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SPECIALTY GRAND CHALLENGE
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Specialty Grand Challenge for Thermal System Design

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INTRODUCTION

Thermal Systems has been an integral part of our society as a main way of providing energy for peoples' day-to-day living as well as industrial activities. Thermal systems are at the heart of energy infrastructure because the generation, distribution, recovery, utilization and storage of energy is related with the transformation, exchange or transfer of thermal heat to another form of energy. Continuous and dedicated efforts from industrial and academic communities have been made to the development of materials, components, equipment, processes and systems for thermal energy technologies, while societal and industrial importance in thermal systems have been fully acknowledged, and its economic benefits have been widely appreciated for generation by generation.

Contrary to scientific achievements made for the improvement of thermodynamic efficiency and economics of thermal systems, little attention has been being paid to the sustainable generation and utilization of thermal energy. Recognition of global climate change and its negative impact on society has driven us to turn our focus on the development of net-zero energy technologies and its implementation in our industrial and district thermal systems. The introduction of policies for cutting CO_2 emissions and a wide range of pledges for achieving net-zero by 2050 from various countries and companies clearly demonstrate urgency and importance of speeding up the transition of conventional thermal systems to sustainable one. However, it is not straightforward in practice to achieve rapid transition to the carbon-free thermal systems. For the last few centuries, the thermal conversion of fossil fuels has played a main role for generating energy, and industrial and domestic energy systems are equipped with devices and units which are optimized with the utilization of combustion heat from fossil fuels. Clean sources of energy, for example, biomass, renewable, hydrogen, etc have different thermodynamic properties and thermo-physical behaviour, which often requires fundamental changes from materials to system integration of existing fossil-fuel-based technologies. Also, most of net-zero energy technologies are not technologically mature to be readily available for end-users or are not economically viable enough to be competitive to fossil fuel-based technologies.

In order to deal with such difficulties and drawbacks related to the introduction of net-zero technologies, various R&D activities should be carried out for achieving the energy-efficient and cost-effective use of renewable energy. When new materials are synthesized or equipment is fundamentally upgraded for net-zero thermal systems, technical advances made from such development should be strategically integrated to the existing energy systems or be evolved to propose new paths for the sustainable utilization of thermal energy for the future. On the other hand, scientific efforts for the development of net-zero energy technologies in these days are made in a multi-disciplinary and multi-scale manner, covering various subjects of natural science and engineering from quantum and molecular simulation to process design and system integration, which demands multi-physics modelling from quantum scale to macro-scale. Under current diverse and complex research environments, "*design*" becomes more a critical and essential discipline than ever for the development of thermal systems technologies, as thermal systems should be "*designed*" holistically to select the most appropriate units, to determine the optimal system configuration and to satisfy multiple objectives, aiming maximum energy efficiency in a most safe working conditions at minimum cost expenditure and environmental emissions.

The effective and systematic design of thermal systems is not only necessary to provide system-wide technical solutions for overcoming scientific challenges, but also to suggest sustainable guidelines for further R&D actions required from scientific communities. This article, first, discusses grand challenges being faced and actions being undertaken for achieving net-zero thermal systems, which is, then, followed by emphasizing the scientific role of design and its importance for shaping future thermal systems.

THERMAL SYSTEMS UNDER NET-ZERO ENERGY MIX

Conventional thermal systems mainly involve thermochemical reactions for converting fossil fuels into energy directly, or other products to be used for energy generation indirectly. The main product from the thermal conversion of fuels is heat which has been a main energy source for industrial manufacturing and domestic applications. The direct supply of heat is not always practical or economic, and the transfer of heat over the distance is widely practiced. The transfer of heat is typically made with the aid of energy carriers, mainly steam and electricity. The conversion of heat to steam demands various supporting facilities, for example, for the treatment of boiler feedwater, the distribution of steam to end-users, the management of steam condensate, etc., and the economy of scale is the important issue for the selection of steam-based heating systems. The use of electricity makes it relatively easy to distribute and transmit to remote end-users and a simple machinery configuration may be maintained, compared to steam-based systems. However, cogeneration of steam and power is common, which is an energy-efficient way of utilizing available heat in practice. A wide range of components, equipment or units are then employed to utilize, exchange, transform or recover thermal energy to another form of energy. In-depth knowledge and a rich database for the creation, design, operation and integration of thermal systems have been accumulated over a long period of time.

