Innovation and advancement of thermal processes for the production, storage, utilization and conservation of energy in sustainable engineering applications

Milan Vujanović[1], Giorgio Besagni[2], Neven Duić[1], Christos N. Markides[3]***

[1] Faculty of Mechanical and Naval Engineering, University of Zagreb, Zagreb, Croatia

[2] Polytechnic University of Milan, Milan, Italy

[3] Clean Energy Processes (CEP) Laboratory, Department of Chemical Engineering, Imperial College London, London, United Kingdom

* Corresponding author. E-mail: milan.vujanovic@fsb.hr

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Abstract

This vision paper accompanies a special issue of Applied Thermal Engineering dedicated to the 16th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES) held in Dubrovnik in 2021, and summarizes a selection of articles presented at the conference. At the focal point are a range of topics related to thermal processes as these arise in energy production, storage, utilization and conservation, covering fundamental research, the development of technical solutions for diverse sustainable engineering applications, technoeconomic analyses, and issues relating to the potential and integration of technologies from higher-level approaches. Thermal processes are the basis of numerous sustainable engineering applications and their understanding and improvement are increasingly required in the context of improved resource use efficiency and reduced environmental impact. Applications of interest include thermal systems used in buildings, thermochemical processes, seawater treatment, thermal storage solutions and renewable energy resource use. Emerging challenges in this space have given an opportunity to scientists, researchers and engineers to actively contribute to the development of relevant technological solutions, which are covered briefly in the present paper.

Keywords: thermochemical processes, thermal storage, thermal systems in buildings, heat pumps, solar thermal systems, seawater treatment

1. Introduction

The Sustainable Development of Energy, Water and Environment Systems (SDEWES) conference series takes the form of regular international gatherings aimed at bringing together leading scientists and professionals tackling problems related to energy, water and environment systems. The conferences have maintained successful cooperation with scientific journals [1], participating in special issue organization, and promoting the development of common scientific topics and research [2]. The 16^{th} SDEWES Conference, which was held from the 10^{th} to the 15^{th} of October 2021 in Dubrovnik, Croatia, brought together 630 scientists, researchers, and experts from 58 countries working in the field of sustainable development. Over 670 oral presentations were given in total, spread over 13 sessions, with 223 onsite participants presenting 219 papers in person.

The *Special Issue* of Applied Thermal Engineering within which the present vision paper is included has been dedicated to the 16^{th} SDEWES Conference. This effort presents an initial cooperation between SDEWES and *Applied Thermal Engineering*, focussing on the application of novel technologies for the advancement of thermal systems. The *Special issue* includes thirteen papers presented at the conference, selected based on the common challenges of improved production, storage, utilization and conservation of energy in sustainable engineering systems. Research covering experimental and computational approaches, fundamental topics and novel applications is included spanning the following five topics: (i) thermal systems in buildings, (ii) thermochemical processes, (iii) seawater treatment, and (iv) thermal storage and renewable energy sources. This vision paper provides an overview of the papers included in the *Special Issue*, as well as a review of current research topics and state-of-the-art applications.

2. Thermal systems in buildings

In accordance with the International Energy Agency (IEA) report for 2020, energy use for buildings amounts to 36% of global energy use combining residential, non-residential, and building construction sectors. CO_2 energy-related emissions for the same sectors amount to 37% of direct and indirect emissions [3]. CO_2 emissions decreased in 2020, but mainly due to the Covid 19 pandemic (closed hotels and restaurants, home office, etc.) and do not signal a new trend but rather a temporary deviation. In the building sector, the most rapid increase in energy usage is for space cooling, emphasizing the need for more efficient systems. Driven by existing emissions reduction policies and government incentives, energy efficiency investment in buildings was boosted in 2020. Almost half of the investments are for the construction of new efficient buildings, while the rest is invested in energy-related retrofits.

