

# ADVANCED THERMOCHEMICAL PROCESS MODEL OF ROTARY KILNS – KILNSIMU

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**Abstract:** Rotary kilns are concurrently used 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. Pigment and cement manufacturing industries among others are using rotary kilns for the thermal treatments of various materials. In the chemical recovery of Kraft pulping rotary kilns are applied for lime recycling. Process simulation software KilnSimu was used to simulate two different cases for lime kiln: one with natural gas and one with gas from bark gasification as fuel. KilnSimu is versatile simulation software that can handle several different kinds of rotary kiln applications with chemical systems consisting of hundreds of phases and species.

**Keywords:** KilnSimu, Lime kiln, Thermodynamic equilibrium, Reaction kinetics

## INTRODUCTION

There is increasing interest in the complex chemistry of the rotary kilns, 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 kiln is the formation of rings due to alkali compounds. The lime kiln is a major component of the Kraft pulp mill recausticizing operation. Sodium hydroxide is mixed with the wood chips, cooked in the digester and recovered in the recovery boiler and then regenerated in the recausticizing plant. This is done by exchanging the sodium in the green liquor (sodium carbonate) from the recovery boiler with the calcium from calcium hydroxide. After the exchange, sodium hydroxide is mixed with wood chips in the digester and the calcium carbonate is calcined to calcium oxide in the rotary kiln. The calcium oxide is then slaked to form calcium hydroxide. The calcium hydroxide is mixed with the sodium carbonate from the recovery boiler and the whole cycle is repeated [1].

While direct measurement from within the kiln is difficult to achieve, process simulation software KilnSimu has been developed by VTT Oy in Finland for describing the different applications with varying multiphase chemistries. Figure 1 shows the schematic diagram of KilnSimu. KilnSimu is commercial software marketed by GTT-Technologies in Germany. In the next chapters KilnSimu and the components it uses are described.

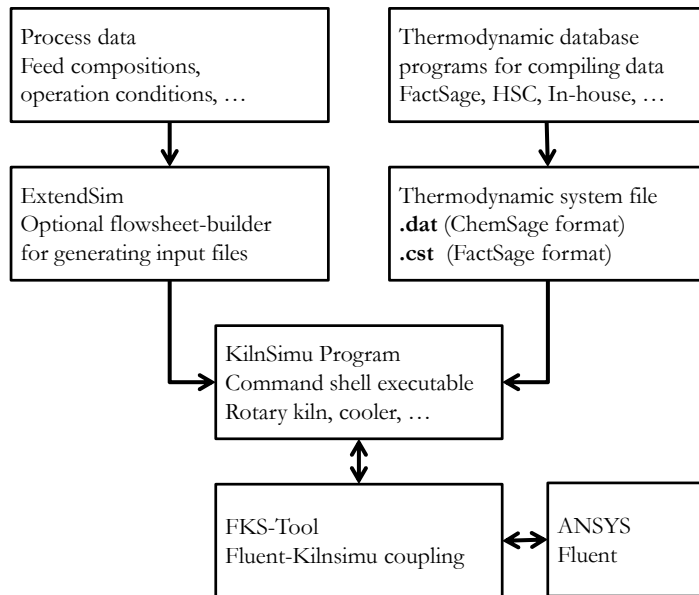


Figure 1 Schematic diagram of KilnSimu program and the components it uses.

KilnSimu combines the calculation of the local thermodynamic equilibrium based on Gibbs free energy method and reaction kinetics with iterative solution of the mass and the heat balance equations. The results are typically axial profiles in the longitudinal direction of the kiln. Additional insight on flame positioning and efficiency can be achieved when this tool is combined to computational fluid dynamics [2].

## ROTARY KILN

Most kilns operate in the counter-current fashion, 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. As a heat source, a fuel burner operating with the primary air is typically used. Schematically the rotary kiln can be divided into drying, heating and reaction(s) zones according to chemical properties of the material [3]. The moisture in the bed feed then is removed in the drying zone. Modern lime kilns contain a preheating system so that the water in the lime mud is removed before it enters the kiln. This increases the energy efficiency of the kiln. Next the temperature of the bed is raised quickly until it reaches the reaction temperature. Lime kiln reactions include mainly the calcination of the limestone particles to lime and the sintering of the lime particles.

### Thermodynamic System

Thermodynamic system consists of elements, phases and species existing in the process (as components in the feed, intermediate and product flows). The first phase is always the gas phase, then follows other liquid or solid mixture phases and pure condensed phases. KilnSimu and the thermodynamic library ChemApp [4] that it uses are compatible with data-files generated by FactSage program [5]. FACT pure and solutions databases were used for the lime system used in this work. It consists of following elements:

- Fuel elements: C, H, O, N, S, P
- Main elements: Ca, O
- Minor elements: Al, K, Mg, Na, Si

Mixture phases consist of liquid and solid salt phases and several pure condensed phases (carbonates, oxyhydrates, sulphates and oxides phases) - all together 171 phases and 258 phase constituents were included. Calcination of limestone to lime requires heat, i.e. it is endothermic and its equilibrium state is dependent on the partial pressure of the carbon dioxide gas. Figure 2 shows the reaction heat and the equilibrium pressure of the  $CO_2(g)$  as function of the temperature.

