Modelling and Simulation of Low Temperature Oxidation Process of Iron Powder

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Metal fuels are gaining increased attention as carbon free energy carries in combustion applications. Unlike conventional fuels with releases carbon dioxide during combustion, metal fuels are oxidized into metal oxides in solid form, which results in zero carbon dioxide emissions. Among various types of metals, iron presents advantages due to its wide availability and similar flame temperatures to conventional fuels. However, the oxidation kinetics and morphology evolution of iron particles in combustion environments are still not well known, limiting accurate prediction of ignition behavior. A validated kinetic model is therefore essential for characterizing powder passivation and ignition readiness, offering a foundation for furnace design. This study presents the mathematical modelling and numerical simulation of the low temperature oxidation of iron powder in oxygen rich environments. In the temperature range of 300-600 °C, oxidation is governed by solid state diffusion of iron ions through the growing oxide shell, in accordance with Wagner's parabolic growth law. As an improvement to the existing models, a spherical shrinking core model was developed in the present study from first principles using Fick's laws of diffusion in spherical coordinates. Simulation results at 500 °C confirmed parabolic growth behavior, with oxide thickness reaching approximately 6.1 µm after 60 minutes. The developed spherical model is also compared with a flat plate model which showed that the spherical shrinking core model predicts oxide layers about 13% thinner, highlighting the importance of curvature corrections. Validation against published thermogravimetric analysis (TGA) data demonstrated excellent agreement, with $R^2 = 0.9950$ and RMSE = 0.139 wt%. The fitted parabolic rate constant was 5.78×10^{-15} m²/s, yielding an effective activation energy of 107.1 kJ/mol, consistent with literature values for Fe_2O_3 formation in the low temperature regime. Parametric studies further confirmed strong Arrhenius temperature sensitivity, with growth rates increasing by three orders of magnitude between 400 °C and 600 °C. By quantifying geometric correction effects and advancing beyond flat plate approximations, the study provides a reliable framework for further improving particle oxidation models. The findings form a foundation for future extensions to multi-layer oxide modelling, Kirkendall void effects, and multi particle oxidation behavior, supporting the development of iron powder as a practical carbon free energy carrier.

Keywords: iron powder oxidation, shrinking core model, Wagner parabolic theory, Fick's diffusion, low temperature oxidation