One of the ways to retrofit old buildings is the integration of renewable energy sources. Old buildings' refurbishment is an important issue, especially in countries with predominantly older residential buildings with inferior energy performance. In the case study presented in Ref. [4], several methods are used to increase the building's thermal efficiency. A dynamic simulation incorporating the use of CO_2

heat pumps for space heating integrated with a photovoltaic (PV) field and Li-ion battery along with improved thermal insulation of the building envelope is investigated. The results show that deploying all refurbishment solutions leads to a 52% energy reduction and 49% of CO_2 reduction per year. From the economic standpoint, the final user will have a payback in 4 years with a Net Present Value over 27 k€. Calise et al. [5] carried out a similar analysis relying on more renewable energy system (RES) implementation. In this research, a novel hybrid RES comprised of building integrated PV panels and a small-scale wind turbine is used. The dynamical model is tested on a case study for a hotel building in which HVAC energy is supplied by an electrically driven heat pump, which is supplied by the hybrid RES. Results show that coupling PV panels and wind turbines enhance the stability of renewable power production, while the heat pump utilization leads to a primary energy demand reduction for building space HVAC and domestic hot water by 30%.

Installing RES into buildings offers a possibility of integrating electric vehicles (EV) in efficient buildings fed by renewables (PV). A future scenario with a dynamic analysis of EV and building integration suggests a substantial reduction of electricity from the grid, leading to 58% of primary energy savings and a 52% of CO_2 emission decrease. However, a case study analysis is dependent on the building location, as is the renewable energy production. It concludes that it is more cost-effective to implement such solutions to areas with more sunny days, e.g., the Mediterranean [6]. Meanwhile, employing the reversible Solid Oxide Cell (rSOC) offers the possibility of integrating RES on a building/district scale. Lamagna et al. [7] conducted a study of integrating rSOC coupled with Li-ion battery with RES for different scenarios in residential and non-residential buildings. The process reversibility between P2H and H2P offers a more flexible system allowing better management of the available energy. Furthermore, rSOC can also be utilized to exploit natural gas or hydrocarbon fuel, not just pure hydrogen, putting it in an advantageous position in energy transition as the next integrated energy system design.

Various process control methods are utilized to achieve cost minimization of space heating/cooling costs. In their experimental research [8], the authors carried out an experimental performance test of the Model Predictive Control (MPC) strategy for space heating while ensuring indoor thermal comfort with a simulated rooftop PV system. The experiment showed predictive controller increases PV self-consumption compared to a conventional thermostat reducing the heat pump electricity cost by 10-17%. Achieved results are significant considering the analysed building lacks a battery for electricity storage. Besides MPC strategies, other process control methods such as deep learning are represented in the smart building control. Applying a deep q-learning (DQN) based control strategy, investigators in Ref. [9] optimized temperature setpoint real-time reset to balance the HVAC energy consumption and indoor temperature. The DQN strategy learns to update the temperature setpoint of air and chilled water supply by interacting with the simulation environment. Results indicate that stable control actions can provide a proper trade-off between HVAC energy consumption and indoor air temperature after 10 DQN training episodes. A study of thermal comfort behaviour employing an artificial neural network (ANN) is presented in Ref. [10]. A predictive surrogate model is generated from the measured data providing a reliable and fast prediction of thermal comfort in naturally ventilated buildings without HVAC. Researchers are using deep learning to predict the thermal behaviour of buildings. Kim et al. trained a convolutional neural network to forecast the temperature and heat flow distribution, while they used a multi-layer perceptron to predict the thermal bridge coefficient. Upon training completion, the thermal behaviour of the building can be predicted just by feeding the building blueprint image and thermal properties into deep learning architecture [11].

3. Thermochemical processes

Many thermochemical conversions and processes are at the core of the industry and our modern world. It is then evident that improvements in these areas can drastically increase the efficiency of our energy use, reduce operating costs, and alleviate the impact on the environment and natural resources.

For example, the utilization of waste heat energy sources has significant potential to improve the efficiency of numerous industrial branches. For low-temperature processes, the supercritical CO_2 Brayton cycle has been found suitable for thermal utilization. Detailed thermodynamical analysis of thermal and exergy efficiencies has been done by Živić and coworkers [12]. They presented their analytical assessment of the Brayton cycle and included turbine and compressor irreversibilities, analysing net work obtained per cycle, along with temperature and pressure ratios. On the practical side, a demonstration plant was investigated in an experimental study with reduced-scale turbomachinery [13]. Here, the optimization of working parameters was performed based on the system characteristics and given external parameters for a conventional cycle design.