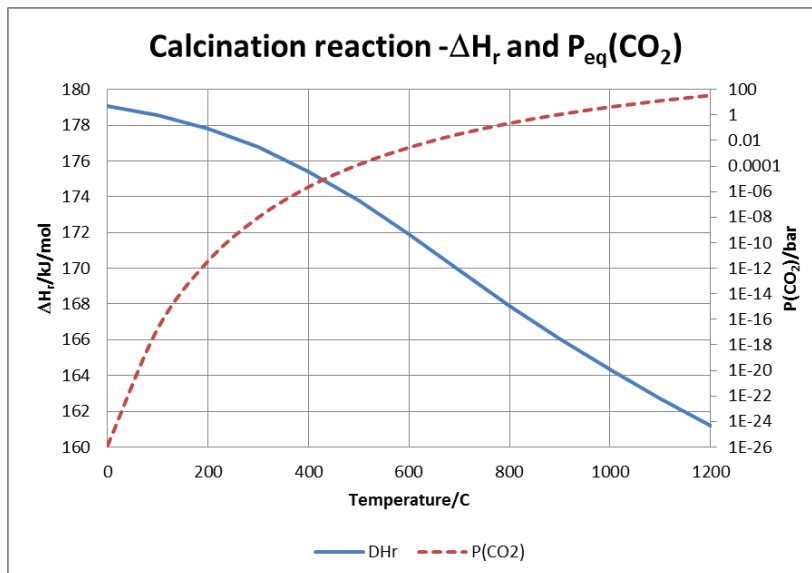


Figure 2 Calcination reaction  $-\Delta H_r$  and  $P_{eq}(CO_2)$  (calculated with thermodynamic data from FactSage 7.0).

Lime system contains many so called non process elements (NPC). They are elements that are either harmful or not useful in the calcination of lime process. These include magnesium, sodium, phosphorous, aluminium and silicon.

### Material Bed

The radial movement of the material 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 or salt (formed at higher temperatures). Figure 3 shows the cross section of the rotary kiln and the material bed.

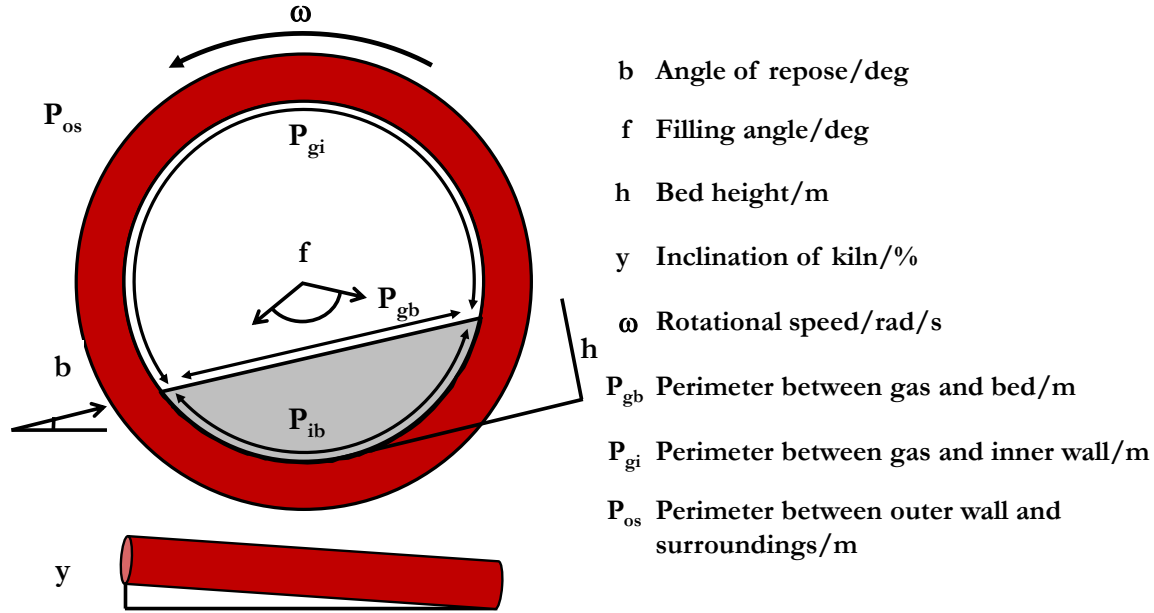


Figure 3 Cross-section of the rotary kiln and the material bed.

The axial velocity of the bed is proportional to inner diameter of the kiln, 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 [6]. If velocity is considered independent on the holdup (valid simplification for long industrial kiln), then in general the axial movement can be given as [7]:

$$v_b = K_b \frac{d_i \omega f(\varphi)}{f(\beta)} \quad (1)$$

where  $K_b$  is the proportional coefficient.

### Mathematical Model

Mostly, the mathematical analysis is based on the heat and mass balance considerations for the counter-current solid and gas streams, to which some specific phase changes were added using assumptions on their reaction kinetics. Mujumdar and Ranade [8] divide the rotary kiln models into two groups. The first group is the conventional solution of one-dimensional material and energy balances for both the condensed bed and gas flows. Such models have been presented e.g. by Manitus et al. [7] for the aluminum oxide kiln and Dumont and Belanger [3] for the titanium dioxide kiln. As the second group one may distinguish the models where a one-dimensional treatise is used to simulate the reactions in the bed region and for the freeboard, a detailed three-dimensional CFD based model is applied [9]. For both groups of the traditional models it is typical that the chemistry of the kiln is presented in terms of selected stoichiometric reactions. To improve the insight on the complex chemical reactions in the bed, one could use thermochemical multiphase approach to recognize the formation of various compounds and phases. A thermodynamic model for the lime calciner used in the

pulp and paper industries was proposed by Backman et al. [10]. KilnSimu represents first group with 1-dimensional material and energy balances combining thermochemical approach and reaction kinetics in a unique way [11].

In KilnSimu heat and mass transfer are assumed to occur in radial direction. Axial heat transfer is neglected and it is assumed that no axial mixing occurs in the material bed or the gas. An axial plug flow model is used for both the bed and the gas. The unknown variables are the temperature of bed, gas, inner and outer wall and the mass flows of bed and gas species. The kiln is assumed to operate in atmospheric pressure.

