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Simulation Research of the Phase change in Ammonia Supply System Based on Amesim

Fuels - Alternative & New Fuels

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ABSTRACT

The most common use of ammonia in CI engines is via pilot ignited dual fuel, where a small amount of diesel is used to ignite a quasi-homogeneous ammonia-air mixture. As characters of ammonia, it is gaseous at room temperature and can be easily liquefied by cooling or pressurization. The experimental research of a single-cylinder ammonia engine shows that the gaseous ammonia is prone to change phase to liquid ammonia in the supply system before being injected into the intake box. Recognizing the phase change influence on the performance and reliability of the engine, this paper explores the impact of key design parameters of the ammonia supply system especially evaporators, buffer and pressure regulators on the state of ammonia by simulation. The 1D flow and thermodynamic simulation is conducted by the Simceter Amesim softerware Two-Phase Flow library. The simulation model is calibrated by the engine test data. Referring to the analysis results, this paper proposes a temperature-pressure cooperative design method which solves the phase change problem efficiently.

1 INTRODUCTION

Climate change is intrinsically linked to sustainable human development and stands as one of the most critical issues in global governance. Since the mid-20th century, CO_2 and other greenhouse gas (GHG) emissions have been identified as the primary drivers of global warming. To mitigate the impact of human activities, such as industrialization and electrification, on the climate system, the international community has progressively established a framework of legal standards. This framework, from the United Nations Framework Convention on Climate Change in 1992 to the Paris Agreement adopted in 2015, aims to regulate and quantify national GHG emission reduction responsibilities. The long-term goal is to limit the global average temperature rise to below 1.5°C compared to pre-industrial levels [1].

As the most economical and energy-efficient mode of transportation, 90% of international trade is facilitated by maritime shipping [2]. With the growth of maritime trade, the CO_2 emissions resulting from ship propulsion are significant and cannot be overlooked. According to a GHG study released by the International Maritime Organization (IMO) in 2020, global shipping emissions increased from 977 million tons to 1.076 billion tons between 2012 and 2018, marking a 9.6% rise. Specifically, CO_2 emissions grew from 962 million tons to 1.056 billion tons, an increase of 9.8%, with their share of global emissions rising from 2.76% to 2.89%. The report also indicated that, without intervention, shipping emissions could reach 1.3 times the 2008 levels by 2050, driven by the growing demand for maritime trade [3]. To accelerate the reduction of GHG emissions in the shipping industry, the IMO adopted the 'IMO Strategy on Reduction of GHG Emissions from Ships' during the 80th session of the Marine Environment Protection Committee (MEPC) in 2023. This strategy sets a target of achieving net-zero emissions around 2050, advancing the goal of 'zero carbon emissions by the end of the century' established during the 72nd session in 2018 by 50 years [4].

To meet these ambitious targets and address increasingly stringent emission regulations and carbon trading mechanisms, researchers have explored various technologies. Among these, the development of zero-carbon and low-carbon fuels such as ammonia, hydrogen, and methanol has become a focal point in the field of power systems, including engines [5].

NH_3 is inherently carbon-free and can be produced through green pathways using renewable energy sources. Compared to H_2, NH_3 is simpler to synthesize, easier to store and transport, and benefits from well-established infrastructure and low costs. Additionally, NH_3 is easily to be liquefied, has excellent anti-knock properties, and a narrow flammability range, making it less prone to explode. Although it is toxic, its naturally pungent odor makes it easily detectable, and its low density allows for rapid diffusion. Under current technological conditions, NH_3 holds greater advantages in terms of applicability, safety, and reliability as a power source for mobile equipment.

Compared to the technical route of direct in-cylinder injection of liquid ammonia, the approach of using a gaseous ammonia fuel supply system with low-pressure port fuel injection (PFI) method requires fewer modifications to traditional diesel engines and existing liquid natural gas (LNG) engines. This method is more cost-effective and easier to maintain, making it more appealing to shipowners. As a result, it has become the mainstream solution for ammonia-fueled engines. Therefore, the ammonia supply system, as a core supporting component, urgently requires focused development.

2 MAIN SECTION

2.1 Engine Test Platform and Ammonia Supply System

To align with the global shipping industry's carbon emission reduction goals and support China's strategic initiatives for energy structure adjustment, Shanghai Marine Diesel Engine Research Institute (SMDERI) initiated a research and development project in 2021 focused on ammonia engines and ammonia supply systems, starting with a single-cylinder ammonia engine as the foundation.

