PROCESS MODELLING TOOLS FOR THE DIGITALIZATION AND DECARBONIZATION OF THE CEMENT SECTOR

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ABSTRACT

Cement production is responsible for 7-8% of global and 25% of industrial CO_2 emissions [1], [2]. These emissions originate both directly via chemical reactions (e.g. calcination) taking place in the process and indirectly via the process energy demands. Process modelling is an important and useful tool that can contribute towards the understanding, development, and implementation of novel decarbonization concepts in the cement sector. In the course of EU Horizon-UKRI funded CO2Valorize project, a novel mineral carbonation process is being developed for the production of supplementary cementitious materials (SCMs) [3]. These materials have the ability to bind CO_2 and can be utilized as a partial replacement of limestone-based clinker. This innovative approach aims to mitigate CO_2 emissions, both by reducing clinker demand (which is responsible for the majority of the carbon emissions) and by utilizing carbon dioxide as a raw material turned into a valuable product.

The scale-up and integration of such novel decarbonization technologies in conventional cement plants requires deep knowledge and understanding of the cement production processes. The main focus of this work is the development of a library of standardized mathematical models for the simulation of the processes inside such plants, with focus on the more carbon-intensive unit operations. The ultimate objective is the creation of a digital simulation tool (based on the mathematical models developed) for environmental and financial evaluation of green investments in the cement sector.

This paper presents first-principles mathematical models for the suspension preheating cyclones and the calciner. The models incorporate mass and energy conservation balances, limestone decomposition kinetics (heat transfer-diffusion limitations, pore efficiency, CO_2 partial pressure effects etc.), fuel combustion kinetics and heat transfer phenomena between the gas and solid phase inside the reactor and the reactor walls (shell and refractory). The resulting Partial Differential-Algebraic Equation (PDAE) system has been implemented in the gPROMS® Advanced Process Modelling environment and solved for various reactor geometries and operating conditions. The simulation results are validated against published data, demonstrating the ability to predict accurately operating temperatures, degree of calcination, gas and solids mass fractions, pressure drop and fuel consumption.

KEYWORDS: Decarbonization, Mathematical Modelling, Process Simulation, Chemical Reaction Modelling, Cement Production

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