Asociación Argentina
de Mecánica Computacional

Resúmenes de Mecánica Computacional Vol II, pp. 229-229
A. Caggiano, G. Etse, P. Folino, M. Goldschmit, M. Pucheta, M. Storti (Eds.)
J. Álvarez Hostos, E.S. Esteban, G. Umbricht, C. Venier (Issue eds.)
Buenos Aires, November 11-14, 2025

THERMOCHEMICAL MODELING OF IRON OXIDE REDUCTION PROCESSES IN FLUIDIZED BED REACTORS

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Keywords: TFM, KTGF, Iron oxide reduction, Fluidized bed, CFD

Abstract.

This study explores the use of computational simulations to analyze the reduction processes of iron oxide powders in fluidized beds. Iron powders are employed as energy carriers; that is, they can be oxidized to release energy and subsequently reduced using renewable energy sources, enabling a closed-loop, carbon-free energy cycle—a clean alternative to fossil fuels. To simulate this process, the Two-Fluid Model (TFM) with the Kinetic Theory of Granular Flow (KTGF) for closure is adopted. This work presents the initial steps in scaling up the computational modeling of such systems, which are typically studied using Lagrangian techniques to capture particle interactions and reaction details. To achieve this, a multiphase (gas-solid) flow involving multiple reacting species is modeled and solved using the OpenFOAM suite. Among the challenges of the study are the complex temperature-dependent reactive dynamics between hydrogen and iron oxides, as well as particle sintering at elevated temperatures. The results demonstrate the capability of the TFM-KTGF approach to capture complex thermochemical phenomena. This represents an initial step toward developing an efficient computational tool for modeling pilot-scale metal fuel fluidization units within a reasonable computational time. Such tools can support the design and optimization of these processes, leading to improved efficiency and reduced operational costs.

ISSN: 3072-7723 DOI: 10.70567/rmc.v2.ocsid8393