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Five Thermal Energy Grand Challenges For Decarbonization

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Roughly 90% of the world's energy use today involves heat over a wide range of temperatures. Here we highlight five of the most impactful problems in thermal science and engineering, which if addressed adequately, have the potential to mitigate climate change at the necessary scale and urgency.

More than 90% of global energy use occurs via heat. Advancing our ability to transport, store, convert and efficiently utilize thermal energy will therefore play an indispensable role in avoiding a > 2°C rise in global average temperature. Even though this critical need exists, there is a significant disconnect between current research in thermal sciences and what is needed for deep decarbonization. The impending effects of climate change demand much greater emphasis on a certain subset of problems that, if successfully solved, will have the most significant impact on reducing green-house gas (GHG) emissions. It is from this perspective that herein, we highlight five grand challenges that we believe experts in thermal science and engineering, in collaboration with intersecting fields, could have meaningful impact on. These were identified based on estimations of the size of their potential impact (i.e., by assessing the fraction of global GHG emissions that could be abated if the technology was maximally successful), as well as the authors' opinions and qualitative assessments of the magnitude of the opportunities for scientific advancement and technological breakthroughs. For example, improving the efficiency of heat engines in the stationary power sector is not highlighted here, despite the fact that it could be impactful, because current heat engines already operate very close to their thermodynamic limits.

1| Thermal Storage Systems

With the increasing penetration of low cost solar and wind electricity, their innate intermittency has hastened the need for low-cost storage over a wide range of time scales, from seconds to multiple days, and even seasonal storage. Current technologies, such as pumped hydroelectricity are geographically limited and lithium-ion batteries (~$80-100/kWh capital cost) are too expensive for the multi-day storage targets (~$3-30/kWh) needed to fully decarbonize the grid.[1,2] If this problem is solved, it could enable full decarbonization of the grid, thereby reducing global GHG emissions by ~ 25%,[3,4] and even greater reductions are possible if electric vehicles (EVs) shift the majority of transportation energy usage to the grid. Thus, *the storage problem* is one of the single most impactful problems to be solved in our energy infrastructure.

Several new thermal energy storage (TES) concepts have been proposed[5,6] and are under various stages of development. While it is relatively easy to convert electricity to heat at a variety of temperatures, the key challenge for TES is the large efficiency penalty associated with the second law of thermodynamics when converting heat back to electricity. However, the key advantage for TES is its potential for low cost (<$20/kWh) at GWh-scale.[5,6] This is because, unlike batteries, where only a small fraction of the atoms that make up the device are actually active species carrying energy, with thermal energy virtually every atom is participating, albeit with much less energy (i.e., meV vs. eV for batteries). Nonetheless, since the specific heat of virtually all materials is the same on a molar basis, at sufficiently high temperatures, TES can make use of extremely abundant and low-cost materials that are impure or even recycled. Although several embodiments have been put forth, they are still early stage and have not yet reached commercial deployment. Thus, there is a need to continue developing more competing embodiments that exploit other thermal storage materials and mechanisms. In particular, it is of utmost importance to develop full system concepts that carefully consider all of the practical issues (e.g., materials degradation and compatibility over time, safety, system integration, transients etc.) that might stifle or prevent commercial deployment. For example, systems that utilize a liquid medium typically have to deal with issues of corrosion and how the liquid will be pumped, which can be very challenging at high temperatures, but a recent demonstration of pumping at 1400°C[7] suggests it is nonetheless possible. For systems that utilize a solid TES medium, the intrinsically transient output as conductive resistance builds up, is inevitable and it is important to consider how this might affect the heat engine. For example, power generating turbines are usually optimized for a specific inlet temperature, and if the TES medium's output decreases during the discharge, it can have a major impact on efficiency.

For space heating/cooling low cost, high gravimetric and high volumetric energy density TES systems can have significant impact on extending the range of EVs, because as much as 35-40% of the electrical battery capacity in EVs can be used for cabin heating/cooling.[8] TES could also play a major role in offsetting heating/cooling loads in buildings as they are expected to be more than 50% of the load in buildings.[9,10] First, buffering heat in the walls of a building could reduce its net energy consumption, by enabling time-shifted matching of internal thermal demand with the diurnal temperature swings of the external natural environment. Second, TES has the ability to make use of inexpensive renewable electricity during its peak production (often oversupply) and storing it in the form most conducive to its final usage – namely as thermal energy for space heating/cooling, instead of storing electricity.

