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Optimization of porous structures via machine learning for solar thermochemical fuel production

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Optimization of the porous structure is essential to achieve high solar-to-fuel efficiency in solar thermochemical fuel production. The porous structure directly converts concentrated solar radiation into heat and facilitates heat and mass transfer, as well as provides sites for chemical reactions. An ideal porous structure is expected to have a large surface area to provide reactive sites, a large mass loading to provide reactants, a small pressure drop in fluid space to facilitate gaseous mass transfer, and uniform solar energy absorption to guarantee thermo-mechanical stability. These optimization objectives demand a comprehensive understanding of the transport and conversion processes in porous structures. The direct 3D multiphysics model based on real morphology is time-consuming and costly to solve. Its further coupling to a conventional optimization algorithm, such as the gradient descent method for structure optimization, is challenging. The triply periodic minimum surface (TPMS) structures are known for their well-defined mathematically controllable morphology and designing flexibility, providing great easiness in structure optimization, so they are introduced into the optimization. In this study, we introduced a machine learning-aided porous structure optimization method for solar thermochemical fuel production. The machine learning tool was used to link the TPMS structures' design parameters with the fuel production performance, temperature gradient, and gaseous flow pressure drop. The training data were calculated from a direct pore-level multiphysics model with various uniform and gradient 3D TPMS structures. The reaction model in this study considered both charge carriers' bulk diffusion and surface reactions, enabling the investigation of the material's kinetics on fuel production performance. The model framework can hence be utilized for porous structure optimization as well as guiding material choices for high-performing solar thermochemical fuel generation.

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References

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