Overview and Outlook of Research and Innovation in Energy Systems with Carbon Dioxide as the Working Fluid

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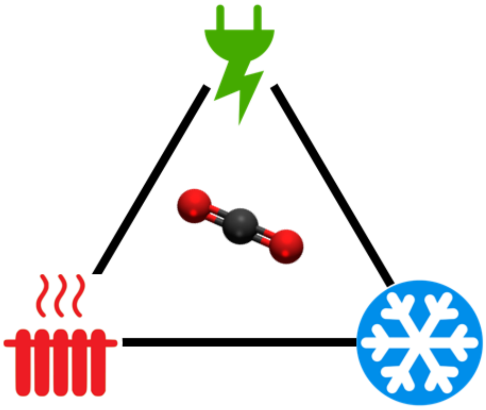
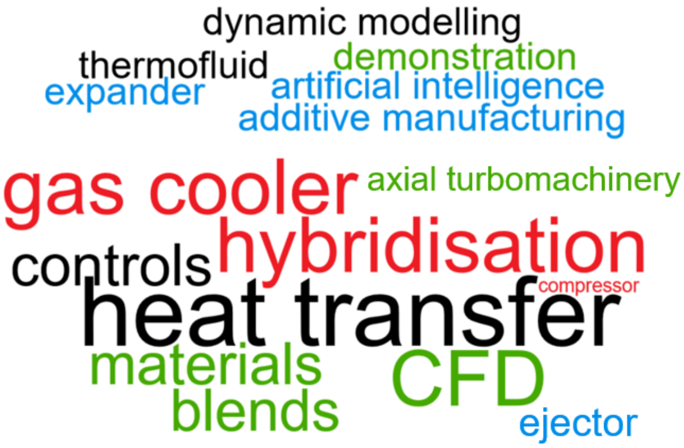
Highlights

- Knowledge gaps for carbon dioxide (CO_2, R744) energy research outlined
- Research is needed along the whole maturity scale of CO_2-based technologies
- Interdisciplinary approaches are required to tackle complex outstanding questions
- Advances in fundamental studies required to enhance current design methodologies
- Technology demonstrations at full scale are critical for mass deployment of the technologies

Graphical Abstract





Keywords

Carbon dioxide (CO_2); R744; refrigeration; heat pump; power generation.

Abstract

Carbon dioxide (CO_2, R744) is a natural working fluid with interesting thermophysical properties that have stimulated strong attention by the academic and industrial communities for a broad range of energy applications. The technology readiness level of CO_2-based energy systems is very diverse due to the increasing consideration that the fluid has been receiving since the 1990s. Hence, the state of the art in CO_2 energy research spans from fundamental thermofluid and chemistry science to commercial system innovations. After a brief compendium on ongoing activities, this paper proposes a roadmap for CO_2 energy research with reference to the cooling, heating and power sectors. The key knowledge gaps and the main challenges at system and component levels are critically discussed. Pathways to advance the understanding and the technological maturity of CO_2 energy systems are also outlined.

1. Introduction

Carbon dioxide, also known with its chemical formula as CO_2 or R744 in industry, has been one of the first working fluids employed in the refrigeration industry, as evidenced by Twining's patent dated 1850 [1,2]. Despite the early uses, during the 1930s CO_2 was gradually displaced by Chlorofluorocarbons (CFCs) Hydrochlorofluorocarbons (HCFCs) and Hydrofluorocarbons (HFCs) that, by operating in the sub-critical region with lower working pressures on the high pressure side of the system, offered better performance than transcritical CO_2 refrigeration systems.

The Montreal protocol entered into force in 1989 and the related actions to mitigate anthropogenic impacts on the environment renewed interest in natural refrigerants and the use of CO_2 [3] which, besides being non-flammable (A1 safety classification) and non-toxic, also has a zero Ozone Depletion Potential (ODP) and a Global Warming Potential (GWP) of one which is negligible compared to the much higher GWPs of alternative working fluids [4]. Soon after its deployment to refrigeration applications, CO_2 has begun attracting increasing attention for heat to power and power to heat applications.