The main technical specifications and parameters of the single cylinder retrofit engine and the ammonia supply system are shown in Table 1 and Table 2, respectively.

Table 1. Test engine specifications

Parameters	Values
Cylinder	1
Bore/mm	270
Rated Speed/rpm	750
Fuel System (Diesel)	Common Rail
Fuel System (Ammonia)	PFI
Brake Mean Effective Pressure (BMEP) /MPa	2.2
Carbon Content Reduction (CCR, @load 20-70%）/%	＞70

Table 2. Ammonia supply system specifications

Parameters (Units)	Values
Mass Flux (kg/h)	0~278
Output Pressure (barA)	1.5~6.0
Filtration Accuracy (μ)	5
Output Temperature (℃)	＞25
Pressure Fluctuation (kPa)	±15

2.1 Ammonia Fuel Characteristics

Ammonia's simple chemical structure, which is devoid of carbon, positions it as a viable alternative to conventional fuels, aligning with the IMO's carbon emission reduction strategy. This holds true whether ammonia is utilized for direct combustion in engines, as a medium for hydrogen storage, or in fuel cell applications.

Ammonia can be liquefied at -33.6°C or under a pressure of 9 barA, making it relatively easy to store and transport. However, due to its lower low heating value (LHV), the required fuel storage volume for ammonia is approximately 2.55 times greater than that of conventional fuels such as heavy fuel oil (HFO). Additionally, given ammonia's toxicity and high reactivity, specific requirements must be established for storage materials, personnel safety protocols, and specialized equipment to ensure safe handling and operation.

Due to its narrow flammability range and slow flame propagation characteristics, ammonia requires specialized ignition methods, such as high-energy ignition or pilot fuel ignition, when used in marine engines. These approaches are essential to ensure reliable and efficient combustion.

Although the combustion of ammonia does not produce CO_2, challenges such as ammonia slip and N_2O emissions may arise due to incomplete combustion efficiency. As a result, it is essential to adjust and optimize the control strategies and combustion processes of traditional engines to address these issues effectively.

The key chemical and physical properties of ammonia are summarized in Table 3, while its thermodynamic data, including saturated curves and phase equilibrium curves, are illustrated in Figure 1 and Figure 2, respectively.

Table 3. Ammonia properties [6].

Properties	Values
Chemical Composition	NH_3
Boiling Point/℃@1 bar	-33
LHV/MJ/kg	22.5
Auto Ignition Temp/℃	630
Flammable Range/ %vol in air	15-33.6
Energy Density/MJ/t	15.7
Volume Comparison HFO (Energy Density)	2.55
Carbon Content	0
Carbon Content Reduction (CCR, compared to HFO)/%	100

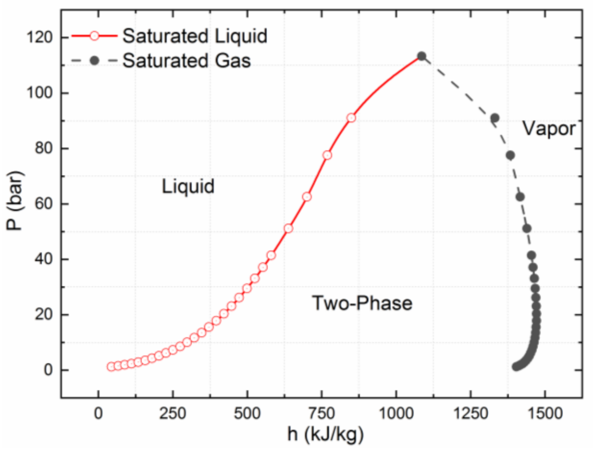

Figure 1. Saturated curve of ammonia (ammonia pressure-specific enthalpy diagram) [7]

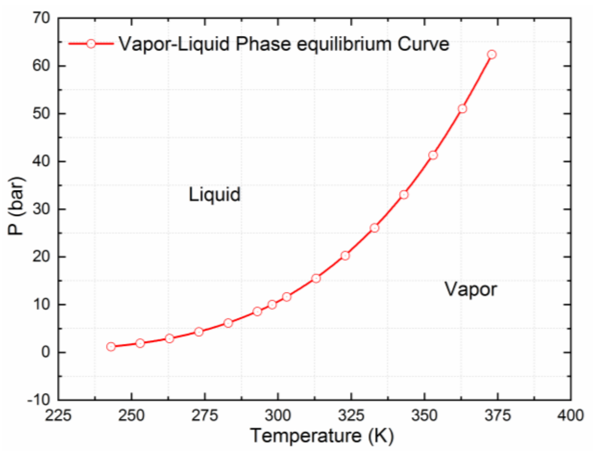

Figure 2. Vapor-liquid phase equilibrium curve of ammonia

2.2 Ammonia Supply System Composition and Working Principle

The primary function of the ammonia supply system is to filter and gasify the liquid ammonia supplied by the ammonia fuel tank. Following pressure regulation, the system delivers the gaseous ammonia to the single-cylinder engine with the precise quantity, temperature, and pressure required for optimal operation.

