Computational Modeling and Design Optimization of a Solar Reactor and the Integration of Supersonic Turbomachinery for Hydrogen Production

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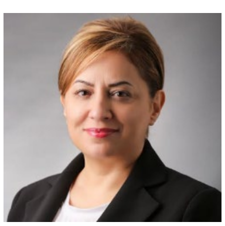
This presentation introduces a patent pending novel solar thermal methane pyrolysis system developed in collaboration with colleagues from the Purdue Experimental Turbine Aerothermal Laboratory (PETAL) of Purdue University School of Mechanical Engineering. The heart of the innovation lies in the integration of a high-speed rotating supersonic turbomachine within the solar thermal reactor, addressing the persistent challenge of carbon deposition during hydrogen production. This patent pending technology utilizes supersonic blades and downstream collector units to enhance energy transfer efficiency, minimize carbon accumulation, and ensure a compact system size with reduced manufacturing costs. The presentation will provide a comprehensive overview of the technology, design and optimization processes of a solar reactor using computational modeling, and describe the non-linear temperature control mechanism of a solar reactor simulating the transient nature of solar power. The presentation outlines the use of computational modeling covering the fluid flow, particle dynamics, heat transfer, and thermochemical reaction for iterative design of a solar reactor. Results of the solar reactor Computational Fluid Dynamics (CFD) simulations are discussed, including turbulence modeling investigations, the particle-gas flow interactions, energy transport, and the High Flux Solar Simulator (HFSS) characterization using an indirect heat flux mapping method, supplemented by an optical modeling through Monte Carlo ray tracing (MCRT) to determine spatial flux distribution and angular characteristics. The initial simulations focus on fundamental thermal fluid dynamics to optimize solar reactor geometry, followed by modeling multi-phase flows considering particulates, radiation, and turbulence. Chemical kinetics modeling utilizes standard techniques, with kinetic parameters for methane pyrolysis referencing Prof. Ozalp's team's prior work. The energy conservation approach for the reactor chamber wall is outlined, involving division into regions for radiation, convection, and conduction, with empirical parameters derived from CFD simulations. The resulting non-linear thermo-chemical dynamics of the solar reactor form the basis for a control-oriented model. This model integrates CFD and experimental results to fine-tune parameters and assess model uncertainty. A heat transfer modeling driven non-linear Model Predictive Control (MPC) system is developed and experimentally tested using an example solar reactor system which exhibited efficient responses to changes in input power, demonstrating its capability to regulate mass flowrate, heat up the reactor, and maintain temperature setpoints. The controller's effectiveness was further validated by shutting off and restarting the flow controller under varying mass flowrates, showcasing its ability to adapt to dynamic conditions.



Nesrin Ozalp is the Founding Department Chair of Mechanical Engineering at Illinois State University. She is also a Full Professor by Courtesy at the School of Mechanical Engineering of Purdue University West Lafayette, and an Associate Editor of ASME Journal of Solar Energy Engineering. She received her Ph.D. from the University of Washington's Mechanical Engineering Department and her MSc in Mechanical Engineering from Stanford University. Dr. Ozalp specializes in the areas of experimental and numerical study of thermal transport processes with particular focus on multiphase convective and radiative heat transfer analysis of solar thermochemical processes with non-linear temperature patterns and turbulent flow dynamics. She is the Lead Principal Investigator of research projects totaling \$5M+. She is the corresponding author of 140+ peer reviewed publications, Co-PI of completed Phase I of Solar Carbon Black commercialization with Fraunhofer, and she has supervised 25 graduate students' theses. She has given 40+ invited/keynote/plenary talks on her research. She is the past chair of ASME Solar Energy Executive Committee, chair of ASME Heat Transfer and Thermal Sciences Education technical committee, Inaugural Executive Committee member of the American Society of Thermal Fluids Engineers, General Chair and/or Technical Program Chair of several ASME and ASTFE conferences on Heat Transfer and Energy Sustainability, and the recipient of many research, teaching, and service awards including the ASME Yellot Award, ASME Dedicated Service Award, Outstanding Reviewer Award by the ASME Heat Transfer Division, and the College-Level Distinguished Teaching Award by the Texas A&M Association of Former Students. Dr. Ozalp is an ASME Fellow and an ASTFE Fellow.