

Simulation of a cement plant using thermochemical and flow simulation tools

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Abstract

As the cement rotary kiln is increasingly used for waste incineration, it features complex transport as well as chemical conditions. An approach of combining CFD and thermochemical equilibrium calculations has been applied in order to numerically model such a kiln. CFD calculations have been carried out including combustion as well as clinkerisation modelling in order to properly map heat and mass transfer. From the achieved results a flow sheet model of the kiln has been derived, picturing chemical processes within the kiln by means of a sequence of thermochemical equilibrium calculations. The flow sheet is capable of predicting incorporation of minor components into the clinker in good agreement with measurement results and clearly indicates formation of vaporisation-precipitation cycles.

Keywords: Thermochemical process modelling, Cement manufacturing process, Rotary kiln

1. Introduction

Most of today's world wide cement production is carried out in rotary kiln plants (see Taylor, 1990). A powdery raw mixture of mainly CaCO_3 , SiO_2 , Fe_2O_3 and Al_2O_3 is passed through a multi-stage cyclone preheater and then fed into the actual rotary kiln. Inside the kiln the raw meal is further heated up to a maximum temperature of about 1250 to 1400 °C by a coal, oil or gas flame. During this process first CaCO_3 is decomposed to CaO and CO_2 (calcination). Together with SiO_2 CaO then forms the two major cement phases $3 \text{CaO} \cdot \text{SiO}_2$ (Alite) and $2 \text{CaO} \cdot \text{SiO}_2$ (Belite). At room temperature, both phases harden after a certain time when mixed with water and so feature the desired cement behaviour. Coming out of the kiln the solid (clinker) has to be cooled down quickly in order to freeze the high temperature phase composition. Throughout the entire process gas and solid flow are directed opposite to each other.

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Practical problems arise from the raw meal as well as the fuel being burdened with considerable amounts of sulphur, alkalies and chlorine. These minor components tend to form volatile compounds that vaporise in high temperature regions in the kiln and then are transported back to cooler regions by the gas flow, where they precipitate again on the raw meal. So these components enrich in vaporisation-precipitation cycles. Furthermore they form a liquid melt when precipitating, which makes the raw meal stick to the kiln walls and by that form coatings which may cause process holdups. This problem becomes even more urgent as increasingly secondary fuels such as waste are being fired for economical reasons. Due to featuring a long residence time at comparably high temperature cement rotary kilns are suitable for waste incineration; yet by increasing input of minor components process behaviour becomes more and more instable.

In the paper at hand that problem is approached by means of numerical simulation of a rotary kiln plant. The chosen modelling method is based on the combination of CFD and thermochemical computations in order to properly map complex transport as well as chemical conditions inside a cement rotary kiln. Computations have been carried out using measurement data from a German cement plant.

2. Modelling approach

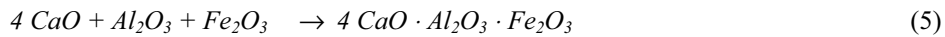
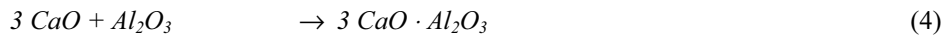
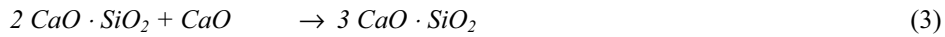
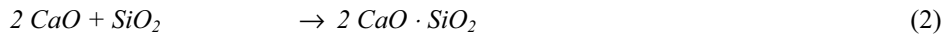
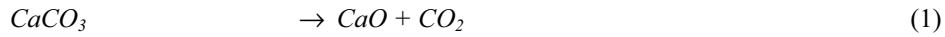
The combination of CFD and thermochemical simulation tools aims at benefiting from the specific strengths of both methods. CFD allows for detailed simulation of mass and energy transport conditions inside the kiln including combustion. However, performing chemical calculations within a CFD environment requires a mass balance equation for each phase to be solved, which results in very high computational costs for complex chemical conditions. An alternative approach to modelling these conditions can be applied, if thermochemical equilibrium can be assumed to establish in certain zones within the kiln. A numerical equilibrium calculation is then assigned to each of these zones. Mass and energy transport conditions are modelled by means of streams interconnecting the equilibrium zones and thus forming a flow sheet model of the kiln. As the flow sheet model needs to be derived from CFD transport calculation results which in turn are strongly influenced by chemical processes, the entire model is solved iteratively.

