]. These systems can achieve high volumetric storage densities and enhanced safety due to the chemical binding of hydrogen atoms, making them attractive for refuelling stations where space constraints may be less critical than in vehicle applications [33] However, solid storage systems typically require elevated temperatures for hydrogen release and may suffer from slow kinetics and limited reversibility, making them less suitable for refuelling stations where rapid hydrogen dispensing is essential for maintaining station throughput and customer satisfaction[34] .

Liquid or cryogenic storage maintains hydrogen in liquid form at extremely low temperatures, typically around -250°C, and has found application in some large-scale refuelling stations, particularly those serving high-volume operations such as bus depots or fleet applications [35]. While this method achieves high volumetric storage densities that can be advantageous for refuelling stations with limited space, the energy requirements for liquefaction and the need for sophisticated insulation systems to prevent boil-off losses present significant challenges for widespread deployment [36]. The complexity and cost of cryogenic storage systems, along with the continuous energy consumption required for maintaining low temperatures, limit their application primarily to specialised refuelling installations where the infrastructure can support the necessary cooling and handling requirements [37].

Gaseous storage, also known as compressed storage, involves storing hydrogen gas at high pressures in specially designed pressure vessels and has emerged as the most mature and widely adopted technology for hydrogen refuelling station infrastructure [38]. Among the three storage approaches, compressed gas storage offers the most practical solution for refuelling stations due to its relatively simple operation, rapid charging and discharging capability, established manufacturing base, and compatibility with existing vehicle refuelling protocols [39]. The technology has been successfully demonstrated in commercial refuelling stations worldwide and continues to benefit from ongoing improvements in materials, manufacturing processes, and operational procedures [40].

The classification of compressed hydrogen storage tanks for refuelling station applications follows established standards that categorise vessels based on their construction materials and design approaches, with considerations for the unique requirements of infrastructure installations [41]. Type I tanks consisting entirely of steel construction are primarily used for stationary refuelling station applications where weight is not a critical concern and where the robust construction provides advantages for long-term durability and maintenance accessibility [42]. These tanks are often employed in refuelling stations for low-pressure storage applications or as backup storage systems where reliability and cost-effectiveness are prioritised over weight considerations. [28].

Type II tanks featuring steel liners with partial composite overwrap offer improved weight characteristics compared to all-steel designs while maintaining cost-effectiveness for specific refuelling station applications. [43]. These tanks find application in refuelling stations where moderate weight reduction is beneficial but where the full performance advantages of composite construction are not required. The hybrid construction provides a balance between performance and cost that can be attractive for infrastructure applications with budget constraints [44]

Type III tanks represent a significant advancement in refuelling station storage technology, incorporating aluminium liners with full composite overwrap that provides substantial weight reduction compared to all-metal designs [45]. These tanks have found widespread application in hydrogen refuelling stations where weight reduction translates to easier installation, reduced structural support requirements, and improved seismic resistance [46]. The aluminium liner provides excellent hydrogen compatibility and corrosion resistance, while the composite overwrap carries the structural loads imposed by high internal pressures [47].

Type IV tanks, characterized by polymer liners fully wrapped in carbon fibber composites, represent the current state-of-the-art for many hydrogen refuelling station storage applications [37]. These tanks offer the highest gravimetric and volumetric storage densities among compressed storage options, making them essential for maximizing storage capacity within the space constraints of urban refuelling stations [16]. The polymer liner, typically made from high-density polyethylene or similar materials, provides a hydrogen-tight barrier while the carbon fibber composite overwrap carries the structural loads imposed by high internal pressures up to 87.5 MPa in refuelling station applications.

The development of Type IV tanks for refuelling station applications has been driven by the need for high-capacity storage systems that can accommodate the large volumes of hydrogen required for continuous station operations [48]. Modern

Type IV tanks for refuelling stations can operate at pressures up to 87.5 MPa and store thousands of kilograms of hydrogen, providing sufficient capacity to serve hundreds of vehicle refuelling operations between replenishment cycles [49]. The manufacturing processes for these large-scale tanks have evolved to incorporate advanced fibre placement techniques, optimised resin systems, and sophisticated quality control measures to ensure consistent performance and safety under the demanding conditions of refuelling station operations [50].

Recent research in hydrogen storage technology for refuelling infrastructure has focused on further improvements in tank design, materials, and manufacturing processes specifically tailored for infrastructure applications [1]. Advanced composite materials with enhanced mechanical properties and improved resistance to hydrogen-induced degradation are being developed to extend tank service life and reduce lifecycle costs for refuelling station operators [14]. Novel liner materials and designs are being investigated to minimise hydrogen permeation while maintaining structural integrity under the cyclic loading conditions typical of refuelling station operations [51]

The integration of smart sensing technologies into hydrogen refuelling station storage tanks represents an emerging trend that promises to enhance safety, performance monitoring, and predictive maintenance capabilities [52]. Embedded sensors can provide real-time information about tank condition, hydrogen purity, pressure and temperature distributions, and potential degradation mechanisms, enabling predictive maintenance strategies and improved operational safety for refuelling infrastructure [53]. These developments are particularly important for refuelling station applications where tank reliability and safety are paramount concerns and where unplanned downtime can significantly impact station availability and revenue [54].

2.2 Hydrogen Refuelling Station Tank Charging Processes

The hydrogen tank charging process in refuelling stations involves the transfer of hydrogen gas from delivery trucks, pipelines, or on-site production systems to the station's high-pressure storage tanks through controlled filling procedures that must accommodate much larger volumes and higher flow rates than vehicle refuelling operations [17]. This process is governed by complex thermodynamic and fluid dynamic phenomena that significantly influence the final state of charge, tank temperature, operational efficiency, and overall safety of the refuelling station [55]. Understanding these processes is crucial for developing efficient charging protocols, ensuring safe operation of refuelling infrastructure, and maximizing station availability and throughput [56].

The thermodynamics of hydrogen refuelling station tank charging are fundamentally governed by the first law of thermodynamics, which relates the change in internal energy of the gas to the work done on the system and heat transfer, but with considerations for the much larger scales and higher flow rates typical of infrastructure operations [15]. During rapid charging of station storage tanks, the compression of hydrogen gas within the tanks leads to significant temperature increases that can exceed safe operating limits if not properly managed through appropriate charging protocols and thermal management systems [14]. The temperature rise is particularly pronounced when the charging process occurs rapidly, as is often required for refuelling stations to minimize delivery truck dwell time and maintain operational efficiency [17].

The Society of Automotive Engineers (SAE) J2601 standard provides guidelines for hydrogen refuelling protocols that, while primarily focused on vehicle refuelling, also inform the development of charging procedures for refuelling station storage tanks [57]. The standard establishes that gas temperature inside tanks should not exceed 85°C during charging operations, and pressure should not exceed 1.25 times the nominal working pressure to ensure safe operation of composite tanks [56]. These limits, based on extensive testing and analysis of tank materials, are designed to prevent thermal and mechanical damage that could compromise tank integrity in both vehicle and infrastructure applications[50].

The refuelling station tank charging process typically involves several distinct phases that differ from vehicle refuelling due to the larger volumes and different operational constraints [49]. The process begins with the connection of delivery equipment and pressure equalization between the supply system and station storage tanks [58]. The main charging phase follows, during which hydrogen is transferred at controlled rates to manage temperature rise while achieving acceptable charging times that minimize delivery truck dwell time and associated costs [48]. The final phase involves pressure equalization and system shutdown, ensuring that the tanks reach their target pressure without exceeding safety limits while preparing the station for normal dispensing operations [4].

Heat transfer mechanisms during hydrogen refuelling station tank charging include both convective heat transfer within the gas and conductive heat transfer through the tank walls, with the relative importance of these mechanisms depending on factors such as charging rate, tank geometry, ambient conditions, and the thermal mass of the station infrastructure [46]. For rapid charging scenarios typical of delivery truck operations, convective heat transfer within the gas typically dominates, leading to relatively uniform temperature distributions within the tank [55]. However, for slower charging processes or larger tanks with enhanced heat transfer capabilities, heat transfer to the surroundings becomes more significant and can help limit temperature rise [45].

The concept of adiabatic charging, where heat transfer to the surroundings is neglected, provides a conservative estimate of temperature rise during station tank charging and is commonly used in preliminary analyses and safety assessments [44]. This assumption is particularly valid for rapid charging scenarios where the time scale of the process is much shorter than the thermal time constant of the tank system, which is typically longer for large refuelling station tanks due to their greater thermal mass [54]. Adiabatic analysis provides an upper bound on temperature rise and is therefore useful for safety assessments and worst-case scenario evaluations in refuelling station design [16].

