Phase chemistry in process models for cement clinker and lime production

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Title
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Abstract
The goal of the thesis is to evaluate if developed phase chemical process models for cement clinker and lime production processes are reliable to use as predictive tools in understanding the changes when introducing sustainability measures.

The thesis describes the development of process simulation models in the application of sustainability measures as well as the evaluation of these models. The motivation for developing these types of models arises from the need to predict the chemical and the process changes in the production process, the impact on the product quality and the emissions from the flue gas.

The main chemical reactions involving the major elements (calcium, silicon, aluminium and iron) are relatively well known. As for the minor elements, such as sodium and potassium metals, sulphur, chlorine, phosphorus and other trace elements, their influence on the main reactions and the formation of clinker minerals is not entirely known. When the concentrations of minor and trace elements increase due to the use of alternative materials and fuels, a model that can accurately predict their chemistry is invaluable. For example, the shift towards using less carbon intensive fuels and more biomass fuels often leads to an increased phosphorus concentration in the products.

One way to commit to sustainable development methods in cement clinker and lime production is to use new combustion technologies, which increase the ability to capture carbon dioxide. Introducing oxy-fuel combustion achieves this, but at the same time, the overall process changes in many other ways. Some of these changes are evaluated by the models in this work.

In this thesis, a combination of the software programs Aspen Plus™ and ChemApp™ constitutes the simulation model. Thermodynamic data from FACT are evaluated and adjusted to suit the chemistry of cement clinker and lime.

The resulting model has been verified for one lime and two cement industrial processes.

Simulated scenarios of co-combustion involving different fuels and different oxy-fuel combustion cases in both cement clinker and lime rotary kiln production are described as well as the influence of greater amounts of phosphorus on the cement clinker quality.

Keywords
Process modelling, phase chemistry, cement clinker, lime, sustainability, CO_2, energy.

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