The ammonia supply system primarily comprises the fuel supply unit (LFSS) and the fuel valve train (FVT), both of which are housed within protective shell packages. Additionally, the system is equipped with self-inspection capabilities, safety interlock mechanisms, leakage alarms, and nitrogen purging functions to ensure compliance with stringent marine regulations.

The function of the LFSS is to deliver gaseous ammonia fuel. It typically consists of a fuel tank, an ammonia supply pump, a heat exchanger, a buffer tank, valves, instrumentation, and a control unit. The FVT is designed to ensure a stable supply of ammonia gas that meets the user-defined temperature and pressure requirements, while also fulfilling safety requirements such as double wall pipe (DWP) ventilation. Figure 3 illustrates the complete composition and functional flow diagram of the ammonia fuel supply system.

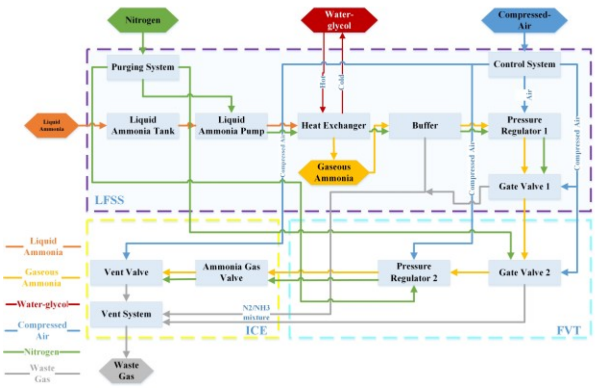

Figure 3. Schematic diagram of the ammonia supply system for the PFI/Low Pressure Direct Injection (LPDI) fuel supply system for the single cylinder engine

- The Liquid Ammonia Diaphragm Pump

The system employs a reciprocating liquid ammonia diaphragm metering pump, driven by an electric motor. The pump has a maximum flow rate of 278 kg/h and an outlet pressure of up to 12.6 barG. Flow regulation is achieved through frequency changes and bypass lines.

- The Heat Exchanger

A plate heat exchanger is used to convert liquid ammonia to gaseous ammonia. The heat transfer medium is water-glycol, with design pressures of 16 barG on the fuel side and 10 barG on the heat transfer medium side.

- The Gaseous Ammonia Buffer

The buffer tank stores gaseous ammonia at a specific temperature and pressure, absorbing pressure fluctuations caused by load changes and discontinuous fuel supply. The project uses a vertical buffer tank with a volume of 0.6 m^3 and a pressure of 21 barG.

- Pressure Regulators

Pressure regulators control valve action according to the host and external control signal in order to meet the ammonia supply pressure requirements. The system's pressure regulators have a diameter of DN50 and can maintain pressure fluctuations within ±15 kPa at an outlet pressure of 5–6 barA.

- The Heat Tracing System

Since the liquid ammonia tank is a pressurized storage vessel, the liquid ammonia pipeline does not require heat tracing to prevent condensation or frosting. However, explosion-proof electric heat tracing, aluminum silicate insulation, and heat insulation coatings are applied to the gaseous ammonia pipeline and buffer tank to prevent liquefaction and ensure system reliability.

- Tubes and Sensors

To address pipeline vibration, noise, and corrosion, the maximum allowable flow velocity for dry gas in the pipeline is set at 25–30 m/s. The pipeline is designed with a pressure loss limit of <2% of the inlet pressure. The pipeline material is 316 stainless steel, with non-metallic components made from ammonia-resistant materials such as perfluoro ether. All sensors are explosion-proof.

2.3 1D Simulation Model of Ammonia Supply System

2.3.1 Modelling and Parameters Settings

Based on the basic composition of the ammonia supply system, a 1D simulation model was developed using Amesim software [8]. The model incorporates the phase transition process of ammonia fuel, with the plate heat exchanger, buffer, and related pipelines characterized using relevant components from the Two-Phase Flow library. To simplify calculations and focus on ammonia's phase changes under varying loads and environmental conditions, the liquid ammonia outlet parameters of the diaphragm pump were used as the simulation inlet boundary. The working principles of pressure regulators and ammonia injection valves were simulated using proportional-integral-derivative control (PID).

