SPU Internal Grant Interim Report

Academic Year & Type of Grant (FRG, SERVE or Innovation): 2014-2015 FRG

PI Name: Daniel J. Keene

Original Title of the Proposal:
Characterizing the Kinetics of Ceria Oxidation for Solar Thermochemical Fuel Production

---

The aim of this research project is to fully determine a mathematical expression for calculating the rate at which the oxygen vacancies of nonstoichiometric ceria are repopulated by the conversion of carbon dioxide into carbon monoxide, which is critical information for designing effective and efficient solar thermochemical reactors. I have previously developed a parameter calibration technique that couples a detailed transport phenomena numerical model with optimization algorithms for the purposes of using them to extract intrinsic kinetic information from existing experimental data. The primary activity for this project was to apply the parameter calibration technique to multiple data sets in order to test the validity of different hypothesized reaction rate expressions. The work carried out during this grant period was performed by the principal investigator only, although Dr. Aaron Dingler provided assistance with some peripheral difficulties that were encountered as described below.

This work is not yet complete and consequently the major findings are still in progress. A considerable amount of effort was required to identify and configure existing resources at SPU to carry out the developed parameter calibration technique. With these resources now in place, I am well positioned for completing this project soon and pursuing further research that will make use of numerical simulations.

The results will be disseminated via a peer-reviewed journal publication, but might also be shared with the solar chemistry community through a technical presentation at an upcoming ASME International Energy Sustainability Conference.

With a complete reaction rate expression for the conversion of carbon dioxide into carbon monoxide using nonstoichiometric ceria, a detailed study of the dynamics of this oxidation step of the ceria cycle can for the first time be performed. There are currently no plans to pursue additional external funding for this work.

There were two primary difficulties that prevented this work from being completed during the grant period. First, the events and aftermath of June 5, 2014 greatly impacted my ability to begin work on this project. When I was able to resume working in my office, I discovered that porting the tools of the parameter calibration technique which I had previously run on Linux workstations to run on my Windows office computer was more complicated than anticipated. CIS was not able to provide support in this endeavor as what I was seeking to accomplish fell outside of their expertise. Thankfully, between his vast knowledge of computer systems and particular fondness for Linux, my genial colleague Aaron Dingler was able to assist me in ultimately establishing the means to carry out my parameter calibration technique.