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A modelling tool selection for decarbonising industrial process heat systems

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ABSTRACT

Industrial Process Heat systems are critical to various industrial processes, representing a significant share of global energy use and emissions. Effective modelling of these systems is essential for evaluating long-term economic and environmental impacts of different technologies. This modelling approach must integrate internal process-specific parameters, such as heat demand dynamics and technological metrics, alongside broader factors like energy costs, emissions policies, and resource availability. This research introduces a comprehensive framework for selecting tools to model industrial process heat systems, focusing on technological, economic, and environmental performance. An initial evaluation of twenty-five tools led to the shortlisting of five based on criteria such as modelling accuracy, scalability, data handling, compatibility with industrial systems, and environmental impacts. Using software engineering principles, a systematic selection process was developed to categorise tools based on essential and desirable capabilities. This framework was validated through an example application, incorporating both technical and practical considerations. The findings highlight the importance of integrating dynamic simulation capabilities with real-time data analysis to improve evaluation accuracy and emphasise user-friendly interfaces to broader industry adoption. The study discusses the framework's applicability, provides key insights, and identifies existing gaps, emphasising the need for adaptable modelling tools to meet evolving industrial requirements. The future applicability of the selection process is discussed, highlighting findings from the capability categorisation, gaps to be addressed, and future trends in modelling these systems. This research contributes to sustainable industrial operations by offering a robust tool selection framework, supporting informed decision-making to reduce emissions and advance industrial sustainability.

1. Introduction

1.1. Process heat energy systems

Industrial Process Heat systems are crucial in many industries, providing key functions such as steam generation, hot water supply, and manufacturing process heating [1]. These systems represent a significant portion of global industrial energy consumption, comparable to energy use in transportation and domestic electricity needs [2]. The industrial sector accounts for roughly 30 % of global CO_2 emissions, making it central to global decarbonisation efforts [3]. However, the reduction of environmental impacts in these systems poses significant challenges due to the complexity of their energy needs and the variability of renewable energy sources [4]. These challenges include uncertainties stemming from the fluctuating nature of renewables and the need to meet varying energy demands amidst regional technological constraints [5]. Additionally, the longevity of primary process heat equipment, such as boilers, often extends beyond their expected lifespan, resulting in lower energy efficiency and increased carbon footprints [6]. Sustainable alternatives are therefore urgently required to address these challenges [7].

The shift towards sustainable energy in industrial settings is not only crucial for mitigating climate change and reducing emissions but also for improving economic growth [8]. This transition faces several obstacles, including fuel diversity, renewable energy unpredictability, and high initial investment [9]. Diverse stakeholders, including policymakers, industry bodies, manufacturers, energy suppliers, and the public, have unique requirements, particularly small and medium-sized industries that struggle with long-term planning [10].

Considering the diverse and complex nature of process heat systems, and the lack of a single tool designed for decarbonising these systems while addressing techno-economic parameters, constraints, and policy implications, a systematic and comprehensive evaluation and selection process is necessary. This study presents a framework for systematically selecting and evaluating modelling tools based on the requirements for

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Nomenclature/abbreviation

CO_2	Carbon Dioxide
EIA	U.S. Energy Information Administration
GHG	Greenhouse Gas
LCA	Life Cycle Assessment
MAC	Marginal Abatement Cost
RETA	Regional Energy Transition Accelerator

decarbonising industrial process heat systems. It considers global, national, regional, and individual business contexts, ensuring that the chosen tool aligns with the specific needs of each scenario. Key criteria include assessing fuel switching options and integrating renewable energy sources. By evaluating tools based on their technical, economic, and environmental capabilities, this framework supports informed decision-making for sustainable industrial process heat systems. It provides stakeholders with a clear and structured method to identify and select the most suitable tools for decarbonising these systems.

The work is organised as follows: Section 2 outlines the initial screening process for identifying suitable tools. Section 3 categorises the capabilities of these tools. Section 4 details the tool selection process and criteria and implements it for an example application. Section 5 presents the analysis results. Finally, Section 6 concludes with key findings and recommendations.

1.2. Modelling tools for industrial process heat decarbonisation

Industrial Process Heat systems are vital in various industries, supporting functions such as steam generation, hot water supply, and chemical reactions. With the evolving energy landscape characterised by fuel diversity and the shift towards renewable energy sources, there is an increasing need for flexible modelling tools [11]. These tools should be adaptable to a range of scenarios and offer strategic insights for effective long-term planning [12].

Several studies have focused on the optimal energy system design for industrial applications, offering valuable insights into modelling tools. Beck et al. [13] developed an optimisation model for retrofitting industrial energy systems, focusing on process scheduling, heat recovery, and energy supply. Applied to a small brewery, their model identifies cost-effective decarbonisation strategies by integrating technologies like photovoltaic modules, heat pumps, thermal energy storages, and electric boilers. However, it does not consider time-sensitive energy supply tariffs or demand profile generation. Atabay [14] created a mixed-integer linear optimisation model for capacity-expansion planning and unit commitment in industrial energy systems. This open-source model identifies cost-optimal configurations for energy-conversion processes and storage techniques, considering time-sensitive prices and peak demand charges. Applied to factories with varying energy demands, the model's flexibility is crucial for detailed process heat system modelling. Nonetheless, it lacks mechanisms for generating dynamic demand profiles and integrating future policy scenarios.

Buoro et al. [15] presented a MILP model for the optimal configuration and operation of a distributed energy supply system in an industrial area, incorporating heat and electricity demands and a district heating network. Their model demonstrates substantial economic and environmental benefits through multi-objective optimisation but does not address time-sensitive energy tariffs or demand charges. Han and Lee [16] described a process integration framework for the optimal design and techno-economic performance of integrated energy supply and CO_2 mitigation strategies, applied to an industrial complex. This framework is essential for evaluating various energy configurations' economic and environmental impacts. Luo et al. [17] proposed a multi-objective MILP model for optimising the number, capacity, and operation of cogeneration systems within industrial utility networks. Their approach considers cost, environmental impact, and exergy efficiency. However, these models are tailored to specific applications and predefined energy types, limiting their adaptability. Voll et al. [18] presented an automated framework for the synthesis and optimisation of distributed energy supply systems (DESS), employing the P-graph approach and a robust MILP formulation. This model supports part-load performance curves but fails to consider demand charges and time-sensitive tariffs for energy supply.

In the context of industrial energy demand, studies like the one by Polemis [19] have utilised cointegration techniques to provide insights into consumption patterns, including those relevant to process heat, and illustrate the inelastic nature of industrial energy demand and the substitution relationships between different energy carriers. Edelenbosch et al. [20] compared long-term energy demand projections, emphasising the need for detailed analysis in industrial sub-sectors. Their study highlights the variations in projected industrial pathways and the implications for energy demand and greenhouse gas emissions, reinforcing the importance of incorporating diverse energy scenarios in models. This comparison provides a comprehensive understanding of the complexities involved in modelling industrial process heat and underscores the need for integrating detailed demand profiles, future policy scenarios, and dynamic pricing mechanisms to enhance the accuracy and relevance of techno-economic analyses.