The 1D simulation model of the ammonia supply system, along with the structure and test operation parameters of its main components, are presented in Figure 4 and Table 4, respectively.

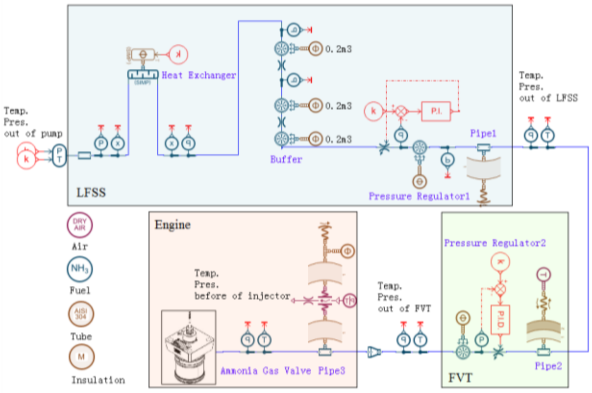

Figure 4. 1D simulation model of ammonia supply system based on Amesim

Table 4. Parameters of the key components in the ammonia supply system on the test conditions

Name	Parameters (Units)
Temperature and Pressure out of Pump	9~12.6 barA, 10~40 ℃
Temperature. of Heat Exchanger	45~75 ℃
Volume of Ammonia Buffer	0.6 m^3, with electric tracing heating and insulation cladding
Target Pressure of the PR1	5~8 barA
Target Pressure of the PR2	3~4 barA
Pipe1	3 m, DN40, with electric tracing heating and insulation cladding
Pipe2	100 m, DN40, buried underground
Pipe3	2 m, DN50, DWP with ventilation

2.3.2 System Calibration

To ensure the accuracy and reliability of the simulation results and guide subsequent design optimization, the simulation model was calibrated. Pressure and temperature measurements of ammonia fuel at the inlet of the FVT and ammonia gas admission valve (AGAV) were compared with simulation results under different loads and ammonia replacement rates, as shown in Figure 5 and Figure 6.

The simulation results closely matched the sensor measurements at ammonia supply flow rates of 25, 54.6, 75.2, and 100.1 kg/h. This indicates that the simulation model accurately reflects the engineering and functional characteristics of the ammonia supply system and can be used for further parameter analysis.

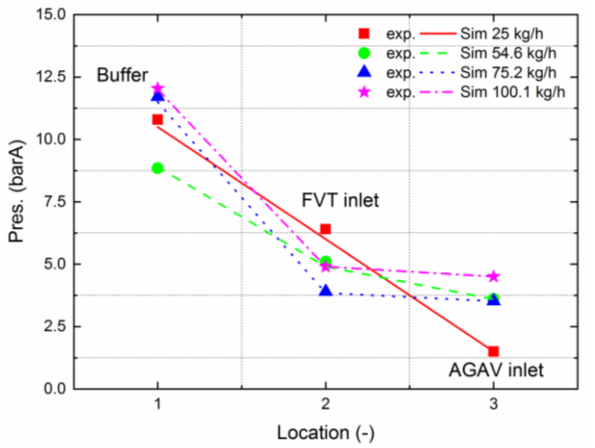

Figure 5. Pressure analysis between experimental and simulation results at different locations with five mass flow rates

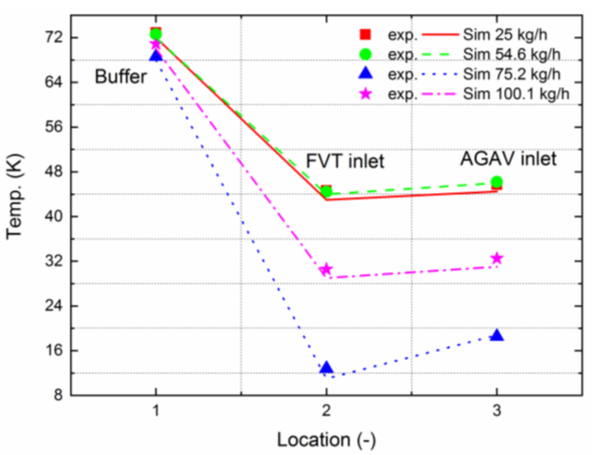

Figure 6. Temperature analysis between experimental and simulation results at different locations with five mass flow rates

2.3.3 Analysis of key parameters affecting ammonia supply temperature

Based on experimental results and theoretical analysis, the mass flow rate, pressure reduction level, environmental heat dissipation rate (HDR), and body heat transfer rate (BHTR) were investigated for their effects on ammonia supply temperature. The outlet pressure of the liquid ammonia diaphragm pump was set to 9 barA, with a supply temperature of 10°C (ambient temperature). Pressure regulator targets were set according to common operating conditions of the single-cylinder ammonia engine. The specific parameter settings are detailed in Table 5.

