KILNSIMU AND CEMENT APPLICATION

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The rotary kiln remains in active use in several industries. The rotary kiln provides an efficient means for both heat and mass transfer in the processing of slurries and other condensed mixtures of particles. Pigment and cement manufacturing industries among others are using rotary drums for the thermal treatments of various materials. In the chemical recovery of kraft pulping rotary drums are applied for lime recycling. Other uses include manufacture of oxides (aluminium, zinc, lead), reduction of ores and waste incineration.

BACKGROUND

There is increasing interest in the complex chemistry of the rotary drums, as many of the raw materials as well as the fuels used as heat sources vary in their chemical composition. This variation may lead to undesired emissions in the off gas or maintenance problems of the kiln. One common problem in lime and cement kiln is the formation of rings due to alkali compounds. An additional challenge is created by the size of the industrial kilns. Due to long residence times, which may exceed 10 hours, controlling and monitoring the kiln is difficult. Thus it is often beneficial to use a reliable simulation model to predict chemical and physical processes in the kiln.

MODEL

Most kilns operate in the counter-current mode, that is, the condensed material is fed into the kiln from the cold ‘feed end’, and is then processed to reacted product by heat transfer from the surrounding hot gas, which is introduced into the kiln from its hot ‘burner end’. The final material product is removed from the hot end. Fraction of exit gas can be circulated back to hot end to improve the heat transfer efficiency. As a heat source, a fuel burner operating with the primary air is typically used.

In KilnSimu there can be any number of bed and gas feed flows – but there must always be at least one bed feed at the ‘feed end’ and one gas feed at the ‘burner end’ of the kiln. If kiln operates in co-current mode then the ‘burner end’ and the ‘feed end’ coincides and the gas flow direction is reversed.

Schematically the rotary kiln can be divided into three zones according to reactions in the material bed [1]:

- Drying zone
- Heating zone
- Reaction zone

If there is moisture in the bed feed then it is removed in the drying zone. While drying the average temperature of the bed stays close to 100 ºC or increases slowly as the heat is consumed in the evaporation of the water. After all the water has been removed the temperature of the bed is raised quickly until it reaches the reaction temperature. Kiln may contain several reaction zones depending on the thermodynamic characteristics of the bed material.

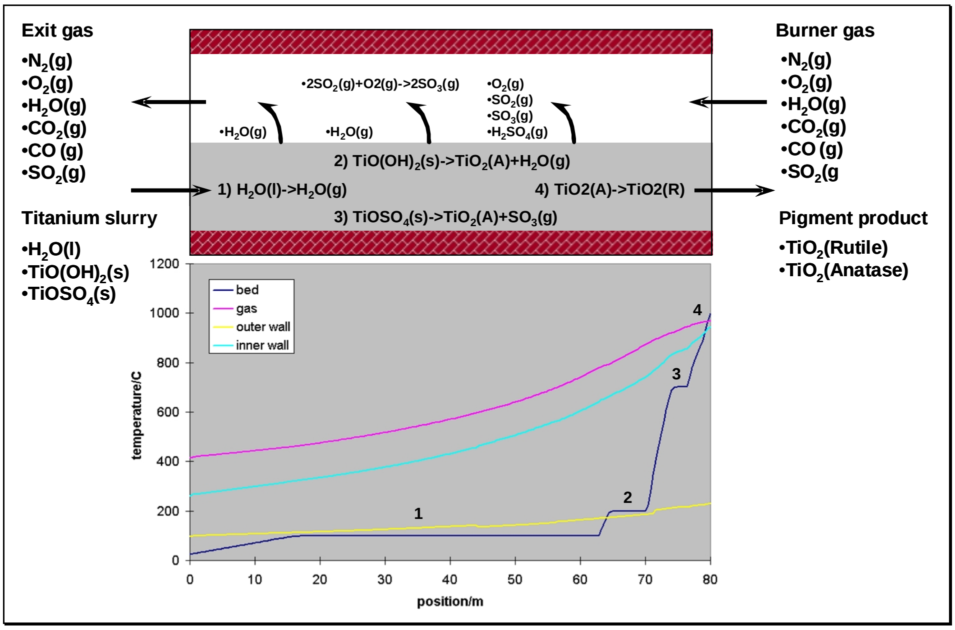

Figure 1: Reaction zones and simulated temperatures in TiO_2 calcination kiln.

