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# Multi-phase thermodynamic modelling of pulp suspensions: Application to a papermaking process

Anna Kalliola, Risto Pajarre, Pertti Koukkari, Juha Hakala and Esko Kukkamäki

**KEYWORDS:** Calcium carbonate, Multi-phase modelling, Papermaking, pH control, Process simulation

**SUMMARY:** During the past decade, multi-phase thermodynamics has been applied to pulp suspensions in order to support calcium chemistry control in neutral papermaking. During this period, multi-phase modelling was initially applied in the development of pulp acidification and pH buffering concepts, and unit operation models have been used to quantify the doses of acidification chemicals and buffering aids. The inclusion of multi-phase chemistry calculation in conventional mass and energy process simulation has enabled the monitoring of the chemistry of large process integrates. The experiences and case examples of multi-phase modelling are reviewed in the present paper.

In the present study, the pH and calcium chemistry of a large process integrate were simulated in conditions that had been previously found to cause problems in paper production. The difficulties were thought to be due to increased dithionite dosing, which had been used to obtain the desired brightness of the paper product. The modelled integrate consisted of two paper machine lines with mechanical and deinked pulp as feed stocks. Simulation of the production of the high brightness grades revealed that a relatively high quantity of solid calcium carbonate is lost under these production conditions. The results improved our understanding of bleaching practices in neutral papermaking.

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Papermaking chemistry is vulnerable to changes in pH, temperature and ion concentrations, as the behaviour of inorganics and organic wood based compounds depend on these properties. One of the key challenges of neutral papermaking derives from the fact that acid conditions accelerate the dissolution of calcium carbonate,  $\text{CaCO}_3$ . This leads to pigment loss, raises the amount of dissolved calcium ( $\text{Ca}^{2+}$ ) and increases foaming ( $\text{CO}_2$ ). A fluctuating concentration of dissolved calcium induces unwanted inorganic and organic precipitation which can reduce production efficiency.

The innovation of carbon dioxide acidification of deinked pulp (DIP) (Laurila-Lumme et al. 2003; Pakarinen, Leino 2000) spurred fresh interest among the

research community in gaining a deeper understanding of neutral papermaking chemistry. At the same time, calcium carbonate became a more common raw material in the production of mechanical pulp dominated paper grades. The pulp and paper producer UPM concluded that the problems of neutral papermaking chemistry can be tackled by improving pH control practices, and that thermodynamic multi-phase modelling could play a role in this development.

In the early 2000s Räsänen et al. (2001), Lindgren et al. (2001) and Nordberg et al. (2001) followed the Donnan theory based approach of Towers and Scallan (1996) and introduced models for predicting metal ion chemistry in pulp suspensions in different process situations. During the same period, a general multi-phase model for pulp suspensions, combining solubility equilibria with both solid and gas phases and Donnan ion exchange equilibria between the pulp fibres and the surrounding aqueous liquid, was introduced by Koukkari et al. (2002). In continuation of this development, the latter research group together with Finnish industry have since focused on investigating practical industrial applications for the multicomponent Donnan method, particularly with respect to modelling the chemistry of neutral papermaking.

Initially, multi-phase modelling was applied to developing pulp acidification and pH buffering concepts. The models were used for the quantification of chemicals (Weaver et al. 2002; Pajarre et al. 2002; Kalliola, Pakarinen 2002). Neutral conversions were also simulated with respect to pH and calcium chemistry (Viitikko, Kalliola 2002). The models were initially produced with a commercial Gibbs energy minimization program, ChemSheet™ (Koukkari et al. 2000; 2001), which proved to be practical due to its multicomponent thermo-dynamic base and easy-to-use spreadsheet interface.

In connection with applying the ChemSheet models, databases and a free-energy minimization subroutine, ChemApp® (Eriksson et al. 1997), were developed to allow the multi-phase Donnan approach to be appended to process simulation programs (Koukkari et al. 2003). One of the extended programs was BALAS® (initial version developed by Kaijaluoto (1984)), a steady-state simulator created especially for pulp and paper processes. For example, this method was used to compare the metal complexing ability and cost efficiency of DTPA with a new chelating agent in the D/Q bleaching sequence (Sundquist et al. 2004).