Table 5. Main Parameter settings for studying output temperature

Name	Parameters (Units)
Temperature and Pressure out of Pump	9 barA, 10 ℃
Temperature of Heat Exchanger	45 ℃
Target Pressure of the PR1	5 barA
Target Pressure of the PR2	3 barA
HDR	-1000/-750/-500/-250/0 W
BHTR	0/250/500/750/1000 W

- Mass Flow

Figure 7 ~ Figure 9 illustrate the simulated outlet temperatures of the buffer, LFSS, FVT, and AGAV inlet under different mass flow rates. Figure 7 shows results without considering HDR or BHTR. Figure 8 includes an HDR of -1000 W without BHTR, while Figure 9 considers a BHTR of 1000 W without HDR.

The results indicate that the outlet temperatures of the buffer, LFSS, and FVT remain relatively stable with increasing mass flow when HDR and BHTR are ignored. However, due to mechanical ventilation in the DWP, the temperature before the AGAV increases slightly with higher flow rates. When HDR is considered, temperatures at all locations except the buffer outlet decrease significantly with increasing flow rates. Conversely, when BHTR is considered, the temperature before the AGAV increases slightly compared to the FVT outlet temperature, with smaller flow rates showing more pronounced temperature increases.

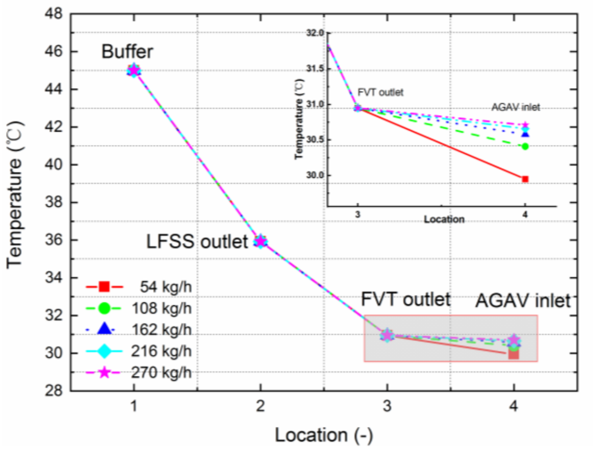

Figure 7. Effects of mass flow on ammonia output temperature without HDR or BHTR

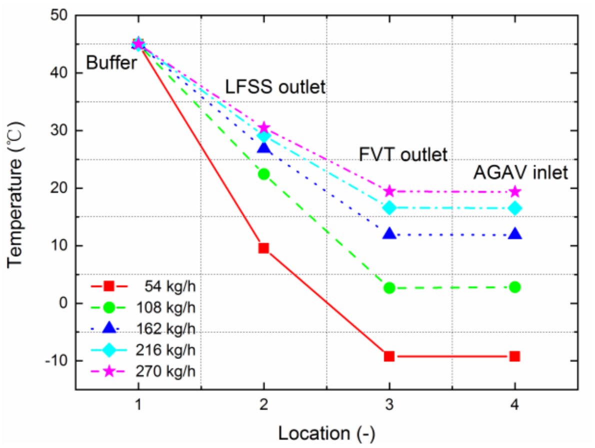

Figure 8. Effects of mass flow on ammonia output temperature with HDR=-1000 W and no BHTR

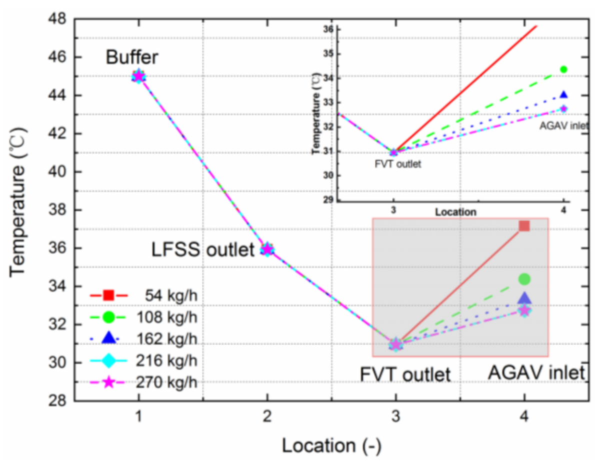

Figure 9. Effects of mass flow on ammonia output temperature with BHTR=1000 W and no HDR