Figure 1 shows the reaction zones and the simulated temperatures in TiO_2 calcination kiln. Example TiO2 kiln has high moisture content in the bed feed and thus very long drying zone.

The Movement of the Material Bed

The radial movement of the bed depends on the holdup of the kiln, its angular velocity and the properties of the bed like its porosity, density and viscosity. Material that consists of dry particles behaves very differently than material that contains liquid phases like free water (at lower temperatures) or partly molten slag (formed at higher temperatures). Figure 2 shows the cross-section of the bed.

When the angular velocity of the drum is low the bed behaves as a solid object, which slides in place as the kiln rotates. The solid particles remain at rest with respect to each other. If the friction between the bed and the kiln wall is high enough, the bed starts moving along the wall as the bed gets stuck to it. When it reaches a point at which the gravitational force is greater than the frictional force it will slide back to the bottom of the kiln. If the friction between the bed and the wall is greater than the friction inside the bed then part of the bed will slump down. These slumping movements will start at the top of the free surface of the bed. When the angular velocity is increased the frequency of the slumping movement is increased. Eventually there is continuous rolling at the surface of the bed.

The axial velocity of the bed is proportional to inner diameter, rotational speed and inclination of the kiln and is inversely proportional to angle of repose of bed. In addition the bed velocity is inversely proportional to the holdup of the kiln [2]. If velocity is considered independent on the holdup (valid simplification for long industrial kiln), then generally the axial movement can be given as [3].

$$v_b = K\frac{d_i \omega f(\psi)}{f(\alpha)} \tag{1}$$

where $f(\psi)$ and $f(\alpha)$ are functions of inclination angle of kiln and angle of repose of bed.

The Mass and Heat Balances

In KilnSimu the rotary kiln is divided into number of axial control volumes (see Figure 3). Each control volume consists of bed, gas, inner and outer wall regions, in which the temperatures and compositions of bed and gas flows and temperatures of inner and outer wall of the kiln are assumed constant.

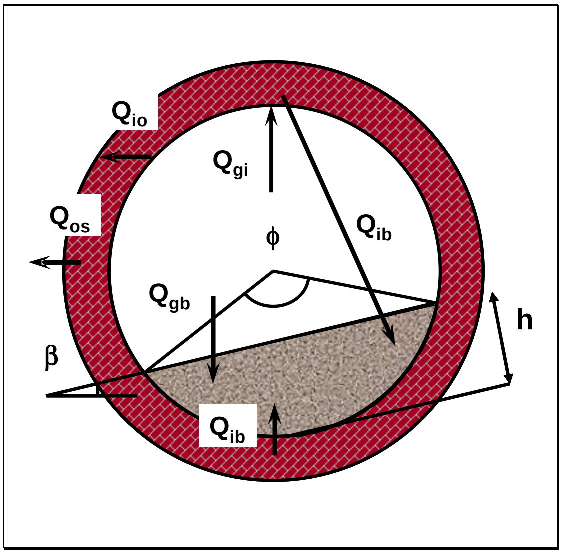

Figure 2: Radial heat flows and bed geometry in rotary kiln.

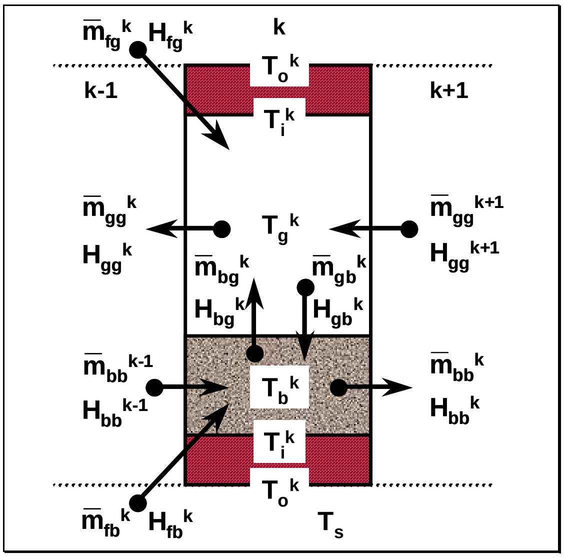

Figure 3: Axial and radial flows to and from a control volume and temperatures in it.