Despite progress to date, the mass scale deployment of CO_2 energy systems is still hindered by technology challenges [5,6]. Latest advances in the technology have been recently reviewed for refrigeration applications [7-13], heat pumps [14-18] and the power generation sector [19-26].

This paper summarises these developments and emerging trends to guide future research initiatives towards further improvement of CO_2 vapour compression refrigeration and heat pumping technologies, and acceleration of the development and commercialisation of CO_2 heat to power technologies.

2. Knowledge and technological gaps

This section recalls the knowledge and technology gaps to be overcome for an increased maturity of CO_2 energy systems. Although some research challenges are not application specific, the brief summary here focuses on three end uses of CO_2 energy systems, namely cooling, heating and power.

2.1. Refrigeration and air conditioning

Refrigeration is the most mature application sector for CO_2 energy systems. Transcritical CO_2 cycles have been historically improved through an extensive research effort that has led to the following technological advances: single-stage compression with oil flooding and an internal heat exchanger, two-stage compression with either compressor intercooling or vapour injection, economisation, sub-cooling, etc. [27]. Barta et al. [28] provided a comprehensive review of the stationary and transport CO_2 refrigeration and air conditioning technologies.

Commercial solutions for CO_2 refrigeration systems are currently available in the market and gained increased popularity for applications at low and moderate temperature climates. The most popular application sector is supermarket refrigeration, in which CO_2 systems have prevailed over systems with alternative refrigerants due to lower footprint and environmental impacts, and capability to achieve low temperatures [29]. At warm climates, CO_2 refrigeration and air conditioning applications experience techno-economic challenges due to the complexity of the transcritical cycles and additional components (e.g. ejectors) that may be required to sustain the efficiency of the whole system [30] during operation at high ambient temperatures; this concept has been clearly addressed in the work of Azzolin et al. [31], presenting an integrated experimental/modelling approach to further develop ad-hoc control strategies to deal with the warm climate issue for CO_2 transcritical cycles. Despite the technical benefits, the high cost of equipment and shortage of technical expertise are key barriers to the application of CO_2 technologies to road transport applications. In this context, further research is needed for the development of new knowledge and tools to advance the efficiency benefits of CO_2 refrigeration systems and reduce further the costs of CO_2 technology. Regardless of cycle architecture, a promising area for research relates to the improvement of the Coefficient of Performance (*COP*) through the replacement of expansion valves with active (expanders) or passive (ejector) devices that can lower the net power input through a recovery or a reduction of the compression work respectively. Although know-how is currently available in these areas, most of the published literature focused on technology development, but not its integration in the whole refrigeration system [32,33]. In this sense, the use of storage technologies, to decouple the demand-side form the supply side, should be further investigated [34]. Unfortunately, the large-scale deployment of ejector-based systems is hindered by the influence of the ejector operation on the performance of the integrated system [35]. To address this, extensive effort towards novel design, optimisation and operation strategies is needed [36]. Barta et al. [37] proposed a design tool for two-phase flow ejectors for vapour compression cycles, whereas Haida et al. [38] experimentally studied performance and instabilities of the R744 vapour compression system equipped with a two-phase ejector. It should be noted that such design tools should consider local-scale fluid dynamics and should be validated against test data [39]. For example, Romei and Persico [40] presented a novel computational fluid dynamics tool to simulate compressible two-phase flows of carbon dioxide operating in the proximity of the thermodynamic critical point and at supercritical conditions. It should be noted that, near the critical point, thermophysical properties of CO_2 are characterized by steep gradients and, in this sense, property tables if used, should have high resolution [41]. Better understanding and prediction of convective boiling heat transfer, two-phase flow patterns and pressure drops are also crucial in achieving accurate and improved design of high-performance CO_2 heat exchangers [42]. To this end, and similarly to ejectors, the use of additive manufacturing technologies could pave the way for new generations of cost-effective CO_2 equipment.