In order to combat climate change, rapid transition for the decarbonization of thermal energy systems is urgently demanded. This can be achieved with various ways: accommodating new energy-generation technologies based on renewable sources, for example, solar and wind energy, replacing fossil fuels with carbon-less or zero-emission energy sources, for example, electrification, hydrogen and biomass energy, or using fossil fuels in decarbonized manner, for example, CCUS (Carbon Capture, Utilization and Sequestration). Other than these measures, IEA (2021) presented another two elements of decarbonization pathways as behavioural changes and energy efficiency. These changes require the fundamental transformation of current mechanisms for energy generation and its utilization in thermal systems, which presents considerable challenges to the design of thermal systems.

CHALLENGES OF THERMAL SYSTEM DESIGN: COMPLEXITY

Knowledge of thermal systems design has been largely built up through investigating system performances and operating characteristics of centralized systems in a steady-state domain, while considerable attention has also been paid to the dynamic behaviour of energy systems and its control. A number of generic design methodologies to support engineers' decisions are readily available and well-established for improving energy efficiency of thermal systems under steady-state conditions. Thermodynamic-based tools, typically, based on the graphical representation of the quantity and quality of available heat or its potential for further use, have been developed, for example, minimizing system-wide energy consumption with the use of Energy Composite Curve (Smith, 2016), designing the heat recovery network using energy pinch concept (Kemp and Lim, 2020), maximizing plant-wide steam recovery with the aid of Site Profiles (Sun et al., 2015). Mathematic-aided tools had been also proposed for dealing with a large-size design problem having complex objectives or multiple constraints, for example, minimizing irreversibility of energy systems with Exergy analysis (Dincer and Rosen, 2020) and optimizing the configuration of thermal systems with superstructure approach (Aguilar et al., 2007).

Due to fast growing contribution from solar and wind energy in energy sectors (IRENA, 2021), thermal systems are being evolved to be more resilient and robust without compromising energy efficiency and cost-effectiveness under the intermittent supply of energy sources and time-dependent end-use of thermal energy. This requires a shift in our design activities from the steady-state evaluation of traditional thermal systems to time-dependent and sequence-oriented modelling, simulation and analysis of net-zero thermal systems. The use of energy-efficient storage of heat and its re-utilization in a time-delayed manner increases design complexities considerably, because the most appropriate way of recovering, storing and reusing available heat should be identified for maintaining high performance of thermal systems through system-wide investigation of multiple units simultaneously.

Technical progress in thermal systems is typically made with the introduction of multi-functional materials, the hybridization of different technologies, the addition of new subsystems for energy-efficient thermal management or decarbonization which results in complexity in system configuration and its operating control.

In the context of development of new thermal systems, it would be invaluable for scientists and engineers to have systematic design methodologies for managing design complexities of net-zero thermal systems effectively, which can support combinatorial decision-making as well as help to gain conceptual insights and design guidelines for complex thermal systems. However, the development of more generic and system-wide design methodologies under highly-integrated and dynamic operating conditions are rather limited, mainly due to numerical complexities related to dynamic equations and its computation, as well as system complexities related to multi-layered integration. Such development allows to screen a wide range of net-zero design options available and to evaluate its techno-economic impact, with which the optimal design of net-zero thermal systems can be systematically identified in confidence, together with strategic selection of operating conditions.

CHALLENGES OF THERMAL SYSTEM DESIGN: SCALE-UP AND SYSTEM DEVELOPMENT

A wide range of design options are proposed, compared, evaluated and modified throughout the whole lifecycle of process development until the flowsheet of thermal systems is finalized and corresponding mass and energy balances are determined. The consideration of design options is made in an iterative and interactive way with all the stages of process development, including laboratory experiments, bench-scale tests, pilot plant tests and demonstration. This interaction is very critical for ensuring system integrity and technical feasibility.

As the prototype or pilot plant is constructed and time-consuming testing with them is carried out, considerable time is inevitably required for process and system development in industries, for example, 8 years from the initial ideas to the commercial-scale production in chemical industries (Vogel, 2005). Although the integrated management of process development activities can reduce the overall duration, the minimization of system development time may not be straightforward, due to unavailability in thermophysical data, uncertainty during system scale-up and incomplete process knowledge. Modular design of units may be an option to increase the production scale or capacity to a certain extent and such flexibility has trade off relationship with economic benefit through the economy of scale.

