



# **Technological and Modelling Progress in Green Engineering and Sustainable Development: Advancements in Energy and Materials Engineering**

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Abstract: Due to a growing number of environmental issues, including global warming, water scarcity, and fossil fuel depletion, the topic of modern materials in energy is becoming crucial for our civilization. The technological advancements that have been observed bring many innovations that significantly impact how energy can be generated, stored, and distributed. Moreover, new opportunities have emerged in energy and materials engineering due to the increasing computational capability of current data processing systems. Methods that are highly demanding, time-consuming, and difficult to apply may now be considered when developing complete and sophisticated models in many areas of science and technology. Combining computational methods and AI algorithms allows for multi-threaded analyses solving advanced and interdisciplinary problems. Therefore, knowledge and experience in this subject, as well as the investigation of new, more efficient, and environmentally friendly solutions, currently represent one of the main directions of scientific research. The Special Issue "Advances in Materials: Modelling Challenges and Technological Progress for Green Engineering and Sustainable Development" aims to bring together research on material advances, focusing on modelling challenges and technological progress (mainly for green engineering and sustainable development). Original research studies, review articles, and short communications are welcome, especially those focusing on (but not limited to) artificial intelligence, other computational methods, and state-of-the-art technological concepts related to the listed keywords within energy and materials engineering.

**Keywords:** sustainability; net-zero emissions; energy efficiency; waste-to-energy; fuels; modelling; optimization; artificial intelligence; bio-inspired methods; simulation; complex systems

## 1. Introduction

Observed climate changes, environmental pollution, the shortage of drinking water, growing demands for energy, and the simultaneous depletion of natural resources force the search for new technologies, including modern materials, which are key to sustainable development. The goal is sustainable development, striving for zero-emission technologies and increasing the energy efficiency of devices. These efforts are accompanied by requirements for selecting and testing new materials.

This work aims to encourage the scientific community to submit work aimed at meeting the above challenges, considering modelling issues and practical technological aspects. The exemplary areas and topics for possible contributions are listed in the next section.



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#### 2. Advancements in Energy and Materials Engineering

In the era of the observed climate change, such clan coal technologies, waste heat application methods, and effective energy conversion systems play a crucial role. However, clean coal technologies and carbon capture and storage pose challenges centered around the efficiency and quality of the materials used [1,2].

Innovations in carbon capture technologies (CCTs), including materials used for CO<sub>2</sub> capture and utilization (CCU) [3,4], artificial-intelligence-driven smart materials [5,6], oxygen carriers [7–10], sorbents in adsorption cooling and desalination systems [8,9], as well as construction materials of energy devices [11–13], play a key role in implementing these technologies on a larger scale and are crucial for achieving the United Nations' Sustainable Development Goals (SDGs) [14].

Thermal fuel conversion, including clean coal fluidized bed technologies, allows various fuels and wastes, including biomass and alternative fuels, to be used [15]. It is impossible not to mention new solutions in the area of energy storage [16–18] and thermomechanical properties, including phase change materials (PCMs) used for thermal energy storage and the modelling of novel composite materials formed by combining PCMs with other materials [19]. In this area, we can also point to innovative approaches using solar energy and heat pumps [20–22], ocean [23,24], and wind [25,26].

In pursuit of the goal of net-zero emission [27,28], waste-to-energy (WtE) technology is becoming more and more important, allowing requirements centered around a circular economy, greenhouse gas reduction [29], and sustainable waste management systems [30,31] to be met.

Recent advances in materials science also include new materials used in refrigeration, including emerging materials and rational strategies in passive daytime radiative cooling (PDRC) [32], thermoelectric devices [33], and adsorption chillers [34]. For example, novel adsorbents and their modifications must perform better in adsorption cooling and desalination systems, including when being blended with nanomaterials.

Progress in materials science and engineering would not be possible without advances in modelling. These advances include, among other things, combustion and co-combustion processes in power boilers, including the use of artificial intelligence methods [35–38]. The issues concern materials, but also the operating conditions and operating strategies of energy devices and systems [39–41].