Lastly yet importantly, improvements in the CO_2 compression technologies are required not only for refrigeration but also for heat pump applications, especially the high temperature ones. In this context, key areas for research relate to volumetric and energy performance improvements, high pressure and temperature ratings, reliability and cost.

2.2. Heat pumps

Despite the early work of Lorentzen in the 1990s, CO_2 heat pumps received significant interest only from the early 2000s, with Japan the pioneering country. Rony et al. [43] presented a comprehensive review of transcritical CO_2 heat pump technologies. It should be noted that the use of heat pumps has been recognized as a preferential pathway toward the decarbonisation of energy systems. The reader may, for example, refer to

Bianchi et al. [44] for an estimation of the waste heat recovery in the European Union industrial sector. Typical uses of CO_2 heat pumps are water and space heating, drying and, more recently, heat integration in industries [45] and electric vehicles [46,47]. As such, the heat is usually supplied at temperatures above the critical point of CO_2 (31.0 °C, 7.38 MPa). Unlike transcritical refrigeration systems, CO_2 heat pumps experience large exergy losses that, over time, have stimulated academia and industry to develop a number of technological innovations that span from an internal heat exchanger to parallel and cascade systems depending on the application and the heat source (air, water or ground) [48]. Furthermore, the use of heat pumps to upgrade the waste heat in industrial applications has sparked an increased consideration but also new challenges.

Besides the need for high-efficiency machines, high temperature heat pumps require new generations of CO_2 compressors whose outlet temperature can exceed 140 °C [49]. This poses challenges to thermofluid science as well as tribology and materials.

Gas cooler design is another crucial aspect to be addressed through fundamental and applied research since these heat exchangers operate in a range where the thermophysical properties of CO_2 experience the largest variation, namely at supercritical pressures (74 - 91 bar) and in a temperature range between 25°C and 65°C [50]. An alternative way to tackle this challenge could be the use of CO_2 blends, e.g. 60% CO_2, 40% C_3H_8 (propane).

The optimisation of the pressure at the outlet of the Electronic Expansion Valve (EEV) is a key parameter affecting the heat pump COP. Adjustable EEVs as well as variable opening ejectors and expanders are all approaches that can lead to efficiency improvements. This requires further research into dynamic simulation and control strategies [51-53]. The hybridisation of conventional heat pumps with solar or geothermal energy may be additional ways to further decarbonise the heating sector but does involve comprehensive investigations.

2.3. Power generation

The use of Rankine or Joule-Brayton cycles for power generation has shown to offer significant potential. In Rankine architectures, CO_2 is conventionally pumped from a sub-cooled liquid state while Joule-Brayton cycles consider gas compressions at lower pressure ratios than those in Rankine cycles [19]. Although pumping a liquid would demand less energy than compressing a gas, in the case of CO_2 this is not always achievable at all operating conditions since it has a low critical temperature, 31.0 °C, and critical pressure of 7.38 MPa. Ongoing research is currently tackling this challenge in two very different ways: a) the use of blends between CO_2 and other compounds, e.g. $TiCL_4$, C_6F_6 [54,55], to shift the critical point above ambient conditions and therefore ensure that the working fluid is still in the liquid phase at moderate heat sink temperatures and, b) the design and control of turbo-compressors to operate slightly above the critical point, where CO_2 experiences low compressibility and, in turn, requires low power to be compressed [56-59]. The CO_2 heat to power research is relevant and spans the whole power generation spectrum: fossil-fuelled, nuclear, waste heat, geothermal and concentrated solar power (CSP) [21].