Conservation of mass for the species in the bed side:

$$\frac{dm_{bj}}{dz} = k_{gbj}P_{bg}m_{bj} - k_{bjg}P_{bg}m_{gj} + R_{bj} \quad (2)$$

where  $R$  is the reaction rate of the species and  $k_{gb}$  and  $k_{bg}$  are the mass transfer coefficients of the species from gas to bed and bed to gas, respectively. For the condensed species the mass transfer from bed to gas equals to dusting (and saltation is used to refer the reverse). For the gas species the mass transfer equals to mixing of the gas flow with the bed surface by convection and diffusion.

Conservation of mass for the species in the gas side:

$$\frac{dm_{gj}}{dz} = k_{bjg}P_{bg}m_{bj} - k_{gbj}P_{bg}m_{gj} + R_{gj} \quad (3)$$

Conservation of energy for the species in the bed side:

$$\frac{dH_b}{dz} = H_{gb} - H_{bg} + P_{gb}\overline{GS}_b\sigma(T_g^4 - T_b^4) + P_{gb}h_{gb}(T_g - T_b) + P_{ib}\overline{S_iS_b}\sigma(T_i^4 - T_b^4) + P_{ib}h_{ib}(T_i - T_b) \quad (4)$$

where  $H_{gb}$  and  $H_{bg}$  are the enthalpy flows from gas to bed and bed to gas,  $h_{gb}$  and  $h_{bg}$  are the heat transfer coefficients between gas and bed an inner wall and bed, and  $\overline{GS}$  is the total heat exchange area between the gas and a surface (bed and inner wall) and  $\overline{SS}$  is the total exchange area between two surfaces (inner wall and bed).

Conservation of energy for the species in the gas side:

$$\frac{dH_g}{dz} = H_{bg} - H_{gb} + P_{gb}\overline{GS}_b\sigma(T_g^4 - T_b^4) + P_{gb}h_{gb}(T_g - T_b) + P_{gi}\overline{GS}_{ib}\sigma(T_g^4 - T_i^4) + P_{gi}h_{gi}(T_g - T_i) \quad (5)$$

Conservation of energy in the inner wall:

$$\frac{dQ_i}{dz} = \frac{2\pi(T_i - T_o)}{\sum_l \frac{1}{\lambda_l} \ln \frac{d_{lo}}{d_{li}}} = 0 \quad (6)$$

where  $\lambda_l$  is the thermal conductivity of a layer.

Conservation of energy in the outer wall:

$$\frac{dQ_o}{dz} = P_{os}\overline{S_oS_s}\sigma(T_o^4 - T_s^4) + P_{os}h_{os}(T_o - T_s) = 0 \quad (7)$$

Equations for the total heat exchange surfaces and heat transfer coefficients are given by Penttilä [12].

Condensed phases and gas species in the bed and the gas flow are divided into inert and reactive parts. Only reactive parts are taken to the equilibrium calculation. General kinetic equation that can be used for the gas-solid and the solid-solid reactions is given as [13]:

$$\frac{dx}{dt} = A_0 \cdot e^{-\frac{E_a}{RT}} \cdot x^m \cdot (1-x)^n \cdot (-\ln(1-x))^p \quad (8)$$

where  $A_0$ ,  $E_a$ ,  $m$ ,  $n$ ,  $p$  are the parameters of the kinetic model and  $x$  is the advancement of the reaction or in this case the reactive part of a phase for the next equilibrium calculation.

The local volume elements of the bed and the gas are described as open thermochemical systems, which transform heat and mass with each other. The equilibrium states of the volume elements are calculated by minimizing their Gibbs energy and by taking into account the heat and mass transfer between the elements and their surroundings. The time-dependent reactions in the bed and the gas flow are taken into account in the Gibbs energy minimization by constraining the fractions of phases taking part in the equilibrium calculation (e.g. inert and reactive parts). The Gibbs energy minimization is done by calling routines in ChemApp library.

Temperatures of bed and gas side and inner and outer wall and flow rates of bed and gas side phase constituents are determined at discrete reference points usually termed a nodal point (node). Each node represents a certain volume, and its temperature and composition is a measure of average temperature and composition of that volume. Usually 100 or so nodes are used in the axial direction. The derivative at the nodal point  $k$  may be approximated as:

$$\frac{m_{bj}^{k-1} - m_{bj}^k}{\Delta z} = k_{gbj} P_{bg} m_{bj}^k - k_{b gj} P_{bg} m_{gj}^k + R_{bj}^k \quad (9)$$

The temperature and the mass flow rates of the gas side are not known in the case of counter-current gas flow. Problem is now a so-called two point boundary value problem with a fixed boundary. With KilnSimu its solution comprises an iterative calculation where first the mass and energy balance equations are solved for the bed side and the inner and outer wall node by node by keeping the gas side temperature profile constant. After solving the bed side the gas side is calculated this time by keeping the bed side and inner and outer wall temperatures as constant. This is repeated until the temperature profiles converge (usually 10-20 iterations are needed).

### ExtendSim Interface

ExtendSim is a powerful simulation tool. Using ExtendSim one can develop dynamic models of real-life processes in a wide variety of fields. ExtendSim can be used to create models from building blocks [14]. A KilnSimu library has been made for ExtendSim so that it can be used as a GUI for designing process flowsheets by drag and dropping process blocks and for inputting the model parameters via dialog windows and controls like text boxes and popup menus. When the model is calculated its flowsheet and parameters are written to a data-file that is then processed by the KilnSimu executable that also handles the simulation of the model.