#### 3. Conclusions

Technological advancements in materials, especially in the energy sector, bring enormous challenges. They also provide an opportunity to create a more sustainable future. Significant progress can be made and contribute to developing solutions in order to achieve net-zero emissions goals through cooperation and by sharing experience and knowledge.

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### References

- Gür, T.M. Carbon Dioxide Emissions, Capture, Storage and Utilization: Review of Materials, Processes and Technologies. Prog. Energy Combust. Sci. 2022, 89, 100965. [CrossRef]
- Liu, E.; Lu, X.; Wang, D. A Systematic Review of Carbon Capture, Utilization and Storage: Status, Progress and Challenges. Energies 2023, 16, 2865. [CrossRef]
- 3. Dziejarski, B.; Krzyżyńska, R.; Andersson, K. Current Status of Carbon Capture, Utilization, and Storage Technologies in the Global Economy: A Survey of Technical Assessment. *Fuel* **2023**, *342*, 127776. [CrossRef]
- Khosroabadi, F.; Aslani, A.; Bekhrad, K.; Zolfaghari, Z. Analysis of Carbon Dioxide Capturing Technologies and Their Technology Developments. *Clean. Eng. Technol.* 2021, 5, 100279. [CrossRef]
- Saleh, T.A. Nanomaterials and Hybrid Nanocomposites for CO<sub>2</sub> Capture and Utilization: Environmental and Energy Sustainability. RSC Adv. 2022, 12, 23869–23888. [CrossRef]
- Zhang, Z.; Zheng, Y.; Qian, L.; Luo, D.; Dou, H.; Wen, G.; Yu, A.; Chen, Z. Emerging Trends in Sustainable CO<sub>2</sub>-Management Materials. *Adv. Mater.* 2022, 34, 2201547. [CrossRef]
- Kim, S.; Annamalai, L.; Lobo, R.F. Silica-Encapsulated Fe<sub>2</sub>O<sub>3</sub> Oxygen Carriers for Selective Chemical Looping Combustion of Hydrogen. *Chem. Eng. J.* 2023, 455, 140919. [CrossRef]
- Ding, H.; Tong, S.; Qi, Z.; Liu, F.; Sun, S.; Han, L. Syngas Production from Chemical-Looping Steam Methane Reforming: The Effect of Channel Geometry on BaCoO<sub>3</sub>/CeO<sub>2</sub> Monolithic Oxygen Carriers. *Energy* 2023, 263, 126000. [CrossRef]
- Chen, J.; Kong, H.; Wang, H. A Novel High-Efficiency Solar Thermochemical Cycle for Fuel Production Based on Chemical-Looping Cycle Oxygen Removal. *Appl. Energy* 2023, 343, 121161. [CrossRef]
- 10. He, Z.; Hou, Y.; Li, H.; Wei, J.; Ren, S.; Wu, W. Novel Chemical Looping Oxidation of Biomass-Derived Carbohydrates to Super-High-Yield Formic Acid Using Heteropolyacids as Oxygen Carrier. *Renew. Energy* **2023**, 207, 461–470. [CrossRef]
- Česánek, Z.; Lencová, K.; Schubert, J.; Antoš, J.; Mušálek, R.; Lukáč, F.; Palán, M.; Vostřák, M.; Houdková, Š. High-Temperature Corrosion Behavior of Selected HVOF-Sprayed Super-Alloy Based Coatings in Aggressive Environment at 800 & deg;C. *Materials* 2023, 16, 4492. [CrossRef]
- 12. Majcher, K.; Musiał, M.; Pakos, W.; Różański, A.; Sobótka, M.; Trapko, T. Methods of Protecting Buildings against HPM Radiation—A Review of Materials Absorbing the Energy of Electromagnetic Waves. *Materials* **2020**, *13*, 5509. [CrossRef]
- 13. Ji, G.; Ding, T.; Xiao, J.; Du, S.; Li, J.; Duan, Z. A 3D Printed Ready-Mixed Concrete Power Distribution Substation: Materials and Construction Technology. *Materials* **2019**, *12*, 1540. [CrossRef]