A variant of the regenerative Joule-Brayton cycle which includes oxy-fuel combustion and carbon capture is the so-called Allam-Fetvedt cycle [60]. The inherent integration of a carbon capture system in the power plant as well as the high efficiency and compactness of sCO_2 power cycles enabled a fast development of this thermodynamic concept into a full-scale demonstration (up to 10MWe). Despite the ongoing sCO_2 projects in the US (STEP, NetPower), the technology readiness level of sCO_2 equipment and systems is still not mature and requires full scale demonstration of the technology in different applications for it to gain the confidence of investors.

With reference to sCO_2 turbomachinery, the knowledge and technology gaps are several and diverse. From a more methodological viewpoint, sCO_2 turbines and compressors are being designed with state-of-the-art numerical tools that were not developed for sCO_2 applications. They rely on the use of unreliable loss correlations that were developed and validated for air turbomachines. Even more importantly, near the critical region, CO_2 experiences strong real gas effects that correlations or simplified equations of state implemented in most of the engineering software do not consider [61]. From a numerical perspective, the large variations of thermophysical properties also lead to solver instability and high computational effort [62,63]. As such, more fundamental studies on flow topology and novel mathematical formulations for the calculation of thermophysical properties of CO_2 and its blends are required to advance current design tools and ensure sound design methodologies. Besides the aerothermal design of sCO_2 turbomachinery, research on bearings, seals and other ancillary equipment is paramount to ensure high net global efficiency of sCO_2 power cycles. In this context, an even more challenging aspect relates to the technology upscaling. In fact, most of the experimental test rigs available worldwide currently employ radial machines which are optimal for small pressure ratios and low mass flow rates. However, beyond 10 MWe, the most suitable design configurations for sCO_2 turbomachines are expected to rely on axial machines, whose operating principle and operational features are different from radial ones, e.g. lower revolution speeds, multi-stage arrangement etc. As such, since the knowledge generated to date cannot be fully transposed from radial turbomachinery, new efforts are required for the study of axial units.

Advances in heat transfer equipment are also crucial for the success of sCO_2 technology. Heat exchangers are responsible for the largest share of the capital expenditure of sCO_2 power systems [64]. This is one of the main reasons why simple cycle layouts have been so far preferred over more complex configurations. The development of sCO_2 heat exchangers is not a trivial task since it must address several challenges that primarily depend on their function within the power cycle. For instance, sCO_2 heaters are critical for materials, recuperators for the heat duty while coolers need to deal with the design shortcomings related to the real gas effects in the critical region [21]. As concerns the heat transfer and flow mechanisms, the influence of buoyancy effects should be considered for the development of empirical correlations and the design of sCO_2 heat exchangers. Moreover, unique universal correlations should be developed to cover a wide range of test parameters and demonstrate the local heat transfer performance [23].

The highly variable pressure and temperature loads, the corrosive behaviour of CO_2 on steel above approximately 550 ˚C, and the likelihood of impurities in the working fluid all require innovations in materials and manufacturing methods for sCO_2 power equipment and systems [65]. Even though nickel and titanium-based alloys are capable of withstanding harsh operating conditions, material and manufacturing costs directly impact the economic viability of sCO_2 power systems [66]. Furthermore, these costs not only relate to the actual components but also affect the installation costs, which can be as high as the cost of the sCO_2 power block, especially in retrofit solutions. To advance the state of the art in this area, additional research is required to characterise existing and novel materials at the operating conditions of sCO_2 power applications. This is crucial especially for direct fired sCO_2 power systems, which are expected to experience pressures up to 300 bar and temperatures up to 1200 °C [67]. As concerns corrosion and erosion resistance tests, new procedures and standards should be developed to accelerate the tests and expedite the research.

The control of sCO_2 power systems is an area not extensively researched at present. This is also due to lack of sufficient information available from the published literature or equipment providers on the geometrical and performance data required to develop low order models. Transient modelling and control are however crucial to ensure the success of sCO_2 power technology, especially in relation to the flexibility feature [68,69]. Besides the challenges related to the optimal control of sCO_2 power blocks during normal operation, more research is needed to assess the operational scenarios at system start-up and shut-down. These regimes are significantly different from the power generation one and involve several ancillary systems, potentially also storage systems, to be included in the modelling platforms [70,71]. As such, more holistic control approach should be considered in future research to outline sound, safe and efficient test and operational procedures.