One fundamental challenge in TES adoption is that there is limited tunability in the usage temperature. For example, if the required temperature is 25°C and the ambient temperature swings above and below 25°C, two different TES materials and systems are needed, which dramatically reduces the utilization of each system, leading to a higher cost. However, Mumme *et al.*[11] recently showed that a material with a perfectly tunable storage temperature can increase the utilization factor of a TES system by a factor of 20. Since the levelized cost of storage (LCOS) is inversely proportional to its utilization factor, tunable thermal storage has the potential to dramatically decrease the LCOS. Advances will require revisiting the thermodynamics of phase transitions to look for ways that such transitions can be manipulated using external fields e.g., an electric field or pressure.[12] For example, Li et al.[12] showed a large effect (~ 10 – 20°C) on the transition temperature by applying pressure in plastic crystals.

2| Decarbonizing Industrial Processes

GHG emissions in the industrial sector comprise more than 15% of global emissions, where the majority is associated with providing heat at temperatures ranging from 100-1000°C.[13] Aside from providing heat, there are many cases where one must also compensate for the thermodynamic driving force associated with forming CO_2, which can only happen in the following ways: (1) electrochemically (e.g., electrolysis), (2) thermally (e.g. pyrolysis), (3) with a reducing agent such as H_2, that is synthesized without CO_2 emissions, or (4) through some combination of the previous three. Although each industry poses its own unique challenges, the most significant industries are: cement, iron/steel, aluminum and hydrogen (H_2), which are each responsible for approximately 10%, 4%, 1%, and 1% of global GHG emissions, respectively. Here, there is an opportunity to redesign these industrial processes so that they utilize low cost, intermittent renewable energy to provide the required heat, the heat can also be localized only where needed, and there is also an opportunity to invent or develop new processes that use one of the aforementioned approaches for thermodynamic compensation.

In the case of cement production, there are CO_2 emissions associated with burning fuel to provide the heat needed for calcination of limestone (~ 40% of the emissions for the process), and the reaction itself also liberates CO_2, primarily when CaO is formed from $CaCO_3$ (~ 60% of the emissions for the process). Conceptually, the process could be redesigned to make use of cheap renewable electricity to supply the heat, via Joule heating. However, abating the other 60% associated with the reaction would require: (a) use of a different reaction; (b) CO_2 capture and sequestration; (c) a new process altogether; or (d) cement itself would need to be replaced by production of another material altogether – via a process that doesn't emit GHGs.

In the case of iron/steel production, carbon or CO is used to reduce iron oxide to iron, thus leveraging the thermodynamic driving force of oxidizing carbon to form CO_2. Initial demonstrations of such alternative approaches using high-temperature electrochemical systems and hydrogen as a reductant have been achieved,[14] but much more effort, attention and funding is needed to make these approaches scalable and cost effective.

The case for aluminum and H_2 production is similar to that of iron/steel, because they again require re-engineering the process to find an alternative thermodynamic driving force. One option for H_2 that is currently being explored is methane pyrolysis, which offers the promise of producing H_2 at competitive costs along with solid carbon, which could be used as construction material. Recently, novel concepts have been proposed,[15] but the topic overall has received minimal attention. Furthermore, it should be mentioned that H_2 itself can be used as a fuel to provide heat, though there are still significant issues associated with the design of and dynamics within H_2 combustors that have not been completely solved.[16] Some of the challenges are significantly higher flashback and auto ignition risk because of the significantly higher flame speed and shorter ignition delay time for H_2 as compared to natural gas. Managing the NO_x emissions from H_2 combustors also requires research in alternate combustor designs.

3| Cooling and Heat Pumping Systems

The global warming potential (GWP) of hydrofluorocarbons (HFCs) which are used as refrigerants is >2000 times that of CO_2. With growing demand of air-conditioning in developing economies and electrification of heating using heat pumps in developed economies, it is expected that the seemingly unavoidable leakage of HFCs alone could single-handedly become a notable fraction (10-40%) of the planet's global warming by 2050.[17] Heating and cooling demands are also expected to dramatically increase the electricity demand. Therefore, affordable and scalable high energy efficiency cooling systems using refrigerants that are non-toxic, non-flammable, have a GWP ~ 1 (i.e. not worse than CO_2) are needed. However currently, there are no viable solutions that meet all these requirements.