- Pressure Reduction

Figure 10 shows the simulated results of ammonia temperature and pressure at the outlet of heat exchanger, LFSS, and FVT, respectively. The system pressure decreases from 9 barA to 3 barA, with a corresponding temperature drop of approximately 14.05°C. The temperature/pressure reduction ratio is about 2.34°C/barA, consistent with the Joule-Thomson effect.

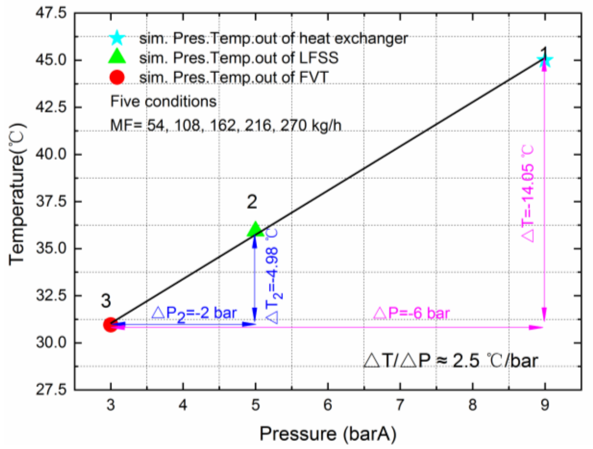

Figure 10. Effects of pressure reduction on ammonia supply temperature

- Heat Dissipation Rate

Figure 11 ~ Figure 13 illustrate the effects of different HDRs (-250 W, -500 W, -750 W, and -1000 W) on the ammonia supply temperature. The negative sign indicates heat dissipation. The results show that temperatures decrease at all locations except the buffer outlet as HDR increases. The most significant temperature drop occurs between the buffer and LFSS outlet due to heat transfer area and pressure regulation.

At a mass flow rate of 54 kg/h, when HDR ≥ 750 W, the FVT outlet temperature reaches the critical phase transition temperature, indicating gas ammonia liquefaction. At a flow rate of 270 kg/h, with a BHTR of 1000 W, the temperature from the FVT outlet to the AGAV increases by 1–1.5°C.

