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Research on Modeling and Simulation Technology of Ammonia Fuel Digital Engine System

Simulation Technologies, Digital Twins and Complex System Simulation

Haopeng Nie, China Shipbuilding Power Engineering Institute CO., LTD

Liwei Li, China Shipbuilding Power Engineering Institute CO., LTD
Teng Liu, China Shipbuilding Power Engineering Institute CO., LTD

ABSTRACT

With the increasing adoption of new fuels such as methanol and ammonia, it has become more challenging to quickly locate and resolve operational faults or potential risks in marine engines. These engines struggle to effectively predict faults and to operate at the optimal performance point in various marine environments. Engine digitalization can help address the needs of marine and engineering professionals by providing solutions to reduce fuel consumption, carbon emissions, and maintenance costs. It can swiftly identify and predict potential faults, ensuring the efficient, safe, reliable, and agile response of ship engines. Therefore, research on digital engines is of great significance and represents a major trend for future development.

In this paper, digital engine is defined, its core concepts and research framework are introduced, and a multi-physics simulation model based on engine knowledge and mathematical physics principles is proposed.

Based on Modelica language, a Multi-physics real-time model of an ammonia fuel engine is established. This simulation model is an important part of digital engine research. The whole machine model includes motion model, combustion model and friction lubrication model. The modeling principle and process of in-cylinder reaction system are introduced emphatically. The model can be used to calculate and predict the real-time operating characteristics of each engine system component, and provide data support for engine control and emission.

1 INTRODUCTION

The shipping industry accounts for 80% of today's global trade transport, and Marine engines as the core equipment of the shipping industry, its operation and maintenance efficiency and cost also occupy a great proportion of ship operation and maintenance. In recent years, with the concept of green shipping and research and development needs more concrete, the Marine engine industry is facing many challenges, mainly including the following three points: 1) the engine can not ensure that different Marine environments are running in the best working conditions, the consumption of fuel consumption, carbon emissions directly affect the ship's comprehensive operating costs; 2) With the popularity of multi-fuel, the operation failure or potential risk of the engine is more difficult to quickly locate and solve, resulting in a further increase in operation and maintenance costs; 3) Today's intelligent operation and maintenance software lacks the learning ability of the multi-physical field real-time prediction model and operation knowledge of the engine, which can not realize the effective prediction of faults and the rapid update of multi-mode information.

Therefore, the solution that can assist the efficient operation of Marine engines, quickly solve the needs of crew/engineers, and accurately predict or locate faults has become a project with wide range of demands and great challenges in the industry. The right solution can greatly reduce the operation and maintenance cost of Marine engines and quickly occupy the market. The traditional research and development model is no longer sufficient to meet the development needs, and a paradigm shift from "traditional design" to "predictive design" is needed [1]. To this end, based on a large number of Marine engine research and development experience, ship maintenance service knowledge and other experience, this paper creates a digital engine core concept and research framework suitable for Marine power, and builds an ammonia fuel digital engine model to provide solutions for reducing fuel consumption, carbon emissions, operation and maintenance costs, and ensure the efficient operation, safety and reliability of Marine engines, and agile response.

Taghavi et al. developed a framework for Marine engine digital twin research to improve the efficiency of ship energy use to solve the problem of excessive growth in energy consumption [2]. Jeon et al. developed a reliability framework for direct test of Marine engines based on a first-principles model. And a method is applied to develop digital twin under the condition of ship engine health. The results show that the reliability of the developed digital twin is guaranteed, the use of digital twin to generate data sets, the development of data-driven anomaly diagnosis model, detection accuracy and recognition accuracy are high, the research is of great significance [3]. Jacek et al. explored the development of a control-oriented digital twin for the Wartsila 4L20 Marine engine. The research results provide a new idea for the feasibility of digital twin in Marine engine field. The obtained fast-running engine model is three times faster than the real-time speed, while the loss of accuracy is within a 5% tolerance of the control output, including the crank Angle resolution of the cylinder pressure [4]. Dmytro et al. proposed that the core component of digital twin is the mathematical model of the working cycle of marine diesel engines. And focused on improving the fuel combustion model, considering the variable value of the average droplet diameter during fuel injection. The results indicate that using an improved combustion model can better adapt the digital twin model to experimental data, thereby more accurately corresponding to the actual engine [5]. Yuanyuan et al. studied the Mean Value Engine Model (MVEM) using three different compressor mass flow models. Research has shown that physics based Kong Song models are a favorable choice for digital twin applications due to their excellent extrapolation ability and low dependence on measurement data [6]. Marios et al. developed a framework that utilizes first principles based digital twins to address the health assessment of ship engines. The results indicate that the developed digital twin helps to effectively map the performance of the entire operating range of the engine under various health conditions, thereby better understanding the current health status of the engine [7]. Stoumpos et al. developed an integrated model that combines detailed engine thermodynamic modeling and control system functional modeling. The results indicate that the developed model can fully represent the behavior of the engine and its subsystems/components, and effectively capture the functionality of the engine control system [8].

This paper introduces the overall framework of digital engine research, and uses digital means to build ammonia host simulation model to improve systemlevel simulation capability. The model includes in-cylinder reaction system, starting system, fuel system, lubricating oil system, intake system, exhaust system, cooling system, transmission system, control system linked with ammonia fuel supply system, etc. It has high execution efficiency, good scalability and upgrading characteristics, can maintain stability during long-term independent operation, and can output in-cylinder temperature and pressure characteristics. The torque, power and speed characteristics of the ammonia fuel main engine, the characteristics of the lubricating oil system, the characteristics of the cooling water system, etc., realize the real-time monitoring of the engine operating parameters.

2 DIGITAL ENGINE OVERALL RESEARCH FRAMEWORK

Digital engine can be defined as: integrated multi-disciplinary, multi-physical quantity, multi-scale engine digital model, which can achieve high-precision and high-fidelity digital analysis and result presentation of the whole engine, system and components in the virtual digital space.

The whole digital engine consists of four main modules: (1) conversational natural language interactive platform. (2) adaptive operation optimization module. (3) predictive operation and maintenance and fault diagnosis module 4) Marine engine knowledge base. See the following chapter for a brief introduction.

