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Engineering thermochemistry: The science critical for the paradigm shift toward carbon neutrality

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ABSTRACT

The global shift toward carbon neutrality, driven by growing concerns about climate change, requires collaborative efforts. While cleaner energy and carbon capture are crucial, addressing some high-carbon-emission industrial processes that significantly and disproportionally contribute to our carbon footprint is more important than ever. Analysis reveals that over 90% of total carbon emissions from human activities are attributed to a few super-emitting thermochemical processes. We urgently need breakthrough technologies and transformative alternatives to combat this excess of carbon dioxide emissions effectively. Engineering Thermochemistry is the scientific discipline that offers both scientifically sound and practical solutions to the pressing carbon neutrality challenges.

1. Introduction

The worldwide transition toward carbon neutrality has gained substantial momentum in recent years. This paradigm shift is propelled by the pressing imperative to confront climate change, necessitating the reduction in the emission of greenhouse gases, primarily carbon dioxide, to curb global warming. The consequence of this global movement has proven to be transformative, and its impact is poised to persistently engender far-reaching and profound transformations across virtually every economic sector and facet of human existence on a global scale. Nonetheless, the journey toward carbon neutrality is intricate and multifaceted, demanding concerted efforts from governments, businesses, and individuals alike. A plethora of strategies and technological solutions have been proposed and explored, encompassing but not limited to the increased utilization of cleaner energy sources, such as solar, wind, and hydropower; enhancements in energy efficiency across various domains, including buildings, appliances, and industrial processes; the widespread adoption of cleaner transportation technologies, exemplified by electric vehicles; the implementation of carbon capture and storage methods, aimed at trapping emissions from industrial processes and power generation; sustainable farming practices, reforestation, and afforestation initiatives; initiatives geared toward shifting individual and collective behaviors, fostering a waste reduction, and the embrace of more sustainable lifestyles. These approaches are necessary as they collectively contribute to achieving carbon neutrality and mitigating the adverse impacts of climate change. Nevertheless, we believe there is an urgent need to clarify which industrial processes are the most carbon-intensive, what innovative technologies are required for these processes, and what scientific principles are needed to enable these innovations to achieve this ambitious goal quickly, efficiently, and economically. This short paper aims to bring these issues up and highlights some of our recent efforts in these areas.

2. Chasing after carbon's superemitters

For carbon emissions, statistical data have indicated that a small number of superemitters are responsible for a disproportionately large share of the emissions. Fig. 1 depicts CO_2 emission statistics from different industrial sectors in China, highlighting that six key sectors, namely coal-fired power plants, residential and industrial coal-fired boilers, iron and steel manufacturing, non-ferrous metallurgical processes, cement production, and lime production, contribute to over 90 % of China's total 10.5 billion tons of carbon dioxide emissions. These industrial processes are crucial in producing energy and materials essential for economic and social development. Therefore, to effectively reduce carbon dioxide emissions and expedite progress toward carbon

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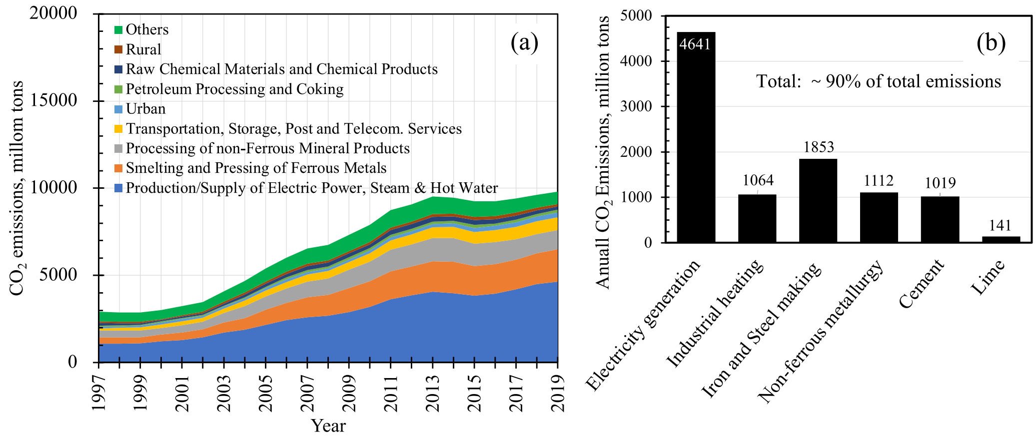

Fig. 1. Carbon dioxide emissions from key industrial sections for the period 1997 to 2019 (a) and from the six superemitters in 2020 (b) in China [1].

neutrality, it is imperative to prioritize technological innovation in these high-emission processes. These processes encompass various industries but share a common characteristic: they all involve thermochemical reactions, such as pyrolysis, gasification, combustion, decomposition, oxidation, and reduction. Despite the different attributes, these thermochemical reactions share a common inherent feature: they are driven or induced by heat and are operated at high temperatures. This commonality underscores the importance of a newly emerging science and technology known as Engineering Thermochemistry, which is critical in guiding our efforts to address carbon emissions.