Computational fluid dynamics (CFD) simulations have been extensively used to study hydrogen refuelling station tank charging processes, providing detailed insights into flow patterns, temperature distributions, and heat transfer mechanisms specific to large-scale infrastructure applications [14]. These simulations can capture complex phenomena such as jet impingement, mixing, and thermal stratification that may occur during charging of large storage tank [57]. However, CFD simulations require significant computational resources and detailed knowledge of boundary conditions, making them more suitable for detailed design studies of specific refuelling station configurations rather than general analysis or real-time control applications [15].

Simplified thermodynamic models, based on lumped parameter approaches, offer an alternative to detailed CFD simulations for understanding fundamental charging behaviour in refuelling station storage tanks [17]. These models treat the tank contents as a uniform system and focus on overall energy and mass balance rather than spatial variations, making them suitable for control system implementation and operational optimization [59]. While less detailed than CFD approaches, thermodynamic models provide valuable insights into system behaviour and can be solved efficiently using standard numerical methods suitable for real-time applications [14].

The heat capacity method, as defined in the SAE J2601 standard, represents a practical approach for estimating end temperatures during refuelling station tank charging [59]. This method considers the actual thermodynamic conditions of both the supply system and station storage tanks to evaluate overall heat transfer and predict final tank conditions [60]. Implementation of the heat capacity method has been shown to reduce end temperature estimates and improve state of charge predictions compared to simpler adiabatic models, making it valuable for refuelling station operational planning [57].

Experimental studies of hydrogen refuelling station tank charging have provided valuable validation data for numerical models and have revealed important insights into the physics of large-scale charging processes [57]. These studies have investigated the effects of various parameters including initial tank conditions, charging rates, hydrogen supply temperature, and tank geometry on final tank state and operational efficiency [59]. The results have informed the development of charging protocols for refuelling stations and have contributed to the establishment of safety standards for infrastructure applications [61].

Recent research has focused on developing advanced charging strategies specifically for refuelling station operations that optimize the trade-off between charging time, temperature rise, and operational efficiency [56]. These strategies may involve variable charging rates, precooling of the hydrogen supply, active thermal management of the tank system, or coordinated charging of multiple tanks to maintain station availability [50]. The goal is to achieve rapid tank replenishment while maintaining safe operating conditions, maximizing storage capacity utilization, and minimizing operational costs for refuelling station operators [49].

2.3 Numerical Simulation Methods for Infrastructure Applications

Numerical simulation has become an essential tool for analysing hydrogen refuelling station storage systems and charging processes, enabling infrastructure designers and operators to investigate complex phenomena that are difficult or expensive to study experimentally on full-scale systems [47]. The choice of simulation approach for refuelling station applications depends on the specific objectives of the study, the level of detail required for infrastructure design and operation, the available computational resources, and the need for real-time implementation in control systems. Simulation methods for hydrogen refuelling station tank charging range from detailed three-dimensional computational fluid dynamics models to simplified ordinary differential equation systems suitable for control system implementation [45].

Computational fluid dynamics represents the most comprehensive approach to simulating hydrogen refuelling station tank charging processes, capable of capturing detailed flow patterns, heat transfer mechanisms, and spatial variations in temperature and pressure within large-scale storage systems [11]. CFD simulations solve the Navier-Stokes equations along with energy and species transport equations to provide a complete description of the fluid behaviour within refuelling station tanks [19]. These simulations can account for complex phenomena such as jet impingement, turbulent mixing, and thermal stratification that may significantly influence the charging process in large storage tanks.

The accuracy of CFD simulations for refuelling station applications depends critically on the quality of the computational mesh, the choice of turbulence models, and the specification of boundary conditions that accurately represent the operating conditions of infrastructure systems [18]. High-quality meshes with sufficient resolution near walls and in regions of high gradients are essential for capturing important physical phenomena in large-scale tanks [20]. Turbulence modelling is particularly important for refuelling station tank charging simulations, as the high velocity jets created during rapid charging typically result in turbulent flow conditions that can significantly affect mixing and heat transfer [62].

Despite their comprehensive nature, CFD simulations require significant computational resources and expertise to set up and interpret correctly, making them more suitable for detailed design studies of specific refuelling station configurations rather than parametric investigations or real-time control applications [11]. The computational cost scales rapidly with the complexity of the geometry and the desired level of detail, which can be substantial for large refuelling station storage systems. Additionally, the results of CFD simulations are sensitive to modelling assumptions and boundary conditions, requiring careful validation against experimental data from infrastructure-scale systems [20].

Ordinary differential equation (ODE) based models offer a computationally efficient alternative to CFD simulations for studying the overall thermodynamic behaviour of hydrogen refuelling station tank charging. These models treat the tank contents as a lumped system with uniform properties and focus on the temporal evolution of average quantities such as temperature, pressure, and mass, making them suitable for control system implementation and operational optimization [20]. While ODE models cannot capture spatial variations within large tanks, they provide valuable insights into fundamental system behaviour and can be solved rapidly using standard numerical methods [61].

The mathematical foundation of ODE-based models for refuelling station tank charging rests on the application of conservation principles to the tank system, with considerations for the unique operating conditions and constraints of infrastructure applications [63]. The conservation of mass requires that the rate of change of mass within the tank equals the mass flow rate into the tank, which may be much higher for refuelling station operations than for vehicle refuelling [64]. The conservation of energy, expressed through the first law of thermodynamics, relates the rate of change of internal energy to the enthalpy flow into the tank and any heat transfer to the surroundings.

MATLAB's ODE suite provides a comprehensive set of solvers for ordinary differential equations, with different methods optimized for various types of problems encountered in refuelling station analysis [65]. The ODE45 function, based on the Dormand-Prince Runge-Kutta method, is particularly well-suited for non-stiff problems and offers a good balance between computational efficiency and accuracy for infrastructure applications [66]. The solver incorporates automatic error control and adaptive step size selection, ensuring reliable solutions while minimizing computational effort, which is important for real-time control applications [3].

The Runge-Kutta methods underlying ODE45 are explicit methods that compute the solution at the next time step based on information from the current time step, making them suitable for problems where the solution does not exhibit extreme sensitivity to small changes in the variables [67]. For hydrogen refuelling station tank charging simulations under ideal gas assumptions, the governing equations are typically non stiff, making ODE45 an appropriate choice for infrastructure applications [68]. The method's stability and accuracy characteristics are well-suited to the smooth, well behaved solutions expected from thermodynamic models of refuelling station operations [35].

The numerical differentiation formulas (NDFs) represent an alternative class of methods for solving ordinary differential equations, particularly suited for stiff problems where implicit methods are required [37]. While not typically necessary for simplified hydrogen refuelling station tank charging models, NDFs may be useful for more complex simulations that include detailed chemical kinetics, rapid heat transfer processes, or coupling with other infrastructure systems [68]. The choice of numerical method depends on the specific characteristics of the problem and the requirements for accuracy and computational efficiency [67].

Error estimation and control are critical aspects of numerical simulation that ensure the reliability of computed results for infrastructure applications where accuracy and safety are paramount [69]. Modern ODE solvers incorporate sophisticated error estimation techniques that monitor the local truncation error and adjust the step size accordingly [3]. This adaptive approach ensures that the solution meets specified accuracy requirements while minimizing computational cost, which is important for both design studies and real-time control applications [70].

Validation of numerical models against experimental data or analytical solutions is essential for establishing confidence in simulation results for refuelling station applications [71]. For hydrogen refuelling station tank charging simulations, validation may involve comparison with experimental measurements of temperature and pressure evolution during charging of large-scale storage systems [3]. Additionally, simplified analytical solutions for limiting cases can provide useful benchmarks for numerical models used in infrastructure design [72].

Sensitivity analysis represents an important component of numerical simulation studies for refuelling station applications, helping to identify the parameters that most significantly influence system behaviour and operational performance [73]. For hydrogen refuelling station tank charging models, sensitivity analysis can reveal the relative importance of factors such as charging conditions, tank geometry, material properties, and operational procedures [74]. This information is valuable for guiding infrastructure design decisions, establishing operational procedures, and identifying areas where improved modelling may be needed [75].

2.4 Composite Materials in Large-Scale Hydrogen Storage Infrastructure

The use of composite materials in hydrogen refuelling station storage applications has revolutionized the design and performance of high-pressure storage systems, enabling significant improvements in storage capacity, operational efficiency, and infrastructure economics while maintaining structural integrity under the demanding operating conditions of commercial refuelling operations [73]. Carbon fibber reinforced polymer (CFRP) composites have emerged as the material of choice for large-scale Type IV hydrogen storage tanks in refuelling stations due to their exceptional strength-to weight ratio, fatigue resistance, and design flexibility that enables optimization for infrastructure-specific requirements [67].

