Fundamental Studies on the Reaction Mechanisms of Oxygen Carriers for CLC/CLOU with Solid Fuels

Chemical looping is considered as a potential energy producing system permitting cost effective efficient CO$_2$ sequestration, and this study concerned chemical processes of importance to the design of oxygen carriers. Experiments were performed to gain better understanding of the metal oxide heterogeneous reaction mechanisms associated with saturated and unsaturated hydrocarbons and with solid carbon. In connection with the experiments, an atomistic scale modeling capability was developed for simulating the chemical reactions associated with metal/metal oxide based chemical looping processes.
**Accomplishments:**

The researchers successfully developed an atomistic-scale simulation method – a ReaxFF reactive force field – for studying the details of CuO and Cu-metal reactions with hydrocarbon-based fuels during fuel cycling. This ReaxFF method was used for a wide range of fuels – including small hydrocarbons and biofuels as well as complex coal-derived fuels like lignite and anthracite. Their simulations revealed the complex reaction kinetics associated with both CuO-reduction and Cu oxidation.

**NETL Collaboration:**

This work did not lead to a specific NETL collaboration. During the first year of the program, a collaboration for students to conduct research at NETL was established. A CRADA between Penn State and NETL was initiated, but due to COVID-19 did not occur.

**Relevant Publications:**


**Benefits:**

The ReaxFF Cu/C/H/O force field parameter set has proven to be highly transferable, where this force field was used to study Cu/graphene interfaces. The study advanced the understanding of the kinetic mechanism of chemical looping using CuO particles with hydrocarbon fuels and solid carbon. It contributed to the development of new carbon capture technologies to reduce carbon emissions in energy conversion. The results also advanced the understanding of the mechanism of low-speed pre-ignition in gasoline engines caused by calcium and magnesium oxide formation of lubrication oil, which limits the engine efficiency. The study also provided a clear answer to why calcium containing lubricants have more low speed pre-ignition than magnesium.

Structure of a CuO nanoparticle after 300 ps of exposure to a hydrocarbon fuel at T=1500K using ReaxFF MD-simulations.