Hybrid modelling approaches, as seen in the study by Murphy et al. [21], combines top-down and bottom-up methodologies, offering a comprehensive perspective on industrial energy systems. Their CIMS model is technologically explicit, behaviourally realistic, and capable of capturing equilibrium feedback, making it a useful tool for policy-makers. This approach aligns well with the multifaceted nature of process heat systems, where various factors, from technological changes to policy implications, need to be considered. However, the model also highlights challenges such as uncertainty in technological change and the significant resources required for detailed behavioural parameter estimation. This reinforces the importance of selecting modelling tools that can incorporate a wide range of parameters, including policy mechanisms, fuel availability, and market dynamics, to effectively evaluate decarbonisation options for industrial process heat systems.

The International Energy Agency's Solar Heating and Cooling Programme (IEA/SHC) has significantly advanced the understanding of solar heat applications in industry, particularly through initiatives like Task 33 [22] and Task 64 [23]. These initiatives explore the potential and integration strategies for solar thermal technologies within industrial processes, underscoring the need for simulation tools that accurately model solar heat integration while balancing technical and economic factors. Building on these insights, recent modelling developments by the U.S. Energy Information Administration (EIA) have further enhanced modularity and flexibility, enabling the exploration of various technology pathways, spatial resolutions, and operational parameters within industrial energy systems. Together, these advancements support the creation of comprehensive, adaptable models that can more effectively capture the multi-dimensional challenges of industrial decarbonisation [24]. However, to fully realise these capabilities, further development and implementation in targeted case studies are essential to demonstrate their full potential and effectiveness in real-world applications.

In addition to these specific studies, comprehensive review papers offer valuable insights into the capabilities of various modelling tools within the broader context of industrial energy systems. Kumar et al. [25] have conducted a thorough examination of energy planning models aimed at sustainable development at the corporate level, critically examining tools designed to enhance overall energy efficiency and reduce carbon footprints across diverse industrial environments. The reviewidentifies seven suitable tools for analysing industrial excess heat and cold recovery, providing a comparative analysis of their capabilities in terms of temporal and spatial resolution, flexibility, and interoperability. Kumar et al. conclude that no single model can meet all requirements universally, thereby underscoring the necessity of selecting modelling tools based on specific criteria such as temporal and spatial resolution and their capacity to integrate diverse energy sources.

Similarly, Laveneziana et al. [26] provide a detailed analysis of techno-economic modelling and optimisation of excess heat and cold recovery in industries, focusing on the economic viability and environmental impact of utilising waste energy in industrial processes. Their review highlights tools that excel in optimising energy recovery and reducing operational costs, while also emphasising the need for tools capable of handling the dynamic and complex nature of industrial energy systems, including the integration of renewable energy sources and advanced energy storage solutions.

While these reviews offer valuable insights, they often fail to address the specific requirements and dynamic nature of industrial process heat systems, necessitating a critical comparison of different technologies to advance decarbonisation efforts. The main challenge here lies in effectively comparing traditional fossil fuel-based systems with sustainable alternatives such as solar thermal or biomass systems. These comparisons are crucial for identifying the most viable solutions and optimal transition timings to more sustainable energy sources. Significantly, no modelling tool currently exists that is specifically designed for this particular task, making the selection of an appropriate tool essential. This is crucial for addressing the unique challenges and requirements of industrial thermal systems, ensuring that decisions are informed by a thorough analysis of all technological options and their impacts.

Moreover, they lack a detailed tool selection process designed for the complexities of modelling these systems. Adapting methodologies from other engineering fields, such as the 'software tool selection process' developed by Sandia National Laboratories [27], can be instrumental in selecting suitable modelling tools for industrial process heat systems. This systematic approach involves gathering and categorising requirements, assessing software quality, and comparing tools against user requirements. Such a method, adapted for the specifics of process heat systems, can guide the selection of tools that effectively address the unique challenges and requirements of industrial thermal systems.

1.3. Objectives, methodology, and scope of the study

The specific objective of this work is the categorisation and documentation of the capabilities of tools suitable for modelling industrial process heat systems. Tools that either possess the potential to be adapted or are inherently well-suited for modelling the complex techno-economic parameters of heating systems, such as boilers, air heaters, and heat pumps, are identified. The aim is the development of a selection process based on the documented capabilities of these tools, to identify the most suitable ones for specific modelling scenarios within this sector.

This will be achieved through.

- Conducting an initial review to identify a range of tools potentially suitable for modelling industrial process heat systems.
- Capability categorisation and tabulation of the identified modelling tools, providing a comprehensive overview of their features.
- Development of a tool selection process, informed by the capability tables, to guide the choice of the most appropriate tools for specific process heat modelling scenarios.
- Demonstration through an example application of the selecting tool process to validate its effectiveness in a real-world setting.
- Analysing and discussing the outcomes of the case evaluation, providing insights, and drawing conclusions from the study.

Despite the enhancement of analytical capabilities through the integration with ancillary software such as MATLAB and EnergyTRADE [28], the focus of this study is primarily on the built-in capacities of the tools. The evaluation process is demonstrated through a case study, which leads to an extensive discussion of the findings. Recognising the dynamic nature of tool development, this work not only presents a contemporary analysis but also establishes a framework for future revisions. This approach ensures that the proposed framework retains relevance in the evolving landscape of modelling tools and their capabilities for accurately predicting the performance of industrial process heat systems.

2. Initial screening process

The initial phase of selecting a modelling tool for industrial process heat systems requires a thorough evaluation of potential options. This process begins with an extensive search of the SCOPUS citation database using keywords such as 'Optimisation model,' 'Energy system modelling,' 'Energy systems analysis,' and 'Energy system model.' To ensure the relevance and up-to-date nature of the tools, the search was limited to literature published after 2010. Additionally, the review of 37 computer models for energy system analysis by Connolly et al. [29], categorises them into simulation and optimisation models, provided a foundational classification. The models evaluated by Groissböck [30], particularly those applicable to industrial heating and electricity optimisation, were considered relevant. Furthermore, articles describing reviews of energy models [31] and the OpenMod Initiative's webpage [32], which offers an overview of models categorised by purpose, scope, and modelling type, were consulted to further support the selection process.

To systematically assess the suitability of these tools, a set of meticulously defined criteria were applied to an initial list of 25 tools, as presented in Table 1. These criteria were developed to ensure that each tool can adequately support the specific demands of industrial process heat systems. For a tool to pass the criteria, it must, according to its design or documented features, demonstrate a clear potential to perform the following essential functions.