The mechanical behaviour of composite materials under hydrogen refuelling station operating conditions involves complex interactions between the fibber reinforcement, polymer matrix, and the hydrogen environment, with considerations for the larger scales, higher pressures, and more demanding duty cycles typical of infrastructure applications [76]. Carbon fibbers provide the primary load-carrying capability of the composite structure, with their high tensile strength and stiffness enabling refuelling station tanks to withstand internal pressures up to 87.5 MPa while accommodating the large volumes required for infrastructure operations. The polymer matrix, typically an epoxy resin system optimized for hydrogen service, serves to transfer loads between fibbers, protect the fibbers from environmental damage, and provide overall structural integrity under the cyclic loading conditions of refuelling station operations [77]. Hydrogen-induced degradation represents a significant concern for composite materials in refuelling station storage applications, as hydrogen molecules can diffuse into the polymer matrix and potentially cause swelling, plasticization, or chemical degradation over the extended service periods required for infrastructure applications [3]. The small size of hydrogen molecules enables them to penetrate into polymer networks more readily than larger gas molecules, potentially leading to changes in mechanical properties over time that must be accounted for in refuelling station design and maintenance planning. Understanding and mitigating these effects is crucial for ensuring long-term durability of composite hydrogen storage tanks in refuelling infrastructure where replacement costs and downtime can be substantial [78].

The multiscale characterization of composite materials has become essential for understanding their behaviour under hydrogen refuelling station operating conditions, which may involve more severe loading and environmental conditions than vehicle applications [79]. Advanced characterization techniques including infrared thermography, X-ray tomography, acoustic emission, and digital image correlation provide insights into damage mechanisms and failure processes at various length scales relevant to large-scale infrastructure applications [80]. These techniques enable researchers to investigate how composites respond under impact and cyclic loading conditions that simulate real-world refuelling station operating environments [81].

Key failure mechanisms in composite hydrogen refuelling station storage tanks include matrix cracking, fibber breakage, and delamination, each of which can compromise the structural integrity of large-scale storage systems and potentially lead to costly infrastructure failures [37]. Matrix cracking typically occurs first under increasing load and can provide pathways for hydrogen diffusion and further degradation, which is particularly concerning for refuelling station applications where tanks may operate continuously for extended periods. Fiber breakage represents a more serious failure mode that directly reduces the load-carrying capacity of the composite structure and can lead to catastrophic failure if not detected and addressed promptly [82]. Delamination, or separation between composite layers, can lead to local stress concentrations and progressive failure that may compromise the integrity of large refuelling station storage systems [43].

The progressive development of damage in composite materials under cyclic loading conditions is particularly relevant for hydrogen refuelling station applications, where tanks experience repeated pressurization and depressurization cycles throughout their service life at much higher frequencies than vehicle applications [83]. Fatigue loading can lead to the gradual accumulation of damage that eventually results in failure, even at stress levels well below the ultimate strength of the material. Understanding fatigue behaviour is therefore critical for predicting refuelling station tank service life and establishing appropriate safety factors and inspection intervals for infrastructure applications [58].

Residual properties following dynamic loading provide important information about the long-term performance of composite materials under real-world refuelling station operating conditions [58]. Impact damage, which may occur during tank installation, maintenance operations, or accidental contact with equipment, can significantly reduce the strength and stiffness of composite materials [37]. Characterizing these residual properties helps establish damage tolerance criteria and inspection requirements for hydrogen refuelling station storage tanks.

The importance of multiscale coupling from macro to microstructure has been recognized as essential for achieving accurate modelling and prediction of composite behaviour in large-scale infrastructure application[48]. Computational models that incorporate details of fibber architecture, matrix properties, and interface characteristics can provide insights into failure mechanisms and guide material optimization efforts for refuelling station applications [84]. These models must account for the complex interactions between different length scales and the influence of manufacturing processes on final material properties in large-scale storage systems [32].

Manufacturing considerations play a crucial role in determining the performance of composite hydrogen refuelling station storage tanks, which may be significantly larger and more complex than vehicle tanks [85]. Filament winding, the primary manufacturing process for large Type IV tanks, involves the precise placement of continuous fibbers under controlled tension to achieve optimal fibber orientation and packing in large-scale structures. Process parameters such as winding angle, fibber tension, and resin content must be carefully controlled to ensure consistent quality and performance across the entire surface of large refuelling station tanks [64].

Quality control and non-destructive testing methods are essential for ensuring the reliability of composite hydrogen refuelling station storage tanks, where failure consequences can be more severe than in vehicle applications. Techniques such as ultrasonic inspection, thermography, and pressure testing are used to detect manufacturing defects and verify structural integrity of large-scale storage systems [48]. The development of in-service monitoring techniques that can detect damage accumulation during refuelling station operation represents an active area of research with significant potential for improving infrastructure safety and reliability [35].

Recent advances in composite materials for hydrogen refuelling station storage applications include the development of new fibber types with improved hydrogen compatibility, advanced resin systems with enhanced barrier properties, and novel manufacturing techniques that enable more complex geometries suitable for large scale infrastructure applications [22]. Nanocomposite materials, incorporating carbon nanotubes or graphene, show promise for improving both mechanical properties and hydrogen barrier performance in refuelling station storage systems [16]. These developments aim to further improve the performance and reduce the lifecycle costs of composite hydrogen storage tanks for infrastructure applications [82].

Although significant progress has been made in hydrogen storage technologies, tank charging protocols, and numerical simulation methods, the literature reveals important gaps when these aspects are considered in the context of **refuelling station infrastructure**. Much of the existing research focuses either on vehicle-scale tanks or on highly detailed CFD studies that are not practical for system-level design. Simplified thermodynamic models exist but are often applied only to small-scale applications or neglect the influence of storage tank volume on charging dynamics. Furthermore, most studies emphasise material behaviour (e.g., composites, liners) rather than the operational thermodynamics of large station tanks under repeated charging cycles. There is limited quantitative analysis of how tank size directly affects **pressure evolution, temperature rise, and refuelling capacity** in infrastructure-scale systems. Addressing this gap is essential for developing safe, efficient, and scalable refuelling station designs that balance storage capacity, thermal management, and long-term durability.

3. Methodology

3.1 Mathematical Model Development for Refuelling Station Storage Systems

The development of a mathematical model for hydrogen refuelling station storage tank charging requires careful consideration of the fundamental physical principles governing mass and energy transport in large-scale infrastructure systems, while accounting for the unique operating conditions and constraints of commercial refuelling operations. The model presented in this study focuses on the thermodynamics behaviour of hydrogen gas within refuelling station storage tanks during charging operations, emphasising the larger volumes, higher flow rates, and more demanding operational requirements typical of infrastructure applications compared to vehicle refuelling. The modelling tank and its properties are shown in Figure 1.

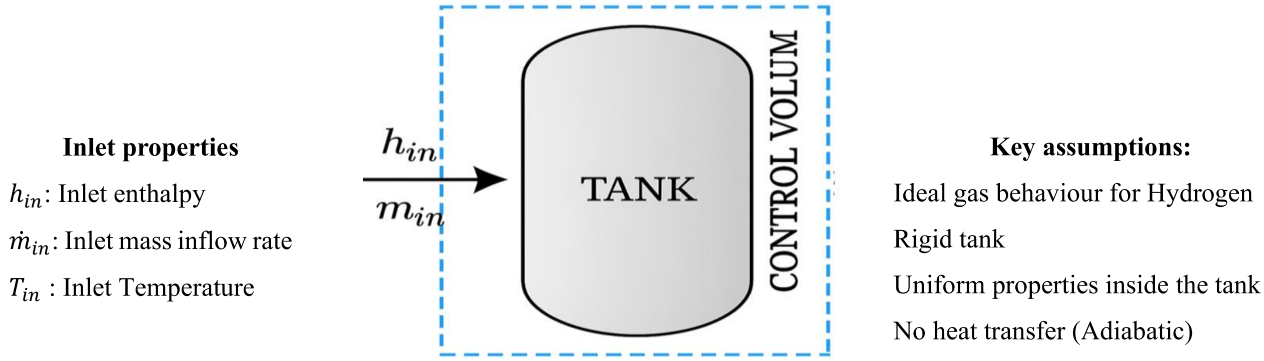

Figure 1: model diagram

The mathematical framework is based on the application of conservation principles to a control volume representing the interior of a refuelling station storage tank, with appropriate assumptions that capture the essential physics while maintaining computational efficiency suitable for infrastructure design and operational optimization. The control volume approach treats the tank contents as a thermodynamic system with well-defined boundaries, enabling the systematic application of conservation laws to predict the temporal evolution of system properties during charging operations. The conservation of mass for the refuelling station storage tank system requires that the rate of change of mass within the tank equals the net mass flow rate into the tank from delivery trucks, pipelines, or on-site production systems. This principle can be expressed mathematically as *in eq. (1)*:

