



## ORIGINAL RESEARCH

# Promoting digital twin technology application for process industry: A novel generation modelling platform and its implementations

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**Abstract**

One key concept of Industry 4.0 is the industrial digital twin (DT)—a virtual replica of physical assets, processes, and systems. DTs optimise operations, enhance productivity, and facilitate innovation across various industries, including manufacturing, energy, healthcare, and transportation. This paper presents a multi-domain and multi-time scale modelling and simulation platform, featuring built-in model libraries that represent diverse physical, chemical, and behavioural properties. A comprehensive system modelling approach and a closed-loop industrial control system based on DTs are developed, showcasing advanced control, optimisation, and system security research capabilities. The architecture and advantages of the novel generation modelling platform are detailed, with specific applications highlighted, underscoring its contributions to the process industry.

**KEYWORDS**

chemical engineering, control engineering, digital twins, electrical engineering, simulation

## 1 | INTRODUCTION

The advent of Industry 4.0 has ushered in an era of unprecedented connectivity, automation, and data-driven decision-making in the industrial landscape.<sup>1,2</sup> At the heart of this transformation lies the concept of the industrial digital twin (DT)—a virtual replica of physical assets, processes, and systems.<sup>3</sup> Industrial DTs have emerged as powerful tools for optimising operations, enhancing productivity, and facilitating innovation across various industries, ranging from manufacturing and energy to healthcare and transportation.<sup>4</sup>

The idea related to DTs was first introduced around the 1960s when NASA started using computer modelling and simulation to create virtual models of physical entities as ‘living models’ of the Apollo mission. The first definition of DT

appeared in 2003 when Michael Grieves presented a study of Product Lifecycle Management: A DT is a digital information structure of a physical system that creates itself as an entity and is associated with the physical system.<sup>5,6</sup> Since then, it has evolved into a versatile technology with applications in diverse domains.<sup>7</sup> A DT encompasses both the physical aspects of an asset or system and its virtual representation, which is continuously updated with real-time data from sensors, IoT devices, and other sources.<sup>8</sup> By bridging the gap between the physical and digital realms, DTs enable organisations to gain deep insights into the behaviour, performance, and condition of their assets, thereby enabling proactive maintenance, predictive analytics, and scenario simulation.<sup>9</sup>

A key component of industrial DTs is the underlying platform that supports their development, deployment, and

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management.<sup>10</sup> DT platforms serve as the foundation for creating and operating DT, providing tools and capabilities for data integration, modelling, simulation, visualisation, and analysis. These platforms typically leverage advanced technologies such as cloud computing, big data analytics, artificial intelligence (AI), and machine learning to deliver scalable, robust, and intelligent solutions. The workflow and architecture of DT platforms and the interaction mechanisms among their core functionalities have been investigated and described by several studies that aimed to standardise DT architectures.<sup>11,12</sup>

In recent years, many world-leading technological companies, including Ansys, AVEVA, Dassault, and Siemens, have actively invested in developing DT platforms tailored to specific industries and use cases. These platforms offer a wide range of features and functionalities, such as virtual modelling and simulation, data ingestion and processing, real-time monitoring and control, predictive maintenance, and collaborative workflow management. Moreover, they are designed to integrate seamlessly with existing information technology and operational technology systems, enabling organisations to leverage their existing infrastructure and investments. Ansys Twin Builder software leverages emulation models to serve as DTs of real technical objects, facilitating a two-way communication in the field of cars and batteries.<sup>13</sup> AVEVA emphasises the necessity for next-generation software to adopt a novel approach in establishing, parameterising, initialising, and solving equation-based simulation models.<sup>14</sup> A prime example of this is AVEVA process simulation, which is primarily tailored for chemical engineers, highlighting its specialised development in this domain.<sup>15</sup> The 3DEXPERIENCE platform of Dassault Systemes features an integrated mathematical modelling application known as Dymola, which enables the resolution of intricate multi-domain system modelling and analysis tasks.<sup>16,17</sup> Siemens Mindsphere drives IoT solutions by harnessing advancements in analytics and AI, enabling the collection of data from connected products, systems, and plants—from the edge to the cloud.<sup>18,19</sup>

Although an increasing number of DT platforms are being developed and launched, most of them have merely focused on a limited number of dimensions or functionalities, hence failing to meet the comprehensive requirements of a commercial multi-timescale DT platform. Further, enabling tools or platforms in related industries often create closed software ecosystems around their respective product systems. This isolation hinders interactions between different tools and platforms, leading to challenges such as difficulties with model or data integration, poor collaboration, compatibility issues, and high usage costs. Motivated by these challenges and requirements, this work attempts to develop a non-causal language-based DT platform that spans multiple time scales, domains and platforms. The main technical contributions made in this work can be summarised as follows:

1. A multi-domain and multi-time-scale modelling and simulation platform have been developed. Its built-in model

libraries cover various industries, effectively representing the physical, chemical, and behavioural characteristics of thermal, electrical, fluid, and mechanical properties across multiple domains. On the other hand, industrial systems such as power systems may simultaneously encompass electromagnetic transients on the microsecond level, electromechanical transients on the millisecond level, and fluid thermal processes on the minute level. The novel generation modelling (NGM) platform is capable of designing and operating models across these diverse time scales within the same system, which underscores its multi-time-scale feature.

2. A comprehensive system modelling approach has been proposed. By employing hybrid modelling and model integration at the granularity of individual equipment units, along with model validation and modification steps, a high-precision DT dynamic modelling system is constructed.
3. A closed-loop industrial control system based on DT models and real control systems has been developed. The model system constructed using DT forms a closed loop with the real control system through I/O mapping technology, accurately replicating the actual operation of the real industrial control system, which can be applied to investigate advanced control, optimisation, and system security research.

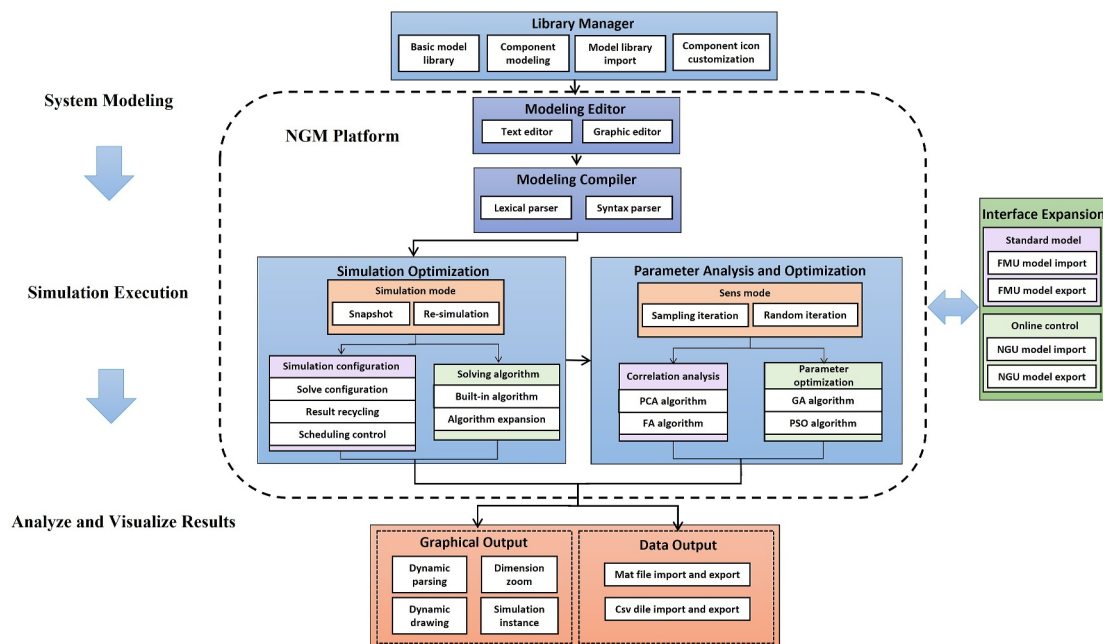
The remainder of this paper is organised as follows: Section 2 describes the architecture, purposes and advantages of the DT platform NGM. The modelling approach of the proposed platform is reported in Section 3. In Section 4, two specific DT applications in various fields using NGM are presented. Finally, Section 5 provides the conclusion.

## 2 | NOVEL GENERATION MODELLING PLATFORM

### 2.1 | Overall architecture

NGM is a multi-domain and multi-time scale DT modelling and simulation platform based on an open-source modelling language Modelica.<sup>20</sup> It is a complete platform for modelling, simulation, control, and optimisation for complex industrial systems, including chemical processes, electrical processes, and utility systems. NGM mainly consists of eight functional modules: NGM Editor, NGM Compiler, NGM Parameter analysis and optimisation, NGM Simulator, NGM FMI2.0,<sup>21</sup> NGM NGU, NGM Model Library Manager, and NGM Graphical Processor, as shown in Figure 1.

The overall architecture design diagram shows the interaction mode and functional division between each module, providing the system with good scalability and maintainability. Specifically, the entire industrial modelling process is divided into three stages: system modelling, simulation execution, and results analysis and visualisation stage. The first stage includes fundamental functions such as modelling editing, modelling analysis, and gallery editing. During the second stage, the system carries out simulation optimisation and parameter analysis



**FIGURE 1** NGM overall architecture. NGM, novel generation modelling.

and optimisation to ensure precise simulation execution. Finally, the system analyses the simulation results and presents them to users through graphical and data outputs. Additionally, the system features the NGM interface expansion block, which allows users to import standard models developed with other software and export models as NGU files.

## 2.2 | Advanced properties of NGM

### 2.2.1 | User-friendly modelling language

In the industrial modelling domain, imperative programming languages such as C/C++ and Fortran are prevalent in existing modelling software.<sup>22</sup> These languages typically intertwine model equations with the solution methods, integrating the solution procedures directly into the model equations. This integration can impose constraints on the models' applicability and scalability. In contrast, using differential algebraic equations (DAEs) in conjunction with a universal solver enhances the reusability,<sup>23,24</sup> transparency,<sup>25</sup> and accuracy<sup>26</sup> of models. By decoupling the equations from the solution methods, this approach allows for more flexible and scalable modelling practices.

Modelica is an open-source, object-oriented, equation-based computer language designed to facilitate the modelling of complex physical systems across various domains. Baharev and Neumaier<sup>27</sup> proposed the possibility of benchmarking commercial software such as Aspen Plus, Aspen Hysys, and ChemCAD by using Modelica for chemical process modelling. Nayak et al.<sup>28</sup> expanded on this idea by developing commonly used chemical engineering models in Modelica and validating their accuracy through comparative simulations with Aspen

Plus and DWSIM. Beyond chemical processes, Modelica is also used to investigate other industrial processes, including electrical engineering, public engineering, and nuclear power systems.<sup>20,29,30</sup> In this context, NGM aims to provide users with a superior Modelica compilation tool that translates Modelica language-based models into C machine code. This tool enhances the usability and performance of Modelica models across various industrial applications.

In the NGM text editor, users can directly develop models using the Modelica language, as depicted in Figure 2. Beyond text-based programming, NGM also supports graphical programming, which visually presents the programme structure and logic, as shown in Figure 3. This visual approach allows users to see the structure and parameters of the model, enhancing readability and modifiability. Compared to traditional text-based programming, the visual approach reduces the learning curve, making it particularly suitable for engineers and researchers to get started quickly. The graphical interface enables users to decompose complex systems into multiple sub-models and build the overall model by connecting these modules. This not only improves programming efficiency but also enhances the reusability and scalability of the models, facilitating rapid iteration and optimisation. Overall, the NGM platform is versatile and applicable across multiple fields. It significantly improves development efficiency and reduces error rates, making it a powerful and practical modelling and simulation platform.