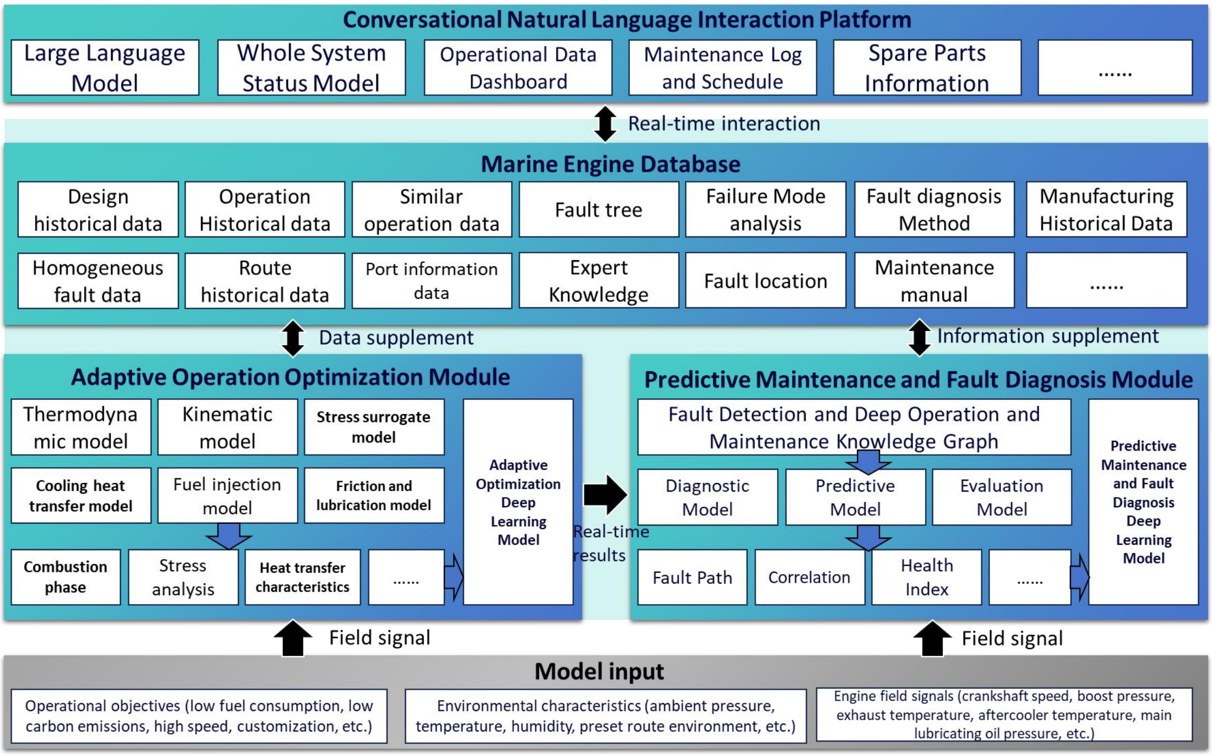

Figure 1. The overall research framework for digital engines

2.1 .Adaptive operation optimization module

This module mainly includes two core units, multi-physical field real-time model and deep learning model, which can predict the state of the engine based on the operation objectives, environmental characteristics and field signals of the engine, and provide an efficient adaptive optimization scheme. The multi-physical field real-time model is established based on engine knowledge and mathematical physics model, including thermodynamic model, etc., and calibrated through engine operation data, which is used to calculate and predict the real-time working characteristics of each engine system component to provide data support for engine control and emission. The deep learning model is based on artificial intelligence technologies such as representation learning and multidimensional feature fusion to model the relationship between navigation requirements, navigation conditions and engine operating parameters, analyze the key factors affecting engine operation, and judge the optimal engine operating parameters under different operating conditions.The development of multi-field modeling integrated technology and new information technology such as big data has made modern supporting technology develop in the direction of accurate calculation, intelligent analysis and complete functions [9].

The adaptive operation optimization module not only reduces reliance on operator expertise but also ensures the system adaptively operates under optimal conditions. While maintaining reliability, it maximizes the reduction of fuel consumption and carbon emissions, achieving environmentally and economically friendly, safe, and efficient operation.

2.2 Predictive operation and fault diagnosis module

This module mainly includes three core units: fault detection and equipment operation and maintenance knowledge graph, predictive operation and maintenance model and deep learning model.

Based on the engine operation and maintenance knowledge base, statistical analysis and multidimensional time series modeling technology are used to mine the symptoms of strong correlation between fault performance, establish the relationship between specific fault types and engine operating parameters, and form the knowledge graph of fault detection and equipment operation and maintenance.

Combining knowledge graph, multi-dimensional time series prediction technology and engine fault diagnosis method, the diagnostic model, prediction model and evaluation model are constructed according to the historical engine operation data. The real-time data obtained from the adaptive operation optimization module is used to predict the trend of failure, such as abnormal wear of parts, flow congestion, fatigue life, etc., and predict the fault risk.

Establish a deep learning model of engine predictive operation and fault diagnosis, input the operating state when the fault occurs into the model, perform rapid fault tracing for a variety of potential abnormal risks, shorten the time of engine fault troubleshooting, and provide targeted guidance for maintenance work, so that engine maintenance and overhaul are more targeted and planned, and reduce operation and maintenance costs.

2.3 Marine engine knowledge base

The knowledge base is a key part of the "Sinan" model, including all kinds of historical data and expert knowledge, interaction with other modules, and continuous closed-loop knowledge supplement. The typical ones are:

Route historical data mainly records the operating environment of the engine in the designated route, including navigation environment, supply information, important historical events, etc.Design historical data mainly records the key characteristic parameters of the designed system and components, including performance parameters, structural parameters, process parameters, etc.The operation history data mainly records the data of each sensor under different working conditions and the engine operation data measured by the multi-physical field model, mainly including the important parameters affecting the operation of each key system and key parts.The knowledge of operation and maintenance manual mainly includes the demolition and construction plan, maintenance plan, inspection and maintenance knowledge of each engine component.The expert knowledge database mainly records the expert knowledge in the field of Marine engines, which mainly includes solutions in aspects such as, performance, combustion, emission, vibration, fault location, etc.