In the following the actually used software tools and the realisation of the modelling approach are briefly described.

2.1 CFD model

For mass and energy transfer computations the finite volume CFD software Cinar ICE by Cinar Ltd. (London, UK) (see Versteeg, 1995) is used. Within Cinar ICE a numerical solution of the Reynolds-averaged Navier-Stokes-equations employing standard k- ϵ -turbulence modelling is calculated. Moreover Cinar ICE offers combustion modelling for any combination of solid, liquid and gaseous fuels (see Lockwood, 1980). What makes Cinar ICE particularly interesting for cement calculations is a 1D-clinkerisation model which is directly integrated into the actual CFD computations (see Yousif, 2002). This model accounts for energy transfer between gas phase, clinker solid and kiln walls as well as for mass transfer from solid phase to gas phase (formation of CO₂ during

calcination). Chemical processes of clinkerisation are assumed to comply with the following reaction scheme:



Temperature dependent reaction kinetics following the Arrhenius-equation are assigned to each reaction. Compared to any other reactions taking place inside the kiln, the above-mentioned are by far the most energy consuming ones. Thus by taking them into account temperature conditions within the kiln can be properly calculated, whereas chemical conditions are more precisely modelled applying thermochemical methods.

2.2 Thermochemical process model

Given an arbitrary reactant composition, the equilibrium composition can be calculated for isobaric and isothermal conditions according to the principle of minimum Gibbs Free Enthalpy (see Adam, 1992, Hack, 1996). In case a real chemical process shall be modelled by such a calculation one has to assure, that thermochemical equilibrium is actually reached i.e., that kinetic inhibitions are negligible. In order to actually perform equilibrium calculations, thermodynamic properties of all phases possibly involved have to be provided by means of a comprehensive database. In this paper, thermochemistry software ChemApp by GTT Technologies GmbH (Herzogenrath) is used.

ChemApp is integrated in flow sheeting environment SimuSage, also by GTT-Technologies. SimuSage provides a collection of building elements such as mixers, splitters and the above mentioned equilibrium calculators, which are interconnected by streams. In order to correctly model transport conditions inside the kiln by means of SimuSage, one first has to identify zones within which thermochemical equilibrium can be assumed to establish. These zones need to feature constant pressure and homogeneous mixing. Moreover, the residence time of the processed material in each zone must be long enough to allow for equilibrium to be reached according to the local temperature.

Due to kiln rotation, the solids bed is subject to intense transverse mixing, which also promotes temperature to be constant over a cross section. Thus it is assumed, that thermochemical equilibrium establishes in every solids bed cross section. Similarly, due to turbulent mixing in the gas phase, equilibrium is assumed in every gas phase cross section. Though this presumption seems to be somewhat simple, especially regarding the flame, it may be accepted as a first approximation.

Considering transport conditions, one may easily distinguish a solid phase flow from the upper kiln inlet towards the flame and a gas phase flow in opposite direction. Though there is some solid to be found in the gas phase (dust) as well as gas in between the solid particles, both phases are distinctly separated from each other. Mass transfer

between both streams occurs due to vaporisation and precipitation of volatile compounds and due to raise and deposition of dust.