In Ref. [14], a supercritical CO_2 (SCO_2) Brayton cycle was modelled in dynamic simulation models, aiming to identify the optimal layout of phases – recompression, reheating, and intercooling. The model was verified against experimental data, and the dynamic response under temperature perturbations was analysed. Additionally, a new layout based on the modelling results was proposed. This work provides valuable guidelines and conclusions on the optimal utilization of system parameters and ways how to maximize efficiency, extraction ratios, and generated power.

On the other hand, more contemporary technological solutions for SCO_2 Brayton cycles include printed circuit heat exchangers. They offer high-pressure resistance and small dimensions and are usually used as a link between primary and secondary loops. Therefore, an evaluation method was developed for heat exchanger efficiency and overall performance [15]. Additionally, the design and utilization of printed circuit heat exchangers as parts of Brayton cycles is still being improved. Lian et al. have designed a new structure for improving heat transfer in printed circuits by combining chemical-etching channels and plate-fin channels for the carbon dioxide and the water side, respectively [16]. The new hybrid design reduces the exchanger size, and increases heat transfer while maintaining structural and stress requirements.

Fluidized bed applications in thermal engineering applications are numerous, as they represent a versatile solution for various issues in energy storage, heat transfer [17], purification technologies, and chemical conversions. For example, fluidized beds were considered in a modelling study for combined wastewater treatment and biogas production, where Metolina and Lopes [18] analysed hydrodynamic characteristics of different reactor designs in which microorganisms fixed on inert particles interacted with organic effluent, producing biogas. Another purification application is the treatment of residue left after flue gas desulfurization via a semi-dry process. De Castro and coworkers [19] tested the upgrading of desulfurization residue in a pilot plant and oxidized it with hot air, turning sulphites to sulphates. Finally, Padula *et al.* [20] proposed a novel approach for using a fluidized bed in a thermochemical battery system powered by concentrated solar thermal.

Still, fluidized beds have been often used in pyrolysis processes, as they provide many advantages such as improved efficiency, reduced energy usage, flexible operating conditions and uniform product quality [21]. Pyrolysis is one of the most interesting thermochemical processes, included in the production of a variety of renewable fuels [22] and their utilization [23]. The work by Hosana *et al.* [24] presented as a part of this *Special Issue* combines these two major topics in a paper on numerical modelling of the fast pyrolysis process in a gas-solid circulating fluidized bed. In their model, process parameters, specularity, and restitution coefficients were tuned, and circulation flow rates, velocities, and heat transfer were assessed.

In searching for the improvement of technological processes, dual systems and chemical looping were established as novel approaches for combining several processes into a single while achieving better efficiency, product, or reducing waste heat. Instead of more conventional combustion approaches [25], chemical looping combustion has been investigated for simultaneous hydrogen and power production with heat recovery [26]. Besides that, mass and energy integration issues are evaluated for the integrated gasification combined cycle for thermochemical looping [27], and the synergy of steam methane reforming, and chemical looping combustion of metal oxides is investigated in the research by Cao and coworkers [28]. Finally, a recent paper included in this *Special Issue* deals with the technical and economic implications of decarbonized flexible hydrogen and power production [29]. The catalytic process [30,31] for biogas reforming is investigated in a chemical looping cycle. Several options were evaluated for carbon capture rate in a technical and economic assessment of a concept, indicating that the iron looping cycle demonstrates significant advantages over calcium looping or methyl diethanolamine chemical scrubbing.

The final topic considered within this Thermochemical Processes section regards waste gas, its thermal utilization, and waste gas-to-energy conversions. As one can imagine, this is yet another important pathway toward increased efficiencies, and savings in industrial applications since waste gases from chemical processes can still contain usable and combustible substances [32]. Additional heat recovery and oxidation of exiting waste gases can introduce fuel savings and reduce the operating costs of the unit.