$$\frac{dm}{dt} = \dot{m}_{in} \tag{1}$$

Where *m* represents the total mass of hydrogen within the refuelling station storage tank, t denotes time, and $\dot{m}_{in}$ represents the mass flow rate of hydrogen entering the tank during charging operations. For refuelling station applications, the mass flow rate may be significantly higher than vehicle refuelling operations to minimize delivery truck dwell time and maximize station throughput. The conservation of energy for the *refuelling* station storage tank system is expressed through the first law o*f* thermodynamics, which relates the rate of change of internal energy within the tank to the energy flow associated with mass transfer and heat transfer to the surroundings. For a control volume with mass flow across the boundaries, the energy equation can be written as eq. (2):

$$\frac{d(mu)}{dt} = \dot{m}_{in}h_{in} - \dot{Q} \tag{2}$$

Where *u* represents the specific internal energy of hydrogen within the tank, h_{in} denotes the specific enthalpy of hydrogen entering the tank, and $\dot{Q}$ represents the rate of heat transfer from the tank to the surroundings. The enthalpy term accounts for the energy carried by the incoming hydrogen stream, which may be at different temperatures and pressures than the tank contents in refuelling station operations.

For the simplified analysis presented in this study, several assumptions are made to reduce the complexity of the governing equations while maintaining the essential physics relevant to refuelling station storage tank charging. The ideal gas assumption is employed, which is reasonable for hydrogen at the moderate pressures and temperatures typically encountered in refuelling station operations, particularly for preliminary design studies and control system development. The adiabatic assumption, where heat transfer to the surroundings is neglected, provides a conservative estimate of temperature rise and is commonly used in safety assessments for refuelling station design . Under the ideal gas assumption, the relationship between pressure, density, and temperature for hydrogen in refuelling station storage tanks is given by the equation of state *as in eq. (3)*:

$$P = \rho RT \tag{3}$$

Where P represents pressure, ρ denotes density, which can be written as $\frac{m}{v}$, R is the specific gas constant for hydrogen (4124 J/kg·K), and T represents temperature. This relationship enables the calculation of pressure evolution during charging based on the predicted mass and temperature within the refuelling station storage tank. The specific internal energy of hydrogen under ideal gas conditions is related to temperature through the specific heat at constant volume as in eq. (4):

$$u = c_v T \tag{4}$$

Where c_v represents the specific heat at constant volume for hydrogen (10180 J/kg·K). This relationship, combined with the conservation equations, enables the prediction of temperature evolution during refuelling station tank charging operations. The specific enthalpy of hydrogen entering the refuelling station storage tank can be expressed in terms of temperature using the specific heat at constant pressure as in eq. (5):

$$h_{in} = c_p T \tag{5}$$

Where c_p represents the specific heat at constant pressure for hydrogen (14260 J/kg·K). For ideal gases, the relationship between specific heats is given by $c_p = c_v + R$, which is consistent with the values used in this study.

Substituting the ideal gas relationships into the conservation equations and applying the adiabatic assumption yields a system of ordinary differential equations that describes the temporal evolution of mass and internal energy within the refuelling station storage tank. The eq. (6) equation, after substituting the relationships for internal energy and enthalpy, becomes:

$$\frac{d(mc_v T)}{dt} = \dot{m}_{in} c_p T_{in} \tag{6}$$

Expanding the left-hand side using the product rule and substituting the mass conservation equation yields:

$$mc_v \frac{d(T)}{dt} + c_v T \frac{d(m)}{dt} = \dot{m}_{in} c_p T_{in} \tag{7}$$

$$mc_v \frac{d(T)}{dt} + c_v T \dot{m}_{in} = \dot{m}_{in} c_p T_{in} \tag{8}$$

$$c_v \frac{d(T)}{dt} = \frac{\dot{m}_{in}}{m} (c_p T_{in} - c_v T) \tag{9}$$

This can be further simplified by expressing the equation in terms of specific internal energy:

$$\frac{d(u)}{dt} = \frac{\dot{m}_{in}}{m} (h_{in} - u) \tag{10}$$

Where $u = c_v T$ and $h_{in} = c_p T_{in}$.

Equations 1 and 10 are a system of ordinary differential equations for refuelling station storage tank charging. These equations describe the temporal evolution of mass and specific internal energy within the refuelling station storage tank during charging operations. The pressure and temperature can be calculated from these primary variables using the ideal gas relationships and the definition of specific internal energy.

3.2 Numerical Implementation for Infrastructure Applications

The numerical solution of the governing differential equations for hydrogen refuelling station storage tank charging is implemented using MATLAB's ODE45 solver, which provides a robust and efficient method for solving non-stiff ordinary differential equation systems commonly encountered in infrastructure thermodynamic analyses. The choice of ODE45 is particularly appropriate for refuelling station applications where computational efficiency and reliability are important for both design studies and potential real-time control system implementation.

The ODE45 solver is based on the Dormand-Prince Runge-Kutta method, which offers fourth-order accuracy with fifth-order error estimation, providing an excellent balance between computational efficiency and numerical accuracy for infrastructure applications. The method incorporates automatic step size control and error estimation, ensuring that the solution meets specified accuracy requirements while minimizing computational cost, which is important for refuelling station operational applications.

The implementation begins with the specification of initial conditions that represent the state of the refuelling station storage tank at the beginning of the charging process. These conditions include the initial mass of hydrogen within the tank, which can be calculated from the initial pressure, temperature, and tank volume using the ideal gas law:

$$m_0 = \frac{P_0 V}{R T_0} \quad (11)$$

Where m_0 represents the initial mass, P_0 is the initial pressure, V denotes the tank volume, and T_0 represents the initial temperature. For refuelling station applications, the initial conditions may vary depending on the state of charge of the storage system and the operational protocols of the facility. The initial specific internal energy is calculated from the initial temperature:

$$u_0 = c_v T_0 \quad (12)$$

These initial conditions define the starting point for the numerical integration and $y_0 = [m_0, u_0]$ represent the state vector for the ODE solver.

The system parameters for refuelling station applications include the tank volume, which may range from several hundred to thousands of litters depending on the station capacity and design requirements. The mass flow rate during charging operations is typically much higher than vehicle refuelling rates to minimize delivery truck dwell time and maximize station operational efficiency. The inlet temperature depends on the hydrogen supply system and may incorporate precooling strategies to manage temperature rise during rapid charging operations. The MATLAB implementation defines the system of differential equations as an anonymous function that can be passed to the ODE45 solver:

```
odefun = @(t,y) [ ...
mdot; ... % dm/dt
(mdot/y(1)) * (h_in - y(2)) ... % du/dt];
```

where mdot represents the constant mass flow rate, h_in denotes the specific enthalpy of the incoming hydrogen, and y(1) and y(2) represent the current mass and specific internal energy, respectively.

The time span for the simulation is specified to cover the duration of the charging process, which for refuelling station applications may range from several minutes to hours, depending on the tank capacity, charging rate, and operational requirements. The ODE45 solver automatically determines appropriate time steps to maintain accuracy while efficiently advancing the solution through the specified time interval. The solution process involves calling the ODE45 solver with the defined system of equations, initial conditions, and time span:

```
[t, y] = ode45(odefun, tspan, y0);
```

The solver returns arrays containing the time points and corresponding solution values for mass and specific internal energy throughout the charging process. These primary variables can then be used to calculate secondary quantities of interest for refuelling station analysis, including temperature, pressure, and density. The temperature and pressure can be calculated from eq. 4 and 3, respectively, and the density of hydrogen as $\rho = \frac{m}{v}$. These calculations provide a complete description of the thermodynamic state of the hydrogen within the refuelling station storage tank throughout the charging process.

Error control and solution accuracy are managed automatically by the ODE45 solver through its adaptive step size algorithm and embedded error estimation. The solver monitors the local truncation error at each step and adjusts the step size to maintain the solution within specified tolerance limits. Default tolerances are typically adequate for refuelling station applications, but can be adjusted if higher accuracy is required for specific analyses.

The computational efficiency of the ODE45 solver makes it suitable for parametric studies of refuelling station charging processes, where multiple simulations with different parameter values may be required to optimize operational procedures or assess system performance under various conditions. The rapid solution times enable the exploration of large parameter spaces and support the development of operational guidelines for refuelling station operators.