### 2.2.2 | Powerful solver

A powerful solver is at the core of a DT platform. NGM effectively handles both rigid and non-rigid, linear and non-

```

Library Browser
Model Name..
Examples
PumpingSystem
Medium
HeatingSystem
DrumBoiler
Tanks
ControlledTankSystem
AST_BatchPlant
Incompres...idNetwork
BranchingDynamicPipes
NonCircularPipes
HeatExchanger
TraceSubstances
Explanatory
...

86 Modelica.Blocks.Continuous.FirstOrder PT1(
87   T=2,
88   InitType=Modelica.Blocks.Types.Init.InitialState,
89   y_start=0)
90   annotation (Placement(transformation(extent={{40,60},{60,80}})));
91
92   Inner Modelica.Fluid.System system(energyDynamics=Modelica.Fluid.Types.Dynamics.FixedInitial)
93     annotation (Placement(transformation(extent=
94       {{60,-96},{80,-76}})));
95   equation
96   connect(userValve.port_b, sink.ports[1]) annotation (Line(points={{74,-30},
97     {77,-30},{77,-28},{80,-28}}, color={0,127,255}));
98   connect(source.ports[1], pumps.port_a) annotation (Line(points={{-80,-70},{
99     -74,-70},{-68,-70}}, color={0,127,255}));
100  connect(valveOpening.y, userValve.opening) annotation (Line(points={{77,10},{
101    98,10},{98,-12},{66,-12},{66,-23.6}}, color={0,0,127}));
102  connect(RelativePressureSetPoint.y, controller.reference)
103    annotation (Line(points={{
104    -79,70},{-60,70},{-60,76},{-42,76}}, color={0,0,127}));
105  connect(controller.y, PumpRPMGenerator.u)
106    annotation (Line(points={{-19,70},{-2,70}}, color={255,0,255}));
107  connect(reservoirPressure.p_rel, controller.u) annotation (Line(points={{20,
108    -13},{20,50},{-52,50},{-52,64},{-42,64}}, color={0,0,127}));
109  connect(reservoirPressure.port_b, sink.ports[2]) annotation (Line(
110    points={{30,-22},{44,-22},{44,-48},{80,-48},{80,-32}},
111    color={0,127,255},
112    pattern=LinePattern.Dot));
113  connect(PumpRPMGenerator.y, PT1.u)
114    annotation (Line(points={{21,70},{38,70}}, color={0,0,127}));
115  connect(PT1.y, pumps.N_in) annotation (Line(points={{61,70},{74,70},{74,30},{

```

FIGURE 2 Novel generation modelling text editor.

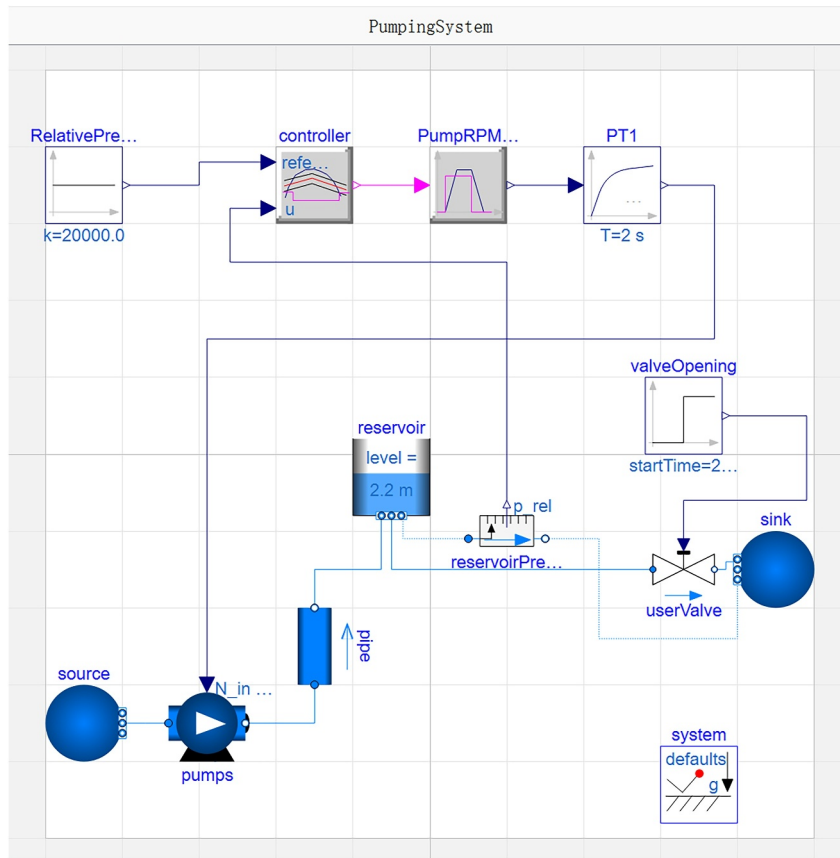
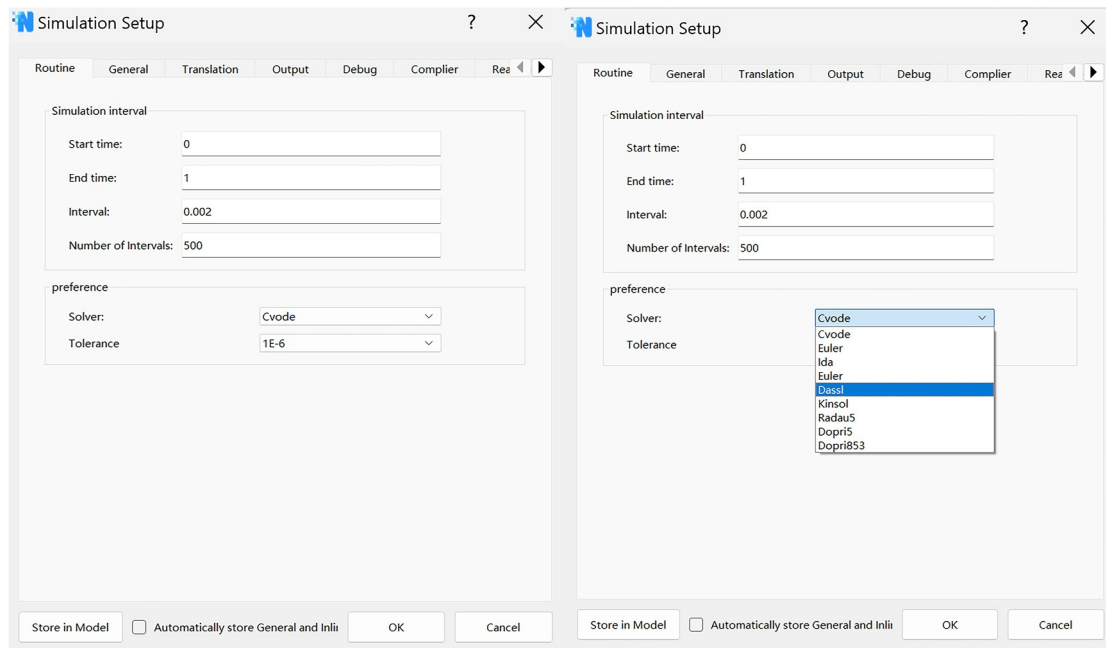


FIGURE 3 Novel generation modelling graphic editor.

linear DAE systems. DAE systems can be categorised into algebraic equation groups and ordinary differential equation (ODE) groups, with Kinsol managing the algebraic equations and Ccode handling the ODEs, as shown in Figure 4.

To address the challenges posed by varying orders of magnitude in data, the solver employs data scaling. Initial values are estimated using nominal values, enabling the handling of a wide range of DAE systems. Additionally, the





**FIGURE 4** Novel generation modelling solver.

solver simplifies problem-solving by requiring only the step size and solving time to be set, without needing to configure the Jacobian matrix of DAE or ODE systems. The solver's capability to partition large DAE systems into multiple smaller blocks for sequential solving helps minimise memory consumption and computing time. This makes it a robust and efficient tool for managing complex DAE systems.

### 2.2.3 | Snapshot

In practical industrial control systems (ICS), an NGU sequence represents a complete production line, with each piece of equipment within the line corresponding to the functional mock-up unit (FMU) instance. During the actual control of sequence operations, the following scenarios may occur: reaching a stable operating condition or a user-desired condition can be time-consuming, requiring the system to quickly restore data to achieve the desired state of sequence operation. Additionally, if the NGU sequence crashes due to extreme operations, the system should be able to restore data to a useable state at a specific time point, ensuring the normal operation of the sequence.

To address these issues, we developed NGU sequence operation snapshots, and users can use the NGU snapshot manager to download, execute, and store snapshots, as illustrated in Figure 5. A snapshot stores all valuable data of the sequence operation at a particular moment. Based on these snapshots, users can quickly achieve condition recovery, switching, extrapolation, and backtracking. This functionality

ensures efficient and reliable control of the production line, even under adverse conditions.

### 2.2.4 | NGU and online control

While applying digital-twins technologies into industrial processes, model exchange and co-simulation are widely employed to allow various models or subsystems of a coupled problem to be simulated in distributed methods.<sup>31</sup> The functional mock-up interface (FMI) is a tool-independent standard for the exchange of dynamic models and co-simulation as well.<sup>32</sup> FMI is successfully adopted by more than 160 popular industrial simulation tools, including Ansys, Matlab, as well as UWintechPro. NGM strictly adheres to the FMI standard and supports virtual electronic control units, advanced co-simulation, and intelligent hybrid models based on both mechanistic and data-driven approaches. By involving the FMI standard, models built on NGM can be exported as FMUs for use in other software platforms, and vice versa. This promotes the flexibility and adaptability of the NGM DT platform and its models.

Building upon the FMU, the NGM platform also incorporates an event scheduling mechanism, defining the serialisable scheduling model units NGU module that follows the IEC 61499 standard. Through the NGU module, seamless online control can be achieved by integrating with the professional control engineering application software platform UWintechPro, as shown in Figure 6. Additionally, the concept of distributed control is introduced, enabling control tasks distributed across different devices or network nodes to be realised through the combination of function blocks and

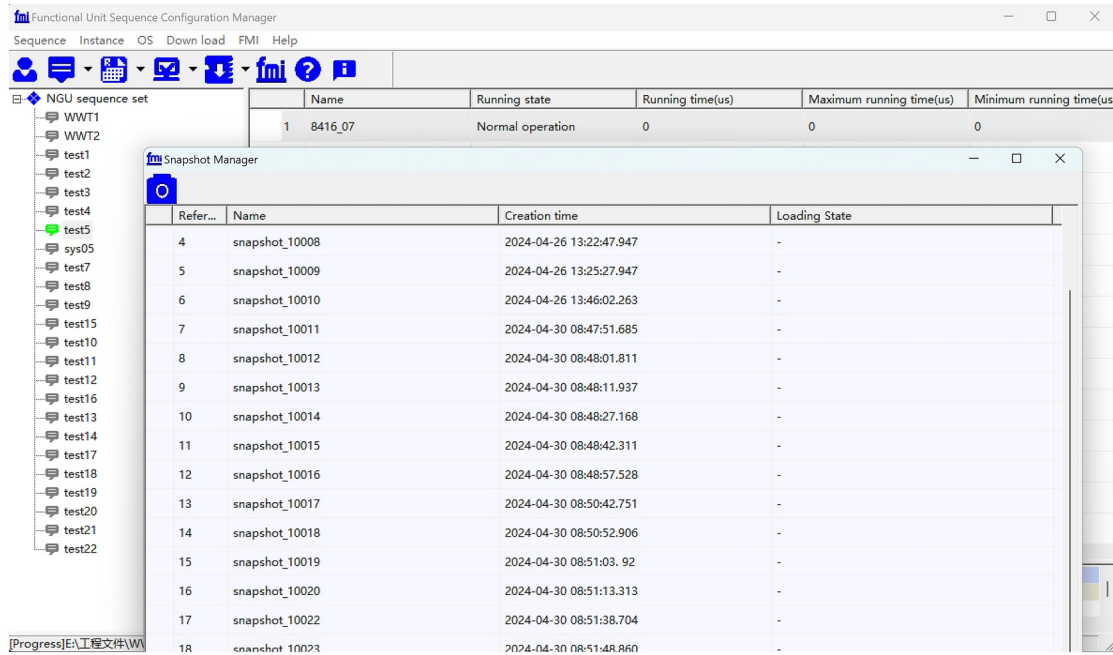


FIGURE 5 Novel generation modelling snapshot manager.

