

Capturing O₂ Desorption through Iso-conversional Kinetics for CFD Application

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Environmental concerns associated with carbon dioxide emissions fostered the emergence of low-emission technologies such as oxy-fuel combustion, where fuel is combusted with nearly pure oxygen instead of air. This commonly requires a separation unit of oxygen from air prior to the combustion chamber. One way to achieve such a separation is to rely on chemical looping redox reactions of a metal oxide (see e.g., Moghtaderi, 2010), during which oxygen contained in air is adsorbed by the metal oxide (i.e., adsorption/oxidation step) and subsequently extracted from the metal oxide (i.e., desorption/reduction step). Due to their good oxygen storage capacities as well as their ability to release oxygen from their lattice arrangements even at relatively low temperatures, in addition to their thermodynamics properties, the metal oxide is often selected within the perovskite families (e.g., Luongo et al. 2020).

The present work examines desorption mechanisms and kinetics of a calcium-doped strontium perovskite at 25% calcium content, with a dependence on the steam content in the desorption environment. Laboratory-scale, low inventory, fixed bed redox cycle experiments were developed and conducted in both dry and steam-based environments for three isothermal temperatures, 450, 500 and 550°C.

The temporal evolution of the conversion extent of the material sample over the redox cycles was obtained through the analysis of the gaseous products of the redox reactions. Then using iso-conversional differential methods, it was found that the Arrhenius parameters exhibit a strong dependence on the extent of conversion during the desorption of this perovskite. In addition, the reconstruction of the reaction model showed that the desorption kinetics are controlled by a three-step mechanism regardless of the desorption environment. Successful *a priori* verifications of the iso-conversional desorption kinetics against the desorption experimental data are shown for both dry and steam-based environments. These indicated that the hypothetical three-step reaction mechanism associated with the conversion extent-dependent Arrhenius parameters clearly capture the desorption dynamics of this perovskite material.

References

Moghtaderi B., Application of Chemical Looping Concept for Air Separation at High Temperatures. *Energy Fuels* 2010, 24, 190-198.

Luongo, G.; Donat, F.; Müller, C. R. Structural and thermodynamic study of Ca A- or Co B-site substituted SrFeO_{3-δ} perovskites for low temperature chemical looping applications. *Phys. Chem. Chem. Phys.* 2020, 22, 9272–9282.