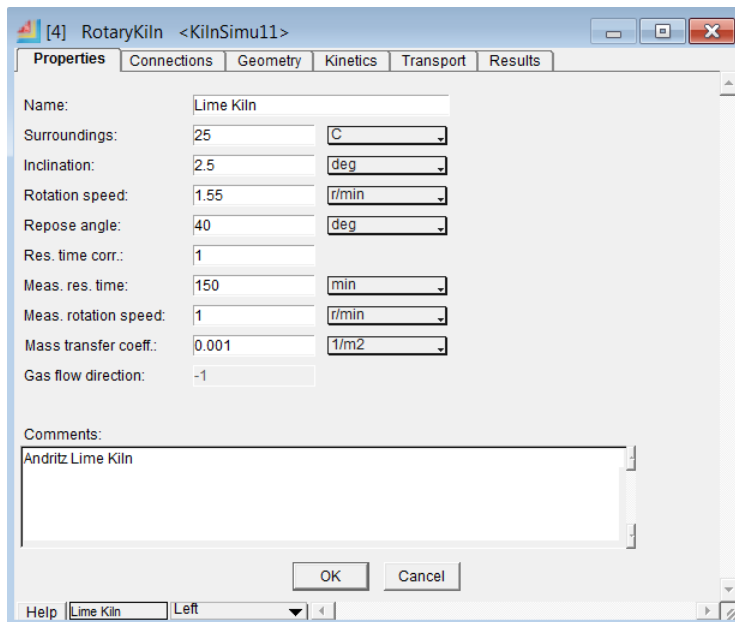


Figure 4 RotaryKiln dialog window.

KilnSimu library contains models for following unit operations (or model blocks in ExtendSim terminology): Calciner (fluidized bed), Cooler, Cyclone, Feed, Tear, Mixer, FixedMixer, Model, Product, RotaryKiln and Splitter. Cyclone and Splitter are flow mixing and separation processes where each phase can be given its own separation efficiency or splitting

factor. Mixer and FixedMixer are general flow mixing processes. Mixer, Splitter and Cyclone include heat loss as input and the temperature of the outgoing flows is solved from the energy balance (enthalpy in – heat out – enthalpy out). FixedMixer includes fixed input temperature for the outgoing flow and the enthalpy change is calculated (useful for checking the heating value of a fuel).

## LIME KILN APPLICATION

Lime mud is washed and dewatered to 70% - 75% dry solids on a lime mud precoat filter or disc filter and is then conveyed to the lime mud dryer, where it is flashed dried and pre-heated prior to being fed into the kiln. The LMD uses kiln exit gases to flash dry the mud in suspension. The mud is completely dried and preheated before it enters the kiln. Higher kiln capacity is possible because there is no drying in the kiln and the entire kiln length is used for additional preheating and calcination.

The lime mud is calcined by heating with oil, gas or other fuels. Most of the calcium carbonate in the lime mud is converted to calcium oxide. The liberated carbon dioxide is removed with the combustion gases, which flow counter currently to the lime mud in the kiln. The lime kiln is a refractory lined, rotating cylinder installed on a slope so the lime will be conveyed from the feed end to the firing end as the kiln rotates. A burner is located at the discharge or downhill end of the kiln and provides the heat for calcining the lime mud. The kiln is supported by roller sets that are located on the top of concrete piers. The kiln shell is rotated by a variable speed electric motor. The kiln shell is sealed by labyrinth seals at the feed-end in the LimeFlash housing and at the firing end in the firing hood. A dam is located near the discharge end of the kiln and is used to increase the retention time in the burning zone of the kiln.

The lime leaving the kiln contains a significant amount of heat. This heat is recovered in a LimeCool. The cooler is used to transfer heat from the product to the secondary combustion air entering the kiln. Lime spills over the dam onto grizzlies that are located in the mouth of chutes that lead to the LimeCool. Smaller lumps pass through the grizzly opening into the cooler. Large lumps remain on the grizzlies until they are broken by the rotation of the kiln. Preheated secondary air passes through the chutes and grizzlies and into the kiln. The LimeCool is installed around the kiln shell over the burning zone and rotates with the kiln. It consists of two concentric shells, which are divided into sectors along the direction of the kiln axis. When hot lime drops into the LimeCool, it enters one of the sectors and is cooled by the counter-current flow of secondary combustion air. The LimeCool is covered by a heat shroud that reduces radiation losses. Secondary air at ambient temperature enters the LimeCool shroud through an annular space around the kiln neck, behind the firing hood.

The secondary air is pre-heated as it flows in the space between the LimeCool and kiln shell and between the LimeCool and the shroud. The preheated secondary air enters the cooler at the uphill end of the cooler. The flow of secondary air recovers kiln shell radiation losses and cools the kiln shell as it passes between the cooler and shell. Part of the preheated air is piped to the primary air fan and is used as preheated primary air in the kiln burner.

The cooled lime leaves the kiln and falls by gravity through a diverter gate and into the product crusher. The lime from the crusher falls into the reburned drag chain conveyor that conveys lime to the bucket elevator and is transported to the reburned lime bin.

The first lime kiln case uses natural gas as a fuel but the second case uses gas from the biomass (wood bark) gasification as a fuel. Atmospheric pressure CFB with preheated air from the LimeCool system is used for the gasification. The moisture content of the bark feed to the CFB riser is 11.6 w-%. The temperature of the exit gas from the cyclone is approximately 700-750 degrees Celsius.

