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Editorial: Role of mathematical modeling in advanced power generation systems

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Editorial on the Research Topic
Role of mathematical modeling in advanced power generation systems

Sustainable development needs the use of alternate sources of energy across the globe. The reduction of carbon emissions (in other words, having a low carbon footprint) depends on the effective utilization of resources and lesser use of fossil fuels. The Sustainable Development Goals (SDGs) decided, during the Paris Agreement, to bring prosperity to all countries across the globe and save the planet. The most prominent goals out of the 17 SDGs related to the current Research Topic are goals 7, 9, 12, and 13. Some of the key targets of Goal 7 include ensuring universal access to affordable, reliable, and modern energy services, substantially increasing the share of renewable energy in the global energy mix, and doubling the global rate of improvement in energy efficiency by 2030. Similarly, Goal 9 talks about building resilient infrastructure, promoting inclusive and sustainable industrialization, and fostering innovation. Goal 12 targets improving energy efficiency and promoting the adoption of sustainable practices in industries. Goal 13 targets limiting global warming to 1.5°C above preindustrial levels by decreasing emissions to half using different technological advancements and behavioral actions. The above four goals can be better achieved by harnessing the advances in mathematical modeling. The present Research Topic was published on 10th February 2022 to call for contributions on how mathematical modeling can play a big role in optimizing energy utilization and reduction of greenhouse gas (GHG) emissions for sustainable industrialization. Around 230 researchers around the globe were contacted for this purpose.

Frontiers in Energy Research in combination with Frontiers in Thermal Engineering published nine articles involving 23 authors from six countries, involving diverse areas of research in mathematical modeling being used in synergy with our objective. Despite the diversity, the six key areas were 1) the optimization of district heating systems (SDG 9), 2) the optimization of safety systems involving condensation in tubes in nuclear power plants (SDG 7, 9, and 12), 3) the optimization of solar photo voltaic modules for power generation (SDG 7, 12, and 13), 4) the characterization of equipment related to thermochemical processing of biomass (SDG 7, 9, 13) 5) the process optimization for CO_2 sequestration during hydrogen production from steam methane reforming (SDG 7, 9, 12, and 13), and 6) mathematical models to predict the identification of personnel who did not wear protective equipment during the construction of power plants (SDG 9 and 12). Mathematical modeling included computational fluid dynamics (CFD) [areas (2), (3), and (4)] and process modeling [area (5)] using commercial software such as Ansys Fluent and Aspen Plus, respectively, while linear programming models were used in studies in area (1) and deep learning models in area (6).

Power plants are classified as coal based, nuclear based, or made of renewables such as solar, wind, or hydro. With the world grappling with climate change Research Topic, power from renewable sources would reduce carbon dioxide (CO_2) emissions, which, in turn, would help in achieving certain SDG targets mentioned earlier. In this context, some important sources of power production include hydrogen and solar photovoltaics. Furthermore, an innovative way of heating rooms can be obtained by optimized district heating.

Hydrogen has emerged as a source of energy and an alternative to fossil fuels. Though green hydrogen (for example, hydrogen production from electrolysis where the electricity is obtained from renewable sources such as solar and wind, *etc.*) is preferred, hydrogen from chemical processes such as steam methane reforming can also be used for energy needs. Thermochemical processes such as gasification of biomass can be used to generate electricity. The particle size distribution in such gasifiers is non-uniform, and the heat and mass transfer effects are different from the ones for uniformly sized particles. The hydrodynamics in such beds depend on geometric and operating parameters and have a huge effect on equipment performance. Experiments are very difficult in such cases, and mathematical modeling is very important. Ganguli and Bhatt have approached the CFD of such gasifiers both in qualitative and quantitative terms. The CFD model developed showed the characteristics of fluidized beds for Geldart B-type particles with seven different binary mixtures. The segregation and mixing of different operating parameters, such as the superficial velocity of fluid, and geometric parameters, such as bed height, were analyzed, and correlations were developed for the minimum fluidization velocity and pressure drop (Ganguli and Bhatt).

District Heating Systems (DHS) involve the combustion of renewable materials (such as biomass) to produce steam and heating buildings through pipe networks. The advanced versions of DHS offer parallel heating and cooling. Sporleder et al. provided a thorough literature review of the DHS systems until March 2022 and found the research gaps that existed in the area of DHS systems. The role of several technologies such as photovoltaics and heat pumps, with their significant contributions (10% and 25%, respectively) to DHS in buildings, was highlighted. The major contribution from the authors was highlighting the fact that the design of large-scale high-temperature DHS into a sustainable system has not yet been looked at. Mathematical modeling has been restricted to using linear programming models for present systems, while for large-scale systems, heuristic models need to be used. The authors recommended that work needs to be majorly undertaken in the direction of 1) the performance improvement of computational efforts using spatial and temporal aggregation and 2) designing a structure for a sustainable supply system that may have an integration of energy converters and heat sources (such as geothermal energy and large-scale heat pumps). These would need multi-objective optimization based on heuristic solvers.