The differential mass and energy continuum equations are discretized accordingly. In steady state the mass and energy balances for the bed and the gas flows and energy balances for the inner and the outer wall in control volume k are given as:

$$\check{m}_{bb}^{k-1} + \check{m}_{gb}^{k} + \check{m}_{fb}^{k} - \check{m}_{bb}^{k} - \check{m}_{bg}^{k} = 0 \tag{2}$$

$$\check{m}_{gg}^{k-1} + \check{m}_{bg}^{k} + \check{m}_{fg}^{k} - \check{m}_{gg}^{k} - \check{m}_{gb}^{k} = 0 \tag{3}$$

$$H_{bb}^{k-1} + H_{fb}^{k} - H_{bb}^{k} + H_{gb}^{k} - H_{bg}^{k} + Q_{gb}^{k} + Q_{ib}^{k} = 0 \tag{4}$$

$$H_{gg}^{k-1} + H_{fg}^{k} - H_{gg}^{k} + H_{bg}^{k} - H_{gb}^{k} - Q_{gb}^{k} - Q_{gi}^{k} = 0 \tag{5}$$

$$Q_{gi}^{k} - Q_{ib}^{k} - Q_{io}^{k} = 0 \tag{6}$$

$$Q_{io}^{k} - Q_{os}^{k} = 0 \tag{7}$$

There is incoming axial bed flow from the previous control volume and incoming axial gas flow from the next control volume. There can be one or more feed flows from the surroundings to the bed and the gas regions. Outgoing flows have the same temperatures and the compositions as in their source regions.

There are also radial flows between the bed and the gas regions in the control volume. The flow from the bed consists of evaporated gas and solid dust carried away with gas flow. The flow to the bed is composed of the gas interacting with the bed surface and solid particles returning back to the bed. In the model the gas phase has a mixing coefficient that determines the fraction of gas interacting with the bed. Also each solid phase has a dusting and saltation coefficients that are used to calculate the mass fractions of the phase constituents transported from the bed to the gas $\check{x}_{bg}^{k}$ and back to the bed $\check{x}_{gb}^{k}$.

The bed and gas flows in the regions are described as thermodynamic systems, which transform mass and heat with each other and their surroundings. Thermodynamic system consists of gaseous and other mixture phases, and number of stoichiometric condensed phases. The equilibrium state of the system can be determined by minimizing its Gibbs energy at constant temperature and pressure. KilnSimu uses ChemApp programming library [4] to calculate the Gibbs energy minimum as well as the enthalpies and heat capacities of the bed and the gas flows.

Bed material consists of particles that are typically at meta-stable state. Most reactions in the bed are gas/solid or solid/solid reactions that are constrained by diffusion and mass transfer in the bed and inside the particles. The composition of the bed flow in a control volume is calculated by combining the equilibrium with time-dependent particle kinetics. The condensed phases in the bed are divided into reactive and inert subsystems by calculating the reaction rates of the phases. Equilibrium is then calculated for the mass flows of the reactive phase constituents only:

$$\check{x}_b^k = \check{A}_0 \exp(-\check{E}_a \big/ RT_b^k)\Delta t^k \tag{8}$$

$$\check{m}_b^k = \check{G}_{\min}\left(T_b^K, P_b^K, \check{x}_b^k\left(\check{m}_{bb}^{K-1} + \check{m}_{fb}^K + \check{m}_{gb}^K\right)\right) + \left(1-\check{x}_b^k\right)\left(\check{m}_{bb}^{K-1} + \check{m}_{fb}^K + \check{m}_{gb}^K\right) \tag{9}$$

$$\check{m}_{bg}^k = \check{x}_{bg}^k \check{m}_b^k \tag{10}$$

$$\check{m}_{bb}^k = \left(1-\check{x}_{bg}^k\right)\check{m}_b^k \tag{11}$$

where $\check{x}_b^k$ are the mass fractions of reactive phase constituents calculated with first order reaction rate equations. Also more complex particle kinetics, like shrinking core model can be used. The composition of the gas flow is calculated in the same way.