Validation of the numerical implementation involves comparison with analytical solutions for simplified cases and verification of conservation principles throughout the simulation. Mass conservation can be verified by confirming that the final mass equals the initial mass plus the integrated mass flow rate over the charging period. Energy conservation can be checked by ensuring that the change in internal energy equals the integrated enthalpy flow into the tank.

The modular structure of the MATLAB implementation facilitates modification for different refuelling station configurations, operating conditions, or analysis objectives. Parameters such as tank volume, mass flow rate, and inlet conditions can be easily adjusted to represent different infrastructure scenarios. Additional physics, such as heat transfer effects or real gas behaviour, can be incorporated by modifying the governing equations while maintaining the same numerical solution framework.

3.3 Simulation Parameters for Refuelling Station Applications

The selection of appropriate simulation parameters for hydrogen refuelling station storage tank charging analysis requires careful consideration of realistic operating conditions, infrastructure constraints, and safety requirements that differ significantly from vehicle refuelling applications. The parameters chosen for this study represent typical conditions encountered in commercial hydrogen refuelling stations while providing a foundation for parametric analysis and operational optimization. Table 1 shows the operating parameters values used in this study.

The tank volume for refuelling station applications is significantly larger than vehicle tanks, reflecting the need to store sufficient hydrogen to serve multiple vehicle refuelling operations between replenishment cycles. For this study, a tank volume of 3000 litres (3.0 m^3) is selected, representing a medium-scale refuelling station storage tank suitable for urban or suburban installations. This volume is consistent with commercial refuelling station designs and provides sufficient capacity to serve approximately 100-150 vehicle refuelling operations, depending on vehicle tank size and target fill level.

Table 2: Operating Conditions for Hydrogen Tank Charging Simulation

Parameter	Symbol	Value/Range	Unit	Notes
Tank type	-	Rigid & adiabatic	-	Not heat or work
Tank volume	V	1.0 – 3.0	M^3	Simulated in 0.5m^3 increments
Initial pressure	P_0	80	MPa	Constant
Initial temperature	T_0	300	K	Same for all tank sizes
Inlet temperature	T_{in}	300	K	Matches initial tank temperature
Inlet mass flow rate	$\dot{m}_{in}$	0.01	kg/s	Constant
Inlet enthalpy	h_{in}	c_vT+RT	j/kg	Ideal gas assumption
Specific gas constant	R	4124	j/(kg-k)	For hydrogen
Specific heat (const. V)	C_v	10180	j/(kg-k)	For hydrogen
Simulation time	t	300	Seconds	Fixed duration
Initial hydrogen mass	M_0	64.80 – 194.4	kg	Calculated from P_0,V,T_0

The mass flow rate during refuelling station tank charging is substantially higher than vehicle refuelling rates due to the need to minimise delivery truck dwell time and maximise station operational efficiency. A baseline mass flow rate of 0.01 kg/s is selected for the primary analysis, representing a moderate charging rate that balances rapid tank replenishment with temperature management considerations. This flow rate corresponds to approximately 36 kg/h, which would enable complete charging of a 3000-liter tank from empty to 70 MPa in approximately 4-5 hours, depending on initial conditions.

The inlet temperature of hydrogen entering the refuelling station storage tank depends on the supply system configuration and may incorporate precooling strategies to manage temperature rise during charging. A baseline inlet temperature of 300 K (27°C) is selected, representing ambient temperature conditions without precooling. This temperature is representative of hydrogen delivered from tube trailers or pipeline systems at ambient conditions and provides a conservative baseline for temperature rise analysis.

Initial conditions for the refuelling station storage tank represent the state of the system at the beginning of the charging process and may vary depending on the operational protocols of the facility. For this study, initial conditions corresponding to a partially charged tank are selected to represent realistic operational scenarios where tanks are replenished before complete depletion. An initial pressure of 80 MPa (800 bar) is chosen, representing approximately 88% of the maximum operating pressure for a 90 MPa service pressure tank with appropriate safety margins.

The initial temperature is set equal to the ambient temperature of 300 K, representing thermal equilibrium conditions that might exist after a period of inactivity or following gradual pressure reduction during normal dispensing operations. These initial conditions result in an initial hydrogen mass of approximately 194 kg within the 3000- litter tank, calculated using the ideal gas law with the specified pressure, temperature, and volume.

The hydrogen properties used in the simulation are based on standard values for gaseous hydrogen under the pressure and temperature conditions relevant to refuelling station operations. The specific gas constant for hydrogen is 4124 J/kg·K, the specific heat at constant volume is 10180 J/kg·K, and the specific heat at constant pressure is 14260 J/kg·K. These values are consistent with ideal gas behaviour and are appropriate for the moderate pressures and temperatures encountered in typical refuelling station charging operations.

The simulation time span is selected to capture the complete charging process while providing sufficient resolution to observe the temporal evolution of system properties. A total simulation time of 300 seconds (5 minutes) is chosen for the baseline analysis, representing a rapid charging scenario that might occur during delivery truck operations where minimizing dwell time is important for operational efficiency. This time span enables the observation of transient behaviour during the initial stages of charging while capturing the approach to steady-state conditions.

The constant mass flow rate assumption employed in this study represents a simplified but realistic approximation of refuelling station charging operations . In practice, the mass flow rate may vary during charging due to pressure differences between the supply system and storage tank, control system responses, or operational procedures. However, the constant flow rate assumption provides a useful baseline for understanding fundamental system behaviour and can be readily modified to investigate more complex charging profiles.

The adiabatic assumption, where heat transfer to the surroundings is neglected, provides a conservative estimate of temperature rise during refuelling station tank charging. This assumption is particularly appropriate for rapid charging scenarios where the time scale of the process is much shorter than the thermal time constant of the tank system. For refuelling station applications, the adiabatic assumption represents a worst-case scenario for temperature rise and is therefore useful for safety assessments and operational limit determination.

The ideal gas assumption employed in this study is reasonable for hydrogen at the pressures and temperatures typically encountered in refuelling station operations. While real gas effects become more significant at very high pressures, the ideal gas model provides adequate accuracy for most practical applications and offers the advantage of computational simplicity. The assumption enables the use of simple relationships between pressure, density, and temperature that facilitate rapid calculation and real-time implementation. The simulation program is available in Appendix A.

4. Results and Discussion

4.1 Refuelling Station Storage Tank Charging Simulation Results

The hydrogen refuelling station storage tank charging simulation was conducted using the mathematical model and numerical implementation described in the previous section, with parameters selected to represent realistic operating conditions for commercial hydrogen refuelling infrastructure. The simulation parameters were chosen to reflect the larger scale and different operational requirements of refuelling station storage systems compared to vehicle applications, with a tank volume of 3000 litres, a constant mass inflow rate of 0.01 kg/s, and an inlet temperature of 300 K representing typical conditions for infrastructure operations. The initial conditions corresponded to a partially filled refuelling station storage tank at 80 MPa pressure and 300 K temperature, representing a realistic operational scenario where tanks are replenished before complete depletion to maintain station availability.

The simulation results demonstrate the fundamental thermodynamic behaviour of hydrogen refuelling station storage tank charging under adiabatic conditions with ideal gas assumptions, providing insights into the temporal evolution of key system variables that are critical for infrastructure design and operation. Three primary variables were tracked throughout the charging process: pressure, temperature, and mass accumulation within the refuelling station storage tank, with their evolution providing important information about charging dynamics and operational characteristics relevant to infrastructure applications. Figure 2 shows Hydrogen Storage Tank Charging Simulation parameters evolution.

