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Derivative-Free Optimization of a Double-Pipe Heat Exchanger for Enhanced Copper–Chlorine Cycle Efficiency

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ABSTRACT

Thermochemical cycles, particularly the copper–chlorine (Cu–Cl) cycle, have emerged as promising solutions for sustainable hydrogen production due to their zero-carbon emissions and high overall efficiencies. Molten cuprous chloride (CuCl) is an important working medium in the four-step Cu–Cl thermochemical cycle for hydrogen production, which offers significant potential for energy recovery. However, residual heat in the molten salt stream often remains underutilized, reducing overall process efficiency. The present work investigates an optimized double-pipe heat exchanger aimed at enhancing heat recovery from molten CuCl to improve the cycle performance. Steam flows through the outer tube to extract heat from molten CuCl in the inner tube, and it can then be utilized in other stages of the Cu–Cl cycle. A comprehensive two-dimensional axisymmetric computational fluid dynamics (CFD) model is developed in COMSOL Multiphysics v. 6.2 software, incorporating fluid flow, heat transfer, and phase change phenomena. The study explores the effects of varied geometric configurations on heat transfer and solidification behavior in both shell and tube domains. The Nelder-Mead algorithm, a well-known derivative-free optimization method, has been employed in this study. This method explores the design space by applying reflections, expansions, and contractions around a simplex of candidate solutions. Each iteration identifies and modifies the least favorable point and converges toward an optimum value without requiring gradient information. Moreover, an adapted mesh refinement approach is used to accurately capture steep gradients in the velocity and temperature fields of the molten salt, due to solidification, which ensures reliable numerical results in those areas. By employing an objective function in COMSOL Multiphysics that maximizes the shell-to-tube Nusselt number ratio while minimizing the shell-to-tube friction factor ratio (via its cubic root), a 59 °C reduction in the average CuCl exit temperature can be achieved. This objective function allows for a balanced design that promotes efficient heat transfer while mitigating excessive pressure drops. Also, the multiphysics model is validated against theoretical data and shows an average Nusselt number error of less than 10% within acceptable limits.