The heat transfer flows in control volume k are calculated as follows:

$$Q_{gb}^k = h_{gb}^k A_{gb}^k \left(T_g^k - T_b^k\right) + \overline{GS_b}^k \sigma\left(T_g^{k4} - T_b^{k4}\right) \tag{12}$$

$$Q_{gi}^k = h_{gi}^k A_{gi}^k \left(T_g^k - T_i^k\right) + \overline{GS_i}^k \sigma\left(T_g^{k4} - T_i^{k4}\right) \tag{13}$$

$$Q_{ib}^k = h_{ib}^k A_{ib}^k \left(T_i^k - T_b^k\right) + \overline{S_i S_b}^k \sigma\left(T_i^{k4} - T_b^{k4}\right) \tag{14}$$

$$Q_{io}^k = 2\pi L^k \left(T_i^k - T_o^k\right) \Big/ \sum_l \frac{1}{k_l^k} \ln\frac{d_{l+1}^k}{d_l^k} = 2\pi L^k R^k \left(T_i^k - T_o^k\right) \tag{15}$$

$$Q_{os}^k = h_{os}^k A_{os}^k \left(T_o^k - T_s\right) + \overline{S_o S_s}^k \sigma\left(T_o^{k4} - T_s^{k4}\right) \tag{16}$$

Forced convective heat transfer takes place between the gas and the inner wall and the bed surface. There are many correlations in the literature [5,6] that can be used to calculate the heat transfer coefficient as a function of gas flow properties, like its velocity, density, viscosity and thermal conductivity. KilnSimu also uses temperature dependent equations for gas species to calculate viscosity and thermal conductivity of the gas flow.

Conductive heat transfer takes place between the inner wall and the bed. So called penetration theory can be used to derive the conductive heat transfer coefficient between the inner wall and the bed [7]:

$$h_{ib} = \frac{2k_b}{\sqrt{\pi \alpha_b \tau_{ib}}} \tag{17}$$

Heat transfer is more efficient the shorter the contact time τ_{ib} between the inner wall and the bed is.

Radiation model consists of radial heat exchange between gray gas and reradiating bed and inner wall surfaces, i.e. radiation between the regions in the control volume. Total energy balance can be written over each region in terms of the radiation arriving at it from all other regions in the control volume (axial radiation is neglected). Radiation equations are written in terms of total exchange factors, which are functions of emissivities and geometries of regions. Total exchange areas can be solved from the resulting system of linear, algebraic equations [8].

The measured emissivity and absorptivity of carbon dioxide and water vapour are tabularized as function of their partial pressures, temperature and mean path length. KilnSimu uses Leckner [9] correlation based on these tables to calculate the emissivity and absorptivity of the gas phase. Also emissivity of the soot particles is included.

SOLUTION

The number of control volumes can be chosen freely but typically it should be between 40-80 for obtaining accurate prediction of the local temperatures and compositions in the kiln. Initially the temperatures and compositions in the control volumes are unknown, only the feed flows into the rotary kiln are known. Rotary kiln is divided into two sides: bed side consisting of bed, inner and outer wall regions and gas side consisting of gas regions. First the initial temperature and composition profiles are estimated for the gas flow. After that the temperatures and compositions of all incoming flows to the bed side in the first control volume are known, including the radial mass transfer from the gas side. Then the bed side temperatures are solved from equations (4), (6) and (7) by using appropriate solver (quasi-Newton method) for non-linear set of equations. Each time the solver changes the bed temperature equations (8) and (9) are calculated to obtain the bed flow composition and enthalpy. After solving the temperatures for the bed side in the first control volume all the flows to the bed side in the second control volume are known. Bed side temperatures and compositions in the second and in all the subsequent control volumes are solved in a similar manner. After that the gas side is calculated by using the previously calculated values for the bed side, including the radial mass transfer from the bed side. Gas flow temperature can be solved from equation (5) by using appropriate root-finding solver. Again each time the solver changes the gas temperature the gas flow composition and enthalpy are calculated. After solving both the bed and the gas side, the procedure is repeated until the temperatures in control volumes converge to their final values, which usually takes 10-20 iterations.