- Capability for Industrial-Scale Modelling: It is crucial that the tool is explicitly designed for or adaptable to industrial-scale applications. This includes the ability to model various process heat technologies such as steam boilers, hot water boilers, air heaters, and heat pumps. This capability ensures that the tool can handle the complex and large-scale requirements typical of industrial systems.
- Technology Flexibility: The selected tool must accommodate a wide range of fuels and emerging technologies. This flexibility is essential to evaluate and integrate diverse energy sources, including renewable options, ensuring the tool's applicability across different scenarios and technological advancements.
- Economic Analysis Proficiency: Effective economic analysis is vital for comparing the costs of alternative technologies. The tool should be capable of evaluating fuel costs, investment requirements, operational expenses, and return on investment timescales. This proficiency ensures that economic feasibility is accurately assessed, supporting sound financial decision-making.
- Emissions Analysis Capability: The tool must analyse emissions from different heating technologies and evaluate the impact of carbon pricing mechanisms. This capability is critical for understanding and mitigating the environmental impact of industrial processes, aligning with global decarbonisation goals.
- Scenario Analysis Skills: The ability to model various future scenarios, including potential changes in energy prices, market conditions, and policy frameworks, is essential. This feature allows stakeholders to anticipate and plan for different futures, enhancing the strategic planning process.
- Dynamic Simulation and Forecasting: Accurate simulation of systems and forecasting future performance are necessary to understand the behaviour of process heat systems under varying conditions. This

Table 1
Structured evaluation of tools based on compliance with established criteria.

Modelling Tool	Criteria Met?	Capability to Industrial Thermal Modelling	Technology Flexibility	Economic Analysis	Emissions Analysis	Scenario Analysis	Sensitivity Analysis	System Sizing Capability	Site-Specific Modelling Capability
Aspen Plus	Yes	Yes	Yes	Assumed	Yes	Assumed	Assumed	Yes	Assumed
Backbone	No	Assumed	Assumed	Assumed	No	Assumed	No	No	No
Balmorel	No	Assumed	Yes	Yes	Assumed	Yes	Assumed	No	Assumed
Calliope	Yes	Assumed	Yes	Assumed	Assumed	Yes	Assumed	Yes	Yes
Dymola	No	Yes	Yes	Assumed	Assumed	Yes	Yes	Assumed	Assumed
EBSILON Professional	No	Yes	Yes	Assumed	Assumed	Yes	No	Assumed	Assumed
ELMOD	No	No	No	Yes	Yes	Assumed	No	No	No
EnergyPLAN	Yes	Yes	Yes	Yes	Yes	Yes	Assumed	Yes	Yes
EnergyScope	No	Yes	Yes	Yes	Yes	Assumed	Assumed	Assumed	Assumed
FICO Xpress	No	No	No	Assumed	No	Assumed	No	No	No
FICUS	No	Yes	Yes	Yes	Assumed	Yes	No	Assumed	Assumed
GAMS	Yes	Assumed	Assumed	Yes	Assumed	Yes	Assumed	Assumed	Yes
HOMER	Yes	Assumed	Yes	Yes	Yes	Yes	Yes	Assumed	Assumed
MARKAL	No	Assumed	Yes	Yes	Yes	Yes	Assumed	No	No
MATLAB/Simulink	No	Yes	Yes	Assumed	Assumed	Yes	Yes	Yes	Assumed
OEMOF	Yes	Assumed	Assumed	Yes	Yes	Assumed	Assumed	Yes	Yes
OSeMOSYS	No	Assumed	Yes	Assumed	Yes	Yes	No	No	No
OpenModelica	No	Yes	Assumed	Assumed	Assumed	Yes	Yes	Assumed	Assumed
PLEXOS	No	Assumed	Yes	Yes	Assumed	Yes	Assumed	Assumed	No
Pyomo	No	Assumed	Assumed	Assumed	Assumed	Assumed	No	Assumed	Assumed
RETScreen	No	No	Yes	Yes	Yes	Assumed	Assumed	No	No
SAM (System Advisor Model)	No	No	Yes	Yes	No	Assumed	No	No	No
TIMES	No	Assumed	Yes	Yes	Yes	Yes	No	No	No
TRNSYS	Yes	Yes	Yes	Assumed	Assumed	Assumed	Assumed	Yes	Yes
Temoa	No	Assumed	Yes	Yes	Assumed	Yes	No	Assumed	Assumed

Table 2
Technical modelling specifications.

Tool	Objective Function Range	Modelling Method	Modelling Interface	Scalability & Integration
OEMOF	Comprehensive	Stochastic	Open-source (Python)	High
TRNSYS	Comprehensive	Deterministic/ Simulation	Open-source (Proprietary)	High
EnergyPLAN	Strategic	Deterministic	N/A	Moderate
Calliope	Comprehensive	Stochastic/ Simulation	Open-source (Python)	High
HOMER	Specialised	Simulation	Proprietary	Moderate

capability supports the development of robust and reliable models, which are essential for effective planning and optimisation.

- System Sizing Capability: The tool must be capable of performing pre-feasibility assessments and determining the appropriate capacity of various system components, including alternative technologies, based on demand profiles and operational requirements. Proper system sizing is crucial for ensuring the efficiency and effectiveness of the process heat systems.
- Site-Specific Modelling: The tool should capture detailed local parameters and conditions, including meteorological data, specific industrial processes and equipment, and the infrastructure upgrades required for implementing new technologies. This capability ensures that the model accurately reflects the unique characteristics and requirements of each site, leading to more precise and applicable results.

The structured evaluation detailed in Table 1 is based on compliance levels drawn from multiple sources [33–57]. These references include explicit documentation, case studies, and examples where the tools have been successfully applied for the specified purposes. Table 1 employs a coding system to indicate compliance levels. Tools marked as "Yes" with no highlight have been verified to fully meet the criteria based on explicit documentation, case studies, or references where the tool has been successfully used for the specified purpose. The "Yes" (light shading) classification is used for tools that technically fulfil a criterion but may do so with significant limitations due to factors such as steep learning curves, high cost, or complexity, which can hinder their effectiveness and ease of use for some users. Tools marked as "Assumed" with no highlight are those that, while not explicitly documented for a particular feature, show strong potential for successful application based on characteristics or functionalities evident in related uses. Tools marked as "Assumed" with light shading are those where there is some evidence or indirect indications that the tool might face limitations in fulfilling certain criteria. This classification often stems from references where the tool has been used but encountered challenges or performance issues in the relevant area. Finally, tools marked as "No" with dark shading have been identified as lacking the necessary capabilities based on clear documentation, case studies indicating their unsuitability, or lack of evidence to show the tool can satisfy the criteria. These tools do not meet the specific criteria needed for effective process heat modelling.

In the context of industrial process heat systems, the selection of an optimal modelling tool is essential for handling complex simulations and analyses. Petro-SIM, COMSOL, ANSYS, and FRNC-5PC, known for their advanced simulations in fluid dynamics and heat exchange, were excluded in the initial screening due to their focus on technical aspects without encompassing economic and environmental assessments [58].

Aspen Plus is robust in chemical process simulation, capable of detailed thermal modelling and supporting a wide range of fuels and technologies, making it suitable for industrial thermal modelling and technology flexibility [59]. It can perform emissions analysis and system sizing effectively [60]. However, its economic and scenario analysis capabilities are less comprehensive, often requiring integration with other tools, and its sensitivity analysis demands significant expertise [61]. Its high cost and steep learning curve limit its practicality for some users [33].

GAMS, MATLAB/Simulink, and Pyomo offer extensive modelling capabilities but share steep learning curves and require significant programming knowledge. GAMS excels in optimisation but needs supplementary tools for economic and emissions analysis [62]. MATLAB/Simulink is robust in dynamic modelling but less intuitive for non-programmers [63]. Pyomo, while powerful for optimisation, also requires additional software for effective economic evaluations [64].