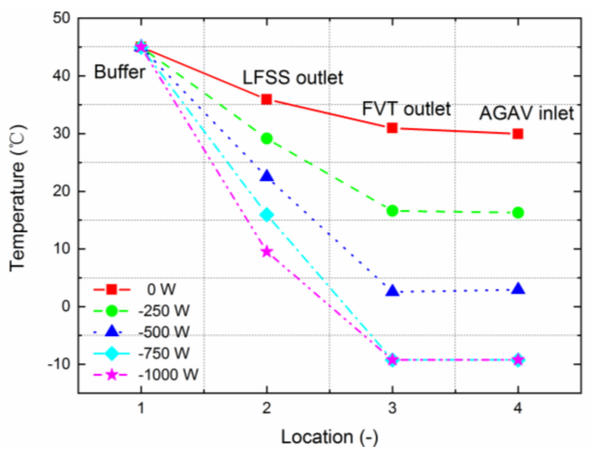

Figure 11. Effects of HDR on ammonia supply temperature at 54 kg/h with no BHTR

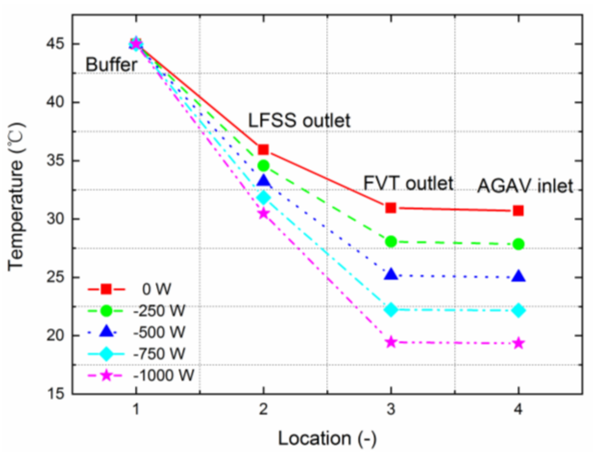

Figure 12. Effects of HDR on ammonia supply temperature at 270 kg/h with no BHTR

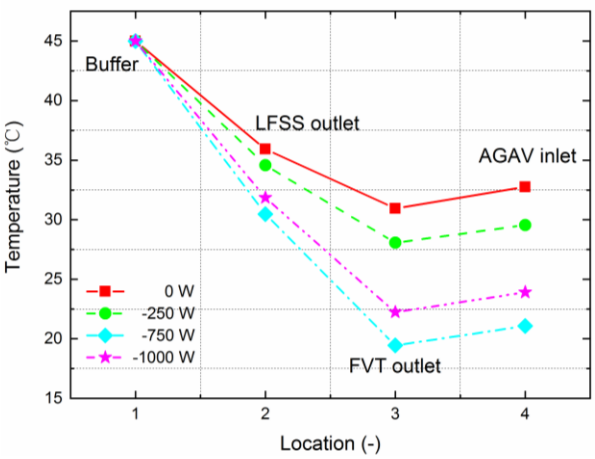

Figure 13. Effects of HDR on ammonia supply temperature at 270 kg/h with BHTR=1000 W

- Body Heat Transfer Rate

Figure 14 ~ Figure 17 show the effects of BHTR (0–1000 W) on ammonia supply temperature at mass flow rates of 54 kg/h and 270 kg/h. BHTR primarily affects the temperature before the AGAV, with more pronounced temperature increases at lower flow rates.

At a flow rate of 54 kg/h, every 250 W increase in BHTR results in a temperature rise of approximately 1.4°C at the AGAV inlet. In contrast, at a higher flow rate of 270 kg/h, the same 250 W increase in BHTR leads to a temperature rise of about 0.6°C. When HDR is considered, the effect of BHTR diminishes. At 54 kg/h with HDR equals to -1000 W, the system liquefies before the FVT exit, and even a BHTR of 1000 W cannot reverse this process.

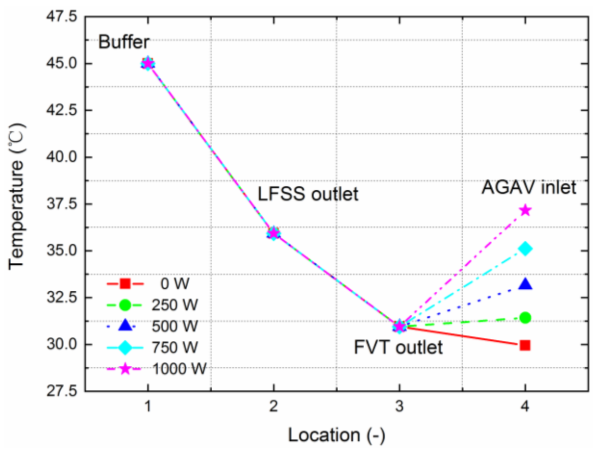

Figure 14. Effects of BHTR on ammonia supply temperature at 54 kg/h with no HDR

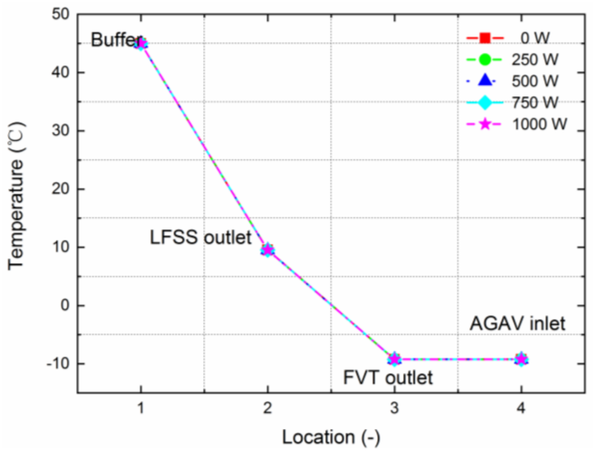

Figure 15. Effects of BHTR on ammonia supply temperature at 54 kg/h with HDR=-1000W