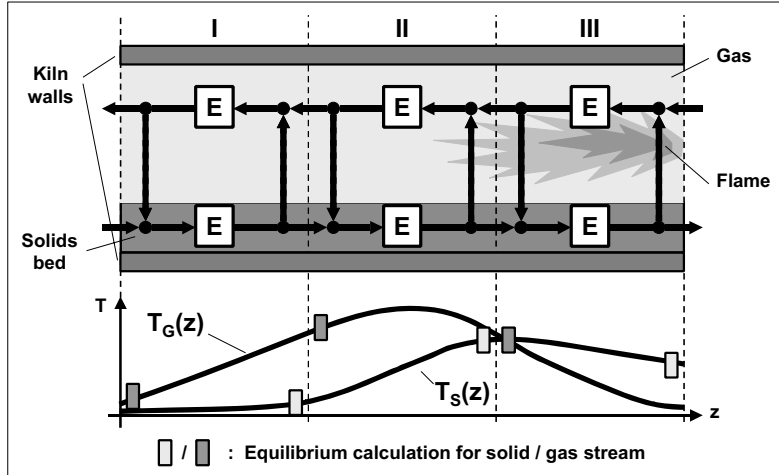


Figure 1. Process flow sheet model of a cement rotary kiln indicating material streams, equilibrium calculations ("E") and qualitative temperature curves for gas (T_G) and solid (T_S) along kiln length z

From these considerations a process model is derived, which is sketched in Figure 1. A longitudinal section of a rotary kiln is shown with the solid entering on the left hand side. Temperature curves for solid and gas are provided by a CFD calculation. The kiln is discretised into three zones of similar structure. When entering the kiln, the raw meal still contains some CaCO_3 , which is decomposed to CaO and CO_2 in kiln zone I. As this reaction is strongly endothermic, the solid temperature rises much slower than in zone II, where the solid is heated up to maximum temperature. In zone III the solid faces comparably cool secondary air from the clinker cooler so that the solid temperature drops again. When passing through a zone, the composition of a material stream is changed by chemical reactions, which are modelled by an equilibrium calculation. This calculation is carried out for the considered stream exiting the zone, i. e. at the zone boundary solid or gas temperature respectively. If an equilibrium calculation for the solid stream turns out a certain amount of volatile compounds to vaporise, these compounds are subsequently cut off and transferred to the gas phase stream. Phases precipitating during a gas phase equilibrium calculation are treated similarly. Splitters following equilibrium calculations are operated in such a way, that a constant dust load of the gas phase and a constant gas load of the solid stream, are being maintained. Calculations have been carried out using a data base which describes 34 mixtures phases (gas phase, Belite i.a.) and 204 stoichiometric compounds from 13 elements. Besides the major components of raw meal (Ca, Si, Al, Fe, Mg) and fuels (C, H, N, O), the data base also includes the secondary components Alkalies (K, Na), Sulphur and Chlorine.

2.3 Calculation procedure

The entire calculation procedure for the rotary kiln model comprises two different steps. The first one is a CFD simulation of the rotary kiln. From the achieved results

temperature curves for gas and solid are derived and fed into the process model, which is subsequently solved iteratively. This approach realises a simple form of one-way coupling between CFD and process simulation.

3. Results and Discussion

Figures 2 and 3 show calculated and measurement results for minor components incorporated into the clinker solid and in the solid at the kiln inlet. Solid composition at

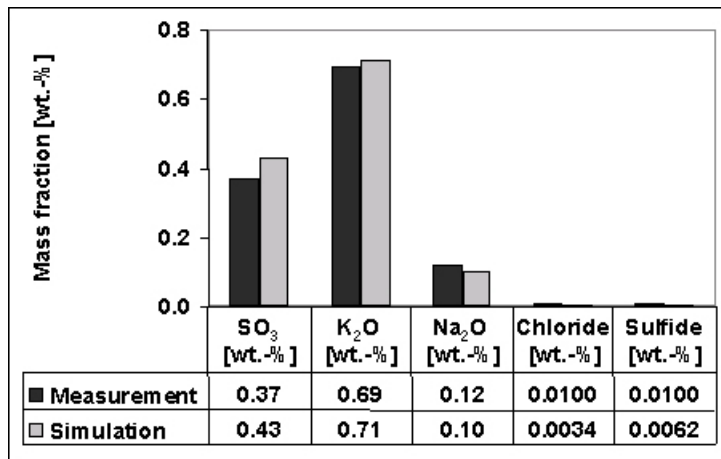


Figure 2. Incorporation of minor components into the clinker

the kiln inlet is strongly influenced by the formation of volatiles' cycles. The measurement results shown in Figure 3 clearly indicate enrichment of minor components compared to clinker as well as to raw meal composition.