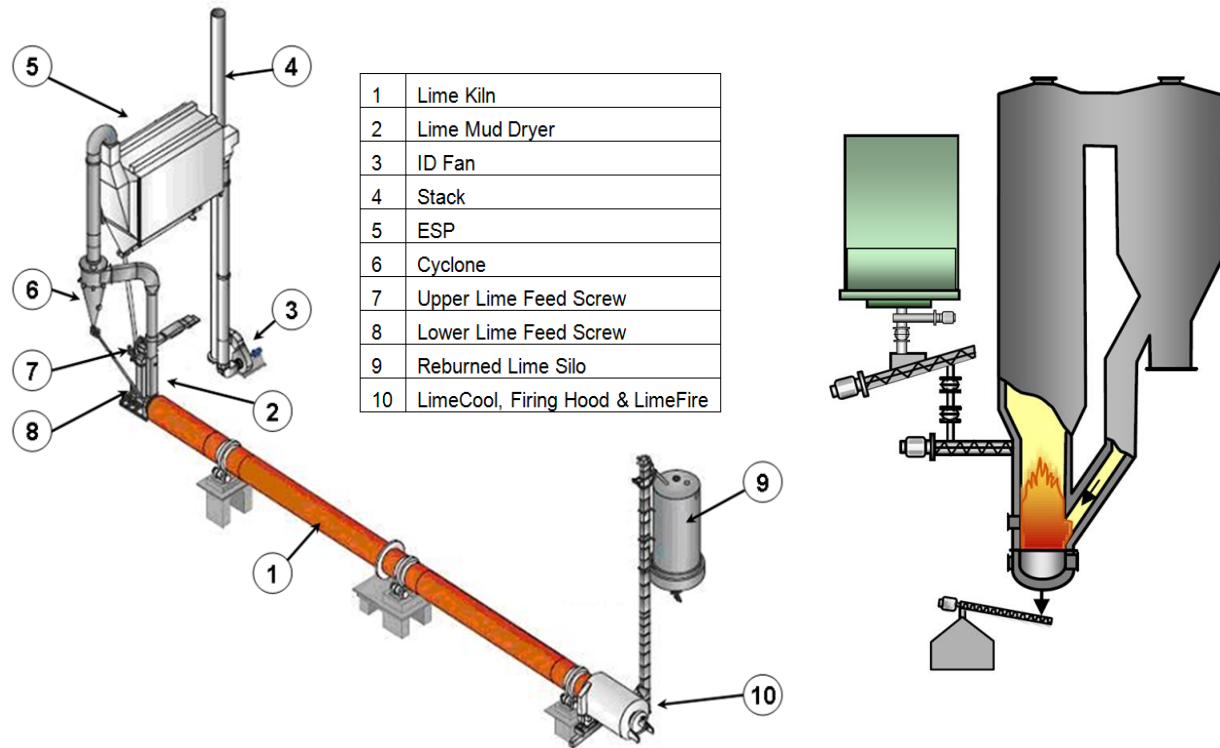


Figure 5 Lime kiln and gasification processes (pictures provided by Andritz).

### Process Model

KilnSimu library for ExtendSim was used to build the process flowsheet. Library does not include all the unit operations specific to lime process like LMD and LimeCool but instead Calciner block was used for the flash dryer, Splitter block for the ESP and the LimeCool. Also extra heat can be entered to each Splitter to take the shell radiation losses into account. Calciner and cyclone blocks were used for the Gasification process.

Lime Mud enters the Lime Mud Dryer block and is heated with the exit gas from the Lime Kiln block so that all the water in the mud is evaporated. Then the gas and lime mixture enters the Cyclone block where typically 85%-90% of the condensed phases are separated from the gas flow. Gas enters the ESP block where typically 99% of the remaining condensed phases are separated. It is also possible to define different separation efficiencies for phases based on their assumed particle sizes for example. Cleaned gas enters the stack and leaves the process. Condensed phases (particles) from the Cyclone enter the Lime Kiln block where the lime is calcined. The lime from the lime kiln enters the Splitter block is partly cooled down by the secondary air before leaving the process.

Optional bark feed and preheated air enter the gasification riser where partial combustion and gasification reactions take place. The exit gas from to cyclone can be connected to the Lime Kiln (as in Fig. 6).