Therefore, means to evaluate this potential for improved efficiency are valuable and need improving. Research by Skvorčinskienė et al. focussed on experimentally testing the waste gases combustion from biomethane production [33]. They investigated low-swirl burners with different geometries designed for sustaining combustion of low calorific value fuels and under syngas enrichment.

Besides improved thermal efficiency, waste gas utilization can also reduce pollutants [34]. For example, combustible Volatile Organic Compounds can successfully be processed in waste gas-to-energy units. Freisleben, Jegla, and Krňávek published their novel graphical-numerical method for evaluating the potential for savings during energy retrofits, which is straightforward and does not require computational resources [35]. Besides being validated against non-linear simulations of the systems, their research provides applicable formulas for possible fuel savings and technological modifications.

4. Seawater treatment

In pursuit of energy sources diversification, non-conventional technologies are taking a more significant place in energy generation, both for the overall energy mix and especially for fringe applications. Ocean energy potential is vast, but the technological solutions exploiting it are still under development and, cost-wise, not competitive. Currently, offshore wind energy is the most developed sea-related technology with the highest capacity [36] but stems from the prior development of onshore wind technologies. Another technology for coastal applications is seawater heat pumps, which are suitable for delivering sustainable heating and cooling for large consumers [37]. Still, other solutions, such as wave converters [38], offshore photovoltaics [39], tidal energy [40], and osmotic energy production (pressure retarded osmosis), are actively being pursued [41].

Oceans can be viewed as extensive heat sources that could be used for power . However, ocean thermal energy conversion (OTEC) technologies require a sufficient temperature gradient between the surface and deep water. Therefore, similarly to all *blue* technologies, the issue is severe location dependency, as micro- and macro locations can severely influence the applicability and feasibility of the implementation [42], and the best locations for the application of OTEC are tropical areas with constant surface water temperatures and suitable bathymetry.

The additional dimension of these novel technologies and an appealing research topic is their combination with different power generation approaches and industrial processes. In this *Special Issue*, Liponi et al. investigated the thermodynamic and economic feasibility of reverse osmosis powered by the thermal energy conversion plant [43].

Clean water supply is becoming an increasingly relevant issue for communities around the world due to higher temperatures, uncontrolled freshwater utilization, and droughts, and for some locations, desalinization can be the only viable approach for ensuring fresh water supply. For example, in a strategy to prepare for prolonged drought periods and build resilience for the future, large desalinization facilities have been built in Australia during the last two decades [44]. The development of desalinization technology is not a novel one but has been revolving around novel ideas, synergies, and locations in recent years, specifically island applications which are especially vulnerable due to lack of bodies of fresh water, isolation, and hotter climates. For island applications (Gran Canaria), Blanco-Marigorta *et al.* have investigated the exergo-environmental impact of reverse osmosis desalinization with a life cycle assessment and concluded that the exergy destruction in the first stages of the reverse osmosis membrane modules is also the highest contributor to the environmental impact [45].

For energy systems with high penetration of renewable sources such as PV and wind, including reverse osmosis desalinization technology can have a synergetic impact on ensuring water supply and smoothing the power generation [46].

On the other hand, a synergetic combination of desalinization and industrial processes can also be achieved. For example, an integration of a solar-geothermal system with water desalinization was investigated by Calise et al. [47]. They presented an innovative polygeneration system for cooling and heating, electricity production, and freshwater supply. Such system would be suitable for islands and remote locations, solving a couple of problems at once by combining the organic Rankine cycle with a medium heated by geothermal or solar and multi-effect distillation for pure water production.

Another study carried out the investigation of RES integration with seawater desalinization and water storage for a small Mediterranean island, where reverse osmosis for freshwater production was powered by PV-generated electricity [48]. By including water storage and improved control strategies, significant savings and fresh water supply have been achieved, reducing dependency on expensive ship-supplied water.