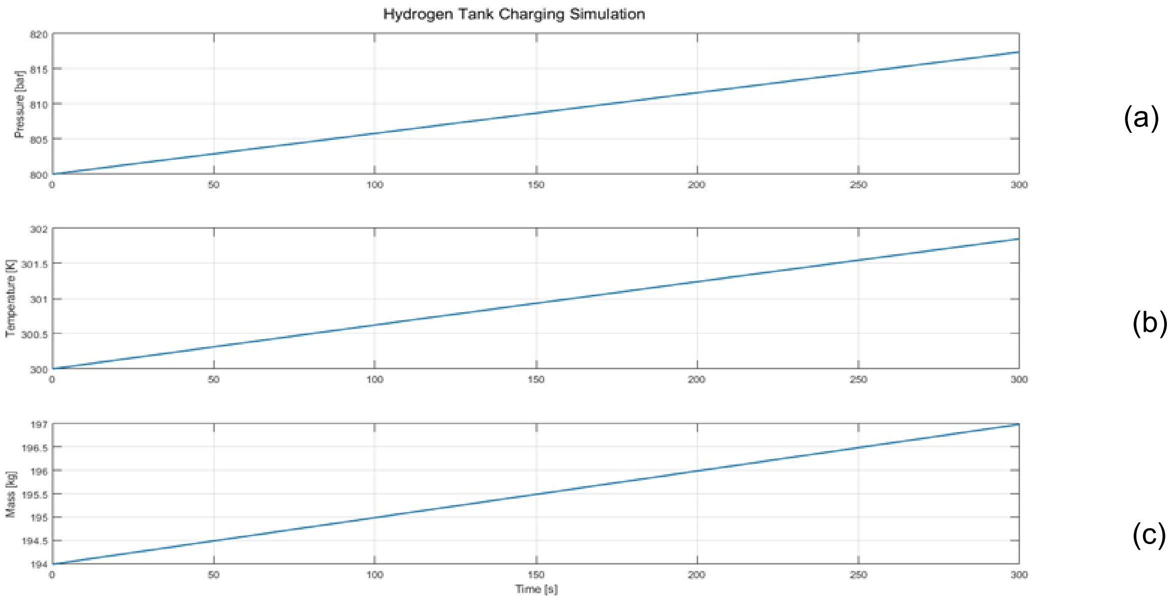

Figure 2: Hydrogen storage tank refuelling parameter evolution; a: Pressure distribution, b: Temperature distribution, c: Mass distribution

Figure 2a: The pressure within the refuelling station storage tank increases from an initial value of approximately 800 bar to 818 bar over the 300-second simulation period, representing an 18-bar increase that is significant for infrastructure operations where pressure management is critical for safety and efficiency. The pressure rise follows a smooth, monotonic curve that exhibits a gradually decreasing rate of increase as the charging progresses, which is characteristic of the ideal gas behaviour under constant mass flow conditions. This behaviour is consistent with the fundamental relationship between pressure, mass, and temperature in refuelling station storage systems, where the pressure increase is driven by both mass accumulation and temperature rise effects.

Figure 2b: The temperature within the refuelling station storage tank increases from the initial value of 300 K to approximately 301.8 K during the charging process, representing a temperature rise of 1.8 K that is modest but significant for infrastructure safety considerations. The temperature rise demonstrates the thermodynamic heating effect that occurs during rapid gas compression and mass addition in large-scale storage systems, which must be carefully managed in refuelling station operations to prevent exceeding safety limits. The relatively modest temperature increase reflects the specific operating conditions chosen for this simulation, including the moderate mass flow rate and the fact that the inlet temperature equals the initial tank temperature, conditions that are representative of well-designed refuelling station charging protocols.

Figure 2c: The mass of hydrogen within the refuelling station storage tank increases linearly from approximately 194 kg to 197 kg over the simulation period, representing a 3 kg increase that corresponds to the product of the mass flow rate and simulation duration. This linear relationship directly reflects the constant mass inflow rate assumption and confirms the correct implementation of the mass conservation equation for refuelling station applications. The total mass increase represents approximately 1.5% of the initial tank contents, which is typical for top-off operations in refuelling station storage systems where tanks are replenished before complete depletion.

The simulation results reveal several important characteristics of the hydrogen refuelling station storage tank charging process under the specified conditions that are relevant for infrastructure design and operation. The pressure increase is primarily driven by mass accumulation rather than temperature rise, as evidenced by the relatively small temperature change compared to the significant mass increase, which is typical for charging scenarios where the inlet temperature is close to the initial tank temperature. This behaviour is characteristic of well-designed refuelling station charging protocols that minimise thermal effects through appropriate temperature management.

The smooth, continuous evolution of all variables indicates stable numerical behaviour and confirms the appropriateness of the ODE45 solver for this type of infrastructure analysis problem. The absence of oscillations or discontinuities in the solution demonstrates that the governing equations are well-posed and that the numerical implementation is robust for refuelling station applications. This stability is important for potential real-time control system implementation, where reliable and predictable behaviour is essential.

The rate of pressure increase shows a gradual decrease over time, which can be attributed to the increasing mass within the refuelling station storage tank. As more hydrogen accumulates, the same mass flow rate represents a smaller fractional increase in total mass, leading to a diminishing rate of pressure rise that is mathematically consistent with the governing equations and physically realistic for the charging process. This behaviour has important implications for refuelling station operational planning, as it indicates that charging rates will naturally decrease as tanks approach full capacity.

The temperature evolution demonstrates the importance of thermal management in refuelling station storage tank charging operations. While the temperature rise in this simulation is modest, it represents the fundamental heating effect that occurs during rapid gas compression and must be considered in the design of charging protocols for infrastructure applications. The temperature increase is directly related to the energy balance during charging and provides insights into the thermal loads that must be managed in refuelling station operations.

The mass accumulation profile confirms the validity of the constant mass flow rate assumption for refuelling station charging analysis and demonstrates the direct relationship between charging time and hydrogen inventory. This linear relationship is helpful for operational planning and inventory management in refuelling station applications, where predicting hydrogen consumption and replenishment requirements is essential for maintaining station availability.

4.2 Effect of Tank Volume on Hydrogen Charging Performance

Parametric simulations were conducted for storage tank volumes from 1.0 to 3.0 m³ (in 0.5 m³ increments) under identical initial conditions (80 MPa, 300 K) and a constant hydrogen inflow of 0.01 kg/s for 300 s. In each case, a total of 3.0 kg of hydrogen is added over the fill. The effect of tank volume is therefore observed primarily in the pressure and temperature responses during charging, as well as the final storage capacity, as detailed below.

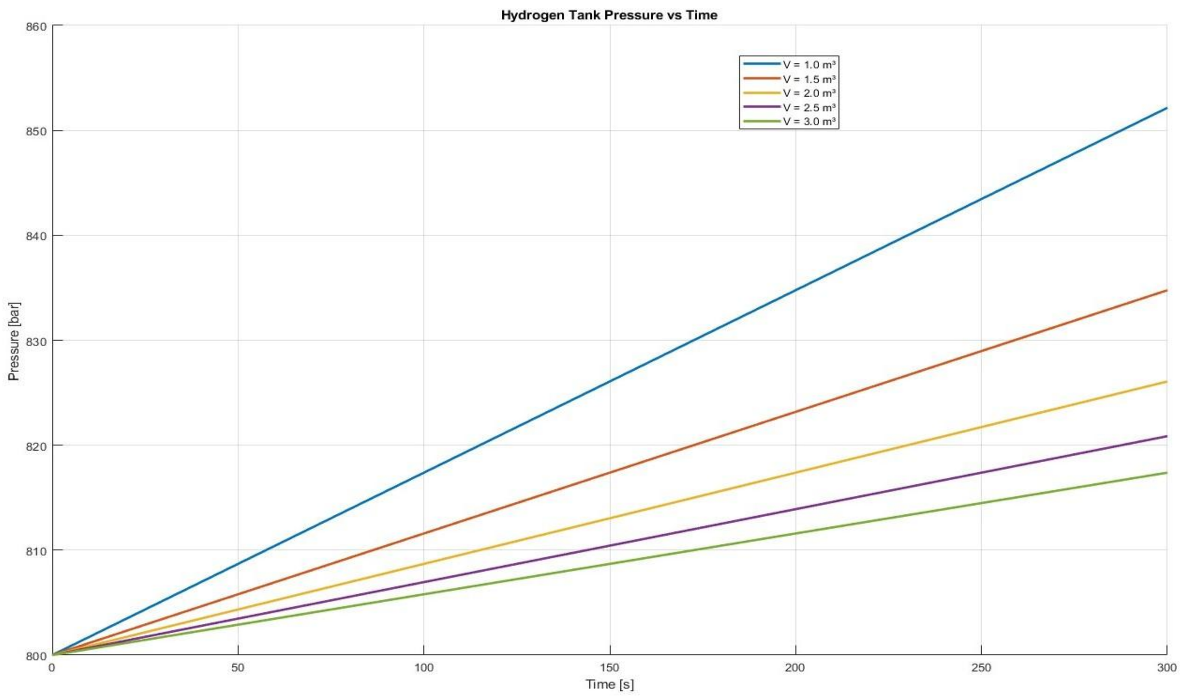

Figure 3:Pressure vs. time during filling for different tank volumes (1.0–3.0 m³)

Figure 3 presents the pressure evolution during filling for each tank volume. All cases begin at the same initial pressure (~800 bar) and exhibit a gradual pressure rise as hydrogen accumulates. However, smaller tanks experience a much sharper increase in pressure: the 1.0 m³ tank reaches about 852 bar by 300 s, whereas the largest 3.0 m³ tank reaches only about 817 bar. The pressure rise is inversely related to volume, consistent with ideal gas behaviour. In practical terms, a larger tank remains more pressure-stable during refuelling, while a smaller tank approaches its pressure limit more quickly.