3. Outlook

Carbon dioxide (CO_2, R744) technology has all the important characteristics to make it one of tomorrow's most attractive energy systems: natural availability, eco-friendliness and inherent safety. Energy systems using CO_2 as the working fluid are today at commercial maturity in the commercial and industrial refrigeration applications for low and medium temperature climates. The strong interest toward the electrification of the heating sector and the need for flexible power generation systems will be additional strategic drivers for CO_2 energy research in the forthcoming decades. However, the diverse technology readiness levels of CO_2 energy technologies call for joint and complementary efforts by academia and industry to advance the state of the art and technology readiness level of heat to power and high temperature power to heat technologies.

The CO_2 refrigeration sector will likely focus on performance and cost optimisations to enable a higher penetration of CO_2 technology in the market. Streamlined design configurations equipped with compact heat exchangers, ejector or expander recovery devices as well as suitable controls for application in any climate zone demand for holistic approaches, whereas advances in thermofluids research will have to support not only the design but also the operation of the CO_2 energy system. In this context, recent advances in artificial intelligence and additive manufacturing technologies could open the way to new design solutions.

Heat pump is a highly promising field for CO_2 technology and research, especially if high-temperature industrial applications are considered. In this area, research will need to focus on novel compression equipment and compact heat exchangers, whose development further requires new fundamental heat transfer knowledge in the supercritical region and in relation to CO_2 blends with other refrigerants. A strong effort on controls is additionally required, especially in the case of solar assisted heat pumps and demand side management.

The ongoing research programmes and the strong interest shown by industry and end users make supercritical CO_2 (sCO_2) power generation one of the key areas where researchers and engineers will focus in the forthcoming years to enhance the maturity and strengthen the competitive position of this technology. Industry and academia will have to collaborate to advance innovation and the state of the art. Industrial efforts will aim at demonstrating sCO_2 power systems at full scale. This will not only build confidence in end users but also develop economies of scale in the manufacture of components. A full-scale demonstrator will however need either private capital or government support to de-risk initial investment. The role of research will be enhancing multidisciplinary knowledge to advance design methodologies and tools. Fundamental research on thermophysical properties and thermofluids should be supported by more applied investigations focused on technology ideation and benchmarking. The harsh operating conditions and the need for bespoke equipment make the development of experimental facilities for sCO_2 power research very difficult due to the high costs involved. Besides a higher engagement from public and private funders, a strong collaborative approach is therefore paramount to develop knowledge networks that can rely on complementary infrastructure rather than individual assets. Academic research will ultimately transfer the knowledge generated through research into educational programmes to develop new generations of talent for the future ahead.

Advisory Board

The Authors are grateful to Professor Piero Colonna, Professor Jacek Smolka and Professor Chi-Chuan Wang who put a great effort to maximise the outreach of the "CO_2-based technologies for heating/cooling and/or power generation and co-generation" virtual special issue.

Acknowledgements

The Authors are grateful to the editorial board of Applied Thermal Engineering as well as to all the authors and reviewers who contributed to the special issue. Aspects of the work reported in this manuscript are funded by the European Union's Horizon 2020 Research and Innovation Programme (Grant No. 680599 – I-ThERM) and the Engineering and Physical Sciences Research Council (EPSRC) of the UK under research grants (i) EP/V001795/1 - Industrial waste heat recovery using supercritical carbon dioxide cycles - SCOTWOHR, (ii) EP/P004636/1 Optimising Energy Management in Industry - OPTEMIN and (iii) EP/K011820/1 - Centre for Sustainable Energy Use in Food Chains (CSEF), an End Use Energy Demand Centre funded by the Research Councils UK.

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