Research is needed to identify/discover and characterize new refrigerants, to develop higher coefficient of performance (COP) low-cost systems that utilize an alternative to HFCs for mechanical vapor compression (MVC) or a completely new type of refrigeration system (non-MVC). There is also a need to develop alternatives that decouple dehumidification from cooling, as the dehumidification load (i.e., a latent heat load) can add significant inefficiency to the system.[18] For example, this could involve compression by electrochemical, instead of mechanical means, or by making use of a different form of entropy change, e.g., via a redox couple, thermoelectricity, thermoacoustics or barocaloric materials[12], combined with membrane-based dehumidification processes. Recently,[19] evaporative cooling has been proposed to provide an additional efficiency boost to MVC based systems, however, it's important to consider how much extra water will be needed, as access to clean water is another global challenge.

4| Long Distance Transmission of Heat

Space and water heating in both residential and commercial buildings are delivered below 60°C. They comprise ~ 8% of primary energy consumption in the U.S. (i.e., ~ 7.75 Quads) and they are responsible for more than 6% of U.S. GHG emissions.[20] In principle, this could potentially be provided by the waste heat available from power plants (~25.4 Quads). However, we cannot transport large amounts of heat over large distances (i.e., order 10 miles) with a small temperature difference (i.e., 1-5°C) or exergy loss. The issue here is one of power density, as the goal is to transport large MW scale heat using minimal equipment/material, so that it is cost effective like an electrical power line. The main difference from transmitting electrical power, however, is that unlike electrical conductivity, which spans ~ 30 orders of magnitude (e.g., silver vs. Teflon), thermal conductivity only spans about 6 orders of magnitude (e.g., air vs. diamond). There is no intrinsic upper bound on thermal conductivity, and thus the discovery of a thermal superconductor[21] would enable long distance transmission of heat, but it is not clear if one can be practically made. Alternatively, one could add enthalpy in an endothermic reaction or phase transition, move the products over long distances and recombine them in an exothermic reaction, which could essentially move heat with potentially small temperature differences. One approach could use a thermochemical heat transfer fluid and storage medium, such as the ammonia dissociation reaction.[22] However, with the advancements in computational chemistry, which enable *ab initio* prediction of reaction enthalpies, it may now be possible to discover[23] other pumpable fluids with reversible chemical reactions, that can be used to move enthalpy. Such long-distance heat transmission could also allow much more effective thermal utilization within large chemical plants, which in general, have not been designed and built to minimize GHG emissions.

5|Variable Conductance Building Envelopes

In the built environment, the requirements for temperature, humidity and indoor air quality are well known and do not change during the day, but the outdoor temperatures and conditions can vary significantly. Langevin *et al.*[24] highlighted that innovations in the building envelope can have a significant impact on decarbonizing the building sector by lowering the demand for cooling or heating. Research is needed to significantly improve insulation, compared to the current materials, in order to thermally isolate the built environment from the external conditions. However, at times it may be prudent to leverage the external environment for the built environment. One approach is to intelligently trigger the modification of the thermal conductance of building envelopes using non-linear thermal devices.[25] For example, this would allow building walls to be insulating on a hot day to prevent heat from leaking in from the outside, but if the temperature drops at night, the walls could intelligently switch to being conducting to allow heat from the building to escape, thereby enabling free cooling. A recent study by Menyhart and Krarti[26] showed that a variable conductance building envelop can lead to energy savings anywhere from 7% to 42% in different cities across the USA, which would be a major impact on reducing GHG emissions. This could also enable on-demand control of envelop-based thermal energy storage. The desired characteristics of a variable conductance envelop are (1) a high on-state and off-state thermal conductance ratio, (2) a very low conductance in the insulating state (off-state), (3) a large number of cycles between on and off states and (4) low power consumption. Enabling a variable conductance envelop will require research in developing cost effective and reliable materials and devices.

Concluding Remarks

Given that 90% of the world's energy use today is based on thermal energy, it seems inconceivable that we can achieve deep decarbonization without technological breakthroughs in thermal science and engineering. Yet, it has not received as much attention from the research community and research funding organizations. Here, we have highlighted five unique challenges in this realm, which if addressed adequately, can each potentially produce gigaton-scale reductions in GHG emissions. Given that energy and climate is one of the defining challenges of the 21st century, we hope this will serve as an intellectual appeal and a call to action for the research community, and we hope these challenges will receive adequate and sustained funding from government, industry and private sources.

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