3. Heat-driven/-induced thermochemical reactions

"Heat" represents one of humanity's earliest recognized and universally harnessed fundamental forms of energy. Throughout history, it has consistently served as the primary force responsible for inducing and driving most of the physical and chemical changes in matter. For example, the myriad evolutionary processes that have shaped Earth over billions of years and the crucial large-scale processing and utilization of resources that underpin contemporary societal development can largely be attributed to "heat" or the thermochemical reactions it induces or drives. It is, therefore, not an overstatement to declare that without "heat," it would be unimaginable how Earth could have evolved to its current state.

Furthermore, without advancements in the study and application of "thermochemical reactions," several pivotal industrial revolutions would not have transpired, and human society would not have attained the material and cultural sophistication we witness today. Our modern society relies heavily on the extensive utilization of heat-induced and heat-driven thermochemical reaction processes, which provide essential elements such as heat, electricity, steam, steel, aluminum, ceramics, and cement, among many other products.

4. Engineering thermochemistry

In the early 19th century, the scientific discipline of "Thermochemistry" emerged as a distinct branch of chemistry. Its primary focus is to qualitatively and quantitatively examine the heat energy generated or absorbed during chemical reactions and phase transitions. Thermochemistry plays a crucial role in assessing the spontaneity and favorability of reactions. However, it is important to note that thermochemistry does not encompass the broader spectrum of fundamental and engineering considerations to make thermochemical reactions practically useful. These considerations include fluid dynamics, chemical reactions, heat transfer, mass transfer, and process and reactor engineering. From a practical standpoint, the successful utilization of thermochemical reactions to produce products with minimized energy consumption, reduced emissions, and maximized efficiency relies heavily on the harmonious integration of these diverse aspects at various scales. This alignment spans individual reactions to reactor design and encompasses entire industrial processes. Achieving this synergy is essential for realizing a future characterized by sustainable and environmentally friendly economic and social development. Furthermore, it enables the seamless transformation of thermochemical industries into low- or zero-carbon emission processes.

In this context, Chinese scientists, led by Professor Guangwen Xu at Shenyang University of Chemical Technology, have proposed an emerging scientific discipline called "Engineering Thermochemistry (ETC)." ETC concentrates on the study of the common attributes of various thermochemical reactions, which have normally been dealt with separately within various distinctly different scientific disciplines and industries. By eliminating the inherent limitations and barriers between different scientific and engineering disciplines, ETC seeks to foster innovation in thermochemical reaction science and technology, developing common transformative theories and core technologies in this

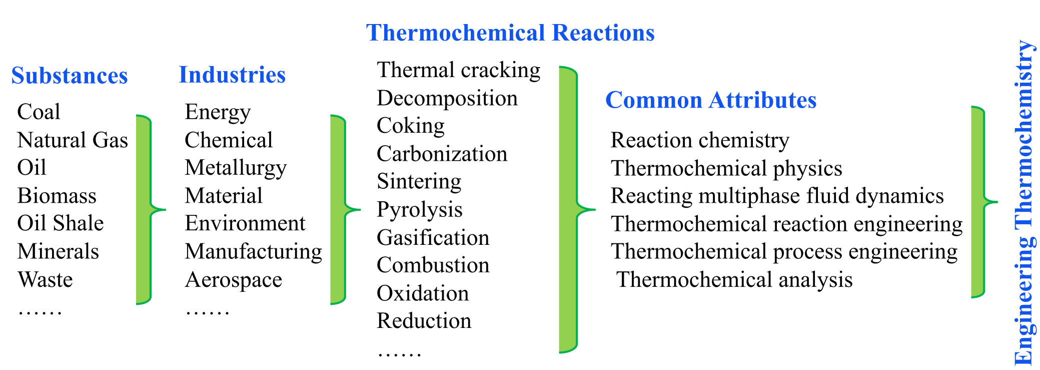

Fig. 2. Engineering Thermochemistry concept and its scientific connotation.

Carbon super-emitters	Pathways	Solutions	CO_2 reduction potential
• Fossil-fuel boilers/motors • Industrial thermal heating • Electric-heating processes ○ Metal smelting ○ Metallurgy silicon ○ Calcium carbide ○ Fused magnesia • High-temperature processes ○ Non-ferrous metals/alloys ○ Ceramics / refractory ○ Glass • Calcination of carbonates ○ Cement ○ Lime, calcined magnesite • Carbon-reducing processes ○ Iron steel ○ Phosphorus	Carbon reduction	✓Increasing power generation efficiency ✓Restructuring industrial combustion systems ✓Replacing electrolytic with carbothermic reactions and electrical heating with thermal energy ✓Reducing thermochemical reaction temperature and time ✓Employing non-carbon thermochemical processes	2–3 billion tons
	Carbon substitution	✓Using non-fossil fuels for thermal power/heat ✓Substituting wastes-pyrolysis oils for crude oil ✓Using hydrogen as a reducing agent in ironmaking	~1 billion tons
	Carbon recycling	✓Carbon dioxide sequestration and mineralization ✓Biochar for soil amendment & charcoal for storage ✓Converting carbonates-derived CO_2 into feedstock	~2 billion tons