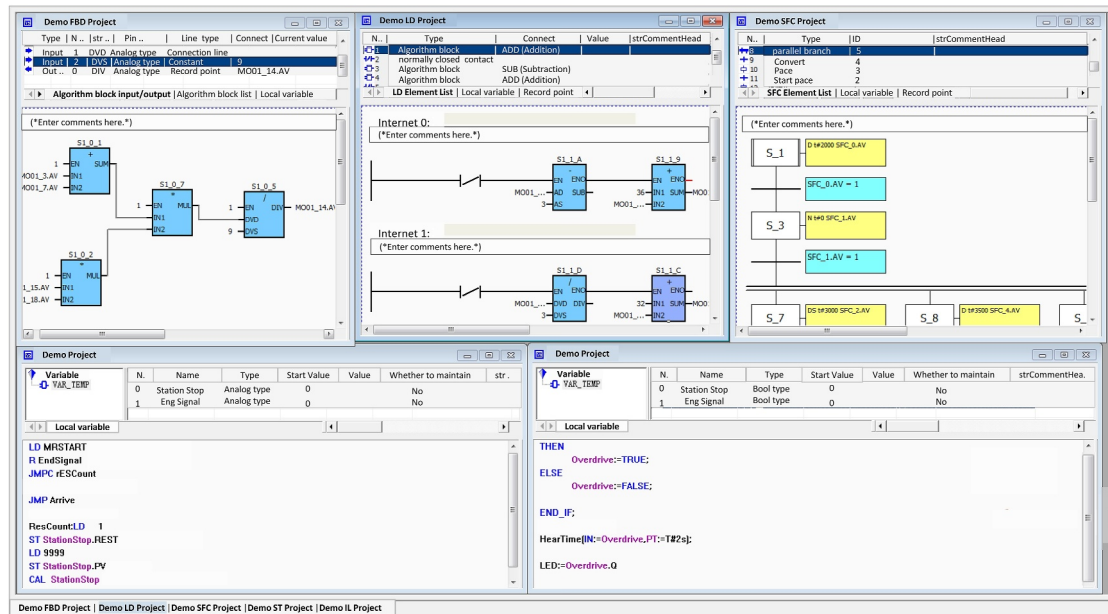


FIGURE 6 Novel generation modelling online control.

events. This approach provides a high degree of freedom in control computation and addresses complex problem-solving requirements.

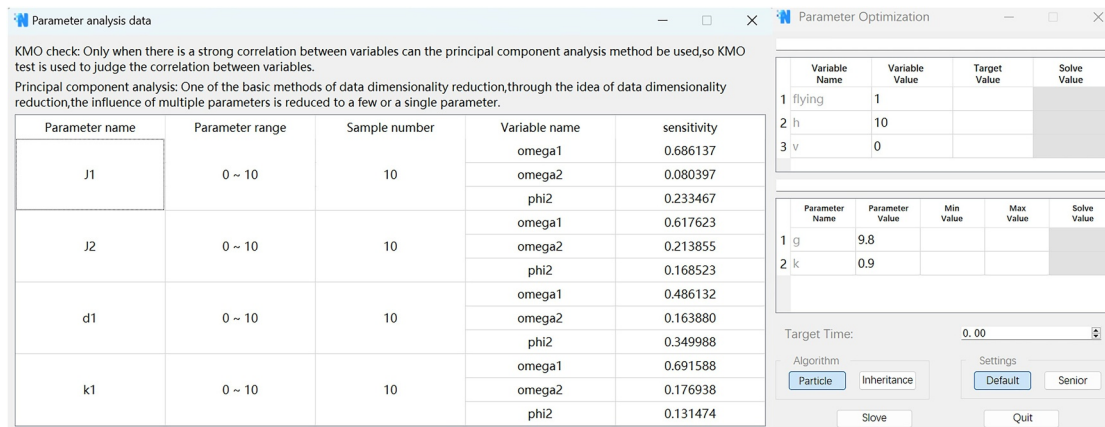
### 2.2.5 | Parameter analysis and optimisation

The NGM platform facilitates comprehensive parameter analysis and optimisation of all variables involved in the model, helping users gain a deep understanding of system behaviour,

optimise design solutions, predict performance outcomes, reduce costs, and enhance work efficiency, as shown in Figure 7.

For parameter analysis, the NGM platform provides algorithms, for example, principal component analysis and factor analysis. These tools offer several advantages in the field of modelling and simulation:

1. Deeper system understanding: By analysing how a system responds to changes in various parameters, users can uncover underlying behavioural patterns and system characteristics.



**FIGURE 7** Novel generation modelling parameter analysis and optimisation.

This insight is crucial for identifying key factors that influence system behaviour and performance.

2. Performance assessment: Parameter analysis allows users to assess the impact of different parameter values on system performance. By quantifying these effects, users can optimise design choices, leading to improved system efficiency, stability, and reliability.
3. Predictive capability: By simulating various scenarios and analysing parameter interactions, users can predict system performance under different operating conditions. This proactive approach helps anticipate potential issues and implement measures to address them, ensuring the system meets performance expectations and operates effectively in real-world settings.

For parameter optimisation, the NGM platform offers heuristic algorithms such as genetic algorithm and particle swarm optimisation. These algorithms provide several benefits:

1. Optimal parameter search: It can help users find the optimal parameter combination in the design space to meet specific performance indicators or constraints, achieving optimal system performance.
2. Automation and efficiency: These algorithms can automate parameter adjustments and optimisations, saving manpower and time, and enhancing work efficiency, especially for complex systems.
3. Multi-objective optimisation: It can simultaneously consider multiple objective functions, assisting users in balancing various performance metrics and achieving comprehensive system design optimisation.
4. Enhanced robustness: These algorithms improve the system's robustness, enabling better adaptability to parameter variations and external disturbances, thereby enhancing system stability and reliability.

In summary, parameter analysis and optimisation are crucial in the process of system design and optimisation. Parameter analysis aids in system understanding and efficiency

evaluation, while parameter optimisation helps users find optimal solutions, automate adjustments, and enhance system robustness. The combination of both guides more effective system design and optimisation efforts.

### 3 | MODELLING METHOD

Model-based system engineering (MBSE) represents a pivotal component within the broader shift towards model-centric methodologies embraced across various industrial engineering disciplines. This paradigm shift highlights the increasing importance of comprehensive models in driving efficiency, precision, and innovation within engineering practices.<sup>33</sup> By integrating MBSE, NGM emphasises the development of DT models that accurately represent the physical, behavioural, and chemical attributes of systems. Additionally, MBSE fosters seamless communication and collaboration among stakeholders using the system model as the definitive source of truth.

This section discusses the modelling of unit equipment, subsystems, and systems, as well as the validation of these systems using NGM:

1. Unit-equipment hybrid modelling: NGM supports the creation of hybrid models that combine the physical, behavioural, and chemical attributes of individual equipment units. This approach ensures a detailed and accurate representation of each piece of equipment within the system.
2. Model integration: NGM facilitates the seamless integration of these unit-equipment models into larger subsystems and full systems. This integration ensures that all components work together harmoniously, reflecting the complex interactions within the real-world system.
3. Model validation: NGM provides robust tools for validating models through comprehensive testing and simulation. This validation process ensures that the models accurately represent real-world systems, providing reliable data for decision-making and performance predictions.

4. Model modification: NGM allows for easy modification of models to reflect changes in design, operation, or environmental conditions. This flexibility ensures that the models remain up-to-date and continue to provide accurate and useful insights throughout the lifecycle of the system.

By integrating MBSE principles into the NGM platform, engineers can easily develop accurate and comprehensive DT systems, enhancing system design and control, improving operational efficiency, and fostering innovation.

### 3.1 | Unit-equipment hybrid modelling

Models of unit equipment in process industries are typically classified into two categories: rigorous mechanistic models and surrogate models. Rigorous mechanistic models are primarily based on fundamental principles such as conservation laws, thermodynamics, kinetics, fluid dynamics, and particle properties. These models accurately represent process characteristics and laws, offering excellent interpretability and extrapolation capability. On the other hand, surrogate models are mainly constructed based on the process data and machine learning algorithms. They offer advantages such as low computational complexity, fast solution speed, and high accuracy within the range of the model's establishment data.

Although rigorous mechanistic models have been extensively studied in the modelling and optimisation of process industrial systems, their complexity and the high cost of establishing complete models can be significant due to the strong coupling, non-linearity, and high dimensionality inherent in such systems. In addition, the significant computational effort required for these models is a challenge. Conversely, while surrogate models have been widely applied in industrial process modelling and optimisation, their poor interpretability, lack of physical meaning, and limited extrapolation capability hinder their reliability in process simulation and control optimisation.

To leverage the strengths of both rigorous mechanistic models and surrogate models, a hybrid modelling approach is advisable. Encouraged by the advantages of this approach, the following steps can be taken:

1. Develop mechanistic models: Initially, develop mechanistic models based on fundamental principles such as reaction kinetics, thermodynamics, fluid mechanics, and mass and heat transfer.
2. Data collection and preprocessing: Collect historical or real-time data from the distributed control system (DCS) system and perform data preprocessing tasks, including data cleaning, data integration, data reduction, and data transformation.
3. Integrate AI algorithms: Use AI algorithms to inject the preprocessed process data into the mechanistic models. Analyse the effects of different AI methods and hybrid structures on the performance of process unit models.

4. Iterate and optimise: Repeat the aforementioned steps for each unit-equipment, continually refining the models to improve accuracy and reliability.
5. Form model libraries: Organise these models into libraries for different process systems, providing a comprehensive resource for future modelling and optimisation efforts.

Through the appropriate incorporation of both rigorous mechanistic models and surrogate models, this hybrid approach can enhance the reliability, efficiency, and scalability of process simulations and control optimisations in industrial settings.

### 3.2 | Model integration

After developing the unit-equipment model libraries, the challenge lies in integrating these unit models into a subsystem or system. NGM addresses this by adopting a multi-level inheritance approach, configuring parameters, and associating combinations of basic unit-equipment-level models from the bottom up.

Firstly, subsystem-level models are developed using a combination of encapsulation and drag-and-drop modelling methods based on the unit-equipment-level models. These subsystem-level models are then integrated into the target system according to the system's topology, thereby achieving system-level model integration, as illustrated in Figure 8.

### 3.3 | Model validation

Model validation is crucial for ensuring that simulation models accurately reflect real-world systems, thereby achieving functional effectiveness and consistency with requirements. This process is essential to ensure that DT models faithfully represent actual systems.

The most common method for model validation involves comparing the simulation results with actual process data or experimental data. However, challenges arise when testing scenarios cannot cover all possible conditions or when it is difficult to comprehensively test certain typical scenarios. These difficulties can make testing hard to control, limiting the ability to effectively and incrementally improve models. Additionally, specific testing tasks can be hard to replicate and are time-consuming and costly.

To address these challenges, validation can also be performed using professional simulation software, industrial design parameters, and industrial process operation data. This approach includes validating both steady-state working points and the dynamic response processes between different steady states. By utilising these additional methods, the validation process can be more comprehensive and efficient.

As shown in Figure 9, NGM supports four types of data to validate models which are historical/real-time data, experimental data, industrial design parameters, and professional software simulation data. We categorise these into two groups:



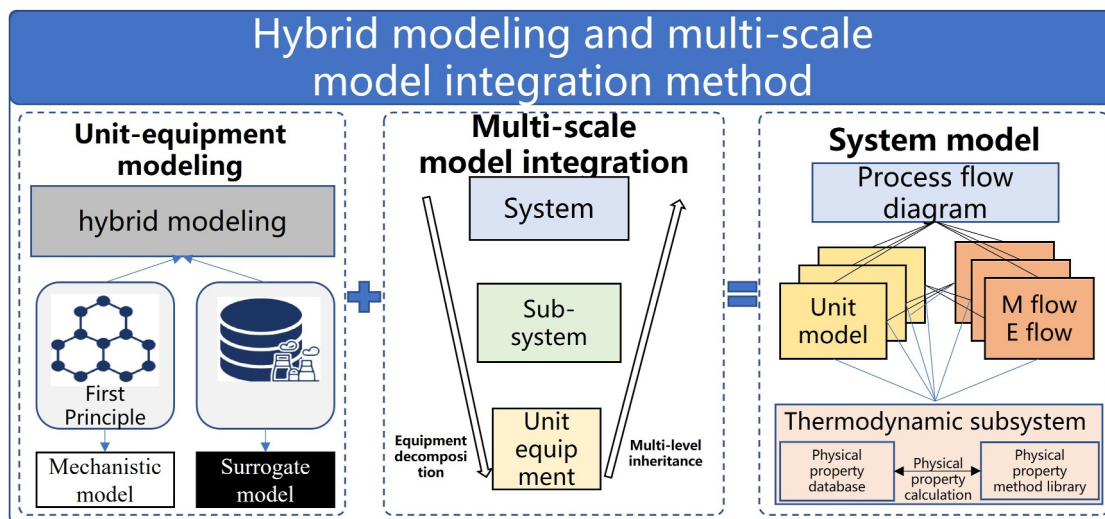


FIGURE 8 Proposed modelling and integration method.