- 14. Olabi, A.G.; Obaideen, K.; Elsaid, K.; Wilberforce, T.; Sayed, E.T.; Maghrabie, H.M.; Abdelkareem, M.A. Assessment of the Pre-Combustion Carbon Capture Contribution into Sustainable Development Goals SDGs Using Novel Indicators. *Renew. Sustain. Energy Rev.* **2022**, 153, 111710. [CrossRef]
- Kijo-Kleczkowska, A.; Gnatowski, A. Recycling of PlasticWaste, with Particular Emphasis on Thermal Methods—Review. *Energies* 2022, 15, 2114. [CrossRef]
- 16. Ajiwibowo, M.W.; Darmawan, A.; Aziz, M. A Conceptual Chemical Looping Combustion Power System Design in a Power-to-Gas Energy Storage Scenario. *Int. J. Hydrog. Energy* **2019**, *44*, 9636–9642. [CrossRef]
- 17. Astolfi, M.; Diego, M.E.; Romano, M.; Abanades, J.C. Integration of a Novel Chemical Looping Combustion Reactor into a Thermochemical Energy Storage System. *Energy Convers. Manag.* **2023**, *291*, 116985. [CrossRef]
- Cormos, A.M.; Petrescu, L.; Cormos, C.C. Techno-Economic Implications of Time-Flexible Operation for Iron-Based Chemical Looping Combustion Cycle with Energy Storage Capability. *Energy* 2023, 278, 127746. [CrossRef]
- 19. Kant, K.; Biwole, P.H.; Shamseddine, I.; Tlaiji, G.; Pennec, F.; Fardoun, F. Recent Advances in Thermophysical Properties Enhancement of Phase Change Materials for Thermal Energy Storage. *Sol. Energy Mater. Sol. Cells* **2021**, 231, 111309. [CrossRef]
- 20. Kijo-Kleczkowska, A.; Bruś, P.; Więciorkowski, G. Profitability Analysis of a Photovoltaic Installation—A Case Study. *Energy* **2022**, *261*, 125310. [CrossRef]
- 21. Pandey, A.K.; Hossain, M.S.; Tyagi, V.V.; Abd Rahim, N.; Selvaraj, J.A.L.; Sari, A. Novel Approaches and Recent Developments on Potential Applications of Phase Change Materials in Solar Energy. *Renew. Sustain. Energy Rev.* **2018**, *82*, 281–323. [CrossRef]
- Goswami, D.Y.; Vijayaraghavan, S.; Lu, S.; Tamm, G. New and Emerging Developments in Solar Energy. Sol. Energy 2004, 76, 33–43. [CrossRef]
- 23. Wang, G.; Yang, Y.; Wang, S.; Zhang, H.; Wang, Y. Efficiency Analysis and Experimental Validation of the Ocean Thermal Energy Conversion with Phase Change Material for Underwater Vehicle. *Appl. Energy* **2019**, *248*, 475–488. [CrossRef]
- 24. Chen, Y.; Yao, Z.; Chen, B.; Liu, Z.; Yang, C. Numerical and Experimental Study of the Ocean Thermal Energy Capture Process Utilizing Metal Foam–Phase-Change Material (PCM) Composites. *J. Energy Storage* **2023**, *67*, 107600. [CrossRef]
- Tirth, V.; Algahtani, A.; Alghtani, A.H.; Al-Mughanam, T.; Irshad, K. Emerging Nano-Engineered Materials for Protection of Wind Energy Applications Photovoltaic Based Nanomaterials. *Sustain. Energy Technol. Assess.* 2023, 56, 103101. [CrossRef]
- Heragy, M.; Kiwata, T.; Hamano, T.; Shima, T.; Ueno, T.; Kono, T.; Ekmekci, A. Experimental Study of Wind Energy Harvesting from Flow-Induced Vibration of Prisms Using Magnetostrictive Material. J. Fluids Struct. 2023, 119, 103910. [CrossRef]
- Rockström, J.; Gaffney, O.; Rogelj, J.; Meinshausen, M.; Nakicenovic, N.; Schellnhuber, H.J. A Roadmap for Rapid Decarbonization. Science 2017, 355, 1269–1271. [CrossRef] [PubMed]
- Moustakas, K.; Loizidou, M.; Klemes, J.; Varbanov, P.; Hao, J.L. New Developments in Sustainable Waste-to-Energy Systems. Energy 2023, 284, 129270. [CrossRef]