Part of the Marine engine knowledge base comes from historical accumulation, part of the resource comes from the actual operation of the associated machine and the prediction of the multi-physics mathematical model.

2.4 Conversational natural language interaction platform

Based on the operational data of marine engines and knowledge base data, a large language model suitable for tasks such as knowledge Q&A and operation control of marine engines is constructed to achieve intelligent human-machine interaction, shorten the human-machine adaptation time, and provide decision support for the intelligent management of marine engines. By using the intelligent agent technology of large language models to parse the technical demands of crew members/engineers, the underlying marine engine knowledge base, adaptive optimization module, predictive maintenance and fault diagnosis module are mobilized to execute corresponding tasks, thereby achieving a more humanized and efficient interaction experience. This enables crew members or engineers to obtain the required information or support more intuitively and conveniently, and better realize the decision-making and control of the engine.

3 DIGITAL MODEL OF AMMONIA FUEL MAIN ENGINE

The multi-physical field real-time model established based on engine knowledge and mathematical physics principles is the key to the research system and the most important basic research. Therefore, the multi-physics real-time model of ammonia fuel engine was first built in this paper, and further research will be conducted based on this model in the future.

Digital engine modeling can be divided into three categories: black box model, physics-based model and gray box model [10].The multi-physics real-time model of ammonia fuel engine is established based on engine knowledge and mathematical and physical models, including thermodynamic models, and calibrated through engine operation data, which is used to calculate and predict the real-time working characteristics of each engine system component to provide data support for engine control and emission.

Modelica language can easily realize the modeling of complex physical systems, and has a relatively mature application in the aerospace field.

MWORKS.Sysplorer software, developed based on the Modelica language, is a multi-domain modeling and simulation platform that integrates the Modelica Standard Library. Building upon this foundation, it incorporates extensions and optimizations to achieve enhanced usability and extensibility. This paper employs MWORKS software to construct a dual fuel main engine model, with the Modelica Standard Library version 3.2.3 selected for implementation.

The engine model includes cylinder Model, cooling System Model, lubrication System Model, turbocharging System Model, starting Air System Model, Power transmission System Model, fuel Control System Model, fuel Oil System Model and emission Calculation Model.The brief functional introduction of each module model is as follows:

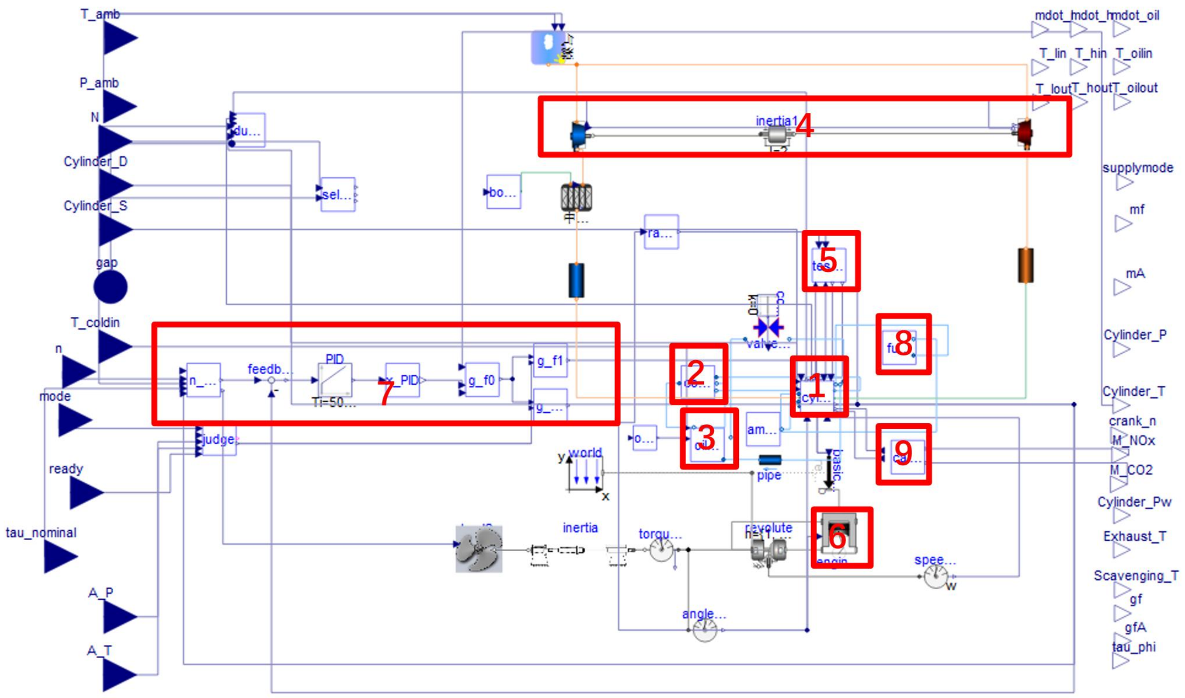

Figure 2. Ammonia fuel main engine model

(1) Cylinder Model

The cylinder model serves as the core module connecting all sub-modules, primarily including the combustion module, scavenging port module, exhaust port module, and in-cylinder working process calculation module. It predicts and calculates curves such as cylinder pressure, cylinder temperature, and heat release rate.

(2) Cooling System Model

This model comprises various heat exchangers like the low-temperature freshwater cooler, main engine lubricating oil cooler, and high-temperature freshwater cooler, along with a thermostat model. The established dynamic thermodynamic model for the ammonia-fueled main engine cooling water system reflects the heat transfer principles of the system.

(3) Lubrication System Model

Components include the lubricating oil sump, lubricating oil pump, lubricating oil cooler, automatic temperature control valve, and temperature regulation controller. This model precisely regulates the temperature and flow rate of lubricating oil entering the main engine.