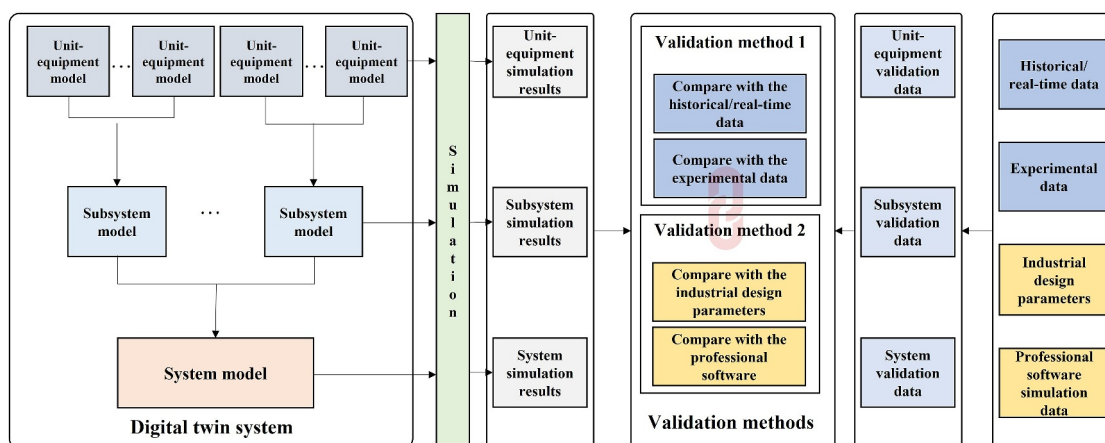


FIGURE 9 Model validation method.

Method 1, based on historical/real-time data and experimental data, is prioritised over Method 2, based on industrial design parameters and professional software simulation data. Users can input their available validation data and specify the data type. Based on the provided data, NGM can automatically select the appropriate method for model validation. This allows users to easily validate models at different scales and evaluate them reasonably.

Once validated, the models can also serve as a benchmark for comparison and validation on other platforms, ensuring consistency and reliability across different environments.

### 3.4 | Model modification

Although actual process data are involved in DT hybrid modelling, unacceptable deviations between the DT models and the actual systems can still occur due to factors such as equipment ageing and process variation. In such cases, model

modification becomes essential to ensure the accuracy of DT models throughout their lifecycle.

The NGM system compares the output of the DT with preprocessed historical records and real-time data streams from the actual industrial equipment to identify deviations, as shown in Figure 10. Using model parameter sensitivity analysis techniques, we identify sensitive parameters. Based on machine learning methods and process expertise, we devise online modification strategies and correction algorithms. These strategies activate the online modification algorithms based on data such as relative deviations. Our platform supports state-of-the-art modification algorithms, including MLP, GCU, LSTM, DNN, RNN, and Transformer. Additionally, we promote the Transformer encoder architecture and developed a new data-driven model called the RP-based channel attention transformer encoder (RP-CATE), designed to generate correction factors for sensitive parameters. Specifically, we first design an RP module to capture the correlation between different samples of the input. Next, a channel attention module is introduced to

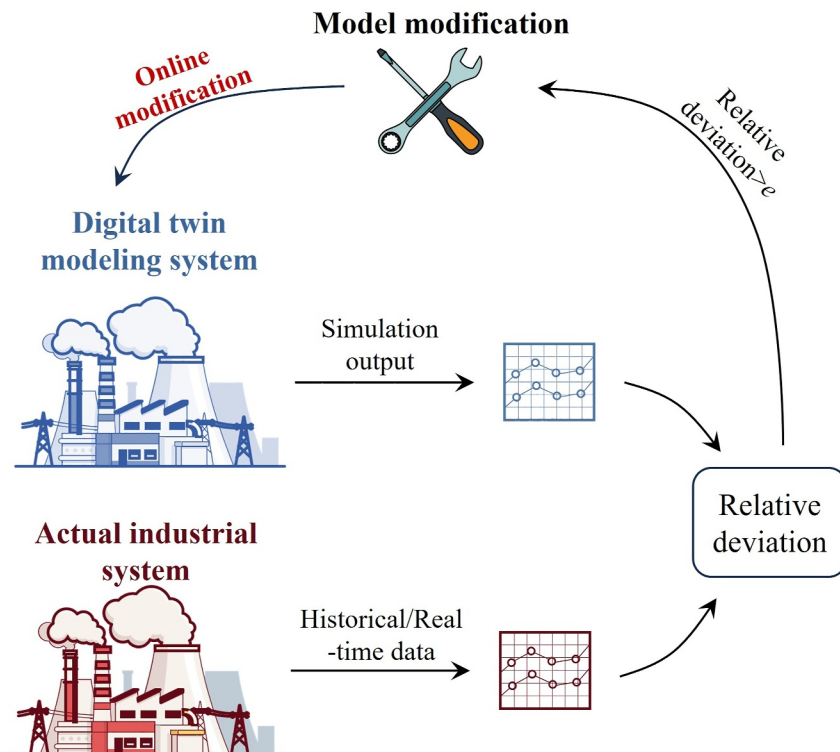


FIGURE 10 Model modification.

generate corresponding attention weights based on the varying contributions of different features of the same sample to the target value. Subsequently, a feedforward module is applied to produce the output of RP-CATE. Finally, a linear transformation is employed to obtain the correction factor of the sensitive parameters. In this way, effective model modifications and adjustments can be achieved.

## 4 | DT APPLICATIONS BASED ON NGM

### 4.1 | CDU of a 10-million-ton refinery

The crude oil distillation unit (CDU), as the primary unit in the refining process, serves as the primary source of raw materials for all refining units. Through an analysis of the process flow diagram (PFD) and pipe and instrument diagram (P&ID) of an actual 10-million-ton refinery's CDU system, we can partition the CDU system into 3 subsystems and 28 unit-equipment components. Initially, 28 unit-equipment models are developed using a hybrid modelling approach and subsequently validated with process data. These unit-equipment models are then integrated into the subsystem models and the overarching system model. Finally, the DT CDU system model undergoes validation in conjunction with a real DCS utilising input/output mapping technology. Through this closed-loop DT-based control system, we can engage in process simulation, control, and optimisation as well as testing for cyberspace attacks and defenses.

#### 4.1.1 | Unit equipment model—Distillation column

Taking the distillation column, the most critical separation equipment in the CDU, as an example, the characteristic parameters of this model are meticulously designed based on the underlying mechanisms. These parameters are detailed in Table 1.

The top column diagram of the distillation column is depicted in Figure 11, where the top section comprises a condenser and a reflux drum. When the vapour mixture reaches the top of the column, it undergoes condensation in the condenser. A portion of the condensed liquid is withdrawn as the top product, while the remaining portion is returned to the rectification column as reflux liquid to support the distillation process. In the proposed design, the top section of the column is considered as the first tray of the rectification column.

The material balance equation for the top section of the column can be described by

$$\frac{dM_D}{dt} = V_R - L_R - D \quad (1)$$

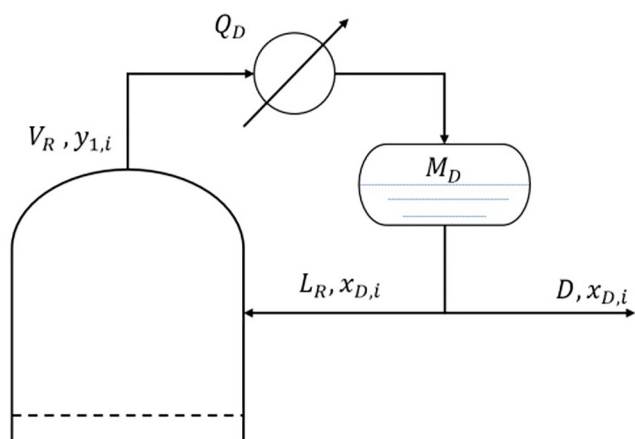
$$\frac{d(M_D \cdot x_{D,i})}{dt} = V_R \cdot y_{1,i} - L_R \cdot x_{D,i} - D \cdot x_{D,i} \quad (2)$$

The phase equilibrium equation:

$$y_{1,i} = k_{1,i} \cdot x_{D,i} \quad (3)$$

**TABLE 1** Distillation column model.

Number	Name	Symbol	Unit
1	Number of components	Nc	
2	Component list	C[Nc]	
3	Boiling point temperature of components	Tb[Nc]	K
4	Column top pressure	P1	MPa
5	Column bottom pressure	PN	MPa
6	Number of trays	Np	
7	Feed tray	Fp	
8	Number of side streams	Ns	
9	Side stream tray(s)	Sp[Ns]	
10	Side stream molar flowrate	Sopt[Ns]	
11	Liquid load on tray	M	mol
12	Liquid load of condenser	M0	mol
13	Liquid load in reboiler	MN	mol
14	Feed molar flowrate	F	mol/s
15	Feed molar composition	x <sub>F</sub> [Nc]	1
16	Feed temperature	TF	K
17	Feed pressure	PF	MPa
18	Vapourisation ratio of feed	e	1
19	Reflux ratio	RR	
20	Bottoms rate	W	mol/s
21	Distillate rate	D	mol/s
22	Condenser heat duty	Q <sub>c</sub>	W
23	Boil-up ratio	BR	1
24	Reboiler heat duty	Q <sub>b</sub>	W
25	Distribution of temperature	T[Np]	K
26	Distribution of pressure	P[Np]	MPa
27	Liquid molar composition	x[Np,Nc]	1
28	Gas phase molar composition	y[Np,Nc]	1



**FIGURE 11** The schematic diagram of the top column.

The summation equation for mole fraction normalisation:

$$\sum x_{D,i} = 1 \tag{4}$$

$$\sum y_{1,i} = 1 \tag{5}$$

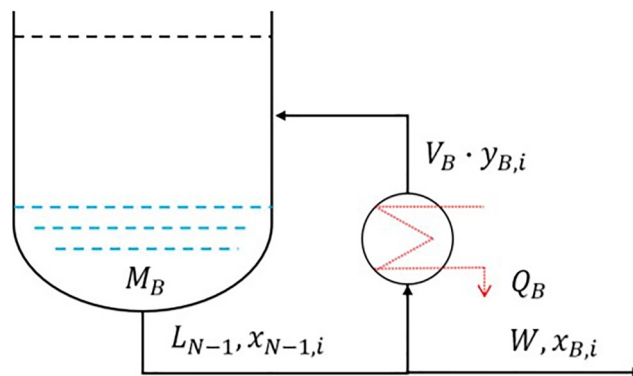
The heat balance equation:

$$\frac{dM_D \cdot (h_l)_D}{dt} = Q_D + L_R \cdot (h_l)_1 - V_R \cdot (h_v)_D - D \cdot (h_l)_D \tag{6}$$

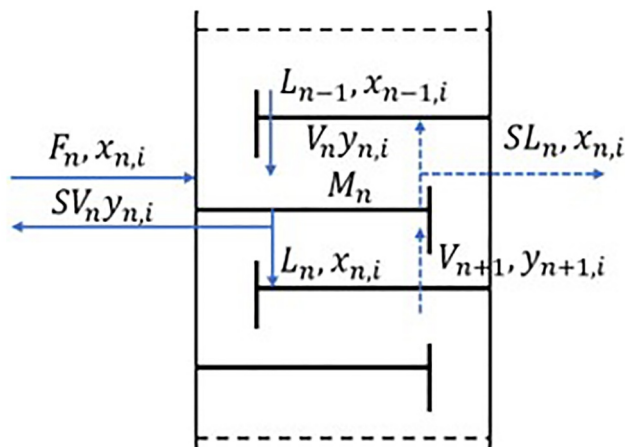
Similarly, the bottom column diagram of the distillation column is depicted in Figure 12. The bottom section comprises a vessel and a reboiler. A portion of the liquid is distilled as the bottom product, while the remainder is heated in the reboiler and vapourised into rising steam, providing heat for the distillation process. In this design, the bottom section is regarded as the last tray of the distillation column.

