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Direct pore-level multiphysical model for solar thermochemical fuel production reactor based on structured porous media

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Solar-driven thermochemical fuel production cycle is one of important route for effective conversion and storing dilute and fluctuation solar energy into value-added fuels. The performance of a thermochemical reactor is largely dependent on the porous media design. The reacting porous media should simultaneously facilitate heat and mass transfer, provide reaction sites, as well as maintain large mass loading. Optimization of porous media structures are essential for further reactor optimization to achieve high solar-to-fuel efficiency. In this study, we developed a fully coupled mulitphysical model in 3D based on the actual morphology of porous media under direct solar irradiation. This model couples solar absorbing in volumetric photo-absorber, fluid flow of inert sweeping gas, multi-mode heat transfer, as well as detailed bulk and surface chemical reactions. The coupled 3D model offers a high fidelity to access the solar-to-fuel performance of various structured porous media. Owing to its 3D nature, the model allows for accurate calculation for the gradient structure design (e.g., artificially introduced anisotropy) to balance mass loading (thermodynamics) and reaction kinetics can be identified. Particularly, a detailed reaction kinetics model including chemical diffusion as well as chemical surface exchange is considered to identify the kinetic limiting regimes for various structure designs. Further, the impact surface roughness factor on the surface kinetics is studied in order to figure out potential of introducing surface modifications in the case of surface limited reaction kinetics.
This study offers a high-fidelity modeling framework for the optimization of porous structures for solar thermochemical applications. The coupled multiphysical model enables to simultaneously coordinate various involved physics including heat and mass transfer, species transport, solar absorption, as well as bulk vs. surface kinetics.

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Participation

Online

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