(4) Turbocharging System Model

Consists of the compressor, turbine, and intercooler. The model controls the air mass flow into the cylinder, compresses intake air, and cools high-temperature air post-compression via the intercooler, enabling dynamic adjustments of intake flow, pressure, and temperature.

(5) Starting Air System Model

Includes the air compressor, starting air reservoir, main starting valve, cylinder starting control valve, and cylinder starting valve. This model simulates the air-starting process of the engine.

(6) Power Transmission System Model

Covers the piston, piston rod, crosshead pin, connecting rod, crankpin, crank arm, and main journal. It analyzes kinematics, dynamics, and structural strength of these components.

(7) Fuel Control System Model

Centered on closed-loop speed control, this system adapts to operational variations or external disturbances to ensure rapid matching between dual fuel supply and engine speed, achieving the preset RPM.

(8) Fuel Oil System Model

The fuel oil pump acts as the intermediary between the fuel oil storage tank and cylinder module. It monitors supply flow from the tank and demand from cylinders to assess fuel consumption in the circuit.

(9) Emission Calculation Model

This module calculates emission flow rates for exhaust components (NO, NO_2, NO_x, CO, CO_2) and tracks urea content variations in the Selective Catalytic Reduction (SCR) system post-treatment

3.1 In-cylinder working process module

The in-cylinder working process calculation module is the core module connecting all sub-modules. It links multiple systems including the scavenging/exhaust system, power system, and fuel system, making it a critical computational module. The following section focuses on explaining the construction principles of the in-cylinder working process.

When building the cylinder model, the cylinder is typically regarded as a thermodynamic system bounded by the inner wall surface of the cylinder liner, the piston crown face, scavenging/exhaust ports, and the fire deck surface of the cylinder head, as shown in Figure 3. By using three fundamental parameters (pressure, temperature, and mass) and solving three governing equations (mass conservation, energy conservation, and ideal gas state equation), the specific state of the working fluid within the system at any moment can be determined.

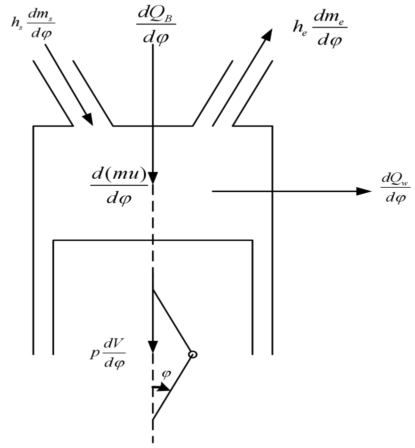

Figure 3. Cylinder working process calculation diagram

3.1.1 Basic differential equation

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The working process in the cylinder is described from conservation of mass, conservation of energy, conservation of momentum and ideal gas state equation respectively. The expressions are as follows:

Mass conservation equation:

$$\frac{dm}{d\varphi} = \frac{dm_s}{d\varphi} + \frac{dm_e}{d\varphi} + \frac{dm_B}{d\varphi} \tag{1}$$

Energy conservation equation:

$$\frac{d(mu)}{d\varphi} = \frac{dQ_B}{d\varphi} + \frac{dm_s}{d\varphi} h_s - \frac{dm_e}{d\varphi} h_e - \frac{dQ_W}{d\varphi} - p\frac{dV}{d\varphi} \tag{2}$$

The derivation simplifies to:

$$\frac{dT}{d\varphi} = \frac{1}{mc_V}\left(\frac{dQ_B}{d\varphi} + h_s \frac{dm_s}{d\varphi} - h_e \frac{dm_e}{d\varphi} + \frac{dQ_w}{d\varphi} - p\frac{dV}{d\varphi} - u\frac{dm}{d\varphi}\right) \tag{3}$$

Ideal gas equation of state:

$$pV = mRT \tag{4}$$

Where: m is the mass of liquid fuel that is not injected into the cylinder, m_s is the mass of air entering the cylinder, m_e is the mass of exhaust gas flowing out of the cylinder, g_f is the amount of circulating fuel injection of the engine, and x is the percentage of fuel combustion in the cylinder; Q_B is the heat released by the combustion of fuel in the cylinder, Q_W is the heat passed into or out through the cylinder walls, u is the specific internal energy, h_s,h_e are the specific enthalpy of the working medium at the inlet and exhaust valve, P is the pressure of the working medium in the cylinder, V is the working volume of the cylinder, T is the temperature of the working medium in the cylinder, R is the gas constant, c_v is the specific heat capacity of the constant volume process, and φ is the crankshaft Angle.

3.1.2 Dual fuel machine working medium characteristics

During the operation of dual fuel engines, the working medium undergoes multiple phase transformations and can be considered as an ideal gas mixture composed of various chemical components. The thermodynamic properties of the working medium significantly influence in-cylinder process characteristics such as combustion heat release rate. Therefore, the calculation of working medium thermodynamic properties has a substantial impact on the accuracy of dual fuel engine modeling and simulation, making its selection the primary computational step. Currently, two methods are commonly used for calculating engine working medium property parameters: one involves semi-empirical formulas to compute working medium characteristics, while the other utilizes chemical reaction equilibrium equations. This paper employs the semi-empirical method for calculating working medium property parameters.

(1)Dual fuel mode parameters

The ammonia replacement rate of the ammonia fuel host in dual fuel mode is calculated as follows:

$$\gamma_A = \frac{m_{d1} - m_{d2}}{m_{d1}} \times 100\% \tag{5}$$

Where γ_A is the ammonia replacement rate; m_{d1} is the fuel consumption of pure diesel mode and m_{d2} is the fuel injection amount of dual fuel mode.

When the replacement rate is set in advance, the fuel injection amount can be calculated according to the fuel consumption under the same working condition.

The amount of ammonia supply is calculated by the equal calorific value method, that is, according to the low calorific value of diesel oil and ammonia, the same heat is converted according to the theoretical complete combustion of fuel:

$$m_A = \frac{\gamma_A \times m_{d1} \times H_d}{H_A} \tag{6}$$

Where m_A is the amount of ammonia supplied; γ_A is the ammonia replacement rate; H_d is Low calorific value of dual fuel injection, 42500kJ/kg; H_A is low calorific value of ammonia, 18,500 kJ/kg.

