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Pore level vs. continuum level model for solar thermochemical fuel production

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For the solar-driven thermochemical fuel production redox cycle, the porous media design significantly determines the solar-to-fuel efficiency and per mass loading conversion efficiency of each redox cycle by governing the heat and mass transfer properties. Thermodynamically, porous media is expected to have a large surface area for fast reaction rate and a large mass loading for high fuel production amount. It has been concluded from the literature that the reduction step is surface area limited in micro/nano powder thermogravimetric study, while the particle size is also reported to become the other limitation as its size gets large enough to hinder the bulk oxygen vacancy diffuse. To optimize the porous media design, a comprehensive modeling framework for Triply periodic minimum surface (TPMS) structures, which are well-known for their mathematic equation-driven modeling and flexibility in design, has been developed to identify the volume-averaging geometrical properties, mass and heat transfer properties in our previous study.

To analyze how the redox reaction is influenced by porous media's structure design, a new continuum level model is developed. It introduces rough surfaces in addition to the millimeter-scale TPMS structure. The surface roughness is simply treated as a correction factor of the surface area, which amplifies the reaction rate. However, this amplification will not influence the reaction equilibrium. The probable impact of porous media structure on bulk diffusivity cannot be observed either. Therefore, we are proposing a pore-level model to capture the mass and heat transfer behavior of extract three-dimensional porous media, coupled to thermochemical reaction with the consideration of bulk diffusion, surface exchange, and gas-phase diffusion. The micrometer-level spheric holes are randomly excavated over the TPMS structure to create the secondary pores (surface roughness). In this model, the surface exchange governing region and bulk diffusion governing region are identified at various combinations of surface area and particle size distribution. Additionally, the particle size is optimized to avoid bulk diffusion limitation.

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References

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Online

Primary authors: Mr XU, Da (Southern University of Science and Technology); Prof. LIN, Meng (Southern University of Science and Technology)

Presenter: Mr XU, Da (Southern University of Science and Technology)

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