System-Level Modeling of Mercury and Sulfur Dynamics in Fluidized Bed Combustion

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ABSTRACT

Coal combustion in fluidized bed constitutes a widely employed technological alternative for energy generation due to its operational flexibility and emission control potential. However, the release of atmospheric pollutants, particularly sulfur oxides and mercury, remains a relevant environmental and regulatory challenge. This work developed a simplified model in Aspen Plus® to represent coal fluidized bed combustion, incorporating fuel decomposition, char oxidation, *in situ* desulfurization, and mercury transformations in both gas and solid phases. The model formulation considered coal decomposition in a yield reactor (RYield), followed by volatile combustion under equilibrium conditions (RGibbs) and fixed carbon oxidation in a stoichiometric reactor (RStoic) at 850 °C. SO_2 capture was represented by limestone addition (Ca/S = 2), with instantaneous calcination and kinetic sulfation. For mercury, homogeneous oxidation mechanisms (Hg/Cl/O) were incorporated in a USER2 block, along with a simplified representation of heterogeneous oxidation/capture also in a dedicated USER2 block, via a solid pseudocomponent "HGASH" (NC-comp). This heterogeneous USER2 block represents mercury adsorbed or chemisorbed on the ash matrix during gas-solid contact, enabling evaluation of its retention in the solid phase within the main reactor. Results indicate that the model qualitatively reproduces O_2, CO_2, NOx, and SO_2 trends, with higher Hg^{2+} formation as a function of chlorine content and additional Hg capture by ashes (~ 20 % of total). Limestone addition reduces SO_2 by ~ 15 %. The methodology provides a basis for parametric analyses and calibration with experimental data, with limitations associated with simplification of heterogeneous kinetic mechanisms and absence of particle size effects.

Keywords: fluidized bed combustion; mercury; homogeneous oxidation; heterogeneous oxidation; Aspen Plus®.

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