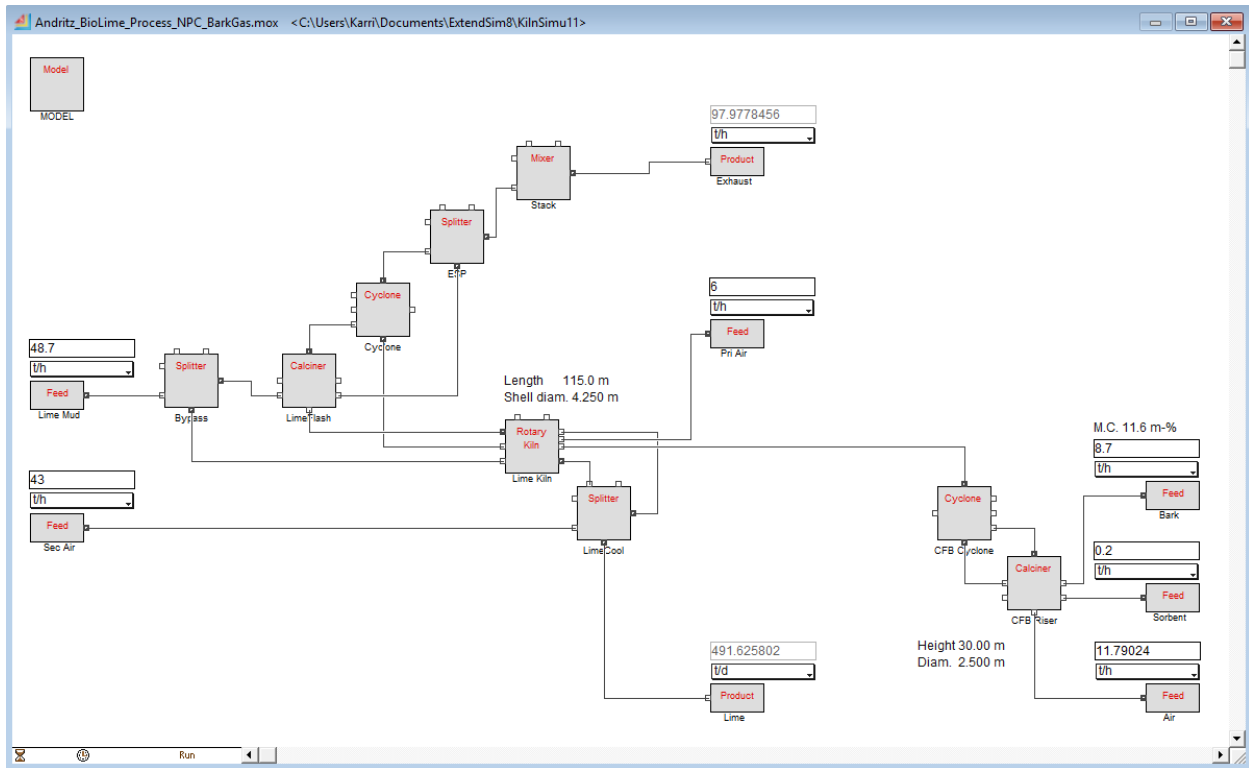


Figure 6 ExtendSim model with the lime kiln and the gasification process (simulation case 2).

## Case Studies

Two simulation cases were calculated. The process data for the cases was provided by Andritz Oy. In the first case the kiln used natural gas and in the second case gas from the bark gasification as fuel (atmospheric pressure CFB with air feed). Otherwise the kilns and their process parameters were almost identical (see Table 1). The lime mud feed was set as 48.7 t/h (1168.8 t/d). This gives production rate that is roughly equal to given 482 t/d rate in case 1 (see Table 1)

Dusting coefficients for the phases were set so that dusting was  $\sim 15$  w-% (of bed feed to the kiln). Dust was separated from the kiln exit gas in the cyclone and the ESP and recycled back to the kiln. Simple first order kinetics was used for all the condensed phases in the bed and the gas sides of kiln to slow down their reaction rates. For example the reaction rate coefficient for the calcination of  $\text{CaCO}_3$  was set as 0.0012 1/s. The calcination was partly controlled by the heat transfer rate from the gas to the bed (and equilibrium calculation) and partly by the given reaction rate.

In the first case 2870 kg/h of natural gas was used. This was equal to 143.5 GJ/h or 7.17 MJ/kg(product) (here product rate is 20 t/h). Natural gas contained 98 w-% methane so it was very clean. In the second case the bark feed rate was set as 7691 kg/h as dry basis (equal to 150.0 GJ/h or 7.50 MJ/kg(product)). Bark contained 3.6 w-% ash (see Table 2). This bark feed rate was set so that it gave the same  $\text{CaCO}_3$  conversion to CaO as natural gas in case 1.

Moisture content of the lime mud was 30 w-% in the first case and 33 w-% in the second case (but 30 w-% was used in both calculations to make the lime mud feed identical). Lime mud composition in dry basis is given Table 2. The composition of the non process elements was not known so suitable values were used (with relatively high Mg and P content as the total NPC measured was 7 w-% in dry basis). Its phase composition was estimated by calculating the equilibrium composition between water, limestone and NPC elements at room temperature and selecting set of stable phases and scaling their mass fractions accordingly (also shown in Table 2).



Table 1 Process parameters (db = dry basis).

<b>Fuel</b>	<b>Natural gas</b>	<b>Bark gas</b>
Kiln type	LMD	LMD
Shell inner diam./m	4.25	4.25
Kiln length/m	115	115
Indination/%	2.5	2.5
Rotation speed/rpm	1.55	1.55
Lime production/t/d	482	475
Lime mud (assumed)		
H <sub>2</sub> O/w-%	30	33
CaCO <sub>3</sub> /w-% (db)	92	92
CaO/w-% (db)	1	1
NPC/w-% (db)	7	7
Exit CaCO <sub>3</sub> /w-%	3	3.9
Kiln exit T <sub>g</sub> /C	723	730
Kiln exit O <sub>2</sub> /w-%	4.1	3.7
Cydone exit T <sub>b</sub> /C	245	265

Table 2 Lime mud composition (NPC = non process elements) and fuel properties (db = dry basis). NPC composition was not known so suitable values were used). Phase composition was estimated with equilibrium between water, limestone and NPC elements. Bark analysis by Andritz, ash composition from Kurkela et.al. [15].

<b>Phase</b>	<b>All/w-%</b>	<b>Dry basis/w-%</b>	<b>Fuel</b>	<b>Natural Gas</b>	<b>Bark gas</b>
H <sub>2</sub> O_liquid(liq)	<b>30.000</b>	<b>0.000</b>	Moisture/w-%	0.000	11.600
CaCO <sub>3</sub> _Calcite(s <sub>2</sub> )	<b>64.400</b>	<b>92.000</b>	Elem. analysis (db)		
CaO_Lime(s)	<b>0.700</b>	<b>1.000</b>	C	74.300	52.000
<b>NPC phases tot.</b>	<b>4.900</b>	<b>7.000</b>	H	24.700	5.700
Al <sub>2</sub> O <sub>3</sub> (H <sub>2</sub> O)_Diaspore(s)	0.091	0.130	N	1.000	0.390
Ca <sub>5</sub> HO <sub>13</sub> P <sub>3</sub> _Hydroxyapat(s)	1.823	2.604	O		38.261
CaSO <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> _Gypsum(s)	0.089	0.128	S		0.035
CaSiO <sub>3</sub> _Wollastonite(s)	0.715	1.021	Cl		0.014
K <sub>2</sub> SO <sub>4</sub> _Solid_Alpha(s)	0.089	0.128	<b>Ash/w-%</b>		<b>3.6</b>
MgCO <sub>3</sub> _magnesite(s)	1.276	1.823	Al <sub>2</sub> O <sub>3</sub> _gamma(s)		3.800
NaAlSi <sub>3</sub> O <sub>8</sub> _Low-Albite(s)	0.179	0.255	CaO_Lime(s)		56.550
Na <sub>2</sub> SO <sub>4</sub> (H <sub>2</sub> O) <sub>10</sub> _solid(s)	0.638	0.911	MgO_Peridase(s)		8.000
<b>NPC elements tot.</b>	<b>1.329</b>	<b>1.899</b>	K <sub>2</sub> O_solid(s)		12.300
Al	0.093	0.133	Na <sub>2</sub> O_Solid-A(s)		0.750
K	0.044	0.063	(P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub> _solid(s)		6.400
Mg	0.404	0.577	SiO <sub>2</sub> _Quartz(l)(s)		11.000
Na	0.130	0.185	S_FC_ORTHORHOMBIC(s)		1.200
P	0.370	0.529	<b>LHV/MJ/kg (db)</b>	<b>50</b>	<b>19.52</b>
S	0.036	0.052			
Si	0.253	0.361			