(2)Instantaneous excess air coefficient

The working medium within the cylinder of a dual fuel engine can be categorized into two distinct phases: pure air and combustion gas. For such a gaseous mixture, its thermodynamic parameters (e.g., specific heat capacity, specific enthalpy) at any given moment during engine operation can be determined by the instantaneous temperature and compositional ratio of the in-cylinder medium. The instantaneous excess air coefficient is conventionally employed to quantify this proportional relationship. The mathematical expression for the instantaneous excess air coefficient is defined as follows:

$$\alpha_\varphi = \frac{m - m_B}{L_o m_B} \tag{7}$$

Where m is the total mass of the working medium in the cylinder, m_B is the mass of the fuel burned in the cylinder before a certain instant, L_0 is the theoretical air amount, (in dual fuel mode is the equivalent theoretical air amount,, $L_0=\gamma_A \times L_A+(1-\gamma_A) \times L_d$, L_A=6.1kg air /kg ammonia, L_d,=14.3kg air /kg diesel).

(3)Instantaneous adiabatic index and instantaneous specific heat capacity at constant

pressure

The formula for the instantaneous adiabatic index is:

$$k_\varphi = 1.4373 - 1.318 \times 10^{-4}\, T + 3.12 \times 10^{-8}\, T^2 - \frac{4.8 \times 10^{-2}}{\alpha_\varphi} \tag{8}$$

For ideal gases, when high temperature thermal decomposition is not considered, the mean specific constant volume heat capacity formula returned by the Justi specific heat capacity table is:

$$c_{Vm\varphi} = 0.14455[-3*(0.0975+\frac{0.0485}{\alpha_\varphi^{0.75}})(T-273)^2*10^{-6}+2*(7.768+\frac{3.36}{\alpha_\varphi^{0.8}}) *(T-273)*10^{-4}+(489.6+\frac{46.4}{\alpha_\varphi^{0.03}})*10^{-2}] \quad (9)$$

(4)Specific internal energy vs. specific enthalpy

The relation between the specific internal energy u and the specific enthalpy h of an ideal gas can be expressed by the thermodynamic identity $h = u + RT$.

The specific internal energy of an ideal gas mixture is a function of temperature and the instantaneous excess air coefficient, $u = u(T, \alpha_\varphi)$. According to the analysis of Eusdibi heat capacity table data, the solution is as follows:

$$c_{Vm\varphi} = 0.14455[-3*(0.0975+\frac{0.0485}{\alpha_\varphi^{0.75}})(T-273)^2*10^{-6}+2*(7.768+\frac{3.36}{\alpha_\varphi^{0.8}}) *(T-273)*10^{-4}+(489.6+\frac{46.4}{\alpha_\varphi^{0.03}})*10^{-2}] \quad (10)$$

3.1.3 Cylinder working volume

By internal combustion engine dynamics, the cylinder volume per instantaneous is:

$$V=\frac{\pi D^2}{4}\left\{\frac{S}{\varepsilon-1}+\frac{S}{2}\left[\left(1+\frac{1}{\lambda}\right)-\cos\left(\frac{\pi}{180}\varphi\right)-\frac{1}{\lambda}\sqrt{1-\lambda^2\sin^2\left(\frac{\pi}{180}\varphi\right)}\right]\right\} \quad (11)$$

Where D is the cylinder diameter, S is the stroke, *λ* is the connecting rod crank ratio, φ is the crankshaft Angle, from the crankshaft at top dead center $\varphi = 0$, °CA.

The change rate of cylinder volume with crankshaft Angle φ is:

$$\frac{dV}{d\varphi}=\frac{\pi^2 D^2 S}{8\times 180}\left[\sin\left(\frac{\pi}{180}\varphi\right)+\frac{\lambda}{2}\cdot\frac{\sin\left(\frac{\pi}{180}\cdot 2\varphi\right)}{\sqrt{1-\lambda^2\sin^2\left(\frac{\pi}{180}\varphi\right)}}\right] \quad (12)$$

Where ε is the compression ratio, $\varepsilon = \frac{V_\varepsilon + V_s}{V_\varepsilon}$, V_ε is the clearance volume; V_s is the working volume of the cylinder, $V_s = \frac{\pi}{4} D^2 S$.

3.1.4 Heat dissipation process around cylinder wall

The cylinder circumference wall is composed of the cylinder head combustion chamber surface, the piston top surface and the wet circumference surface of the cylinder liner. The hot gas in the cylinder transfers heat to the coolant through the cylinder circumference wall. The heat dissipation rate of the working medium in the cylinder to the surrounding wall of the cylinder is:

$$\frac{dQ_w}{d\varphi}=\sum_{i=1}^{3}\frac{dQ_{wi}}{d\varphi}=\sum_{i=1}^{3}\alpha_g\cdot A_i\left(T-T_{wi}\right) \quad (13)$$

Where α_g is the instantaneous average heat transfer coefficient, A is the heat transfer area, T is the instantaneous temperature of the working medium in the cylinder, T_{wi} is the average wall temperature, *i*=1, 2, 3, respectively representing the cylinder head, piston and cylinder liner.

The instantaneous average heat transfer coefficient A was determined by Eichelberg formula:

$$\alpha_g = 2.1*10^{-3}\sqrt[3]{C_m}*\sqrt{PT} \quad (14)$$

Where P is the pressure of the working medium in the cylinder, T is the temperature of the working medium in the cylinder, and C_m is the average speed of the piston.

3.1.5 Cylinder combustion process

The instantaneous heat release rate of fuel combustion in the cylinder can be calculated by the following formula:

$$\frac{dQ_B}{d\varphi}=g_f\bullet H_u\bullet\frac{dx}{d\varphi} \quad (15)$$

Where Q_B is the instantaneous heat release; g_f is the fuel supply of the engine per cycle; H_u is the low calorific value of fuel combustion; x is the percentage of fuel combustion; $dx/d\varphi$ is the fuel combustion rate.

