INTEGRATED MODELING OF UCG REACTORS: A REVIEW BASED ON ASPEN PLUS AND ANSYS FLUENT SIMULATIONS

A Mini Project Report

In Partial Fulfilment of the Requirement for Award of Degree of

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<u>CERTIFICATE</u>

Certified that the Major Project Report entitled *"Integrated Modeling of UCG Reactors: A Review Based on Aspen Plus and ANSYS Fluent Simulations"* submitted by Rahul Das, Muskan Ojha, Nathan of B.Tech. 4th Semester, in partial fulfillment of the requirements for the award of degree in Bachelor of Technology (B. Tech) in Chemical Engineering, is according to the students their own investigation carried out by them in the Department of Chemical Engineering, School of Studies of Engineering & Technology, GGV, during the session 2024-25.

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ABSTRACT

Underground Coal Gasification (UCG) is a sophisticated in-situ method that translates unmined coal to fuel gas (syngas) by pumping in oxidizers like air, oxygen, and steam into the coal seam. This project examines UCG with double modeling methods: process-level modeling with Aspen Plus and transport-reaction-level modeling with ANSYS Fluent (CFD), with a view of discovering system dynamics and improving syngas yield.

The Aspen Plus model was established with principal reactor blocks—R-Yield, R-Stoic, and R-Gibbs—to model coal drying, pyrolysis, combustion, and gasification processes. Non-conventional coal was specified with a fixed proximate and ultimate analysis. Simulations were conducted with varying gasifying media (air, O_2, and steam-oxygen mixtures). The outcomes indicated that syngas quality was greatly enhanced by steam-oxygen mixtures, with a notable increase in hydrogen and CO concentration, and realized improved Cold Gas Efficiency (CGE). Sensitivity analysis indicated best operating temperatures between 900–1100°C, where there was a balance of conversion and energy output.

ANSYS Fluent, in parallel, was employed for performing CFD-based modeling of the UCG cavity. A 2D geometry was established with suitable meshing and appropriate boundary conditions for oxidant flow and heat loss. Species transport, volumetric chemical reactions, and heat transfer mechanisms were included in the model. Simulation outputs showed in-depth physical events like paths of gas flow, temperature pattern, reaction front progress, and rock–gas interaction. Steam utilization also had an effect on where hotspots occur and the gas residence time in the cavity.

In summary, the research proves that Aspen Plus is best suited for system-level optimization, whereas CFD allows for detailed analysis of reactor internal behavior. Future proposals involve integrating both tools in co-simulation environments and using AI-based optimization for real-time UCG process control.