Figure 7 and 8 show the calculated temperature, lime (CaO/(CaCO<sub>3</sub>+CaO)) conversion and Salt-liq profiles for case 1 and case 2, respectively.

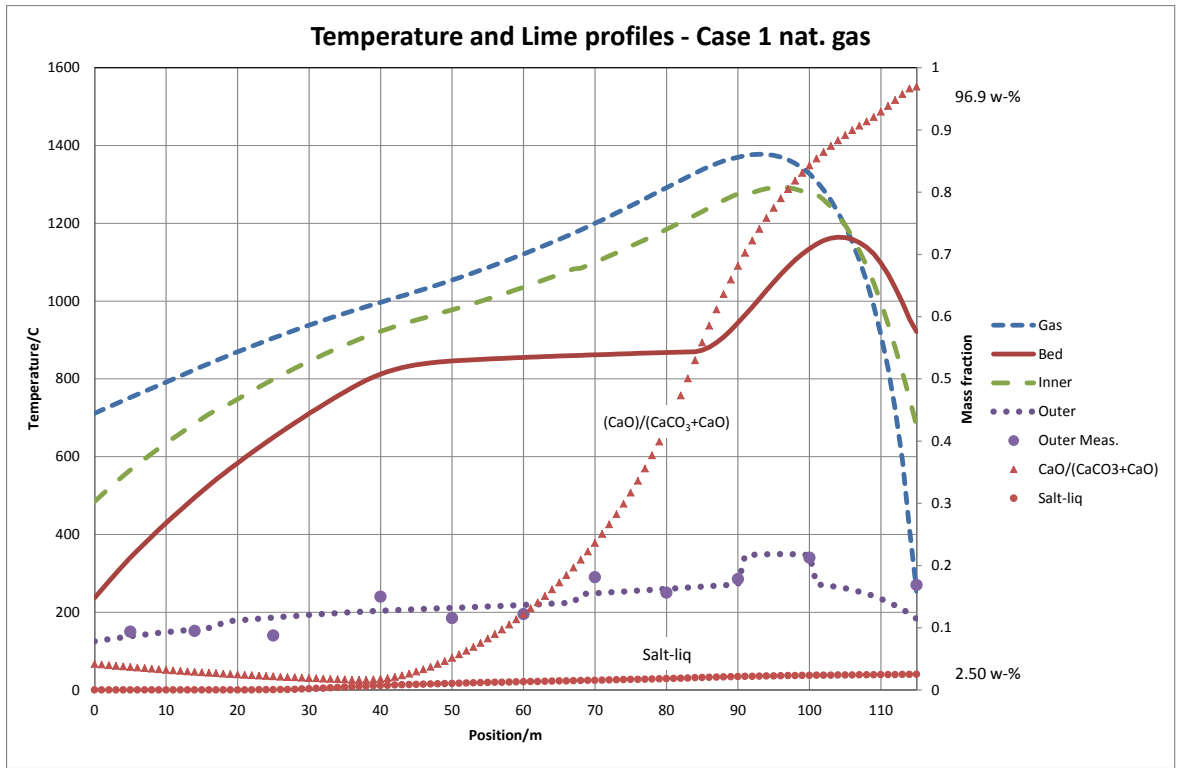


Figure 7 Kiln temperature, lime ( $\text{CaO}/(\text{CaCO}_3+\text{CaO})$ ) conversion and Salt-liq profiles in case 1 with natural gas.