The paper by Liponi and coworkers combines previous topics and analyses a mix of desalinization and power generation on an island location, where synergetic effects can provide additional benefits. For an island with stable and warm surface temperature levels, but also sufficient ocean depths, OTEC can be used for utilization of temperature gradient, while reverse osmosis could reduce water scarcity in remote areas. The coupling of OTEC and reverse osmosis desalinization is beneficial as the process requires a substantial amount of power, which thermal conversion can supply almost constantly and without carbon emissions. A thermodynamical and economic study of such system has been performed, including choices between working fluids (ammonia and R1234yf), heat exchanger materials (stainless steel and polyvinylidene difluoride), and a sensitivity analysis such as depth and operating temperatures. For the analysed location, the efficiency and economic viability of the system are high, which indicates suitability for similar applications.

Besides energy production and freshwater supply, another seawater-related topic in the overlap of engineering and sustainable development can be of interest. Following the International Maritime Organisation's imposed restrictions on the allowed sulphur in heavy fuel oil powering ships, flue gas desulfurization was established as one of the main solutions. Gas scrubbing is an established technological process used for gaseous pollutant removal with liquid reagents, and its application is being expanded to different fields, for example, biogas upgrading by amine solution scrubbing [49] or chemical regeneration of solutions by anaerobic biofilm scrubbing [50]. However, more conventional applications such as sulphur dioxide scrubbing from flue gases still account for the majority of use cases [51]. One of the scrubbing liquids that can be used is seawater, as it has increased absorption ability due to alkalinity and dissolved ionic species [52]. The spray used for the dispersion of seawater droplets represents one of the crucial sections of the whole system, and its modelling and optimization remain among the most challenging technological problems [53]. For one desulfurization system, Pan et al. investigated droplet entrainment and behaviour in an experimental investigation [54], and Panão et al. looked into the thermal-fluid assessment of multijet atomization for spray applications [55], which is an important basis for a thorough understanding of mass transfer between droplets and the gas phase. For example, Bešenić and coworkers, in their investigation on an individual droplets scale, analysed sulphur dioxide absorption by numerical modelling and application of different mass transfer modelling approaches [56]. Related work on evaporation characteristics of desulfurization wastewater has been performed by Liang et al. by combining modelling work with experimental measurements [57]. Additionally, the evaporation rate was correlated to different nozzle types, and parameters in a modelling investigation focussed on the droplet behaviour [58].

Among the work presented at the SDEWES Conference, a paper concerning this topic has been published in the present *Special Issue*, dealing with the analysis of the mass transfer for the engineering application. Grinišin et al. presented their investigation of droplet behaviour for seawater spray scrubbing [59], where they focussed on a critical issue of mass transfer between gas and liquid phase. They developed a numerical model and included an improved model for determining mass transfer, with better sensitivity and accounting for more physical properties of droplets.

5. Thermal storage and renewable energy sources

The search for optimization possibilities of thermal industrial applications covers multiple directions, macro-, and micro-scales, and aims to integrate new synergies and renewable sources of energy. Heat pumps, for example, are a widely used and mature technology, but the research on optimization and novel applications is still underway. Ground heat pumps already represent a commercial solution for heating and cooling, but investigations of the coefficient of performance under different material choices, soil parameters, and design are costly, and significant improvements can contribute to future technological solutions [60]. Optimization of heat pump operation and implementation can also be investigated on large scales, considering exergetically optimal use of heat recovery and design in sustainable buildings [61]. The work by Ceglia and coworkers focuses on energy consumption in buildings by using ground source heat pumps and numerically simulates a system with thermal storage based on experimental data [62]. The analysis includes irreversibility in the system by a hardware-in-the-loop simulation and provides valuable conclusions regarding exergoeconomic prices for end-users.