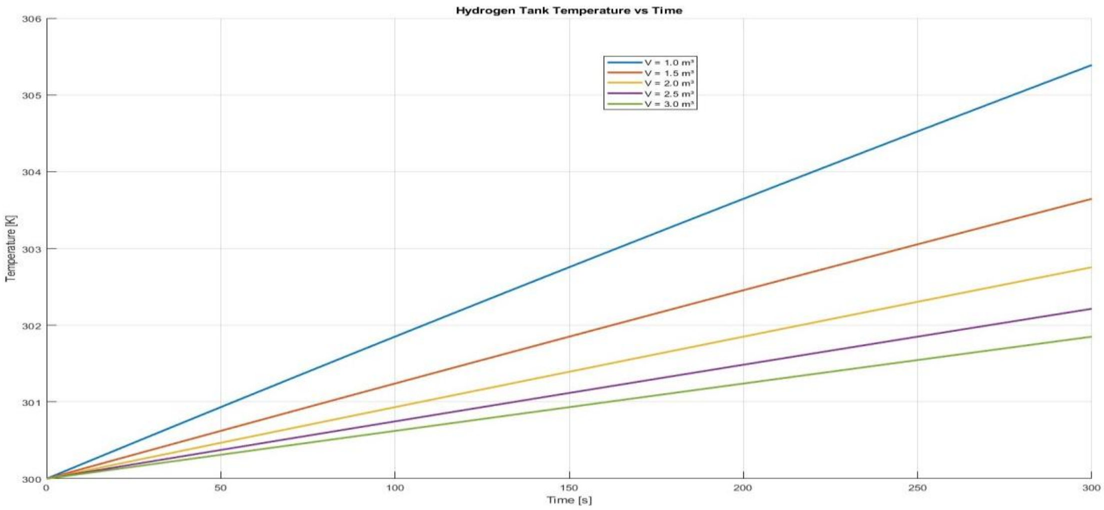

Figure 4:Gas temperature vs. time during filling for different tank volumes.

Despite the large pressure differences, the gas temperature inside the tank rises only modestly in all cases (Figure 4). Starting from 300 K, the temperature increases due to adiabatic compression and internal energy gain, but it reaches relatively low peak values by the end of the fill. The smallest tank (1.0 m³) warms to about 305 K after 300 s. In contrast, the largest (3.0 m³) finishes at about 302 K. This mild temperature rise is volume-dependent: a smaller volume yields a slightly higher temperature increase, while a larger volume absorbs the energy with minimal thermal effect. All temperature profiles tend toward a plateau by 300 s, indicating that the rate of temperature increase diminishes as the tank's mass grows.

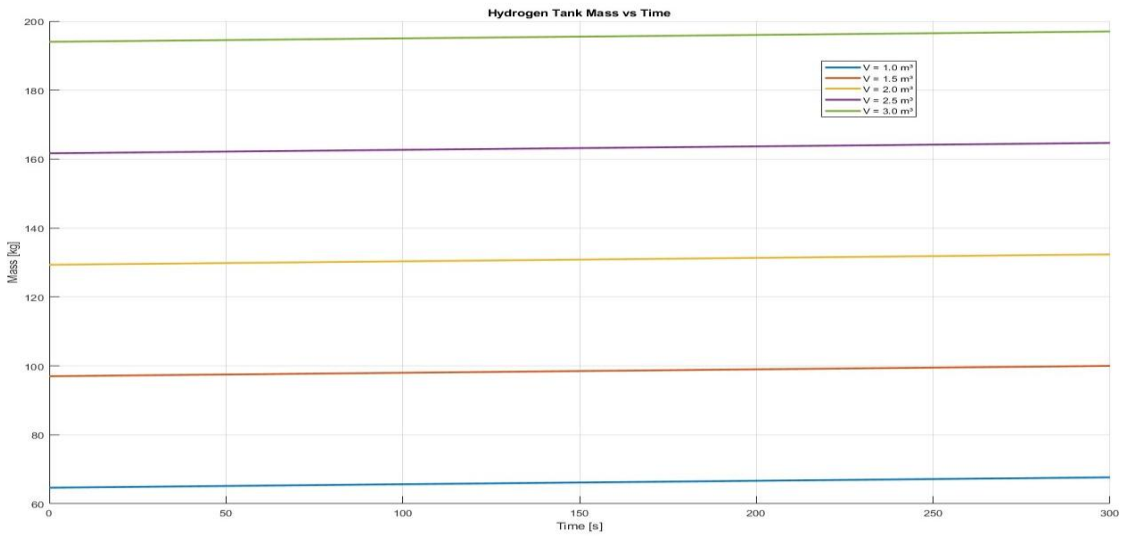

Figure 5: Hydrogen mass vs. time for different tank volumes

Figure 5 illustrates that all cases have nearly identical mass accumulation profiles, given the uniform inflow rate. The hydrogen mass in each tank increases linearly with time, with only vertical offsets due to different initial inventories. By the end of the 300s fill, every tank has gained 3.0 kg of hydrogen, yielding final stored masses ranging from ~67.7 kg in the 1.0 m³ tank to ~197.0 kg in the 3.0 m³ tank. Table 2 summarises these final results, including the equivalent number of 6-kg car tanks. Larger tanks store more hydrogen (up to ~32 car fills) and end at a lower pressure, whereas the smallest tank holds only ~11 car fills but at a much higher pressure. This outcome highlights the trade-off involved: smaller volumes lead to greater pressure and temperature excursions, while larger volumes provide greater capacity with a more moderate pressure rise. Tank volume is therefore a critical design parameter for balancing storage capacity and pressure constraints in hydrogen refuelling systems.

Volume (m³)	Final Pressure [bar]	Final Temp [K]	Final Mass [kg]	Cars Refueled (6 kg each)
1.0	852.15	305.39	67.66	11

1.5	834.77	303.65	99.99	16
2.0	826.08	302.76	132.32	22
2.5	820.86	302.21	164.66	27
3.0	817.38	301.85	196.99	32

Table 3: Final pressure, temperature, stored mass, and equivalent refuelling capacity after 300 s of charging for various tank volumes.

5. Safety and Engineering Implications for Refuelling Station Operations

5.1 Temperature Management in Refuelling Station Infrastructure

What the simulations seem to suggest is that the size of the hydrogen storage tank plays a surprisingly important role in how temperatures behave during filling. Smaller tanks, like the 1.0 m³ case, ended up with noticeably higher gas temperatures, roughly 5 K above the ambient. Larger tanks, up to 3.0 m³, barely nudged beyond 301–302 K. The reason is that in the small tank, there's just not enough gas or wall material to absorb the heat that builds up from gas compression. So the temperature spikes quickly. A bigger tank, on the other hand, acts like a buffer. It spreads out the thermal load, keeping things relatively stable.

Now, while these temperature levels are still comfortably below safety limits (typically around 85 °C or 358 K), the implication is clear: small tanks may require closer temperature monitoring or even active cooling to prevent local hotspots. Larger tanks, by contrast, offer more thermal breathing room, which not only helps with safety but can also make the hydrogen denser and easier to handle during transfer. It's not a dramatic insight, but it's a practical operational point that engineers can't ignore.

5.2 Pressure Management and Infrastructure Safety

Pressure trends during filling tell a similar story. In the simulation, the small 1.0 m³ tank shot up from 80 MPa to around 85.2 MPa. By contrast, the 3.0 m³ tank only climbed about 1–2 MPa under the same conditions. The additional volume gives it more slack. Less of the total capacity is displaced with each kilogram of gas, so the pressure builds more slowly and predictably.

From an engineering perspective, this difference isn't trivial. Smaller tanks probably need slower fill rates, smarter control systems, and tighter cutoff thresholds to avoid pressure relief valves kicking in unnecessarily. Larger tanks are more forgiving; they absorb the pressure load without raising alarms. But that doesn't mean they're always the better option. Space, cost, and usage profile all matter. Still, the trend is clear: bigger tanks help maintain a safer pressure envelope during fast fills.

5.3 Structural Integrity and Infrastructure Durability

Pressure and temperature aren't just numbers on a gauge; they translate directly into stress on the tank walls. In the 1.0 m³ scenario, the combination of higher peak pressure and sharper temperature rise creates a more aggressive loading situation. Hoop and axial stresses climb proportionally with pressure, and the warmer gas means the inner wall wants to expand more than the outer wall, introducing thermal gradients and stress mismatches.