The material balance equation for the bottom section of the column can be described by

$$\frac{dM_B}{dt} = L_{N-1} - V_B - W \tag{7}$$



**FIGURE 12** Schematic diagram of the bottom column.



**FIGURE 13** The schematic diagram of the trays.

$$\frac{d(M_B \cdot x_{B,i})}{dt} = L_{N-1} \cdot x_{N-1,i} - V_B \cdot y_{B,i} - W \cdot x_{B,i} \quad (8)$$

The phase equilibrium equation:

$$y_{B,i} = k_{B,i} \cdot x_{B,i} \quad (9)$$

The summation equation for mole fraction normalisation:

$$\sum x_{B,i} = 1 \quad (10)$$

$$\sum y_{B,i} = 1 \quad (11)$$

The heat balance equation:

$$\frac{dM_B \cdot (h_l)_B}{dt} = Q_B + L_{N-1} \cdot (h_l)_{N-1} - V_B \cdot (h_v)_B - W \cdot (h_l)_B \quad (12)$$

Lastly, the schematic diagram of the trays is shown in Figure 13. As the vapour phase ascends through the rectification section, the lighter components in the vapour phase are continuously purified, leading to an increasing concentration of light components in the vapour phase and yielding light component products at the column top. In the stripping section, the liquid phase moves towards the bottom vessel under the influence of gravity, with lighter components continuously transferring from the liquid phase to the vapour phase, resulting in a concentration of heavy components, ultimately producing heavy component products at the bottom vessel.

The material balance equation for each tray can be described by

$$\frac{dM_n}{dt} = L_{n-1} + V_{n+1} + F_n - L_n - V_n - SL_n - SV_n \quad (13)$$

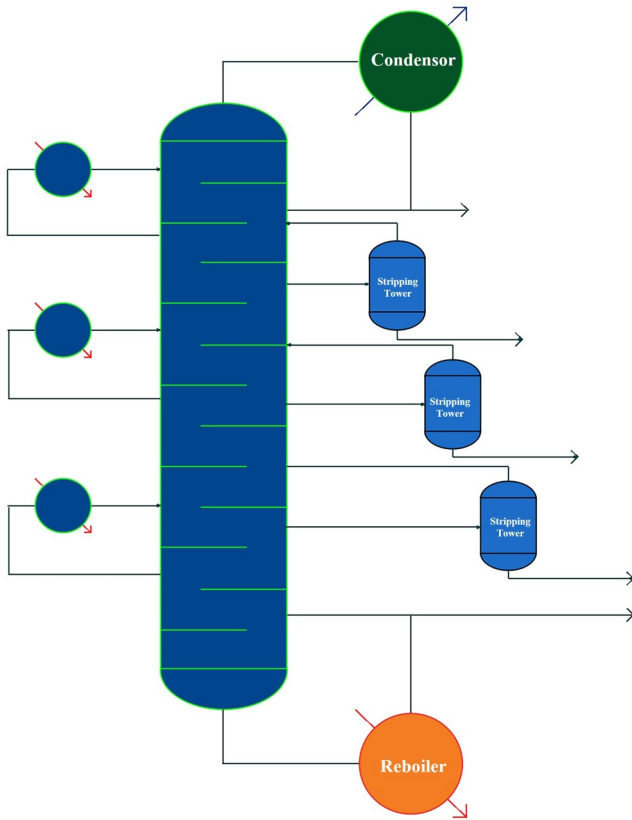


FIGURE 14 Distillation column model.

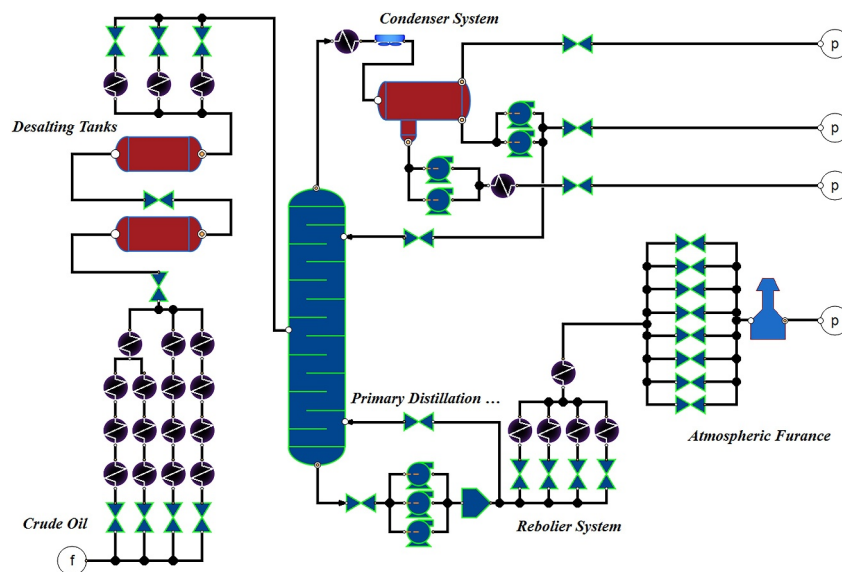


FIGURE 15 Primary distillation subsystem model.



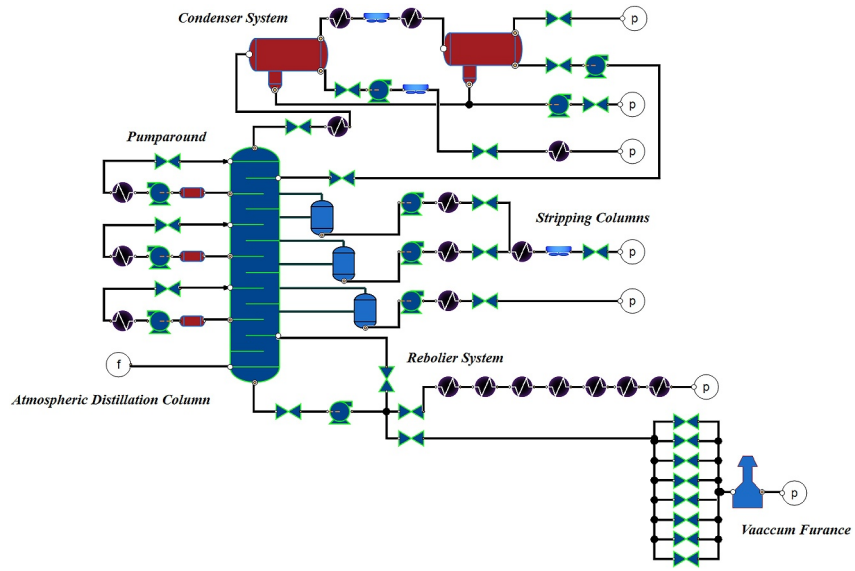


FIGURE 16 Atmospheric distillation subsystem model.

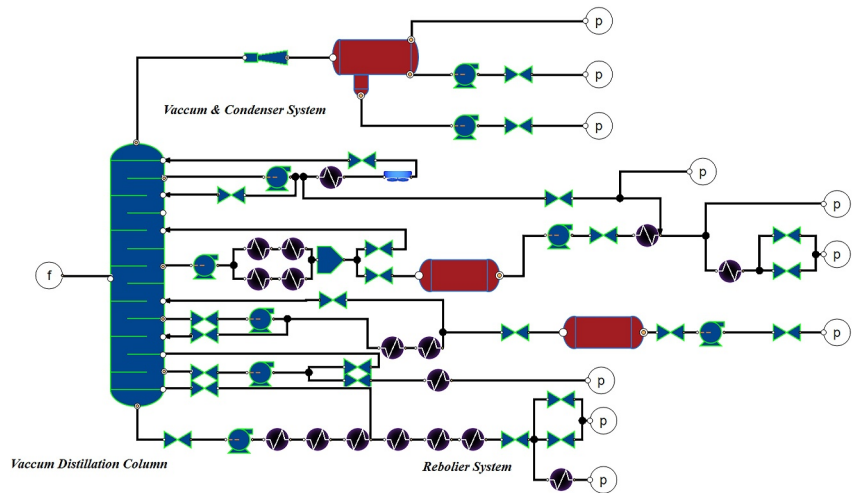


FIGURE 17 Vacuum distillation subsystem model.

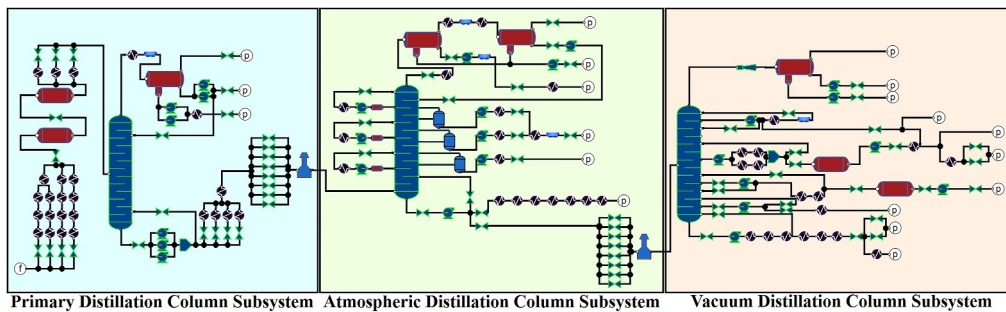


FIGURE 18 Crude oil distillation unit system model.

**TABLE 2** Equipment parameters of the atmospheric distillation subsystem under condition I.

Number	Name	Symbol	Unit	Numerical value
1	Number of components	Nc		10
2	Component list	C[Nc]		See tab. 4.3
3	Boiling point temperature of components	Tb[Nc]	K	See tab. 4.3
4	Column top pressure	P1	MPa	0.13
5	Column bottom pressure	PN	MPa	0.15
6	Tray number	Np		10.00
7	Feed tray	Fp		9.00
8	Number of side streams	Ns		3.00
9	Side stream tray(s)	Sp[Ns]		10.00
10	Side stream flowrate	Sopt[Ns]	mol/s	150.00
11	Liquid load on tray	M	mol	150.00
12	Liquid load of condenser	M0	mol	0.13
13	Liquid load of reboiler	MN	mol	0.15

$$\frac{d(M_n \cdot x_{n,i})}{dt} = L_{n-1}x_{n-1,i} + V_{n+1}y_{n+1,i} + F_n x_{n,i} - L_n x_{n,i} - V_n y_{n,i} - S L_n x_{n,i} - S V_n y_{n,i} \quad (14)$$

The phase equilibrium equation:

$$y_{n,i} = \eta_n k_{n,i} x_{n,i} + (1 - \eta_n) y_{n-1,i} \quad (15)$$

The efficiency equation for a distillation tray can be expressed as follows:

$$\eta_n = \frac{y_{n,i} - y_{n-1,i}}{y_{n,i}^0 - y_{n-1,i}} \quad (16)$$

The summation equation for mole fraction normalisation:

$$\sum x_{n,i} = 1 \quad (17)$$

$$\sum y_{n,i} = 1 \quad (18)$$

The heat balance equation:

$$\frac{dM_n(h_l)_n}{dt} = L_{n-1}(h_l)_{n-1} + V_{n+1}(h_v)_{n+1} + F_n h_f - L_n(h_l)_n - V_n(h_v)_n - S L_n(h_l)_n - S V_n(h_v)_n \quad (19)$$

Using Equations (1)–(19), we can construct the mechanistic model for the distillation column, as shown in Figure 14. Leveraging this mechanistic model, we implement the FANN method to refine it, resulting in a hybrid model that provides satisfactory simulation results when compared with Aspen Plus.