- Islam, A.; Teo, S.H.; Ng, C.H.; Taufiq-Yap, Y.H.; Choong, S.Y.T.; Awual, M.R. Progress in Recent Sustainable Materials for Greenhouse Gas (NOx and SOx) Emission Mitigation. *Prog. Mater. Sci.* 2023, 132, 101033. [CrossRef]
- Karmakar, A.; Daftari, T.; Sivagami, K.; Chandan, M.R.; Shaik, A.H.; Kiran, B.; Chakraborty, S. A Comprehensive Insight into Waste to Energy Conversion Strategies in India and Its Associated Air Pollution Hazard. *Environ. Technol. Innov.* 2023, 29, 103017. [CrossRef]
- Lee, J.; Lin, K.Y.A.; Jung, S.; Kwon, E.E. Hybrid Renewable Energy Systems Involving Thermochemical Conversion Process for Waste-to-Energy Strategy. Chem. Eng. J. 2023, 452, 139218. [CrossRef]
- Gao, W.; Chen, Y. Emerging Materials and Strategies for Passive Daytime Radiative Cooling. Small 2023, 19, 2206145. [CrossRef] [PubMed]
- 33. Cao, T.; Shi, X.L.; Chen, Z.G. Advances in the Design and Assembly of Flexible Thermoelectric Device. *Prog. Mater. Sci.* 2023, 131, 101003. [CrossRef]
- 34. Xie, W.; Hua, W.; Zhang, X. Research Progress on Synthesis and Adsorption Properties of Porous Composite Adsorbents for Adsorption Cooling and Desalination Systems: A Mini-Review. *Energy Fuels* **2023**, *37*, 4751–4768. [CrossRef]
- Krzywański, J.; Rajczyk, R.; Nowak, W. Model Research of Gas Emissions from Lignite and Biomass Co-Combustion in a Large Scale Cfb Boiler. *Chem. Process Eng.* 2014, 35, 217–231. [CrossRef]
- Muskala, W.; Krzywański, J.; Czakiert, T.; Nowak, W. The Research of CFB Boiler Operation for Oxygen-Enhanced Dried Lignite Combustion. *Rynek Energii* 2011, 92, 172–176.
- Muskała, W.; Krzywański, J.; Rajczyk, R.; Cecerko, M.; Kierzkowski, B.; Nowak, W.; Gajewski, W. Investigation of Erosion in CFB Boilers. *Rynek Energii* 2010, 87, 97–102.
- Ongar, B.; Beloev, H.; Georgiev, A.; Iliev, I.; Kijo-Kleczkowska, A. Optimization of the Design and Operating Characteristics of a Boiler Based on Threedimensional Mathematical Modeling. *Bulg. Chem. Commun.* 2023, 55, 153–159. [CrossRef]
- 39. Li, Y.; Wei, C.; Liu, X.; Zhang, Z.; Wan, J.; He, X. Application of Gasification Slag in Construction Materials and High Value-Added Materials: A Review. *Constr. Build. Mater.* **2023**, 402, 133013. [CrossRef]
- Montagnaro, F.; Zaccariello, L. Performance Assessment of a Demonstration-Scale Biomass Gasification Power Plant Using Material and Energy Flow Analyses. *Energy* 2023, 284, 129327. [CrossRef]
- 41. Ge, Y.; Ding, S.; Zhang, W.; Kong, X.; Kantarelis, E.; Engvall, K.; Pettersson, J.B.C. Impacts of Fresh Bed Materials on Alkali Release and Fuel Conversion Rate during Wood Pyrolysis and Char Gasification. *Fuel* **2023**, *353*, 129161. [CrossRef]

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