Only a few studies concerning chemistry modelling of large-scale processes or rigorous physico-chemical phenomena in pulp and papermaking have been reported. Gu et al. (2004a; 2004b; 2004c) demonstrated that the metal profiles of real mill processes, including bleach plant, thermomechanical pulping, and kraft chemical

recovery, can be predicted by incorporating multi-phase, multicomponent equilibrium calculation (SOLGASWATER) in process simulations (WinGEMS). However, these studies did not include the Donnan effect in free energy minimization, but assumed that metals bound to pulp-binding ligands, and initially measured the formation reaction constants of each notable reaction between the pulp fibres and different metals in the system. Tarvo et al. (2008) applied the concept of two liquid phases (Donnan model) in the phenomenon models applied to kraft pulp bleaching chemistry. Sundman et al. (2008) stated that in an excess of NaCl higher amounts of divalent metal ions, such as  $\text{Ca}^{2+}$  are adsorbed onto cellulosic fibres than predicted by the Donnan model. Thus, in combination with the Donnan equilibrium, specific metal ion–fibre surface complexes  $(\equiv\text{COO})_2\text{Me}$  were assumed to form. Recently, Dionísio De Oliveira et al. (2010) applied a process simulation (WinGEMS) in combination with Donnan-type non-specific binding of ions and a competitive adsorption equation for specific binding (the NICA-Donnan model) to predict the metals distribution in the case of bleach plant closure.

The theory and methods of multi-phase thermodynamics of pulp suspensions are reviewed by Kangas et al. (2012). The objective of the present paper is to review the studies conducted with multi-phase models while improving the control practices of neutral papermaking chemistry. The latest study in this field is discussed in most detail. The study aimed to identify the process stages that had a major contribution to  $\text{CaCO}_3$  dissolution in a papermaking integrate consisting of two neutral paper machines and thermomechanical pulp (TMP) and deinking processes. Sodium dithionite,  $\text{Na}_2\text{S}_2\text{O}_4$  was applied in pulp bleaching, and production difficulties were often experienced with greatly increased dithionite dosing.

## Methods

### Multi-phase modelling of pulp suspensions

The papermaking furnish consists of an aqueous suspension containing pulp fibres and inorganic pigments. The furnish can be considered as a multi-phase system since it has at least four different phases (gaseous, aqueous, fibre, solid) and tens of different chemical constituents. The salient feature here is that the fibre itself forms a chemically active entity, as fibres from different sources have different levels of acidity. A separate fibre phase can thus be assumed, consisting of fibre-bound acidic groups and the water absorbed by the fibre. These properties lead to a so-called Donnan equilibrium between the fibre and its surrounding filtrate phase (Towers, Scallan 1996) and will strongly influence any simulations aimed at determining the chemical state of the fibre suspension. *Fig 1* illustrates a typical multi-phase system of pulp suspension. In addition to the fibre-bound acids ( $\text{Acid}^- + \text{H}^+$ ,  $\text{AcidH}$ ), the fibre phase includes the same constituents as the aqueous phase. Electro-neutrality is applied for both fibre and aqueous phases.

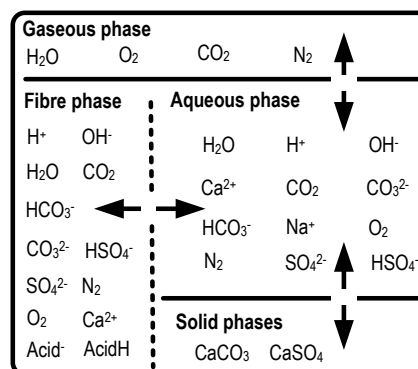


Fig 1. A typical multi-phase system with four separate phase types and multiple constituents (adopted from Kangas et al. 2012).

