Special Issue

Mathematical Modeling and Simulation of Catalytic Processes for Sustainable Energy Conversion and Environmental Applications

Message from the Guest Editors

While there exists huge knowledge and experience on the kinetics of catalytic reactions, other process variables. Given the great number of state variables and process design variables, mathematical modeling and simulations are often the only way to lead comprehensive studies to optimize the process.

In this view, it is a great pleasure for us to announce a call for contributions to a Special Issue entitled "Mathematical Modeling and Simulation of Catalytic Processes for Sustainable Energy Conversion and Environmental Applications". This Special Issue will welcome contributions centered on detailed modeling, down to CFD detail, as well as block modeling and real-time process simulation and optimization. Moreover, experimental data in support of the simulation outcome would be most welcome.

Potential topics include but are not limited to mathematical modeling and simulation of:

- Chemical reactors for synthesis of renewable fuels;
- Chemical reactors for gas-to-power applications;
- Water purification systems;
- Systems for pollutant removal;
- Fuel cells.

Guest Editors

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Deadline for manuscript submissions

closed (10 October 2021)

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Editor-in-Chief

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Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.6 days after submission; acceptance to publication is undertaken in 2.7 days (median values for papers published in this journal in the first half of 2025).

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