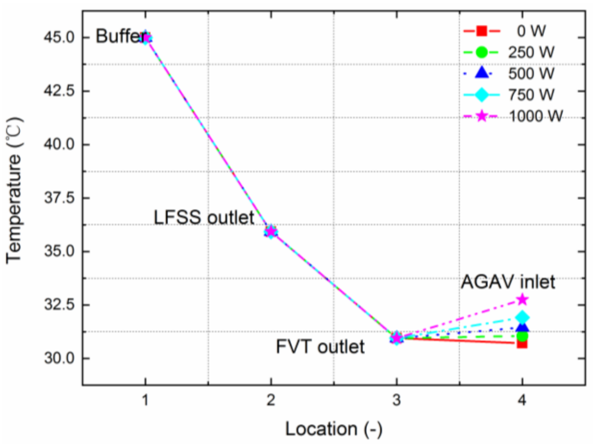

Figure 16. Effects of BHTR on ammonia supply temperature at 270 kg/h with no HDR

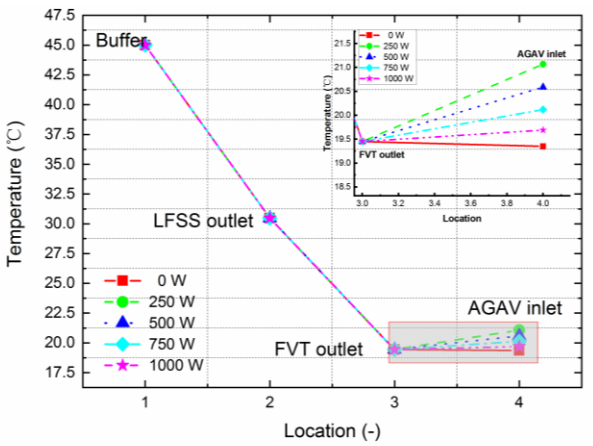

Figure 17. Effects of BHTR on ammonia supply temperature at 270 kg/h with HDR=-1000W

2.4 Ammonia Supply System Temperature/Pressure Control

Unlike LNG, ammonia can easily reach its phase transition critical point. If the system's pressure and temperature control are mismatched, gaseous ammonia may liquefy due to pressure increases, temperature decreases, or insufficient heating insulation. This can reduce the corrosion resistance of system components and pipelines, absorb significant heat during regasification, and potentially damage valve group sensors, ultimately degrading system performance.

To prevent these issues, the ammonia supply system must ensure that the temperature of all components and pipelines downstream of the gasifier remains above the liquefaction temperature of ammonia at the corresponding pressure, based on the engine's maximum pressure requirements. Additionally, pressure stability must be maintained, and pressure fluctuations minimized.

Simulation results indicate that mass flow rate, pressure reduction, HDR, and BHTR significantly influence ammonia outlet temperature. Due to the system's structural composition and functional characteristics, temperature changes in the LFSS are more pronounced, while the positive effects of BHTR are limited. Therefore, during the design process, PID control can be used to regulate the output pressure of the liquid ammonia supply pump and the buffer's set pressure, corresponding to the LFSS supply valve opening.

3 CONCLUSIONS

Based on the structure and functional principles of the ammonia supply system, this paper investigates the temperature and pressure characteristics of the system using 1D simulation software Amesim and the Two-Phase Flow simulation database. The simulation model is calibrated with experimental data obtained from single-cylinder ammonia engine tests.

The simulation results reveal that the ammonia supply mass flow rate, pressure reduction, HDR, and BHTR significantly influence the ammonia supply temperature. Specifically, the outlet temperature of ammonia decreases with reductions in mass flow rate and BHTR, while it increases with decreases in pressure reduction and HDP.

Therefore, both target pressure and design temperature must be considered simultaneously during system design. To achieve this, a PID control strategy can be employed to appropriately set and regulate the output pressure of the liquid ammonia supply pump and the buffer's set pressure, corresponding to the opening of the LFSS supply valve. This approach ensures optimal system performance and stability.

4 ACKNOWLEDGMENTS

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5 DEFINITIONS, ACRONYMS, ABBREVIATIONS

AGAV: Ammonia Gas Admission Valve

BHTR: Body Heat Transfer Rate

BMEP: Brake Mean Effective Pressure

CCR: Carbon Content Reduction

DWP: Double Wall Pipe

FVT: Fuel Valve Train

GHG: Green House Gases

HDR: Heat Dissipation Rate

HFO: Heavy Fuel Oil

IMO: International Maritime Organization

LFSS: Low Flashpoint Fuels Supply System

LHV: Low Heat Value

LNG: Liquid Natural GAS

LPDI: Low Pressure Direct Injection

MEPC: Marine Environment Protection Committee

MF: Mass Flow

PFI: Port Fuel Injection

PR: Pressure Regulator

PID: Proportional-Integral-Derivative control

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