None of this necessarily breaks the tank, but over time, repeated cycling under these harsher conditions can fatigue materials faster, especially around welds, ports, or other geometric features where stress tends to concentrate. So even if design codes are met, the long-term durability could be compromised unless those factors are anticipated.
Larger tanks, again, fare better. Their gentler pressure ramp and minimal temperature change lead to a more uniform stress distribution. The wall materials don't get pushed as close to their limits, which can translate into longer service life and fewer maintenance headaches. That said, it's easy to get overly confident with bigger tanks. Even they aren't immune to fatigue, especially if external factors like vibrations, ambient temperature swings, or inconsistent fill protocols come into play.

6. Conclusions

This thesis has presented a numerical analysis of hydrogen refuelling station storage tank charging processes through the development and implementation of a thermodynamic simulation model tailored for infrastructure applications. The research has achieved its primary objectives of understanding the thermodynamic behaviour during hydrogen refuelling station tank charging and providing a computational framework for analysing various operating conditions and design parameters relevant to commercial hydrogen infrastructure operations.

The mathematical model developed in this study, based on ideal gas assumptions and adiabatic conditions, has proven effective for capturing the essential physics of hydrogen refuelling station storage tank charging processes. The model successfully describes the temporal evolution of pressure, temperature, and mass within large-scale storage tanks through a system of ordinary differential equations that can be solved efficiently using standard numerical methods. The implementation using MATLAB's ODE45 solver has demonstrated excellent numerical stability and computational efficiency, making the approach suitable for both detailed infrastructure analysis and parametric studies relevant to refuelling station design and operation.

The simulation results for different tank volumes revealed significant insights into the relationship between storage capacity and thermodynamic response. For a 3.0 m^3 tank charged over 300 seconds with a constant mass inflow rate of 0.01 kg/s, the pressure increased from 80 MPa to 81.74 MPa, representing a modest 2.18% increase. The temperature rose from 300 K to 301.85 K, an increase of 1.85 K. The hydrogen mass increased from 194.40 kg to 196.99 kg during this charging period. In contrast, when the tank volume was reduced to 1.0 m^3 under identical conditions, the thermodynamic response was more pronounced. The final pressure reached 85.22 MPa, representing a 6.53% increase from the initial 80 MPa, while the temperature climbed to 305.39 K, an increase of 5.39 K from the initial 300 K.

Parametric analysis revealed how system behaviour changes with tank volume, despite constant flow conditions. Smaller tanks showed sharper pressure and temperature rises, while larger tanks exhibited smoother responses. These insights reinforce the importance of volume as a design lever in infrastructure planning. Though mass flow rate and inlet temperature were held constant in this study, the results suggest that strategies like precooling may be especially useful in small-volume systems to manage thermal loads.

The safety and engineering implications are clear: smaller tanks, while space-efficient, demand tighter control over temperature and pressure and may require additional thermal management. Larger tanks, by contrast, offer greater storage capacity and inherent buffering, which improves operational stability and system longevity. The study confirmed that, under the simulated conditions, safety thresholds were not exceeded, with all temperature increases remaining well below the 85°C safety limit and pressure increases staying within acceptable bounds of 1.25 times the nominal working pressure.

The research has identified several key contributions to the field of hydrogen infrastructure technology. First, the simplified thermodynamic model provides a computationally efficient tool for understanding fundamental charging behaviour and conducting preliminary design evaluations specifically for refuelling station applications. Second, the parametric analysis has quantified the relationships between operating parameters and system performance, guiding optimization of charging protocols and operational procedures for infrastructure facilities.

The limitations of the current study provide opportunities for future research and model improvements specifically targeted at infrastructure applications. The ideal gas assumption becomes less accurate at very high pressures, where real gas effects become significant, suggesting the need for more sophisticated equations of state for high-pressure refuelling station applications. The adiabatic assumption may overpredict temperature rise for slow charging processes or systems with enhanced heat transfer, indicating the potential value of incorporating heat transfer models that account for the larger thermal masses and different heat transfer characteristics of infrastructure-scale storage systems.

Future research directions should focus on extending the model to address these limitations while maintaining computational efficiency suitable for infrastructure applications. The incorporation of real gas effects through appropriate equations of state would improve accuracy for high-pressure refuelling station operations. The addition of heat transfer models would enable more accurate predictions for a broader range of charging scenarios encountered in infrastructure applications. The development of spatial models that account for temperature and concentration gradients would provide insights into mixing and stratification effects that may be more significant in large-scale refuelling station storage tanks.

The work presented in this thesis represents a significant step forward in the numerical analysis of hydrogen infrastructure systems and provides a valuable tool for researchers, engineers, and practitioners working in the field of hydrogen technology and infrastructure development. The combination of theoretical development, numerical implementation, and practical validation demonstrates the potential for computational modelling to contribute to the advancement of sustainable energy technologies and the transition toward a hydrogen-based economy supported by robust and efficient refuelling infrastructure.

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Appendices

Appendix A: MATLAB Code Implementation for Refuelling Station Applications

```
function hydrogen_tank_variable_volume()
    % Constants
    T_in = 300;              % Inlet temperature [K]
    R = 4124;                % Specific gas constant [J/kg·K]
    cv = 10180;              % Specific heat at constant volume [J/kg·K]
    h_in = cv * T_in + R * T_in;  % Inlet enthalpy [J/kg]
    P0 = 80e6;               % Initial pressure [Pa]
    T0 = 300;                % Initial temperature [K]
    u0 = cv * T0;            % Initial internal energy [J/kg]
    mdot = 0.01;             % Mass inflow rate [kg/s]
    t_end = 300;             % Simulation time [s]
    car_capacity = 6;        % Each car uses 6 kg of H2
    volumes = 1:0.5:3;       % Tank volumes [m^3]
    t = linspace(0, t_end, 500);
    dt = t(2) - t(1);
    % Initialize result matrix
    results = zeros(length(volumes), 5);

    %% === Pressure Plot ===
    figure;
    hold on; grid on;
    for i = 1:length(volumes)
        V = volumes(i);
        m0 = (P0 * V) / (R * T0);
        m = zeros(1, length(t));
        u = zeros(1, length(t));
        m(1) = m0;
        u(1) = u0;
        for j = 2:length(t)
            dm_dt = mdot;
            du_dt = (mdot / m(j-1)) * (h_in - u(j-1));
            m(j) = m(j-1) + dm_dt * dt;
            u(j) = u(j-1) + du_dt * dt;
        end
        T = u / cv;
        P = m .* R .* T / V;
        P_bar = P / 1e5;
        plot(t, P_bar, 'DisplayName', sprintf('V = %.1f m³', V), 'LineWidth',2);
        % Store results
        final_mass = m(end);
        final_temp = T(end);
        final_press = P_bar(end);
        num_cars = floor(final_mass / car_capacity);
        results(i,:) = [V, final_press, final_temp, final_mass, num_cars];
    end
    xlabel('Time [s]');
    ylabel('Pressure [bar]');
    title('Hydrogen Tank Pressure vs Time');
    legend;

    %% === Temperature Plot ===
    figure;
    hold on; grid on;
```

```
    for i = 1:length(volumes)
        V = volumes(i);
        m0 = (P0 * V) / (R * T0);
        m = zeros(1, length(t));
        u = zeros(1, length(t));
        m(1) = m0;
        u(1) = u0;
        for j = 2:length(t)
            dm_dt = mdot;
            du_dt = (mdot / m(j-1)) * (h_in - u(j-1));
            m(j) = m(j-1) + dm_dt * dt;
            u(j) = u(j-1) + du_dt * dt;
        end
        T = u / cv;
        plot(t, T, 'DisplayName', sprintf('V = %.1f m³', V), 'LineWidth',2);
    end
    xlabel('Time [s]');
    ylabel('Temperature [K]');
    title('Hydrogen Tank Temperature vs Time');
    legend;

    %% === Mass Plot ===
    figure;
    hold on; grid on;
    for i = 1:length(volumes)
        V = volumes(i);
        m0 = (P0 * V) / (R * T0);
        m = m0 + mdot * t;
        plot(t, m, 'DisplayName', sprintf('V = %.1f m³', V), 'LineWidth',2);
    end
    xlabel('Time [s]');
    ylabel('Mass [kg]');
    title('Hydrogen Tank Mass vs Time');
    legend;
    %% === Print Results ===
    fprintf('\n%-10s %-20s %-20s %-20s %-20s\n', ...
        'Volume', 'Final Pressure [bar]', 'Final Temp [K]', 'Final Mass [kg]', 'Cars Refueled');
    for i = 1:size(results,1)
        fprintf('%-10.1f %-20.2f %-20.2f %-20.2f %-20.0f\n', ...
            results(i,1), results(i,2), results(i,3), results(i,4), results(i,5));
    end

end
```