Fig. 3. The approaches and potentials of ETC in reducing carbon emissions through thermochemical reaction processes [1,7].

field to produce value-added products efficiently, economically, and environmentally friendly. As conceptually illustrated in Fig. 2, ETC studies fundamental and engineering aspects of thermochemical reactions, including chemistry, physics, multiphase fluid dynamics, reaction engineering, and process engineering, seeking to comprehend the intricate interactions and interdependencies among different forms of heat, heat transfer, mass transfer, and substance transformation. Through precise control and harmonious coordination between heat and reactions across different scales and scopes, ETC offers solutions to the substantial challenges encountered by existing thermochemical industries, notably the issues of high energy consumption and emissions. Consequently, it is pivotal in driving significant theoretical and technological transformations within thermochemical reactions and processes. To promote the development of ETC, a world-class research organization dedicated to ETC was established and registered in Vancouver, Canada, in 2022 [2], following the creation of the Special Division of Engineering Thermochemistry under the Chemical Industry and Engineering Society of China in 2018 [3].

Since its conceptual inception in 2018, "Engineering Thermochemistry" has emerged as a pivotal scientific foundation for advancing progress in thermochemical reactions. A recent specialized Xiangshan Science Conference, themed "Engineering Thermochemistry: Interdisciplinary and Scientific Frontiers," has further ignited the interest and attention of numerous experts in related fields. Professor Mingyuan He, an academician of the Chinese Academy of Sciences and a professor at East China Normal University, emphasized that ETC is the fundamental science that plays a crucial role in achieving the goal of carbon neutrality. He pointed out that, from a chemical perspective, the effective utilization of carbon energy hinges on maintaining a balance between carbon and hydrogen, necessitating a series of reactions to break and reassemble these molecular bonds. Whether it involves breaking down large molecules into smaller ones or synthesizing smaller molecules into larger ones, ETC assumes a critical and, at times, irreplaceable role in numerous processes. All participating experts at the conference concurred that scientific and technological innovations related to thermochemical reactions are pivotal for achieving low-carbon development because they believed that without addressing the issue of carbon dioxide emissions from thermochemical reactions, particularly those with high emissions, the attainment of carbon neutrality remains an exceedingly challenging endeavor.

5. Engineering thermochemistry for carbon emission mitigation

Following extensive research into technologies capable of effectively reducing carbon emissions on a scale ranging from tens of billions to hundreds of billions of tons [4–6], Professor Guangwen Xu and his colleagues at Shenyang University of Chemical Technology have identified three key pathways for achieving this goal: carbon reductions, carbon substitutions, and carbon recycling (Fig. 3). These strategic solutions have been comprehensively detailed in their recent research papers [1,7]. These publications have expounded upon the scientific significance of Engineering Thermochemistry and outlined its potential avenues and capabilities for advancing progress toward the carbon neutrality agenda through technological innovation. By showcasing specific exemplary processes, they have effectively demonstrated how and why ETC can play a pivotal role in revolutionizing carbon super-emitting processes to reduce carbon emissions substantially. As depicted in Fig. 3, with a targeted emphasis on technological innovations aimed at mitigating carbon emissions from major carbon emitters through strategies involving carbon reduction, carbon substitution, and carbon recycling, it is estimated that China could potentially reduce approximately 5–6 billion tons of CO_2 annually. This significant reduction would bring the country closer to achieving carbon neutrality. It is evident that ETC provides invaluable scientific support for driving the transformative shift towards carbon neutrality. Ultimately, while driving the achievement of carbon neutrality goals, ETC also facilitates and promotes substantial technological revolutions and paradigm shifts in various critical industrial processes, such as steel, cement, and carbonate processing. These transformations shift these industrial sectors from the traditional paradigm that prioritizes process efficiency to a new paradigm that emphasizes both process efficiency and environmental friendliness.

6. Conclusion

In conclusion, the pursuit of carbon neutrality is a global imperative to combat climate change. Addressing high-carbon-emission industrial processes is essential to achieve this goal. Engineering Thermochemistry offers a transformative approach by integrating scientific and engineering disciplines to improve energy efficiency and reduce the carbon emissions of heat-driven/-induced thermochemical reactions. By focusing on carbon reduction, substitution, and recycling in high-emission processes, ETC can contribute to significant reductions in carbon emissions. The potential for reducing 5–6 billion tons of CO_2 annually in China highlights the pivotal role of ETC in advancing carbon neutrality. ETC provides invaluable scientific support for this paradigm shift towards a more sustainable and environmentally friendly future.

CRediT authorship contribution statement

Zhancheng Guo: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Conceptualization. **Shiwei Wang:** Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **Dingrong Bai:** Writing – review & editing, Conceptualization.

Declaration of Competing Interest

The authors 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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