However, more fundamental improvements of used technologies are still being investigated and provide attractive research topics. This *Special Issue* includes a paper by Huang *et al*. [63], reporting on a modelling study of refrigerant behaviour in parallel multi-channel geometry of heat exchangers. In their research, the authors have investigated the two-phase flow of R1233zd(E) and provided a visualization of narrow channels. They showed the dependency of the calculated void fraction on different inlet configurations and provided coupling between experimental methods and numerical analysis for reducing the dimensions of heat exchangers in heat pump systems. Previous work on a similar topic was provided by Masiukiewicz and Anweiler, who experimentally measured two-phase flow phenomena in mini-channel structures [64]. Novel configurations of micro-channels were also investigated by Venkiteswaran *et al.* in computational fluid dynamics (CFD) simulations of heat and fluid flow [65], as well as applications and behaviour of two-phase flow in small channels with injections [66].

Besides integration with the ground as a heat container, another obvious synergy combination can be achieved by using low-temperature heat from solar thermal applications. Heat pumps can use various sources of power, and the comparisons and suitability for different applications are being investigated [67]. Economic analysis of different low-temperature heat supplies is presented and assessed based on parameters such as surface area, cost, and power supply intermittency in work by Caballero-Esparza and coworkers [68], where they indicated that parabolic trough collectors display considerable advantages compared to competing technologies. Additionally, novel approaches for solar energy conversion and utilization are being developed. For example, vertical design of solar thermal collectors with increased thermal energy production [69], or novel triangular solar thermal plate design suitable for buildings integration and utilization of facades [70].

On the cooling side of thermal industrial applications, heat-driven chillers can also utilize low-temperature heat from thermal collectors. Parametric analysis of one such system is given by Tawalbeh *et al.* [71], in a study of system parameters and component design, along with a comparison to a geothermal heat source. Multiple studies of solar heating and cooling systems have been published, with Buonomano and coworkers modeling absorption and adsorption chillers driven by concentrating photovoltaic/thermal solar collectors [72] and Aneli *et al.* [73] analysing the performance of an adsorption chiller driven by solar energy in present *Special Issue*. By searching for the influence of operating temperatures on efficiency, they have demonstrated that photovoltaic/thermal panels—providing both electricity and heat power for chillers—can improve the flexibility of a system.

By including various intermittent renewable heat sources in the power generation mix, the need for balancing supply and demand becomes a great issue. The phase change is yet another thermodynamical process that can be used in industrial heat storage applications. For example, seasonal heat storage included in a district heating system with a heat pump was presented by Sorknæs [74]. He provided an hourly-basis simulation method for the dynamical analysis of yearly thermal losses in a system with thermal storage. The usage of phase change in novel applications was also shown in a paper included in this *Special Issue.* Mendecka and coworkers presented an interesting solution for the utilization of volumetric expansion during the phase change by including a waste heat power plant that alleviates the losses due to solar tracking by providing additional mechanical work from storage medium expansion [75]. Finally, another top-level research paper considered the optimization of power-to-heat technologies and heat storage by advanced metaheuristic optimization algorithms, genetic algorithms, and particle swarm optimization [76]. These models derive optimal schedules for heat pump-based grid-edge technologies and aim to achieve operational cost reductions for consumers and localized implicit demand-side flexibility.

6. Conclusion

This vision paper accompanies a *Special Issue* of Applied Thermal Engineering dedicated to the 16th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), held from the 10th to the 15th of October 2021 in Dubrovnik, Croatia. It presents and discusses topics covered in a selection of articles presented at the conference related to promising technological solutions aimed at engineering sustainable systems for future society, specifically focussed on thermal processes as these arise in energy production, storage, utilization and conservation.

Thermal processes are the basis of numerous sustainable engineering applications, and their understanding and improvement are increasingly required in the context of improved resource use efficiency and reduced environmental impact. Applications of interest include thermal systems used in buildings, thermochemical processes, seawater treatment, thermal storage solutions and renewable energy resource use. Diverse approaches from fundamental research to the development of technical solutions for a range of sustainable engineering applications, technoeconomic analyses, and issues relating to the potential and integration of technologies from higher-level approaches are included. An overview is given od the development of existing and established technological solutions, as well as of novel applications and innovative heating, cooling, electrical energy and water production integration. It is concluded that improvements of relevant processes have the potential to lead to significant economic benefits, as well as reduced climate impact and damage to the environment.

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