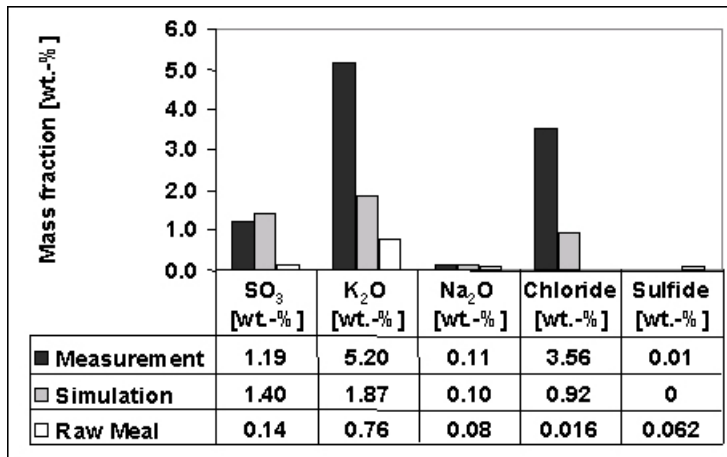


Figure 3. Minor components in the solid at the kiln inlet

The minor components' behaviour in the kiln strongly depends on how their volatility varies with temperature. The highest solid and the lowest gas temperature in the kiln mainly determine the incorporation of minor components into the clinker and the

formation of cycles. Thus calculating these temperatures inaccurately directly leads to incorrect chemical results.

Figures 2 and 3 indicate the most accurate results for Na-compounds, because the volatility of these substances only weakly varies with temperature in the considered temperature range. However, regarding K- and Cl-compounds (mainly KCl is formed), computational and measurement results do only fit each other by an order of magnitude. Moreover, the kiln temperature profiles and therefore as well the formation of cycles strongly depend on the plant operating conditions. As minor component cycles may cause plant holdups, volatile compounds are occasionally removed from the process e.g. by drawing off gas at the kiln inlet. Thus cycle buildup is a dynamic process and can only be mapped tententially by the steady state approach shown here, even more due to the exact plant operating conditions being unknown.

4. Conclusions

Regarding the above-shown results, a combination of thermochemical and CFD calculations appears to be a proper way to approach the complex chemical and transport conditions in a cement rotary kiln. In order to practically apply this method to real plants, e.g. to predict effects of changing raw meal and fuel composition on process behaviour, it needs to be further assessed, especially to increase quantitative accuracy. In order to account for varying plant operating conditions it should be extended to transient calculations.

The method shown in the paper at hand has already been applied to an LD converter by Traebert (2001) and a bio mass fired power plant by Modigell et al. (2003). Since these three works indicate a combination of CFD and thermochemical computations to be able to properly model complex processes, it is a perspective to realise automatic two-way coupling between these two modules. In order to do so, first criteria have to be found by means of which equilibrium zones within the considered reactor can be distinctly defined.

References

- Adam, G. and O. Hittmair, 1992, Wärmethorie, Vieweg (in German).
- Hack, K. (editor), 1996, The SGTE Casebook – Thermodynamics at Work, The Institute of Materials.
- Lockwood, F.C., A.P. Salooja and S.A. Syed, 1980, A prediction method for coal-fired furnaces, *Combustion and Flame*, 38(1):1-15.
- Modigell, M., D. Liebig, M.Weng and B. Sundermann, 2003, Prozessmodellierung eines Biomasseheizkraftwerkes, VDI-Berichte 1750 (in German).
- Taylor, H.F.W., 1990, *Cement Chemistry*, Academic Press.
- Traebert, A., 2001, *Methodik zur Modellierung von Hochtemperaturprozessen*, PhD thesis, RWTH Aachen (in German).
- Versteeg, H.K. and W. Malalasekara, 1995, *An introduction to Computational Fluid Dynamics*, Longman.
- Yousif, S., T. Abbas and F.C. Lockwood, 2002, Mathematical modelling of combustion and cement/lime formation processes in rotary kilns fired with conventional and alternative fuels, in 12th International Cement Conference and Exhibition (AUCBM), Morocco, 24-27. October 2002.