APPLICATION

Cement manufacturing is one of the most widely used industrial processes involving a rotary kiln unit operation. Cement process has two main variations: a wet process and a dry process. In the wet process a suitable mixture of raw materials is fed into the rotary kiln in the form of slurry, which may have water content of 30 to 40%. In the dry process this “raw meal” is first dried with exhaust gas from the rotary kiln and then heated in a precalciner system typically consisting of several cyclones and riser duct that is fuelled with coke to calcine the limestone. Cyclones collect dust from the kiln’s exhaust gas and mix that with partially calcined raw meal, which is then fed into the kiln at about 800 °C. The advantage of the dry process is its lower fuel consumption and thus it is the main choice for cement manufacturing today. Figure 4 shows an example of the dry process.

VTT has provided Ube Industries, a Japanese cement manufacturing company, with a KilnSimu model for rotary kiln and clinker cooler unit in the dry cement process. Ube Industries has three cement factories in Japan with combined production capacity of nine million tons of cement per year. Ube Process Technology Research Laboratory has combined KilnSimu with Aspen® flowsheet model to describe the whole cement manufacturing process.

There is interest of using alternative fuels in the cement process as additional heat sources and for waste incineration in the rotary kiln and the riser duct. Typical candidates in the Ube factories are waste plastics (including pachinko panels), oils, tyres and even tatami mats! These additional fuels may have a high content of volatile elements like sulphur and chlorine, which react with alkali metals to form sulphates and chlorides. These then accumulate to the process through alternate vaporization at the hot end and precipitation at cold end of the kiln and in the cyclones and cause cyclone clogging and ring formation and accelerated brick damage in the kiln.

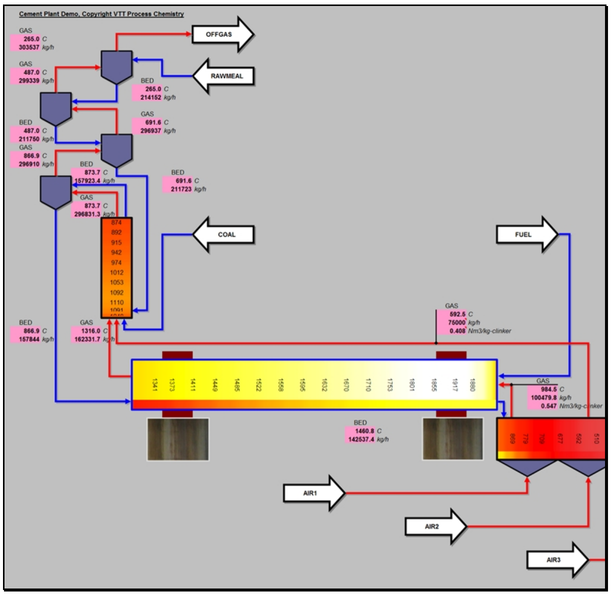

Figure 4: Cement process with a precalciner.

KilnSimu cement model contains a full thermodynamic description of the phases and phase constituents in the cement system. These include gaseous species, liquid slag and solid mixtures and around 100 stoichiometric condensed phases. The mixture of raw materials consists of calcium carbonates, silicon oxides, aluminium oxides and iron oxides respectively occurring as limestone, sand, clay, bauxite, laterite, etc. In the precalciner most of the calcium carbonate is first calcined to calcium oxide or lime at 800-900 °C. Then in the kiln lime reacts with other raw materials at 1200-1450 °C to form calcium and iron silicates and aluminates that are the main components in the burned product called cement clinker.

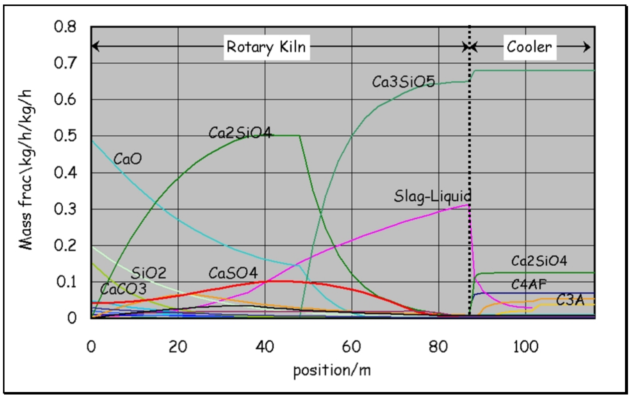

Figure 5: Simulated axial bed flow composition.