**TABLE 3** Parameters for pseudo-components.

Pseudocomponent	Boiling point temperature	Relative density
CP1	334.69	0.63
CP2	360.01	0.65
CP3	391.95	0.67
CP4	421.76	0.68
CP5	452.08	0.70
CP6	480.66	0.71
CP7	510.18	0.73
CP8	538.94	0.74
CP9	568.63	0.76
CP10	597.85	0.77

#### 4.1.2 | Subsystem modelling and system modelling for CDU

By adopting the aforementioned method, we developed a total of 28 unit-equipment models for CDU systems, including the distillation column, regulation valve, heat exchanger, and heating furnace. Utilising the multi-level inheritance and module packaging features of these DT models, and connecting them according to the PFD and P&ID, we established three subsystem models and an overall system model for the CDU, as shown in Figures 15–18.

#### 4.1.3 | Subsystem model validation

Taking the atmospheric distillation subsystem model as an example, we carry out comparative studies under three

different operating conditions to validate the accuracy of this subsystem model. The calculation method of relative deviation is shown in Equation (20), where  $E_{s,i}$  represents the steady-state deviation of each test item in the tested system.  $y_{obj,s,i}$  stands for the actual operational values of each test item of the physical object, and  $y_{mod,s,i}$  denotes the steady-state operational results of each test item in the model.

$$E_{s,i} = abs\left(\frac{y_{mod,s,i} - y_{obj,s,i}}{y_{obj,s,i}}\right) \times 100\% \quad (20)$$

The operating condition I can be described by Tables 2–4. Based on the parameters mentioned earlier for the atmospheric distillation subsystem model, we conduct simulation studies and compare the results with their benchmark. It is important to note that the benchmark used in this study is the simulation results of Aspen Plus under identical circumstances. The validation results are presented in Table 5 and Figure 19.

Similarly, the operating condition II can be described by Table 6.

**TABLE 4** Atmospheric distillation system input variables under operating condition I.

Number	Name	Symbol	Unit	Numerical value
1	Feed flow rate	F	mol/s	400.00
2	Feed molar component	xF[Nc]	1	{0.0029, 0.011, 0.11, 0.13, 0.13, 0.13, 0.13, 0.13, 0.13, 0.13}
3	Feed temperature	TF	K	502.00
4	Feed pressure	PF	MPa	0.15
5	Reflux ratio	RR		2.00
6	Bottoms rate	W	mol/s	120.00
7	Number of side streams	Sp[Ns]		{2, 4, 6}
8	Side stream tray(s)	Sopt[Ns]	mol/s	{0, 0, 0}

**TABLE 5** Comparison of key parameters in atmospheric distillation column under condition I.

Number	Name	Symbol	Unit	Aspen plus	NGM	Error (%)
1	Temperature of tray 1	T[1]	K	414.60	415.07	0.00
2	Temperature of tray 2	T[2]	K	433.60	434.27	0.00
3	Temperature of tray 3	T[3]	K	444.58	445.22	0.00
4	Temperature of tray 4	T[4]	K	451.15	451.70	0.22
5	Temperature of tray 5	T[5]	K	456.12	456.56	0.22
6	Temperature of tray 6	T[6]	K	461.13	461.41	0.00
7	Temperature of tray 7	T[7]	K	467.51	467.37	0.21
8	Temperature of tray 8	T[8]	K	478.25	476.75	0.21
9	Temperature of tray 9	T[9]	K	501.83	497.44	1.00
10	Temperature of tray 10	T[10]	K	521.17	520.34	0.19
11	Pressure of tray 1	P[1]	bar	1.27	1.27	0.00
12	Pressure of tray 2	P[2]	bar	1.29	1.29	0.00
13	Pressure of tray 3	P[3]	bar	1.31	1.31	0.00
14	Pressure of tray 4	P[4]	bar	1.34	1.34	0.00
15	Pressure of tray 5	P[5]	bar	1.36	1.36	0.00
16	Pressure of tray 6	P[6]	bar	1.38	1.38	0.00
17	Pressure of tray 7	P[7]	bar	1.40	1.40	0.00
18	Pressure of tray 8	P[8]	bar	1.43	1.43	0.00
19	Pressure of tray 9	P[9]	bar	1.45	1.45	0.00
20	Pressure of tray 10	P[10]	bar	1.47	1.47	0.00

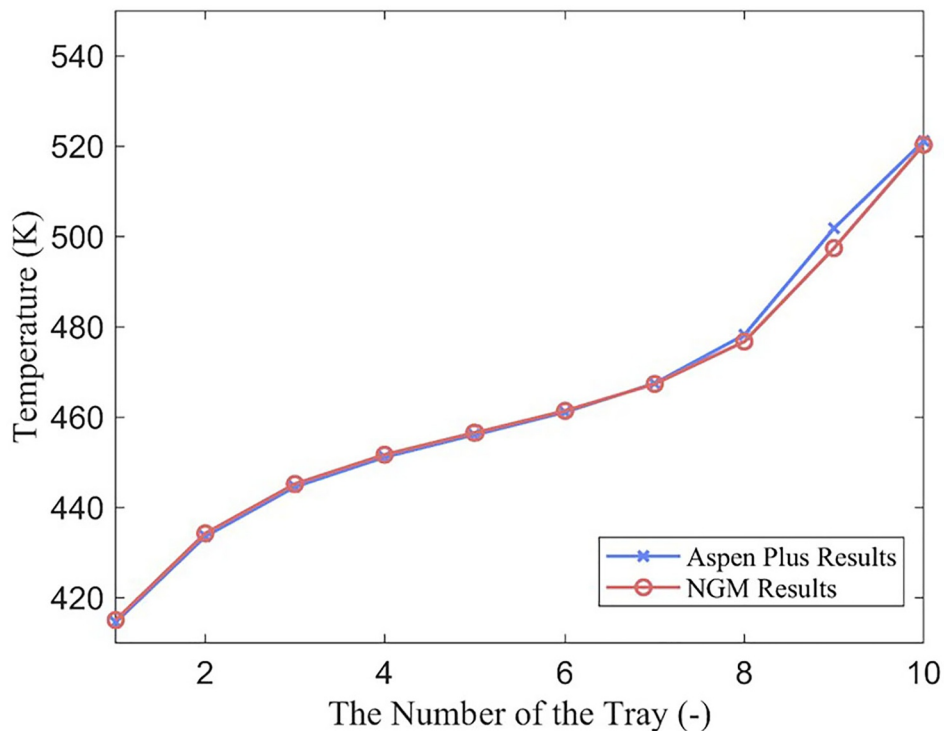
Abbreviation: NGM, novel generation modelling.

The simulation results are presented in Table 7 and Figure 20.

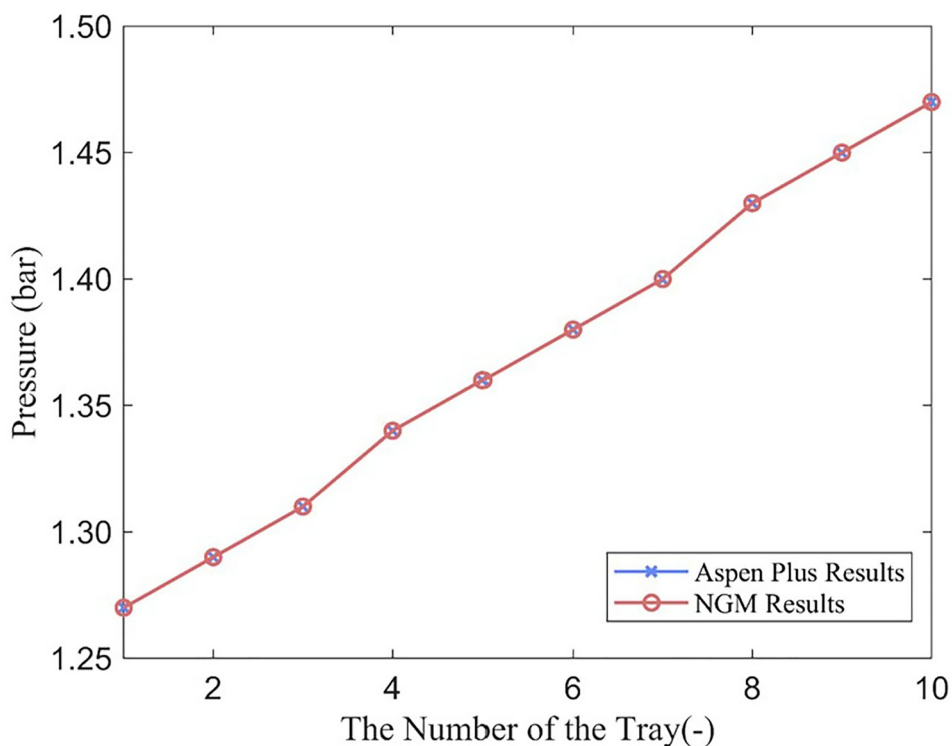
The operating condition III can be described by Table 8.

The validation results are presented in Table 9 and Figure 21.

According to the comparison results, we can simply conclude that the proposed modelling system can achieve



(a) Tray temperature distribution comparison<sup>e1</sup>



(b) Tray pressure distribution comparison<sup>e1</sup>

FIGURE 19 Comparison of key parameters in atmospheric distillation column under condition I.



satisfactory simulation results compared with Aspen Plus, which is the most professional and prevalent simulation software in chemical engineering.

## 4.2 | 25 MW CFB thermal power unit

### 4.2.1 | The DT model for the CFB

The circulating fluidised bed (CFB) power plant plays a crucial role in power generation due to its low pollutant emissions,

wide fuel adaptability, and high combustion efficiency, leading to widespread adoption globally.

In this study, a DT model of an actual 25 MW CFB power plant is developed using the NGM platform. Initially, 13 unit-equipment models are created using a hybrid modelling approach, encompassing key components of the CFB power plant such as valves, furnaces, steam turbines, condensers, deaerators, and pumps. The characteristic parameters of these unit-equipment models, like pipe flow resistance and fan characteristic curve coefficients, are determined from the specifications and design data of the actual equipment. Next,

**TABLE 6** Atmospheric distillation system input variables under operating condition II.

Number	Name	Symbol	Unit	Numerical value
1	Feed flow rate	F	mol/s	400.00
2	Feed molar component	xF[Nc]	1	{0.0029, 0.011, 0.11, 0.13, 0.13, 0.13, 0.13, 0.13, 0.13, 0.13}
3	Feed temperature	TF	K	502.00
4	Feed pressure	PF	MPa	0.15
5	Reflux ratio	RR		2.00
6	Bottoms rate	W	mol/s	120.00
7	Number of side streams	Sp[Ns]		{2, 4, 6}
8	Side stream tray(s)	Sopt[Ns]	mol/s	{0, 28.79, 33.97}

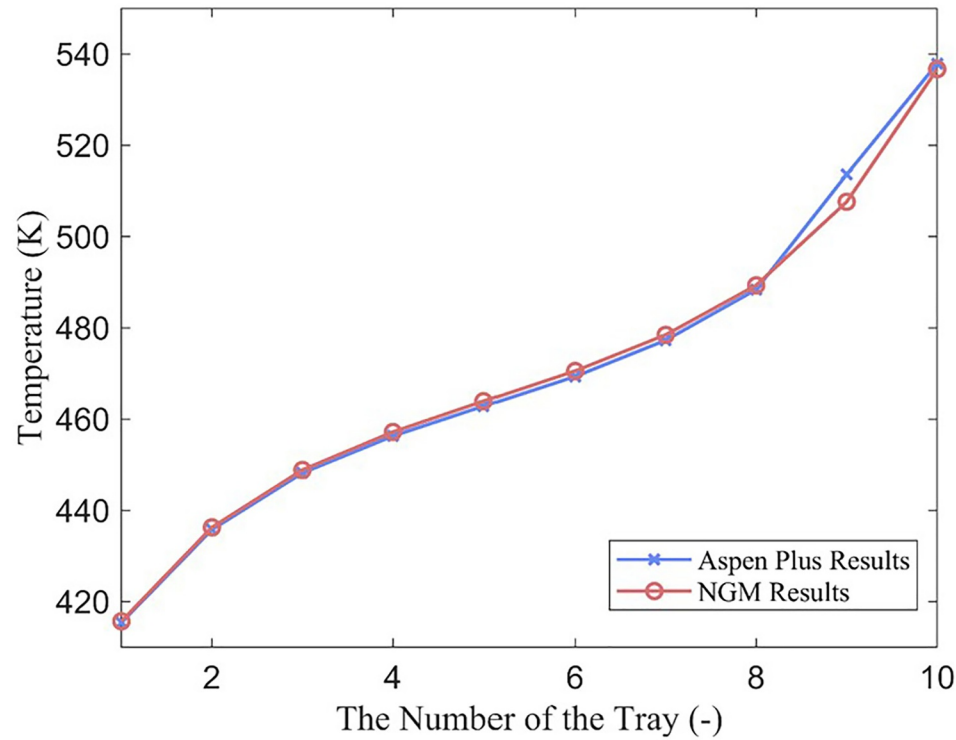
**TABLE 7** Comparison of key parameters in atmospheric distillation column under condition II.