Nuclear power plants also face the challenge of accidents with the risk of radiation coming out into the atmosphere and causing huge damage to life and property. Passive containment cooling systems (PCCS) in nuclear power plants have innovative condensers in which film condensation takes place in the presence of non-condensable gases such as air or helium. The non-condensable gases cause a decrease in condensation, while the wavy effects of the film cause an enhancement in condensation. However, for many decades, research work has been carried out largely through experimental measurements and analytical modeling. Li et al. performed two-phase CFD simulations using the volume of fluid (VOF) approach to visualize the effect of non-condensable gases on the condensation process. The authors found that for small concentrations of non-condensable gases (5%–10%), the boundary layer of the non-condensable gas layer decreased with the time period of condensation. For lower concentrations of the non-condensable layer, the thermal resistance of the film could be 20%–26%. Another study on such condensers focused on the distribution of steam in specially designed heat exchangers for safety systems in nuclear power plants. These exchangers absorb the heat during shutdown operations or during accidental conditions of nuclear power plants. Ganguli and Pandit carried out single-phase CFD simulations to understand the distribution of steam in such exchangers for higher pressures ranging from 10 to 70 bar since nuclear power plants operate at these pressures. The authors developed a new correlation to find the heat transfer coefficient from the Chilton Colburn analogy. The friction factor was obtained from the pressure drops for the different operating conditions of the condenser.

Safety Research Topic are of prime importance, and during the construction of large power plant sites, it becomes difficult to keep track of them. A case study related to the safety of personnel during the construction of a power plant, in which a deep learning model instead of a manual method was employed to ensure whether each and every personnel was abiding by rules, was developed by Chen et al. The authors developed a deep learning model (modified convolution neural network) to identify the safety of power workers. This included the detection and identification of safety helmets, work clothes, and safety gloves for each worker automatically without manual intervention. The application of this algorithm to real-life scenarios ensured that the algorithm was able to identify the staff who did not wear safety equipment as per the rules and regulations provided to them.

The steam methane reforming (SMRs) process produces hydrogen and a lot of carbon dioxide (CO_2), which must be prevented from emitting into the atmosphere. One of the methods is capturing CO_2 using carbon capture storage and utilization (CCSU). Pellegrini et al. carried out process simulations using ASPEN Plus (with necessary modifications to incorporate mass transfer with reaction and changes in the thermodynamics of the system) to design units for treatment of PSA tail gas by washing with methyldiethanolamine (MDEA). They used a combination of absorber and regenerator for removing the CO_2. The authors chose seven different designs of the absorber and carried out sensitivity analyses of the operating parameters to understand the maximum removal of CO_2 with the conservation of energy and minimum energy change. The developed model gave promising predictions for the implementation of the suggested modifications. While steam methane reforming is one of the oldest and most effective processes for hydrogen production, there has been considerable work on process intensification, especially in advanced reactor configurations. The current status of advanced reactors for hydrogen production in SMR was reviewed by Ganguli and Bhatt. A comparison of the reactors based on residence time, surface area, scale-up, coke formation, conversion, space velocity, and yield of hydrogen was presented. Furthermore, all the recent kinetic models and coke formation mechanisms were listed. The authors concluded that all the reactors considered had their own strengths. However, implementation on a large scale had a few challenges. Microreactors were shown to be of higher potential in terms of higher yields and lower residence times.

Nassar et al. developed an innovative three-dimensional numerical analysis to understand the view factors of solar PV for arrangement in solar photovoltaics (PV) to increase energy yields. The authors conducted a sensitivity analysis on the tilt angles of solar PV modules placed in different rows for receiving a range of solar irradiations. The primary reason for taking up such a study was the insufficient amount of received radiations on these panels due to the hindrance of PV panels ahead of them. The objective was to improve the performance of PV panels for different incident radiations. The model developed by the authors could accurately estimate the reduction in the incident solar rays and reduction in energy yields in the second and third rows of the PV channels. The model was tested for energy yields with data from different regions of the world. The authors claimed that the model was a viable alternative to other available models [such as the crossed-strings method (CSM)] that failed for the conditions considered for the undertaken study.

In conclusion, it has been observed that mathematical models can play a key role in design optimization and the optimization of safety systems in cities and power plants, such as solar or nuclear. For example, optimization using linear programing in DHS was able to reduce the carbon footprint of cities and contribute to not only low carbon emissions but also building resilient infrastructure. CFD models have shown good promise to predict modifications in both geometric and operating variables, which aided in the optimization of 1) biomass gasifier designs, 2) the distribution of steam under high pressure ensuring a robust design of safety systems in nuclear power plants, and 3) solar PV panel arrangements for better power generation using renewable energy. Deep learning models were proven to be of exceptional use for identification to ensure the safety of personnel. Process modeling using Aspen Plus was able to optimize the process of CO_2 sequestration by optimizing the design of key equipment in the process, such as absorbers, while deep learning models were able to accurately identify personnel who did not wear protective equipment during the construction of a power plant, which was not possible by manual intervention. This provides us with more confidence about the role of mathematical models in achieving the targets of the specific SDGs mentioned at the start of the editorial.

Author contributions

AG: Conceptualization, Formal Analysis, Methodology, Writing–original draft, Writing–review and editing. MT: Writing–review and editing. SD: Writing–review and editing. MD: Writing–review and editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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