Thermodynamics of CeO_2 Thermochemical Fuel Production

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ABSTRACT

Ceria (CeO_2) is a very diverse material which has found many applications due to its unique properties. At high temperatures it is an oxide conductor and is also noted for its oxygen storage and redox properties.

In this work we focus on its redox properties. Ceria has been heavily investigated for its use in converting heat energy to fuels. It can be thermally reduced at high temperatures, releasing oxygen.

$$CeO_2 \xrightarrow{heat} CeO_{2-\delta} + \frac{\delta}{2} O_2 \quad \text{Ceria reduction T} \approx 1600° C$$

The reduced ceria can then be used to split H_2O or CO_2.

$CeO_{2-\delta} + \delta H_2O \rightarrow CeO_2 + \delta H_2$	Water splitting	T $\approx 900° C$
$CeO_{2-\delta} + \delta CO_2 \rightarrow CeO_2 + \delta CO$	CO_2 splitting	T $\approx 900° C$

Carbon monoxide and hydrogen can be combined to form denser diesel type fuels using the Fischer-Tropsch process.

Analytical model of the high temperature CeO_2 redox system.

In this work an analytical model of the reduction and oxidation of CeO_2 was developed by the author. It predicts both equilibrium composition and reaction rates over a wide range of temperatures and oxygen partial pressures.

It was developed from the basic properties of the reaction and the parameters were fixed using equilibrium data from the literature and experimental data obtained by the author of Ceria oxidation and reduction.

The model was then used to perform an in-depth thermodynamic study of the ceria cycle. It predicts the equilibrium composition of ceria in an oxygen atmosphere, which combined with the known properties of H_2O and CO_2 splitting, gives all the necessary information to calculate the extent of each reaction for a given set of conditions.