Fuel combustion percentage x represents the ratio of the mass of burned fuel to the amount of circulating fuel supplied at a crankshaft Angle, calculated as follows:

$$x=\frac{m_B}{g_f}\times 100\% \quad (16)$$

For dual fuel engines, the triple Wiebe functions are selected to accurately simulate in-cylinder heat release patterns. The first two Wiebe function curves represent diesel combustion processes, specifically the premixed combustion phase and diffusive combustion phase respectively. The third Wiebe function curve characterizes the premixed combustion process of ammonia fuel. The fuel mass fraction burned and fuel combustion rate in the triple Wiebe formulation are calculated as follows:

$$x_d = x_1 + x_2 \tag{17}$$

$$x_A = x_3 \tag{18}$$

$$\frac{dx}{d\varphi} = \frac{dx_1}{d\varphi} + \frac{dx_2}{d\varphi} \tag{19}$$

$$\frac{dx_A}{d\varphi} = \frac{dx_3}{d\varphi} \tag{20}$$

$$x_1 = \left[1 - e^{-6.908\left(\frac{\varphi-\varphi_B}{\varphi_1}\right)^{m_1+1}}\right] Q_1 \tag{21}$$

$$x_2 = \left[1 - e^{-6.908\left(\frac{\varphi-\varphi_B-\Delta\varphi_2}{\varphi_2}\right)^{m_2+1}}\right] Q_2 \tag{22}$$

$$x_3 = \left[1 - e^{-6.908\left(\frac{\varphi-\varphi_B-\Delta\varphi_3}{\varphi_3}\right)^{m_3+1}}\right] Q_3 \tag{23}$$

$$\frac{dx_1}{d\varphi} = \left[6.908\frac{m_1+1}{\varphi_1}\left(\frac{\varphi-\varphi_B}{\varphi_1}\right)^{m_1} \cdot e^{-6.908\left(\frac{\varphi-\varphi_B}{\varphi_1}\right)^{m_1+1}}\right] Q_1 \tag{24}$$

$$\frac{dx_2}{d\varphi} = \left[6.908\frac{m_2+1}{\varphi_2}\left(\frac{\varphi-\varphi_B-\Delta\varphi_2}{\varphi_2}\right)^{m_2} \cdot e^{-6.908\left(\frac{\varphi-\varphi_B-\Delta\varphi_2}{\varphi_2}\right)^{m_2+1}}\right] Q_2 \tag{25}$$

$$\frac{dx_3}{d\varphi} = \left[6.908\frac{m_3+1}{\varphi_3}\left(\frac{\varphi-\varphi_B-\Delta\varphi_3}{\varphi_3}\right)^{m_3} \cdot e^{-6.908\left(\frac{\varphi-\varphi_B-\Delta\varphi_3}{\varphi_3}\right)^{m_3+1}}\right] Q_3 \tag{26}$$

Where x_d is the percentage of diesel combustion, x_A is the percentage of ammonia combustion, C is the combustion starting Angle, m_1 , m_2 and m_3 are the combustion quality index of combustion processes 1, 2 and 3, φ_1 , φ_2 and φ_3 are the duration angles of combustion processes 1, 2 and 3, $\Delta\varphi_2$ and $\Delta\varphi_3$ are the hysteresis angles of combustion processes 2 and 3 relative to process 1. Q_1 and Q_2 are fuel fractions of diesel premixed combustion process and diffusion combustion process, respectively, and $Q_1 + Q_2 = 1$; Q_3 is the fuel fraction of ammonia combustion process, $Q_3 = 1$ in dual fuel mode and $Q_3 = 0$ in pure diesel mode.

3.1.6 Analysis of each stage of the in-cylinder working process

The working cycle of internal combustion engine can be divided into four stages: compression, combustion, expansion and air exchange. At different stages, the differential eq. 1 and eq. 2 can be simplified appropriately.

(1)Compression process

In the compression process, the intake valve and exhaust valve have been closed, ignoring the leakage loss of the intake valve, exhaust valve and piston ring, the quality of the working medium in the cylinder can be considered to remain unchanged:

$$\frac{dm_s}{d\varphi} = 0 \quad \frac{dm_e}{d\varphi} = 0 \quad \frac{dm_B}{d\varphi} = 0$$

the mass conservation eq 1 is simplified as:

$$\frac{dm}{d\varphi} = 0 \tag{27}$$

During the compression process, no gas flows into the cylinder and mixes with the working medium, and there is no combustion reaction, so $\frac{dQ_B}{d\varphi} = 0$. Eq 3 can be simplified as:

$$\frac{dT}{d\varphi} = \frac{1}{mc_V}\left(\frac{dQ_w}{d\varphi} - p\frac{dV}{d\varphi}\right) \tag{28}$$

(2)combustion phase

In the combustion stage, intake and exhaust valves are closed, $\frac{dm_s}{d\varphi} = 0$, $\frac{dm_e}{d\varphi} = 0$, but fuel is gradually burned, so eq 1 can be simplified as:

$$\frac{dm}{d\varphi} = \frac{dm_B}{d\varphi} = g_f \cdot \frac{dx}{d\varphi} \tag{29}$$

In the combustion phase, the equation 3 can be simplified as:

$$\frac{dT}{d\varphi} = \frac{1}{mc_V}\left(\frac{dQ_B}{d\varphi} + \frac{dQ_w}{d\varphi} - p\frac{dV}{d\varphi} - u\frac{dm}{d\varphi}\right) \tag{30}$$

After substituting eq 15 and eq 29 into eq 30, the equation can be arranged as:

$$\frac{dT}{d\varphi} = \frac{1}{mc_V}\left[\frac{dQ_w}{d\varphi} - p\frac{dV}{d\varphi} + g_f(H_u - u)\frac{dx}{d\varphi}\right] \tag{31}$$

(3)Expansion stage

In the expansion stage, the intake valve and exhaust valve are closed, there is no fuel combustion, the quality and composition of the working medium in the cylinder remain unchanged, and the instantaneous excess air coefficient remains unchanged, equal to the value at the end of combustion. Therefore:

$$\frac{dm_s}{d\varphi}=0 \quad \frac{dm_e}{d\varphi}=0 \quad \frac{dm_B}{d\varphi}=0$$

In the expansion stage, both eq 1 and eq 3 can be reduced to the same form as in the compression stage, namely equations eq 16 and eq 17.