MARKAL, TIMES, and OSeMOSYS are designed for long-term, macroscopic energy system planning. MARKAL focuses on economic aspects and energy market interactions, suitable for policy analysis but lacks the granularity needed for detailed, site-specific industrial heat plant modelling [65]. TIMES offers a more detailed representation of energy technologies but remains oriented towards macroscopic analyses rather than specific operational details of industrial heat systems [66]. OSeMOSYS excels at exploring energy scenarios and policy options on a national or regional level but does not focus on detailed industrial heat plant modelling [67]. These tools' optimisation models are tailored for large-scale strategic energy analyses, making them less suitable for granular modelling required for industrial process heat technologies, particularly in areas such as system sizing and site-specific modelling.

OpenModelica and Dymola are powerful tools requiring significant modelling expertise. They face challenges with economic and emissions analysis, needing extra libraries or tools. OpenModelica, with its open-source community support, demands high user expertise and is not specifically designed for economic or scenario analysis [68]. Dymola excels in dynamic simulation and sensitivity analysis but is complex and less accessible for certain industrial applications, requiring extensive expertise and additional modules for comprehensive economic and emissions analysis [69]. Both tools are less suitable for site-specific modelling due to their general nature and complexity in integrating detailed local parameters.

Balmorel and EnergyScope are designed for energy system modelling but do not target site-specific industrial heat systems. Their broad focus on national or regional energy systems lacks the necessary detail for industrial process heat technologies. Similar to OSeMOSYS and TIMES, Balmorel does not have predefined technologies for modelling industrial process heat [25]. EnergyScope, while proficient in economic and emissions analysis, lacks granular detail for site-specific modelling and sensitivity analysis [70].

Backbone excels in scenario and sensitivity analysis but lacks detailed thermal modelling and site-specific assessments due to its primary focus on broader energy system optimisation rather than specific industrial processes [34]. EBSILON Professional is strong in industrial thermal modelling and scenario analysis but limited in technology flexibility and site-specific capabilities because it is designed for power plant simulations [71]. ELMOD is robust in economic and scenario analysis but not suited for detailed thermal modelling as it focuses on electricity market simulations [72].

FICO Xpress offers powerful optimisation but lacks comprehensive features for industrial applications. It requires extensive customisation and additional software for detailed economic and emissions analysis, making it less practical for users without significant programming expertise. Its primary focus on optimisation rather than integrated energy system modelling limits its suitability for detailed industrial process heat system simulations [73]. FICUS provides flexibility in modelling but is limited in technology flexibility and site-specific capabilities due to its general approach to energy systems [43]. PLEXOS excels in electricity market simulations but lacks focus on industrial thermal modelling and site-specific assessments [74]. RETScreen specialises in economic and emissions analysis but lacks detailed thermal modelling and site-specific capabilities because it is designed for evaluating renewable energy projects [75]. SAM is strong in economic and emissions analysis for renewable projects but not industrial heat systems, as it focuses on renewable energy performance and financial modelling without the necessary depth for industrial heat technologies [76]. Temoa excels in scenario analysis but lacks detailed thermal modelling and site-specific assessments because it is designed for broader energy system optimisation, not specific industrial applications [77].

The initial screening process has shortlisted five tools—OEMOF, TRNSYS, EnergyPLAN, Calliope, and HOMER—for further evaluation based on their capabilities in modelling industrial process heat systems. The next step will involve a detailed examination of these tools to determine their particular features and their suitability for modelling industrial process heat systems.

3. Categorisation of modelling tool capabilities

To assist in the precise selection of a modelling tool for industrial process heat systems, detailed evaluations were conducted for the five selected tools. These assessments focus on capabilities crucial for determining each tool's effectiveness in specific industrial applications.

1. Technical Modelling Specifications
2. Input Data Requirements and Support Capabilities
3. Output Capabilities and KPI Presentation
4. Economic and Financial Analysis Capabilities
5. Sustainability and Environmental Impact Assessment
6. Practical Considerations

These capabilities are instrumental during the tool selection process, providing insight into each tool's capacity to meet the requirements of a specific industrial process heat system analysis. This categorisation is described in greater detail in Section 5, where it forms the basis of the framework for selecting the most appropriate modelling tool for a specific case study.

3.1. Technical Modelling Specifications

The selection of an appropriate modelling tool is influenced by its technical specifications, which determine its effectiveness and alignment with process heat system analysis requirements [11]. The objective function range guides analysis goals like cost minimisation or emissions reduction, with versatile tools offering a comprehensive range [78]. The modelling method should match system complexity: deterministic methods for stable systems [79], stochastic methods for handling uncertainties [80], and simulation-based approaches for capturing dynamic behaviours [81]. The modelling interface impacts flexibility, accessibility, and integration potential [82]; common interfaces like Python and MATLAB offer broad compatibility and customisation [83], while proprietary interfaces may limit integration [84]. Scalability and integration are crucial for adapting to different system sizes and complexities, enhancing the tool's utility across various applications [85].

TRNSYS's combination of deterministic and simulation-based methods, along with its extensive objective function range, makes it highly effective for detailed and dynamic process simulations in complex heat systems [86]. However, its proprietary interface and the need for FORTRAN knowledge may present challenges in terms of accessibility and data integration. Since TRNSYS 18, a built-in compiler aids in the development of new types, partially mitigating these challenges [87]. Conversely, OEMOF, with its stochastic modelling approach and Python support, offers flexibility and user-friendliness, though it may require users to have proficiency in statistical methods for effective application [48].

EnergyPLAN's strategic focus is suitable for high-level planning [88] but may lack detail for specific processes. Calliope's combination of stochastic and simulation methods provides versatility [89], while HOMER specialises in renewable systems but may not be as comprehensive for industrial heat applications [90].

3.2. Input data requirements

Accurate and detailed input data directly impact the reliability of model outputs [84]. Demand profile generation evaluates the tool's ability to create dynamic demand profiles, essential for capturing industrial heat usage variations [91]. Data input flexibility assesses the tool's capability to handle diverse data types and formats [92]. Embedded functions and libraries assess built-in features that support modelling for process heat applications and enable integration with expandable open-source resources [93]. Table 3 presents a comparative overview of the selected modelling tools, highlighting their diverse input data support capabilities.

TRNSYS excels in handling extensive time-series data, enabling the creation of dynamic demand profiles with hourly or sub-hourly data over extended periods. It includes a wide range of pre-configured components and modules for simulating various energy system aspects [87], which can be customised for specific industrial process heat systems. TRNSYS integrates with external data sources like weather data and production schedules, facilitating realistic demand profiles that account for external influences on energy consumption [94]. This capability allows for the simulation of complex scenarios, reflecting the dynamic nature of industrial operations.

OEMOF is highly flexible and capable of handling various data types well. Still, it lacks extensive pre-configured modules specifically designed for industrial process heat applications, making it more suited for broader energy system analyses [95]. EnergyPLAN, offers moderate data input flexibility, supporting macro-level analysis with strategic rather than operationally detailed functions [96]. Calliope's flexibility in handling diverse data inputs and formats is notable, though it still depends on user-provided demand profiles, missing detailed industrial heat usage variations [97]. HOMER requires detailed input data, including hourly electricity and thermal demand values, which are critical for creating realistic demand profiles [90].