The ion exchange and ionic equilibria in pulp–water systems can be described quantitatively when the overall ionic composition, accounting for anions, cations, ionic species and fibre charge, is known. The nature of the cellulose fibre wall in ionic media as a negatively charged polyelectrolyte phase determines the equilibrium ion distribution. The amount of fibre-bound water is conventionally known as the water retention value, WRV (measured according to ISO 23714:2007). The characterisation of the charge properties is performed by potentiometric acid–base (Laine et al. 1994; Räsänen et al. 2001) or conductometric (Katz 1984) titration methods. Together with the electroneutrality condition, this data can be combined with the multicomponent equilibrium data of the suspension. The thermodynamic data then accounts for possible precipitates as well as the effect of the gaseous phase, and multi-phase equilibrium procedure for the suspension can be applied. The theory covers the charge properties of different fibres, their ion exchange behaviour in terms of pH and the ionic composition of the suspension.

The chemical state, i.e. the ionic composition of the two aqueous phases, the solubilities of the various compounds and the pH of the solutions can be determined based on either equilibrium constant or Gibbs energy data (Kangas 2009; Koukkari et al. 2002, see also Pajarre et al. 2006). For practical simulation purposes, the Gibbsian approach has proven to be the best calculation method (Kangas et al. 2011). The approach involves the minimisation of the Gibbs free energy of the system in terms of the molar amounts and chemical potentials of its constituents. Chemical potentials are computed using the standard-state and the excess term of the chemical potential of the constituent. This thermodynamic data is obtained from the literature/handbooks or from existing commercial data bases. To solve the minimisation problem, the multi-phase system (e.g. in *Fig 1*) is defined in a form of stoichiometric matrix with constituents as rows and system components (C, O, H, S, Ca,  $e^-$ , etc.) as columns (see *Table A2*, Kangas et al. 2012). The set of equations thus obtained is iteratively solved until convergence is reached. Hence, in the Gibbsian approach it is not necessary to define the individual reactions as in the method applying equilibrium constants.

## Multi-phase calculation in process simulation

The compatibility of thermodynamic Gibbs energy solvers, such as ChemApp®, allows their combination with other simulation programs. The extension of BALAS® with multi-phase reactor modules provides a tool for extensive and diversified process studies which take into account the process chemistry. Streams in the simulator carry the components which will serve as inputs to the equilibrium calculation module and, likewise, the simulator handles the reactor outputs. An example of a process stream with a given conditions and constituents is presented in *Fig A1* (Appendix 1). *Fig A2* (Appendix 1) presents an editing window of the equilibrium module (ChemApp reactor) in which the fibre-bound water and fibre acids are determined. After conducting the simulation pH, carbonate alkalinity, heat balance and conductivity of the system are shown in the editing window. Use of the ChemApp multi-phase reactor module in any fibre-liquid separation calculation, such as dewatering element, correctly reallocates the metals between the two aqueous phases, i.e. the fibre-bound water and the filtrate phase.

## Building a model

### Unit operation models

Initially, the unit operation multi-phase models were produced with ChemSheet™. Typical process stages modelled included the machine chest, broke chest or tower, and pulp bleaching or acidification. The data for the model included the  $pK_a$  values of the fibre acids and the corresponding charge, the fibre consistency, and the water retention value (WRV) of the fibre types. The inorganics data, i.e. the quantity of the filler or pigment, was adjusted in the model based on ash measurements provided by the mill. The model input also included known chemicals, acids or bases, entering the process stage.

### Process integrate

In the present study, an integrate of two paper machines (PM A and PM B), TMP and deinking processes was modelled with BALAS®, to which the multi-phase

Table 1.  $pK_a$  values and the corresponding charge of fibre material in TMP and DIP.

pka	TMP unbleached	TMP bleached	DIP
3.6	65.3	74.6	82.2
5.6	23.8	39.5	40.4
9	45.1	44.5	37.0

subroutine (ChemApp®) was appended. The mass (fibre, filler i.e. 525 & 925 °C ash, and water) and energy balances were adjusted in the process model prior to the extension of the multi-phase reactor modules. A schematic model of the integrated process and the most important phenomena with respect to the process chemistry are shown in *Fig 2*.

The process chemistry was validated in the model by using the conditions in which the production of the low brightness target paper grades was conducted on both PM lines. Fibre acid properties (*Table 1*) were included in the multi-phase reactor modules based on acid-base titrations (Räsänen et al. 2001). The quantities of chemicals, acids or bases entering the process were used as model inputs. As dithionite bleaching was carried out at six different stages in the process integrate (in the DIP and TMP processes as well as at the PMs), special attention was given to the sulphur chemistry. The molar proportions of the species ( $Na^+$ ,  $HSO_3^-$ ,  $HSO_4^-$ ) formed from the dosed dithionite were adopted from the study by Malkavaara et al. (2000). Oxidation of (bi)sulphite to (bi)sulphate was included in the model.