Number	Name	Symbol	Unit	Aspen plus	NGM	Error (%)
1	Temperature of tray 1	T[1]	K	415.42	415.69	0.24
2	Temperature of tray 2	T[2]	K	435.78	436.27	0.00
3	Temperature of tray 3	T[3]	K	448.20	448.86	0.22
4	Temperature of tray 4	T[4]	K	456.29	457.18	0.22
5	Temperature of tray 5	T[5]	K	462.84	463.93	0.22
6	Temperature of tray 6	T[6]	K	469.33	470.54	0.43
7	Temperature of tray 7	T[7]	K	477.28	478.46	0.21
8	Temperature of tray 8	T[8]	K	488.40	489.32	0.20
9	Temperature of tray 9	T[9]	K	513.61	507.62	1.17
10	Temperature of tray 10	T[10]	K	537.89	536.67	0.19
11	Pressure of tray 1	P[1]	bar	1.27	1.27	0.00
12	Pressure of tray 2	P[2]	bar	1.29	1.29	0.00
13	Pressure of tray 3	P[3]	bar	1.31	1.31	0.00
14	Pressure of tray 4	P[4]	bar	1.34	1.34	0.00
15	Pressure of tray 5	P[5]	bar	1.36	1.36	0.00
16	Pressure of tray 6	P[6]	bar	1.38	1.38	0.00
17	Pressure of tray 7	P[7]	bar	1.40	1.40	0.00
18	Pressure of tray 8	P[8]	bar	1.43	1.43	0.00
19	Pressure of tray 9	P[9]	bar	1.45	1.45	0.00
20	Pressure of tray 10	P[10]	bar	1.47	1.47	0.00

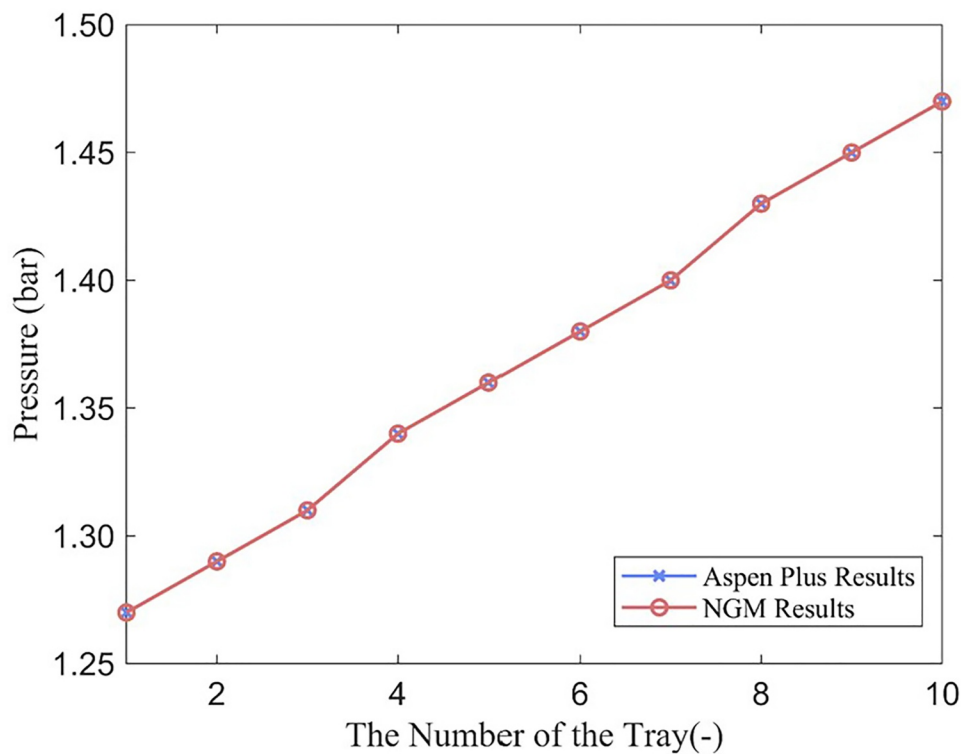
Abbreviation: NGM, novel generation modelling.

following the PFD, these unit-equipment models are sequentially connected to form the comprehensive system model for the CFB power plant, as illustrated in Figure 22. This digital

replication covers the combustion system, steam turbine system, condenser system, and feedwater system, effectively describing the entire boiler water-steam circuit of the CFB



(a) Tray temperature distribution comparison



(b) Tray pressure distribution comparison

FIGURE 20 Comparison of key parameters in atmospheric distillation column under condition II.

power plant. The system model considers valve openings and the rotation rates of pumps and fans as input variables. By adjusting these inputs, the model can perform continuous dynamic simulations of various operating conditions of CFB power plants. Additionally, these input variables serve as control instructions outputted from the DCS, enabling the system model to achieve online control, which will be detailed in the following section.

#### 4.2.2 | Application of snapshot

During the operation of the DT model, snapshots can be taken at any time using the snapshot function. These snapshots can be loaded at startup to initialise the model with specific operating conditions or loaded during runtime to switch between different operating conditions. In the practical application, the constructed 25 MW CFB power plant system model is

**TABLE 8** Atmospheric distillation system input variables under operating condition III.

Number	Name	Symbol	Unit	Numerical value
1	Feed flow rate	F	mol/s	400.00
2	Feed molar component	$x_F[Nc]$	1	{0.0029, 0.011, 0.11, 0.13, 0.13, 0.13, 0.13, 0.13, 0.13, 0.13}
3	Feed temperature	TF	K	502.00
4	Feed pressure	PF	MPa	0.15
5	Reflux ratio	RR		2.00
6	Bottoms rate	W	mol/s	120.00
7	Number of side streams	Sp[Ns]		{2, 4, 6}
8	Side stream tray(s)	Sopt[Ns]	mol/s	{23.88, 28.79, 33.97}

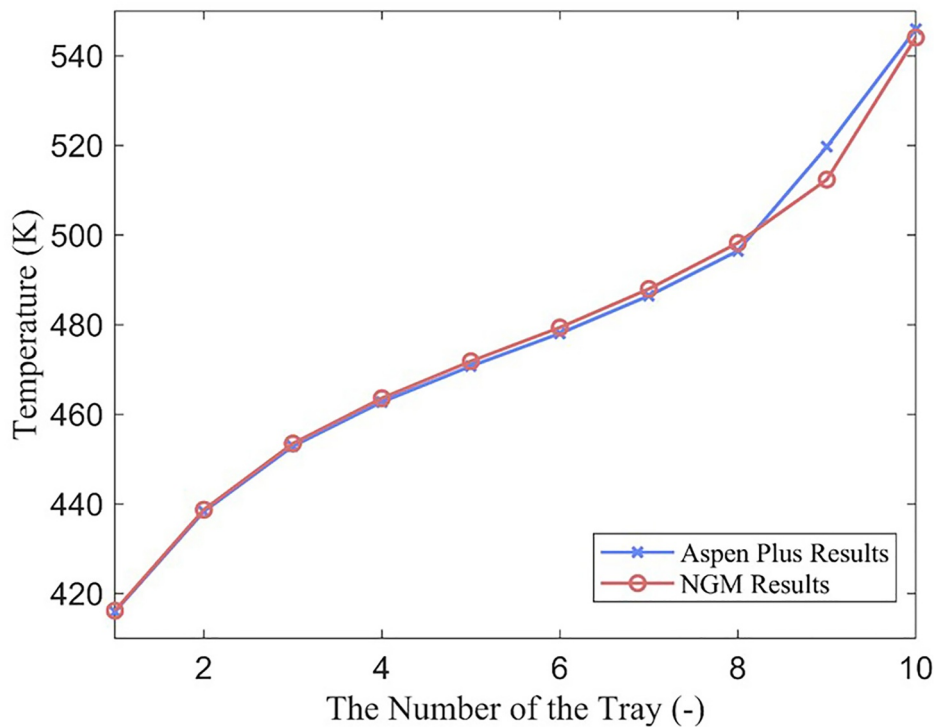
**TABLE 9** Comparison of key parameters in atmospheric distillation column under condition III.

Number	Name	Symbol	Unit	Aspen plus	NGM	Error (%)
1	Temperature of tray 1	T[1]	K	415.97	416.18	0.00
2	Temperature of tray 2	T[2]	K	438.31	438.71	0.23
3	Temperature of tray 3	T[3]	K	452.89	453.49	0.00
4	Temperature of tray 4	T[4]	K	462.75	463.60	0.22
5	Temperature of tray 5	T[5]	K	470.75	471.84	0.21
6	Temperature of tray 6	T[6]	K	478.05	479.38	0.21
7	Temperature of tray 7	T[7]	K	486.45	487.98	0.41
8	Temperature of tray 8	T[8]	K	496.46	498.25	0.40
9	Temperature of tray 9	T[9]	K	519.70	512.38	1.54
10	Temperature of tray 10	T[10]	K	545.93	544.08	0.37
11	Pressure of tray 1	P[1]	bar	1.27	1.27	0.00
12	Pressure of tray 2	P[2]	bar	1.29	1.29	0.00
13	Pressure of tray 3	P[3]	bar	1.31	1.31	0.00
14	Pressure of tray 4	P[4]	bar	1.34	1.34	0.00
15	Pressure of tray 5	P[5]	bar	1.36	1.36	0.00
16	Pressure of tray 6	P[6]	bar	1.38	1.38	0.00
17	Pressure of tray 7	P[7]	bar	1.40	1.40	0.00
18	Pressure of tray 8	P[8]	bar	1.43	1.43	0.00
19	Pressure of tray 9	P[9]	bar	1.45	1.45	0.00
20	Pressure of tray 10	P[10]	bar	1.47	1.47	0.00

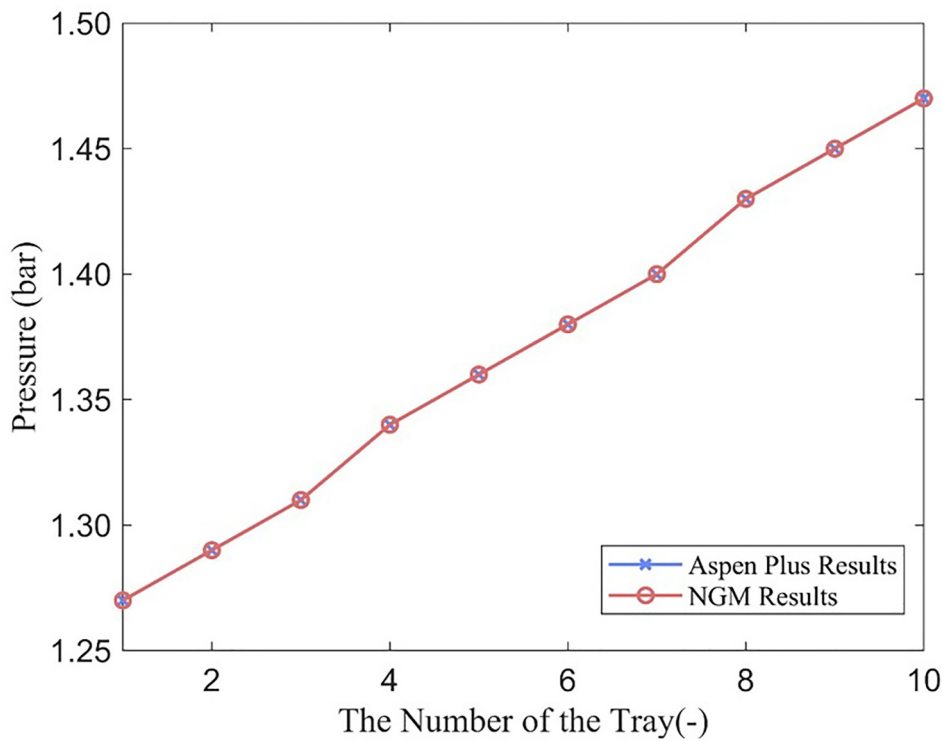
Abbreviation: NGM, novel generation modelling.

exported via the NGM platform to generate a system-level NGU. This NGU is then loaded into UWintechPro for startup and operation. By adjusting operational commands, the

model is operated at turbine maximum continuous rating, turbine heat acceptance (THA), and 75% THA conditions, with snapshots stored for each condition, as shown in



(a) Tray temperature distribution comparison



(b) Tray pressure distribution comparison

FIGURE 21 Comparison of key parameters in atmospheric distillation column under condition III.