3.3. Output capabilities and KPI presentation

Interpreting modelling results is crucial for accuracy and actionable insights [98]. Effective output capabilities and Key Performance Indicator (KPI) presentations translate complex data into comprehensible insights, aiding stakeholders in making informed decisions toward sustainable energy solutions [99]. Table 4 compares the selected modelling tools based on these parameters.

OEMOF offers competent presentation of cost and emissions KPIs, with moderate visualisation that supports energy system optimisation [48]. TRNSYS stands out with dynamic visualisation and detailed KPI presentation, enabling comprehensive thermal scenario analysis over time [100]. EnergyPLAN's strategic focus is reflected in its moderate visualisation tools and macro-level KPIs, which are well-suited for broad energy scenario evaluations [88]. Calliope provides excellent scenario visualisation and good KPI presentations, incorporating renewable integration, making it versatile for both overarching and site-specific analyses [101]. Finally, HOMER excels with high-quality visualisation and comprehensive KPIs for hybrid and renewable scenarios [90].

Table 3
Input data support capabilities.

Tool	Demand Profile Generation	Data Input Flexibility	Embedded Functions and Libraries
OEMOF	User-provided; not inherently generated	High; handles various industrial data types	Limited; primarily focuses on energy system components
TRNSYS	High capability; detailed industrial process simulation	High; adaptable to complex setups	Extensive; includes process heat simulation components
EnergyPLAN	User-provided; general energy system focus	Moderate; apt for macro-level analysis	Moderate; more strategic than operationally detailed
Calliope	User-provided; suited for broader energy scenarios	High; flexible across different energy models	Moderate; more energy systems, less industrial process
HOMER	User-provided; focus on energy systems	Moderate; for hybrid and renewable systems	Moderate; includes renewable and conventional components

Table 4
Comparison of output capabilities.

Tool	Data Visualisation and Reporting	KPI Presentation	Scenario Comparison Capabilities
OEMOF	Moderate; energy system focus	Moderate; cost and emissions	High; energy system optimisation
TRNSYS	High; dynamic visualisation	Detailed, system metrics	High; time-based thermal scenarios
EnergyPLAN	Moderate; strategic focus	Basic; macro-level	High; broad energy scenarios
Calliope	High; scenario visualisation	Moderate; includes renewables	High; macro and site-specific analysis
HOMER	High; for hybrid/ renewable systems	Detailed, Covers hybrid and renewable systems	High; hybrid and renewable scenarios

3.4. Economic and financial analysis capabilities

The economic and financial dimensions of modelling industrial process heat systems are critical, particularly for small and medium-sized industries where the economic viability of transitioning to sustainable technologies is a deciding factor but challenging due to limited data and complex long-term planning [5]. A modelling tool that can implement analyse the economic impact of policy changes is indispensable [102]. Table 5 compares the selected modelling tools based on their economic and financial analysis capabilities, highlighting their strengths and suitability for industrial process heat system modelling.

OEMOF uses built-in modules for cost breakdown and sensitivity analysis, offering robust assessments of carbon pricing impacts through scenario modelling by incorporating various carbon pricing schemes and their potential economic impacts over time [48]. While it allows users to simulate and compare policy scenarios, handling many scenarios could require significant resources and expertise due to its complexity. TRNSYS enables precise lifecycle savings assessments and dynamic scenario-based economic evaluations by including time-varying economic inputs, fluctuating fuel prices, and changing operational conditions. This dynamic approach facilitates comprehensive economic feasibility studies under various future scenarios, allowing for detailed comparisons [100]. Despite its strengths, TRNSYS might be complex to set up for multiple scenarios, potentially requiring substantial user input and detailed configuration.

EnergyPLAN offers broad strategic economic evaluations and general lifecycle cost overviews [88], but may have moderate flexibility for new scenarios due to its predefined frameworks, making it less suitable for detailed multi-scenario analysis. Calliope excels in scenario-based evaluations with advanced sensitivity analysis and detailed economic assessments [89], but its complexity could demand significant expertise and time for multiple scenarios. HOMER performs robust lifecycle cost analysis and detailed capital cost breakdowns, making it effective for hybrid and renewable energy systems [90]. However, managing numerous complex scenarios might require advanced configuration and a thorough understanding of the tool.

3.5. Sustainability and environmental impact assessment

Sustainability and environmental impact assessment are crucial in selecting a modelling tool that evaluates the transition to sustainable and environmentally friendly energy solutions [103]. By assessing tools based on their ability to support renewable integration, quantify emissions, and comply with regulations, the most suitable options for aligning with sustainability objectives can be identified. Table 6 compares the selected tools, highlighting their strengths and suitability for modelling industrial process heat systems in alignment with these critical sustainability goals.

Table 5
Comparison of economic and financial analysis capabilities.

Tool	Lifecycle Cost Analysis	Capital/Operational Cost Analysis	Fuel Price Sensitivity	Carbon Pricing Impact	Economic Scenario Analysis	Economic Modelling Flexibility
OEMOF	Detailed analysis	Detailed in-depth breakdown	Comprehensive highly responsive	Comprehensive impact assessment	Comprehensive modelling	Comprehensive highly adaptable
TRNSYS	Detailed modelling	Detailed precise evaluation	Moderate sensitive to changes	Detailed assessment	Detailed scenario analysis	Detailed adaptable modelling
EnergyPLAN	General overview	Basic cost analysis	Moderate sensitivity	Basic analysis	Basic scenario focus	Moderate adaptability
Calliope	Detailed lifespan analysis	Detailed cost breakdown	Comprehensive sensitivity	Detailed evaluation	Comprehensive scenario modelling	Comprehensive highly flexible
HOMER	Comprehensive analysis	Detailed cost breakdown	Comprehensive price analysis	Detailed impact study	Comprehensive wide-ranging analysis	Comprehensive highly adaptable

Table 6
Sustainability and environmental impact assessment.

Tool	Renewable Energy Integration	Emissions Analysis & Reduction	Lifecycle Environmental Impact	Policy Regulation Compliance	Scenario-Based Sustainability Analysis
OEMOF	Moderate effective renewable integration	Moderate emissions modelling	Comprehensive impact assessment	Comprehensive regulatory adaptability	Detailed future scenario analysis
TRNSYS	Detailed renewable system mod.	Detailed emissions reduction analysis	Moderate impact evaluation	Moderate policy adaptation	Detailed scenario comparison
EnergyPLAN	Moderate renewable energy support	Moderate emissions impact analysis	Detailed environmental assessment	Comprehensive regulatory compliance	Moderate scenario evaluation
Calliope	Detailed renewable energy focus	Detailed emissions strategy modelling	Detailed overall impact assessment	Comprehensive policy and regulation fit	Comprehensive sustainability scenarios
HOMER	Moderate renewable energy use	Moderate emissions analysis	Moderate lifecycle evaluation	Moderate policy compliance	Moderate future sustainability analysis

OEMOF can be coupled with life cycle assessment (LCA) tools to assess the environmental impacts of energy systems throughout their entire lifecycle. The LCA procedure within OEMOF follows steps like goal and scope definition, inventory analysis, impact assessment, and interpretation, ensuring a comprehensive environmental evaluation [104]. TRNSYS offers advanced capabilities for sustainability and environmental impact assessment by integrating renewable energy sources, modelling emissions, and performing lifecycle environmental impact evaluations over the system's operational life [105]. It supports renewable energy systems like solar-assisted desiccant cooling [87].