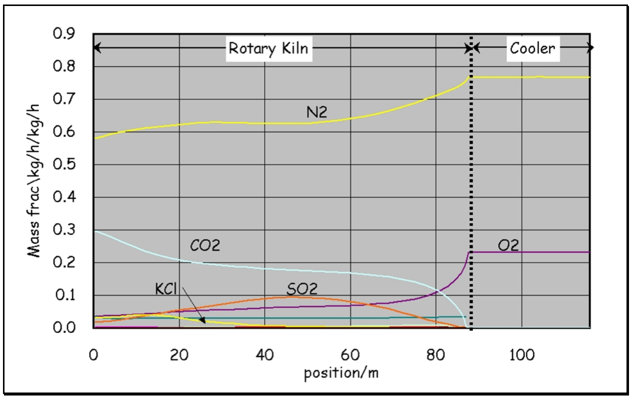

Figure 6: Simulated axial gas flow composition.

A special version of KilnSimu was prepared with a clinker cooler unit which is used for cooling the clinker from the rotary kiln and also for pre-heating the air going into the kiln and the riser duct. Cooler is typically a grate kiln where air is blown from the bottom of the cooler through the grates and the clinker in a cross current fashion. The clinker cooler is also divided into number of control volumes in a similar way as the rotary kiln.

Figure 5 shows simulated axial bed flow composition profile and Figure 6 shows simulated axial gas flow composition profile. Bed flow direction is from left to right and gas flow direction is from right to left. Figures include results for both the rotary kiln and the clinker cooler.

CONCLUSIONS

The simulation yields axial temperature profiles for the bed, the gas and the inner and outer walls. In addition, axial phase compositions of the bed and gas flows are calculated. Results can be used to optimize fuel consumptions with different material feed capacities and to study the effect of using various fuels. Other uses are optimizing the gas circulation and other energy factors including the kiln geometry. KilnSimu is also well suited for kiln scale-up.

In cement case KilnSimu model was successfully used to predict the cement clinker crystal formation and composition and to estimate the circulation of sulphate and chlorine species in the precalciner and rotary kiln. Results can be used for making a correlation between the brick damage rate and the behaviour of sulphates and chlorides.

SYMBOLS

A	Heat transfer area.
$\check{A}_0$	Vector of frequency factors of phase constituents, () 1/s.
d	Diameter, () m.
Δt	Residence time (L/v), () s.
$\check{E}_a$	Vector of activation energies of phase constituents, () J/mol.
G	Gibbs energy, () J/mol.
$\check{G}_{\min}$	Function that returns vector of mass flows of phase constituents at equilibrium, () kg/s.
$\overline{GS}$	Total exchange area between gas and surface, () m^2.
h	Heat transfer coefficient, () W/m^2-K
H	Enthalpy flow, () W.
k	Thermal conductivity, () W/m-K
K	Proportionality constant, () 1/rad.
L	Length, () m.
$\check{m}$	Vector of mass flows of phase constituents, () kg/s.
P	Pressure, () Pa.
Q	Heat flow, () W.
R	Thermal resistivity, () m-K/W.
R	Gas constant, () 8.314472 J/mol-K
$\overline{SS}$	Total exchange area between two surfaces, () m^2.
T	Temperature, () K.
v	Velocity, () m/s.
$\check{x}$	Vector of mass fractions of phase constituents, ().

Greek symbols

α	Thermal diffusivity ($k/c_p\rho$), () m^2/s.
β	Angle of repose, () rad.
ϕ	Filling angle, () rad.
σ	Stefan-Bolzmann constant, () $5.67032\cdot10^{-8}$ W/m^2-K^4.
τ	Contact time (β/ω), () s.
ω	Angular velocity, () rad/s.
ψ	Inclination angle, () rad.

Subscripts And Superscripts

b	Bed
f	Feed
g	Gas
i	Inner wall
o	Outer wall
s	Surroundings, surface
k	Control volume
l	Wall layer

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