As active, rapid and thorough implementation of net-zero technologies in our society is necessary in order to meet our goals of net-zero ambition by 2050, cutting development time of net-zero thermal systems as practically down as possible would be highly desired. Various aspects in process development can be supported with computer-aided design and high-performance computing. Computational chemistry is widely used to compute structures, properties and interactions of molecules, which allows to identify novel chemicals or materials, or to predict chemical phenomena or physical properties. Computer-aided materials design based on molecular dynamics, machine-learning techniques, etc., is also useful to understand material's chemistry and physics at atomic levels, which supports the exploitation of functional materials and finds the tailored-made novel materials. With these developments, considerable effort and time required to gather thermodynamic and physical properties, or to search for innovative next-generation energy materials, can be significantly saved.

The design of thermal systems includes the selection of materials or components or units to be used, the choice of the most appropriate configuration and the determination of adequate integration between subsystems, and the strategic balancing act between economic gains and practicality. Hence, the development of new thermal systems inherently involves the investigation of a large number of promising design options, which demands not only resources but also time. Computer-aided process design can play an important role to contribute to the reduction of development time. Combinatorial decision-making can be systematically assisted by mathematical optimization, which can perform complex economic and/or environmental trade-offs for key design variables and suggest the optimal system structures and operating conditions, considering constraints and practical limitations. Repetitive experimentation and time-consuming manual pilot tests required during the system development phase can be effectively minimized with the aid of theoretical computation and simulation.

It is believed that the scientific progress in automated design tools for thermal systems would be one of key research areas to be focused, because such development enables us to fully appreciate the sustainable benefits of net-zero thermal energy and to significantly enhance the uptake of net-zero thermal technologies in industries and communities.

CHALLENGES OF THERMAL SYSTEM DESIGN: HYDROGEN AND ELECTRIFICATION

Fossil fuels has been a main player in power and energy sectors. Due to threats related to climate change and urgent needs for clean energy, renewable electricity is expected to be the main contributor for the power industry and hydrogen is considered as one of main energy carriers for the future. Traditional thermal systems are mainly based on the heat generated from the combustion of fossil fuels, which is further exploited for power generation. For example, thermal systems in manufacturing industries typically includes steam boilers, gas turbines and furnaces based on fossil fuels, and steam and power generated is then distributed and serviced for various units in the plant.

The fuel switching from fossil fuels to hydrogen and renewable electricity requires drastic transformation of current thermal systems. Existing combustion and thermal technologies should be adapted to accommodate heat generation from the burning of hydrogen or to facilitate the utilization of hydrogen-derived fuels in energy generation. Great care should be given for the replacement of combustion-based heat supply with electricity-based one in industrial manufacturing, because the production is heavily interacted with heat supply and, furthermore, the supply of heat or its recovery is an in-built element of production systems.

Very active engagement of various industries for the implementation of electrification has been observed, including cement, steel, refinery, chemical, etc, in which a wide range of electricity-driven technologies, for example, electrode boiler, electrified heater[1] and heat pump are considered. Although a range of technologies for fuel switching and industrial electrification has high TRLs (Technology Readiness Levels)

[1]Electrified heating includes induction heating, electric arc heating, infrared heating, plasma heating, microwave heating and resistance heating.

and are available for commercial applications, significant "design" work is still needed for industrial implementation (Element Energy & Jacobs, 2018). The introduction of hydrogen-based heating and electrification in industries affects not only individual energy balance for unit levels, but also fuel balances and utility management for the whole system, which requires the identification of the most economic combination for low-carbon technologies among possible routes or options. As the optimal solution for the integration of hydrogen energy and electrified heating is highly likely to be very application-dependent and case-specific, scientific needs for improving our skills and know-hows in system design are clearly necessary for the development of thermal systems technologies.

CONCLUDING REMARKS

Climate change demands urgent actions to be taken for the development of net-zero thermal technologies with significant impacts on and contribution to building a low-carbon society. Key technical challenges being faced in the academic and industrial communities of thermal systems design are discussed, which author would like to take as opportunities rather than difficulties. The "Thermal System Design" section of "Frontiers in Thermal Engineering" publishes original theories and rigorous research results of all aspects of process design and system integration for thermal systems. The "*design*" of thermal systems represents the creative act of defining the types and features of thermal energy in the form of products or processes, which can systematically and effectively support scientific decision and engineering judgement for achieving sustainable solutions for thermal systems. It is, therefore, believed that this "Thermal Systems Design" section is vital to provide original contribution to the knowledge and to bring new breakthroughs in thermal management and engineering. Also, this section will play a key role in providing an exciting forum for our researchers and engineers by sharing the innovation, research, development and demonstration of thermal systems design.

AUTHOR CONTRIBUTIONS

The author confirms being the sole contributor of this work and has approved it for publication.

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