EnergyPLAN facilitates comprehensive system-wide planning and long-term impact assessments through its holistic approach to energy system modelling, including interactions between different sectors for thorough environmental evaluations and regulatory compliance [88]. Calliope offers high flexibility in renewable energy integration and advanced emissions strategy modelling, supported by robust optimisation algorithms and high temporal and spatial resolution. This enables detailed sustainability scenario analysis and environmental impact assessments. While Calliope does not directly conduct LCA, its capabilities support such assessments through integration with external LCA tools and databases [101]. HOMER simulates and optimises system configurations, aiding in evaluating the economic and environmental viability of renewable energy solutions. HOMER's lifecycle evaluations further support renewable energy integration and policy compliance, making it versatile for future sustainability analysis [90].

3.6. Practical considerations

Practical considerations significantly influence the tool's feasibility and ease of adoption in real-world industrial settings, where resources and expertise may vary [106]. Key factors include accessibility, cost, support, academic or commercial origins, user-friendliness, and expertise development requirements. Accessibility encompasses how readily users can obtain and start using the tool, whether it's freely available or requires purchase [102]. Cost includes initial and ongoing expenses, with commercial tools often being more expensive, impacting affordability [107]. Support refers to the quality of resources like manuals, videos, training, forums, and direct assistance [30]. The tool's academic or commercial nature can indicate its target audience and cost structure [108]. User-friendliness assesses the ease of use and intuitiveness of the tool, important for industries without specialised modelling teams [109]. Expertise development looks at the time and effort needed to become proficient with the tool, affecting its practicality for industries with limited training resources [30]. Table 7 provides a comparative analysis of these practical considerations across the selected modelling tools.

OEMOF is accessible and free but requires significant expertise, posing challenges for researchers with limited modelling experience [110]. TRNSYS, while providing robust support, may be cost-prohibitive for smaller research projects but includes all source codes, making it potentially open source with comprehensive support [87]. EnergyPLAN offers balanced accessibility and support, suitable for cost-effective solutions with moderate learning requirements [88]. Calliope is highly accessible as an open-source tool but demands considerable learning investment, which can be challenging for researchers with limited training resources [111]. HOMER is user-friendly with comprehensive support, making it ideal for researchers seeking ease of use, although its cost might be a barrier for smaller research projects [90].

4. Tool selection process

A systematic tool selection process was devised to facilitate the identification of the most suitable modelling tool for techno-economic analysis and environmental assessment of industrial process heat systems. This methodical approach, inspired by the rigorous framework provided by Sandia National Laboratories [27], has been customised to address the unique technical, economic, and environmental factors associated with the comparison of technologies.

4.1. Establishing evaluation criteria and quantitative scoring

In the initial stage, the modelling tools' capabilities, as outlined in Tables 2–7, are classified as 'essential', 'desirable', or 'not applicable'. This approach facilitates a detailed quantitative analysis, essential for

Table 7
Practical considerations.

Tool	Accessibility	Cost	Support	Academic/ Commercial	User-Friendliness	Expertise Development
OEMOF	Open source; downloadable	Free	User manual, videos, training, online forum	Academic	Medium	High investment required
TRNSYS	Open source; downloadable	5060 USD* (single user)	Comprehensive user manual, online forum	Commercial	High	Significant investment in time to gain proficiency
EnergyPLAN	Free; browser-based or downloadable	Free	User manual, online forum, contact details	Academic	Medium	Moderate investment required
Calliope	Open source; downloadable	Free	User manual, training, online forum	Academic	Medium to high	High investment required
HOMER	Commercial; downloadable	500–1500 USD	Comprehensive user manual, videos, training, online forum	Commercial	High	Moderate investment required

identifying critical features for techno-economic and environmental evaluations. This scoring mechanism is designed to be flexible, accommodating the specific conditions and demands of the site under review. It considers regional resources, environmental factors, and policy frameworks, thereby underscoring the process's adaptability to the unique geographical and regulatory context of the location. The methodology prioritises input data flexibility and other pertinent features based on the site's distinct requirements, ensuring an exhaustive and precise tool selection process for informed, scenario-specific decision-making. The evaluation of each capability follows a scoring system of 2, 1, or 0, according to its alignment with 'essential' or 'desirable' criteria. Fully satisfied 'essential' capabilities receive a 2, partially met a 1, and unmet a 0. 'Desirable' capabilities are scored similarly, with full satisfaction earning a 1 and unmet a 0, while 'not applicable' capabilities are omitted to streamline the analysis.

For instance, consider the necessity for a tool to furnish demand profiles, weather data, and renewable generation supply profiles from limited input data, such as location and demographics. Such capabilities would be considered 'essential', with the tool's ability in these areas scored accordingly. Conversely, if a user possesses existing data for demand, weather, and renewable generation (e.g., from monitored data), these capabilities become 'not applicable' and are excluded from further analysis. If the sourcing and generating of this input data are feasible but require significant effort, these capabilities would be marked as 'desirable', with scores assigned based on the tool's efficacy. This detailed scoring system is demonstrated in Table 8 through a simplified case study example, which will be described in more detail in the following section.

4.2. Example application of the modelling tool selection process: New Zealand

The application of the tool selection process and evaluation criteria developed in this study is demonstrated through a case study of New Zealand's industrial process heat systems. In New Zealand, process heat accounts for a significant proportion of energy consumption and emissions, with fossil fuels like coal and gas being the primary sources [112]. Process heat contributes to approximately 8 % of gross emissions in New Zealand. Fossil fuels, particularly coal and gas, supply 56 % of process heat and are responsible for emitting 8.8 million tonnes of CO_2 in 2020, which is about 29 % of the country's overall energy emissions [113]. The manufacturing industry is the largest consumer of process heat, utilising it predominantly for low to medium-temperature needs [114]. The importance of transitioning to sustainable heating solutions is underscored by New Zealand's commitment to emission reduction goals [115], necessitating a deeper understanding of energy consumption patterns across various sectors [116].

The current energy landscape for process heat in New Zealand is marked by a reliance on fossil fuels, contributing substantially to emissions [113]. However, there is a growing interest in alternative sources like electricity, bioenergy, and geothermal energy [116]. The imbalance in emissions contribution between different fuel types, such as the disproportionate impact of coal compared to its usage, highlights the need for a strategic shift towards more sustainable heating solutions [117].

The extensive use of boiler systems in New Zealand, often extending beyond their intended lifespan, presents both challenges and opportunities for technology transition to renewable energy sources like biomass and electricity [118]. These alternatives, essential for the country's decarbonisation efforts, encounter like biomass's significant storage needs due to its lower energy density and the fluctuating biomass market [119], as well as the variability in electricity generation from hydroelectric power sources, which can impact reliability [120]. There is a significant gap in comprehensive evaluations of these alternatives, especially for site-specific needs [121]. The deployment of advanced modelling tools, capable of simulating diverse technological, economic, and policy scenarios, is essential for a thorough evaluation. These tools could play a key role in facilitating the seamless integration of new technologies through comprehensive economic and environmental analyses, adjusting to changes, and making informed decisions that are in harmony with New Zealand's unique industrial landscape and supportive of policies like the Emissions Trading Scheme and governmental initiatives [122].