Figure 23. Loading different snapshots allows for rapid switching between operating conditions, significantly reducing wait times and enhancing operational efficiency.

The snapshot function enables the preservation of instantaneous snapshots of power production conditions, facilitating the switching of operational scenarios. This capability allows for the testing and evaluation of industrial controls under different operating conditions.

### 4.2.3 | A real-time closed-loop control system based on the DT model

Constructing a real-time closed-loop control system requires both the model-side, centred on the DT model, and the control side, centred on the DCS. Additionally, the I/O mapping system serves as the bridge between the model and the control system, connecting them through physical interfaces.

On the model side, a DT model of the 25 MW CFB power plant is employed, with the generated NGU loaded into UWintechPro and connected to model-side I/O hardware. On the control side, the power plant's DCS control system, also built using UWintechPro, is connected to control-side I/O hardware. Physical connections establish I/O mapping between the control-side and model-side I/O hardware, enabling effective interaction and data transfer between the control system and the DT model.

In a real-time closed-loop control system, control commands are issued by the control system, converted into current or voltage signals by control-side hardware, and transmitted via physical connections to model-side hardware. Upon receiving these signals, the model-side hardware converts them into analogue or digital signals for the model to process. The model then performs calculations based on the received control commands and generates simulation results. These results are transmitted back to the control system through I/O mapping, ensuring that the monitored data accurately reflects real-world performance, as shown in Figure 24.

This setup enables the physical reconstruction of a 25 MW CFB power plant, facilitating advanced control, real-time optimisation, and integrated industrial control security investigations for this type of power plant.

## 5 | CONCLUSIONS

In conclusion, this paper proposes a multi-domain and multi-timescale DT platform for industrial processes, referred to as the NGM platform. The platform features a user-friendly modelling language, a powerful solver, snapshots, NGU, online control, and tools for parameter analysis and optimisation, enabling it to deliver exceptional performance in modelling, simulation, control, optimisation, fault diagnosis, and ensuring the safety and security of ICS. Additionally, this paper illustrates

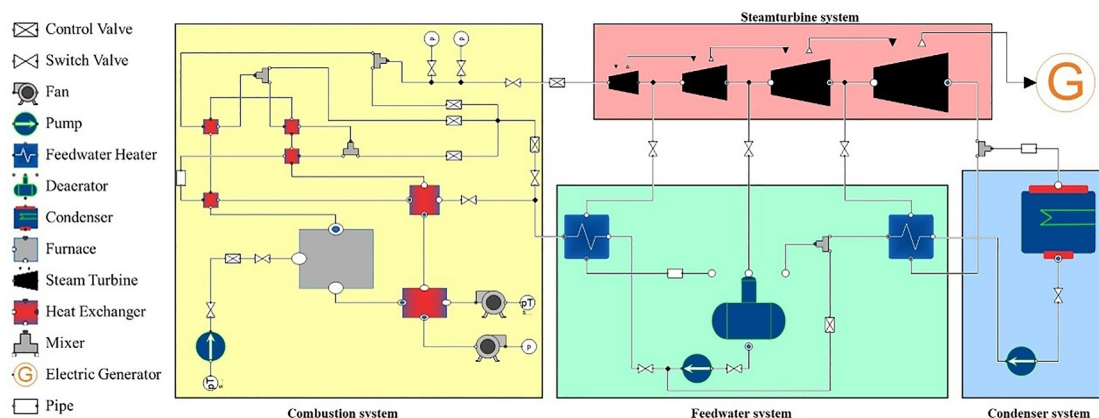


FIGURE 22 The unit-equipment models (left) and the system model (right) of the 25 MW circulating fluidised bed power plant.

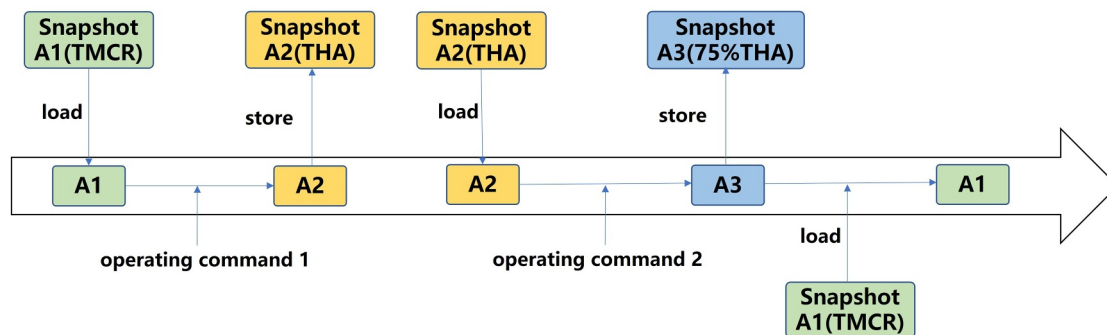


FIGURE 23 The schematic diagram of the snapshots.

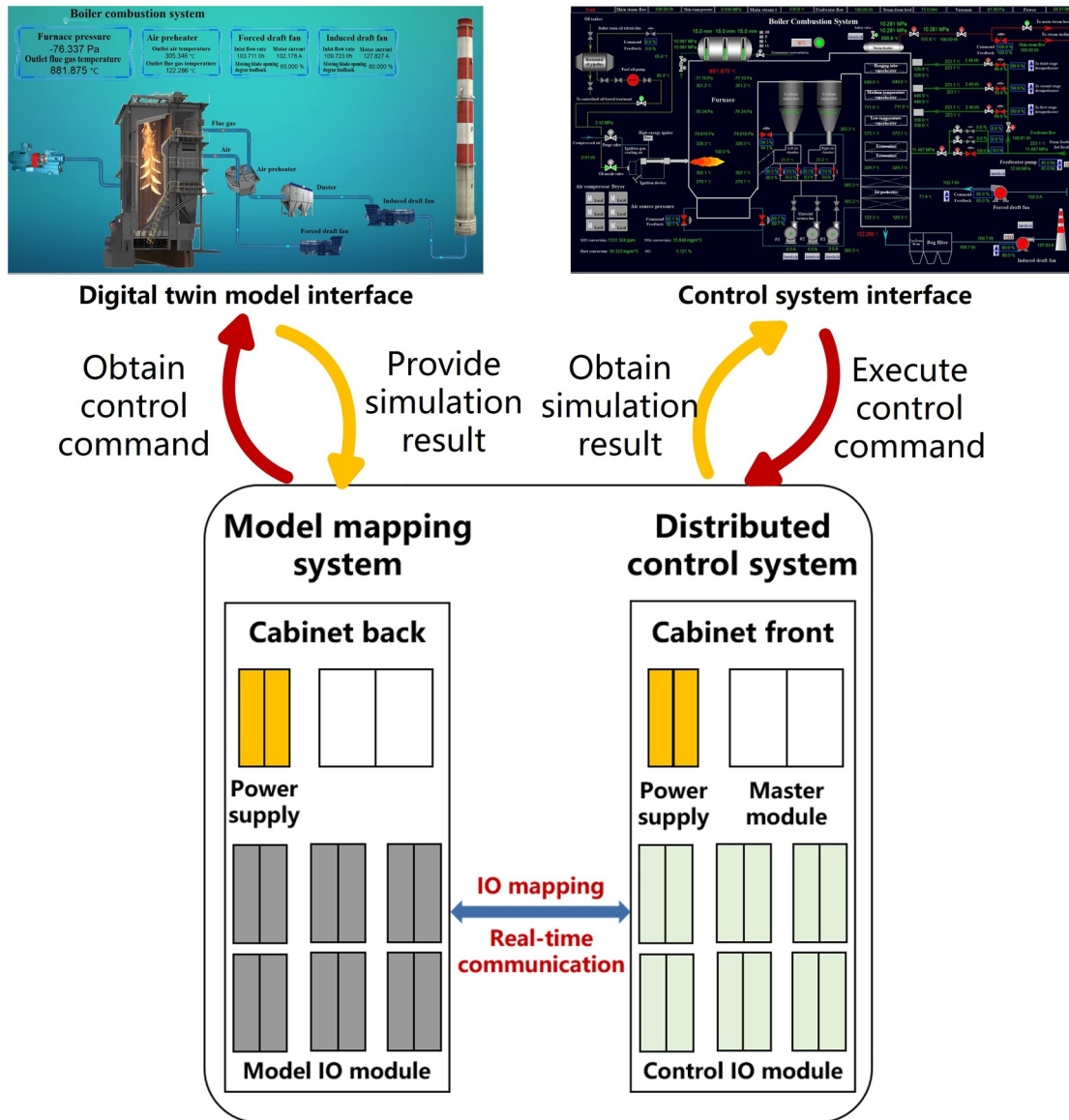


FIGURE 24 Real-time closed-loop control system.

the modelling procedure based on NGM. By employing a hybrid modelling method for unit equipment and integrating them into subsystem and system models, NGM facilitates the creation of transferable, scalable, and reconfigurable unit-equipment models as well as high-fidelity system models.

Finally, the proposed platform and method have been applied to two prevalent industrial applications. In the CDU case, the development of a DT system model based on NGM is detailed, and its accuracy is verified through comparison with Aspen Plus. In another instance, I/O mapping technology is used to achieve real-time closed-loop control systems for a 25 MW CFB thermal power unit, enabling the potential investigation of advanced control, multi-objective optimisation, and system security. In a nutshell, this work can provide a reference for further research efforts to explore future directions based on the proposed NGM platform and modelling method.

## AUTHOR CONTRIBUTIONS

**Yinan Zhang:** Conceptualisation; methodology; validation; software; data curation; writing – review & editing; writing – original draft; formal analysis; investigation. **Wenhai Wang:** Investigation; conceptualisation; supervision; funding acquisition; resources. **Qiang Yang:** Writing – original draft; writing – review & editing; investigation; funding acquisition. **Xiaoyu Tang:** Conceptualisation; methodology; writing – original draft. **Wei Ruan:** Writing – original draft; supervision; formal analysis. **Yingze Li:** Methodology; conceptualisation; software; visualisation. **Surong Daerji:** Methodology; software; validation; formal analysis. **Xiang Zhang:** Methodology; validation; visualisation; writing – original draft. **Yuqi Ye:** Methodology; software; writing – original draft; validation. **Jiawei Huang:** Methodology; software. **Junjie Li:** Methodology; software. **Yu Yang:** Methodology; software. **Xinyao**

Wu: Methodology. Haoran Yang: Validation. Tianyu Cao: Validation.

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## CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

## DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

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