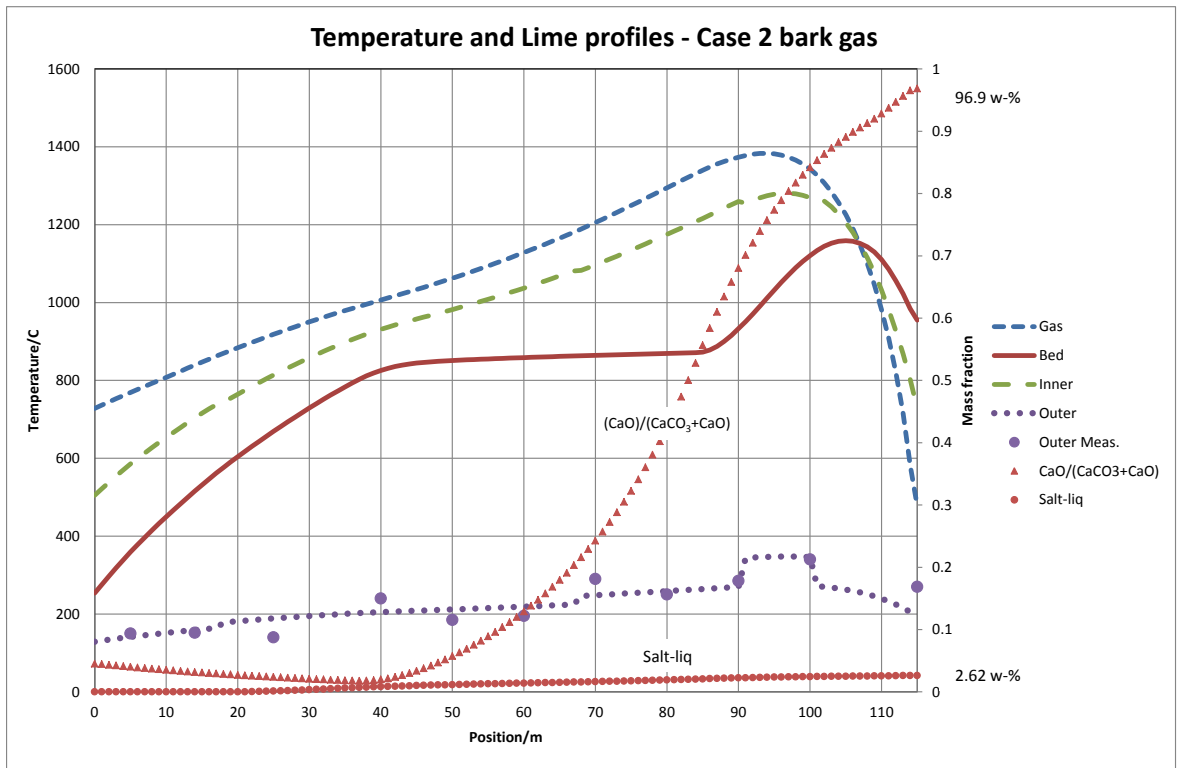


Figure 8 Kiln temperature, lime ( $\text{CaO}/(\text{CaCO}_3+\text{CaO})$ ) conversion and Salt-liq profiles in case 2 with Bark gas.

## CONCLUSIONS

KilnSimu was used calculate two different cases for the lime kiln: one with natural gas and one with gas from bark gasification as fuel. The process data for the cases was provided by Andritz Oy. Lime mud feed rate (48.7 t/h) and composition (see Table 2) were identical in both cases. Table 3 shows comparison between some calculated and measured values.

Table 3. Comparison between some calculated and measured values.

Param.	Case 1		Case 2	
	Meas.	Calc.	Meas.	Calc.
Exit CaCO <sub>3</sub> /w-%	3.0	3.1	3.9	3.1
Exit Tg/C	723.0	711.4	730.0	728.2
Cyclone exit/C	245.0	237.3	265.0	253.3
Exit O <sub>2</sub> (g)/w-%	4.1	4.0	3.7	4.4

In case 1 the total air feed rate to the kiln was 64.0 t/h (primary + secondary) and the calculated production rate was 480 t/d. The feed rate of the natural gas was 2.87 t/h (143.6 GJ/h). There was a good agreement between calculated and measured values. This was accomplished by fine tuning model parameters like calcination reaction rate coefficient, bed emissivity and gas to bed mass transfer coefficient which all are user inputs and affect the gas and bed temperature profiles. Same values were also used in case 2.

In case 2 the total air feed rate to the kiln was 49.0 t/h (primary + secondary) and the calculated production rate was 492 t/d. (higher rate was due to ash in the bark). The feed rate of the dry bark was 7.69 t/h (150.0 GJ/h). The maximum average gas temperature inside the kiln was lower in case 2 than in case 1 (1359 °C versus 1378 °C) but on the other hand the exit gas temperature (728 °C versus 711 °C) and flow rate (83.4 t/h versus 81.0 t/h) were higher. The flow rate of the bark gas from the gasification unit was 20.7 t/h and its temperature was 724 °C.

Currently KilnSimu does not contain any parameter optimization or goal seeking routines so finding the optimal set of process parameters must be done manually which in some cases might take a long time. Other than that KilnSimu is versatile simulation software that can handle several different kinds of rotary kiln applications with chemical systems consisting of hundreds of phases and species and up to 15-20 elements including trace elements. KilnSimu is especially suitable for situations where changes in chemical composition of some feed flow like the fuel should be studied.

## SYMBOLS

$A_0$	Frequency factor [1/s]
$d$	Diameter [m]
$D$	Kiln diameter [m]
$E_a$	Activation energy [J/mol]
$\overline{GS}$	Total heat exchange area between gas and a surface [m <sup>2</sup> ]
$h$	heat transfer coefficient [J/m <sup>2</sup> -K]
$h$	Height [m]
$H$	Enthalpy flow [J/s]
$K_b$	Proportional coefficient []
$k$	Mass transfer coefficient [1/m <sup>2</sup> ]
$m$	Mass flow [kg/s]
$P$	Perimeter [m]
$Q$	Heat flow [J/s]
$R$	Reaction rate [kg/s]
$\overline{SS}$	Total heat exchange area between two surfaces [m <sup>2</sup> ]
$t$	Time [s]
$T$	Temperature [K]
$z$	Axial dimension [m]

v	Bed velocity [m/s]
x	Mass fraction []

### Greek symbols

$\beta$	Repose angle [rad]
$\phi$	Filling angle [rad]
$\psi$	Inclination [%]
$\lambda$	Thermal conduction [J/s-m-K]
$\sigma$	Stefan Boltzmann constant [J/s-m <sup>2</sup> -K <sup>4</sup> ]

### Subscripts

b	Bed
g	Gas
i	Inner wall
j	Species
o	Outer wall

### Superscripts

m	Reaction rate parameter
n	Reaction rate parameter
p	Reaction rate parameter

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