Insights from the Heat Demand Database [123], Regional Heat Demand Database (RHDD), and the Regional Energy Transition Accelerator (RETA) [124], initiatives by the New Zealand Energy Efficiency and Conservation Authority (EECA), provide a foundational understanding of energy use across various regions. These resources, along with additional data from publicly available reports and industry-specific studies, offer broad insights into energy demand patterns and technology adoption. However, the data lacks the granularity required for detailed modelling, particularly concerning site-specific operational parameters of boilers, such as load variability, efficiency profiles, and operational hours. This limitation poses challenges for accurate demand profile simulations and highlights gaps in targeted data collection by governmental agencies. Addressing these gaps requires a flexible modelling framework capable of integrating hybrid approaches, such as stochastic modelling, which are particularly effective in compensating for limited or incomplete datasets. Such frameworks can ensure robust analyses and more reliable insights into the transition to sustainable energy systems.

A detailed review of the technical specifications of the modelling tools, as summarised in Tables 2 and is crucial for evaluating process heat users in New Zealand. These tools offer objective functions addressing operational efficiency, cost-effectiveness, and sustainability. Modelling methods are pivotal in managing uncertainties and capturing dynamic system behaviours. While flexibility in programming languages like Python and MATLAB aids customisation, seamless integration with industrial settings is paramount. Scalability and integration capabilities ensure the tools' applicability to diverse system complexities and emerging technologies, supporting both site-specific and broader regional or national analyses.

The input data requirements, detailed in Table 3, are crucial for comparing heating technologies. Accurate demand profiles are key to capturing the diverse energy use patterns of both traditional and sustainable systems. Modelling tools must simulate techno-economic parameters, such as biomass reliability and hydroelectric power variability, while remaining effective with limited data, particularly across varying industrial scales. Generating hourly or sub-hourly demand profiles is essential for precise sizing studies and leveraging time-of-use electricity tariffs, potentially making electrification more competitive with fossil fuels. Flexibility in data input is equally critical to accommodate diverse formats and ensure adaptability to New Zealand's industrial landscape. While embedded functions and libraries support the process, priority should be given to accurate demand profiling and input flexibility.

Enhanced data visualisation and reporting, as highlighted in Table 4, are critical for helping stakeholders interpret complex results, supporting informed decision-making, and advancing initiatives like the GIDI Fund. Effective tools must clearly convey the costs and benefits of sustainable technologies to align with New Zealand's renewable energy goals. Scenario comparison capabilities are equally essential, offering valuable insights into system.

The economic analysis outlined in Table 5 encompasses lifecycle cost analysis, sensitivity to fuel price fluctuations, carbon pricing impacts, and economic scenario evaluation. An effective tool must assess the economic viability of each technology, considering capital investments, operational expenses, and necessary infrastructure upgrades for integrating new solutions. This comprehensive approach enables industries in New Zealand to make informed decisions by balancing upfront costs with long-term benefits, fostering sustainable and cost-effective process heat solutions. While economic modelling flexibility is valuable, priority should be given to accurately evaluating lifecycle costs, sensitivity to key variables, and scenario-based impacts.

Sustainability and environmental considerations, as detailed in Table 6, are critical for aligning with New Zealand's environmental standards and sustainable energy goals. Key factors include renewable energy integration, emissions analysis and reduction, and compliance with policy regulations. These elements are essential for enabling modelling tools to support the transition to sustainable energy, quantify emissions reductions, and adhere to evolving environmental policies. Additional factors, such as lifecycle environmental impact assessments and scenario-based sustainability analyses, provide deeper insights into the ecological effects and long-term viability of energy solutions. Incorporating Marginal Abatement Cost (MAC) calculations is also vital for evaluating the cost-effectiveness of emissions reduction strategies, ensuring a balanced approach that integrates economic and environmental priorities.

Practical considerations, outlined in Table 7, are crucial for ensuring a tool's applicability in New Zealand's industrial contexts. Key factors include feasibility, cost-effectiveness, robust support, accessibility, and ease of use. The ability to incorporate real-time data enhances the framework's responsiveness, while open-source tools offer greater flexibility and promote higher adoption rates through customisation and accessibility. Engaging local stakeholders further ensures practical relevance and user satisfaction. Additionally, investing in user training and capability building enhances the tool's effectiveness, making it both technically robust and practically viable for diverse industrial applications.

The scoring system in Table 8 quantitatively assesses each tool, focusing on those that demonstrate comprehensive analysis capabilities required in New Zealand. Each tool's overall score is calculated by aggregating its performance across all criteria. The average score, determined by dividing the total scores of all evaluated tools by the number of tools, serves as the benchmark for comparison. In this analysis, tools scoring below the average value of 35 are classified as 'Fail', while those scoring above this threshold are classified as 'Pass'. This clear demarcation ensures that our focus is directed towards tools that demonstrate the highest capability for the comprehensive analysis required in New Zealand. By explicitly defining the average score, we provide a transparent basis for evaluating and comparing tool suitability.

5. Discussion

The evaluation of tools for modelling process heat in New Zealand, as summarised in Table 8, provides critical insights into their applicability

Table 8
Scoring of modelling Tools for New Zealand case study.

	Evaluation Criteria	OEMOF	TRNSYS	EnergyPLAN	Calliope	HOMER
Objective Function Range	**E**	2	2	1	2	1
Modelling Method	**E**	1	2	1	1	1
Modelling Language	**D**	1	0	0	1	0
Demand Profile Generation	**E**	1	2	0	1	0
Data Input Flexibility	**E**	2	2	1	2	1
Embedded Functions & Libraries	**D**	1	1	0	1	0
Data Visualisation & Reporting	**E**	2	2	1	2	2
KPI Presentation	**E**	2	2	1	2	2
Scenario Comparison	**E**	2	2	2	2	2
Lifecycle Cost Analysis	**E**	2	2	1	2	2
Capital/Operational Cost	**E**	2	2	1	2	1
Fuel Price Sensitivity	**E**	2	2	1	2	2
Carbon Pricing Impact	**E**	2	2	1	2	1
Economic Scenario Analysis	**E**	2	2	1	2	1
Economic Modelling Flexibility	**E**	1	1	0	1	1
Renewable Energy Integration	**E**	2	1	1	2	1
Emissions Analysis & Reduction	**E**	1	2	1	1	1
Lifecycle Environmental Impact	**D**	1	2	2	1	1
Policy Regulation Compliance	**D**	1	1	1	1	0
Scenario-Based Sustainability	**E**	1	1	2	2	1
Tool Accessibility	**E**	2	2	2	2	1
Tool Cost	**E**	2	0	2	2	1
Tool Support	**E**	2	2	2	2	1
User-Friendliness	**E**	1	2	2	1	2
Expertise Development	**E**	1	2	1	1	2
Met Essential Capabilities		Pass	Pass	Fail	Pass	Fail
Overall Score		39	41	28	40	28

D = Desirable, E = Essential.

and feasibility. Tools such as TRNSYS, Calliope, and OEMOF meet the essential capability threshold, demonstrating potential for either building the New Zealand process heat model directly on their platforms or leveraging their approaches, modules, or methods within a customised modelling framework. In contrast, HOMER and EnergyPLAN scored below the threshold, reflecting significant limitations in addressing sector-specific requirements. This analysis highlights the importance of modularity, flexibility, and integration capabilities to effectively manage the complexity of industrial energy systems, underscoring the value of open-source modelling approaches.