(4)Ventilation stage

In the air exchange stage, the volume of the cylinder changes with the Angle of the crankshaft, the exchange of mass and heat exists in the cylinder and the outside world at the same time, and the thermal process in the cylinder is very complicated.

① Pure exhaust stage

From the opening of the exhaust valve to the opening of the intake valve. In this stage, $\frac{dm_s}{d\varphi}=0$, $\frac{dm_B}{d\varphi}=0$, the eq 1 is simplified as follows:

$$\frac{dm}{d\varphi}=\frac{dm_e}{d\varphi} \tag{32}$$

Similarly, eq 3 is simplified as:

$$\frac{dT}{d\varphi}=\frac{1}{mc_V}\left[\frac{dQ_w}{d\varphi}-p\frac{dV}{d\varphi}+(h_e-u)\frac{dm_e}{d\varphi}\right] \tag{33}$$

② Intake and exhaust stack phase

From the opening of the scavenging port to the closing of the scavenging port. In this stage, fresh air enters the cylinder and exhaust gas is discharged from the cylinder. There is no combustion reaction in the folding stage of the valve, that is, $\frac{dQ_B}{d\varphi}=0$, $\frac{dm_B}{d\varphi}=0$. The mass conservation equation in the cylinder at this stage is:

$$\frac{dm}{d\varphi}=\frac{dm_s}{d\varphi}+\frac{dm_e}{d\varphi} \tag{34}$$

Eq 3 simplifies to:

$$\frac{dT}{d\varphi}=\frac{1}{mc_V}\left[\frac{dQ_w}{d\varphi}-p\frac{dV}{d\varphi}+(h_s-u)\frac{dm_s}{d\varphi}+(h_e-u)\frac{dm_e}{d\varphi}\right] \tag{35}$$

③ Post-exhaust stage

From the scavenging port is closed until the exhaust valve is closed. In this stage, $\frac{dm_B}{d\varphi}=0$, $\frac{dm_s}{d\varphi}=0$, eq 1 is simplified as:

$$\frac{dm}{d\varphi}=\frac{dm_e}{d\varphi} \tag{36}$$

Ignoring the influence of α_φ, eq 3 is simplified as follows:

$$\frac{dT}{d\varphi}=\frac{1}{mc_V}\left[\frac{dQ_w}{d\varphi}-p\frac{dV}{d\varphi}+(h_e-u)\frac{dm_e}{d\varphi}\right] \tag{37}$$

3.1.7 in-cylinder reaction system model

Based on Modelica language and the modeling principle introduced above, the completed overall model of the in-cylinder reaction system is shown in Figure 4.

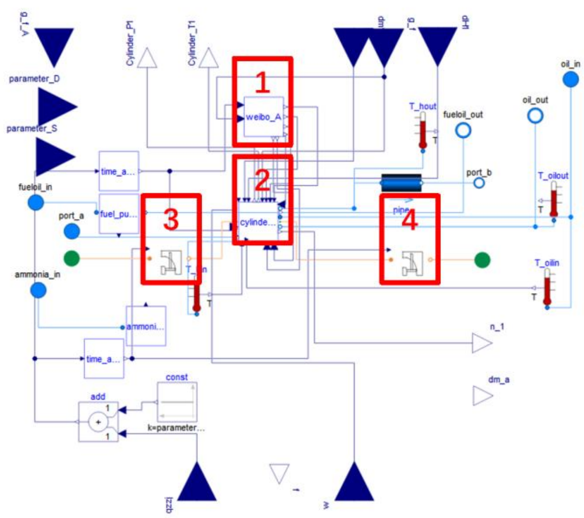

Figure 4. In-cylinder working process model

The in-cylinder working process module mainly includes combustion module, intake valve module, exhaust valve module and in-cylinder working process calculation module. The calculation simulation of each device is carried out, and the in-cylinder working process module is further integrated. The cylinder model of the ammonia fuel main engine can simulate the changing trend of engine performance parameters when pure diesel combustion is switched to ammonia-diesel dual fuel combustion, and the established in-cylinder working module is feasible to be applied to engineering prediction.

4 RESULTS

The multi-physics real-time model of ammonia fuel engine has high execution efficiency, good scalability and upgrade characteristics, can maintain stability during long-term independent operation, can output cylinder temperature and pressure characteristics, torque, power and speed characteristics of ammonia fuel main engine, ammonia fuel/oil fuel supply characteristics. Flue gas flow, composition and temperature characteristics, intake/exhaust system characteristics, lubricating oil system characteristics, cooling water system characteristics, etc. realize real-time monitoring of engine operating parameters.

Under a specified operating conditions, the speed variation curve of the engine starting process and the compressed air volume variation curve are illustrated in Figures 5~6. During air starting, compressed air is delivered into the cylinders to propel piston movement for diesel engine ignition. The air supply valve is closed once the engine reaches the starting speed, thereby validating the model's effectiveness through these curves. Figures 7~12. present the parameter variations during the engine operation from startup to stabilized target speed, including speed variation, power output, lubricating oil outlet temperature, high-temperature cooling water outlet temperature, in-cylinder pressure, and compressor outlet pressure. The data demonstrate that the dynamic responses of the integrated engine model and its subsystem parameters align with theoretical principles, confirming the model's validity. Consequently, this model exhibits excellent predictability by enabling continuous computation of results at each time step.