TRNSYS demonstrated exceptional simulation capabilities, making it ideal for detailed thermodynamic process analysis and renewable energy integration. Its utility in modelling complex systems like solar-assisted process heat or high-temperature heat pumps is noteworthy. However, its reliance on a FORTRAN-based architecture and proprietary design limits seamless integration with modern tools and open-source libraries, restricting its flexibility in large-scale scenario management and iterative analyses. The steep learning curve and technical expertise required further limit its accessibility for rapid assessments or non-expert users. While well-suited for site-specific thermal analysis, additional tools are often needed to comprehensively address techno-economic aspects. In New Zealand, where biomass and electricity dominate renewable energy options, TRNSYS's versatility supports advanced integration scenarios. However, its lack of scenario management, interoperability with modern platforms, and user accessibility highlights the need for refinement and supplementary integration layers.

Calliope, with its robust capabilities in renewable energy system analysis, excels in scenario comparison and system optimisation, making it a valuable tool for high-level energy transition planning. Its flexible framework supports diverse objectives and constraints, allowing for customisation in renewable integration scenarios. However, Calliope's deterministic nature and simplified representation of thermal processes mean it lacks the granularity required for detailed modelling of process heat systems with complex hybrid configurations. While its open-source nature enhances adaptability, integrating Calliope into a broader framework for industrial applications would require significant modifications, such as adding modules for high-temperature heat processes or hybrid energy systems.

OEMOF provides a modular, open-source framework that supports extensive customisation for techno-economic analysis across diverse energy systems. While it excels in flexibility and adaptability, its lack of native capabilities for modelling high-temperature industrial process heat systems—often characterised by dynamic loads and complex thermal processes—limits its immediate applicability to the sector. Addressing these gaps would require significant user-driven development, including the addition of specialised modules or integration with external libraries. However, OEMOF's compatibility with broader frameworks and its potential for hybrid modelling approaches enhance its value for flexible system analysis. This adaptability positions OEMOF as a resourceful tool for integrating diverse energy systems but highlights the need for complementary tools to meet the specific needs of industrial process heat applications.

EnergyPLAN and HOMER excel in macro-level energy planning and hybrid renewable system optimisation, but both fall short in addressing the unique demands of industrial process heat systems. EnergyPLAN's deterministic framework, reliant on predefined inputs, restricts its capacity to model dynamic, site-specific scenarios or adapt to varying operational conditions. Similarly, while HOMER is effective in hybrid electrical system optimisation, it lacks the functionality to model high-temperature thermal processes or intricate hybrid configurations required for industrial applications. Although useful for preliminary designs and large-scale planning, neither tool offers the scalability or depth needed for detailed, site-specific industrial process heat analysis, limiting their broader applicability in this domain.

A significant challenge in assessing energy modelling tools lies in their validation against real-world data. Most tools have not been rigorously benchmarked against empirical datasets, especially for industrial process heat systems like steam boilers, heat pumps, and air heaters. Instead, many rely on design assumptions, raising doubts about their accuracy and practical applicability. Complex factors such as dynamic loads, maintenance patterns, and site-specific conditions often go unaddressed. The absence of standardised validation protocols and peer-reviewed examples further limits objective evaluation and comparison. Overcoming these challenges requires integrating high-resolution operational data, developing diverse industrial case studies, and adopting standardised benchmarking frameworks. Hybrid modelling approaches that combine deterministic sizing with stochastic demand variability are essential for aligning tools with real-world conditions.

Emerging tools that enhance modularity and flexibility, such as BlueSky [24], a prototype recently released by EIA, while requiring further evaluation and implementation, exemplifies a new paradigm in energy modelling. BlueSky's modular architecture supports the integration, adoption, or modification of capabilities from various tools, making it adaptable to diverse use cases. This flexibility facilitates hybrid modelling approaches, enabling detailed analyses across multiple scales and scenarios. By addressing specific limitations of other tools, BlueSky can serve as a unifying platform for integrating diverse data streams, conducting scenario analyses, and delivering both site-specific and regional outputs. Additionally, its capacity to incorporate real-time data and leverage advancements in artificial intelligence, including large language models, underscores its potential for automated scenario generation, enhanced demand profile simulation, and dynamic synthesis of insights from multiple tools. Future research should explore BlueSky's potential to foster a more integrated and efficient modelling ecosystem, advancing the capabilities of energy systems analysis.

6. Conclusion

Decarbonising the industrial sector presents a significant challenge that demands precise and robust modelling tools to support strategic decision-making. This study reviewed 25 energy system modelling tools, identifying five with potential for technical, economic, and sustainability analysis of industrial process heat systems. The tools' capabilities were systematically categorised to form a structured selection process, offering guidance for analysing New Zealand's process heat systems. Key strengths, limitations, and opportunities for improvement were discussed, highlighting gaps in applicability and the need for enhanced tool development.

A systematic selection process remains essential to identify and customise tools to meet specific requirements. Ensuring tools operate effectively at site-specific and regional levels will be vital for advancing New Zealand's transition to low-carbon industrial energy systems. Tools like TRNSYS, Calliope, and OEMOF show promise for site-specific and scenario-based modelling but do not fully address the diverse and complex requirements of industrial process heat systems in New Zealand. While TRNSYS excels in thermodynamic simulation, Calliope offers flexibility for energy transition planning, and OEMOF provides modularity for customisation, all require significant refinement to improve usability, adaptability, and thermal process modelling. This underscores the importance of tools capable of integrating detailed site-specific analysis with broader energy system objectives.

Future research should focus on validating these tools with empirical data and conducting high-resolution case studies tailored to New Zealand's industrial energy systems. Hybrid modelling approaches, leveraging the strengths of multiple tools, present an opportunity to address these gaps. Platforms like Project BlueSky exemplify this direction, with their modular architecture and real-time data capabilities offering a promising framework for scalable and adaptable modelling ecosystems.

CRediT authorship contribution statement

Ahmad M. Lahijani: Conceptualization, Methodology, Writing – original draft. **Michael D. Protheroe:** Funding acquisition, Review & Editing, Supervision. **Michael Gschwendtner:** Review & Editing, Supervision.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Michael D. Protheroe reports financial support was provided by Auckland University of Technology. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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During the preparation of this work the authors used the services of ChatGPT in order to enhance the English language quality. The usage of ChatGPT was instrumental in refining the clarity and readability of our text. Subsequent to employing this tool, the authors meticulously reviewed and revised the manuscript to ensure accuracy and integrity of the content. The responsibility for the final publication content rests entirely with the authors.

Data availability

No data was used for the research described in the article.

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