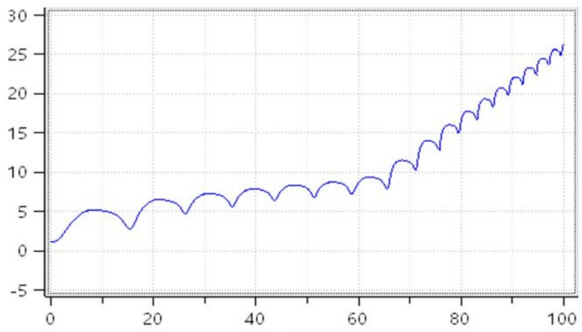

Figure 5. Start-up speed curve

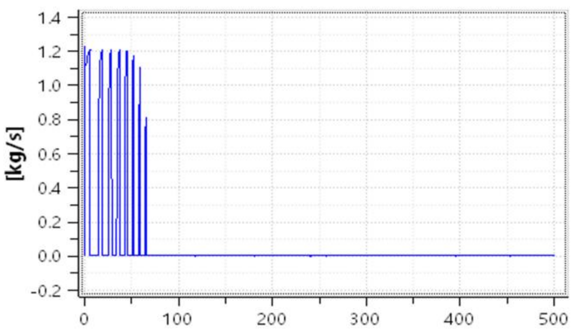

Figure 6. Compressed air flow curve during start-up

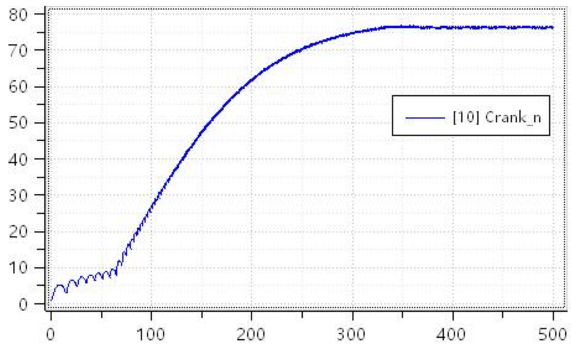

Figure 7. Engine speed change curve

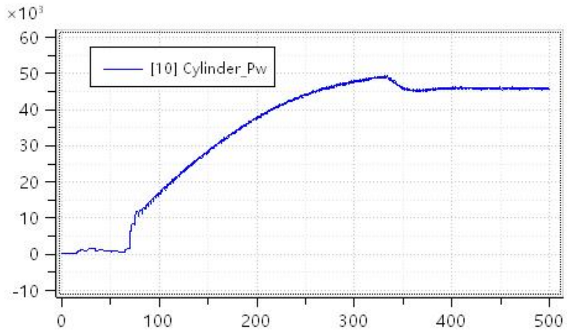

Figure 8. Engine power change curve

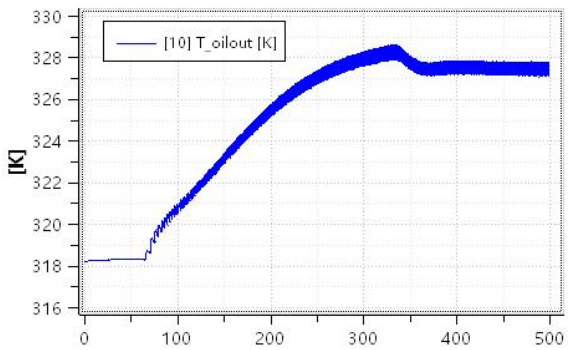

Figure 9. Oil outlet temperature curve

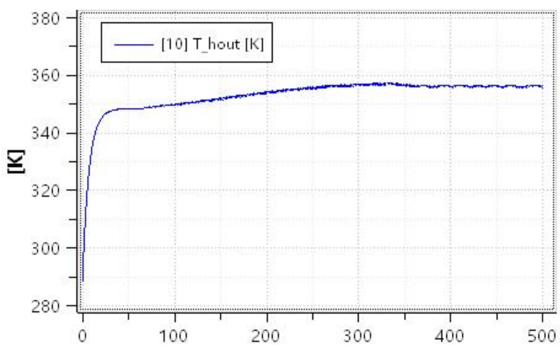

Figure 10. Cooling water outlet temperature curve

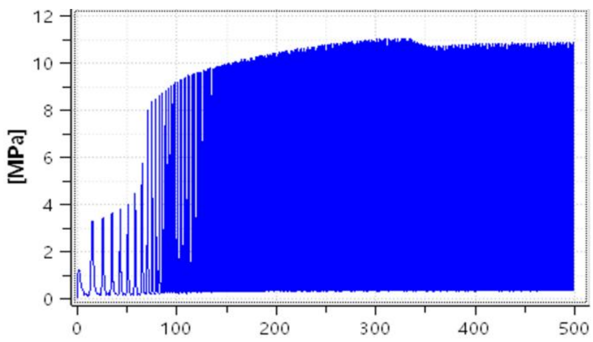

Figure 11. Cylinder pressure curve

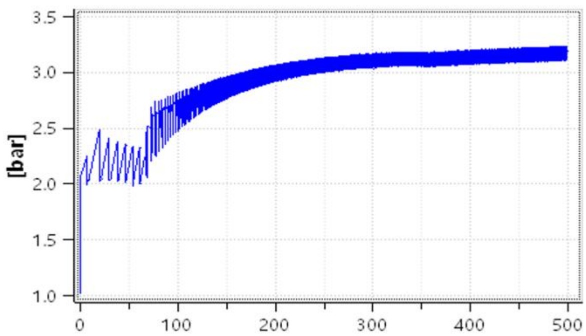

Figure 12. Compressor outlet pressure curve

5 CONCLUSIONS

(1) Marine engine digitalization is a technical solution developed for the future needs of Marine power operation and maintenance, aiming to break the traditional ship engine operation and fault diagnosis. Through the application of engine digitization, Marine engines can achieve efficient operation, safety and reliability, and agile response, promote the intelligent development of Marine power industry, and make positive contributions to the construction of a green and intelligent future Marine traffic system.

(2) Based on the research framework of Digital Engine, built a multi-physics real-time model of ammonia fuel engine based on Modelica language, and introduced the modeling principle of the in-cylinder reaction system, including combustion module, intake valve module, exhaust valve module and in-cylinder working process calculation module. The model has high execution efficiency, good scalability and upgrade characteristics, and can maintain stability during long-term independent operation.

(3) The complete multi-physics real-time model of ammonia fuel engine has relatively complete calculation functions, which can output the main calculation results of engine thermodynamics and dynamics, and has important application significance for engine performance prediction and optimization.

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