The primary metals entering the process within the raw materials (TMP: sample taken just after main refining; DIP: sample taken from the storage chest just after drum pulping of recycled paper) were adjusted in the model based on inductively coupled plasma atomic emission spectroscopy (ICP-AES) analysis. The pulp and filtrate (and fresh water) samples, numbering approx. 100 in total, collected for the initial mass balance modelling were filtered immediately after sampling, first with black ribbon filter paper and thereafter with 0.2  $\mu m$  membrane to obtain a liquid phase sample, which was analysed for metals ( $Ca^{2+}$ ,  $Mg^{2+}$ ,  $Na^+$ ,  $K^+$ ,  $Al^{3+}$ ) and anions ( $SO_4^{2-}$ ,  $Cl^-$ , and  $HCO_3^-/CO_3^{2-}$ ) by ion chromatography (IC) and capillary electrophoresis (CE). This data was finally used to validate the concentrations of cations and anions in the model.

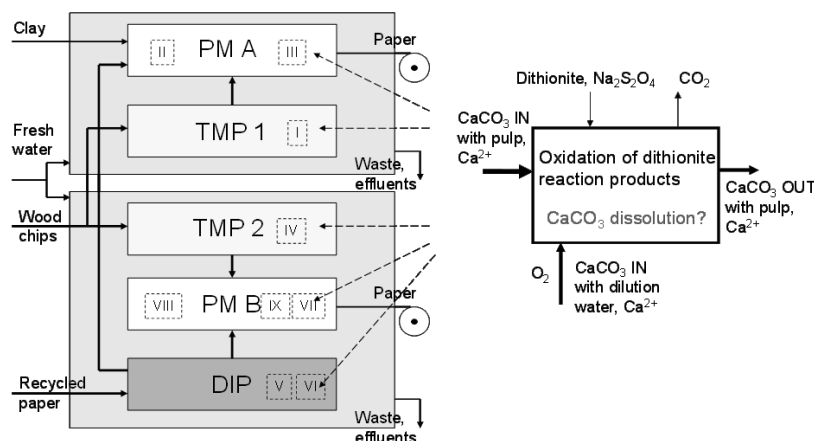


Fig 2. A schematic process model of a papermaking integrate subjected to a study with the main focus on combined  $CaCO_3$  and sulphur chemistry. Each block (PM A, TMP 1, etc.) represents a large process model. In nine sub-processes, marked with I-IX (bleaching stages, broke circulations and short circulations of the PMs), the loss of solid  $CaCO_3$  was quantified.

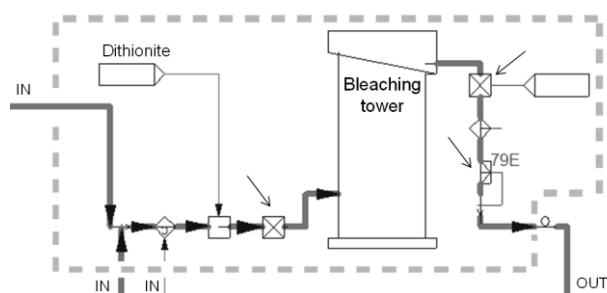


Fig 3. A sub-process (PM B bleaching, VII) subjected to the quantification of the loss of solid  $\text{CaCO}_3$ . Dotted line defines the balance area. The units computing the multi-phase equilibrium are marked with arrows.

The amounts of  $\text{CaCO}_3$  and clay entered in the model were based on 525 and 925 °C ash determinations (TAPPI T 211) performed on the collected samples. Deinked pulp normally also contains other inorganic pigments in addition to  $\text{CaCO}_3$  and clay. However, only  $\text{CaCO}_3$  was considered in the multi-phase calculation. The other pigments were assumed to be inert and were introduced as clay in the model.

In addition to the mill measurements and analyses, experience and literature based assumptions were applied in the model. These include, e.g., furnish aging induced formation of acids in broke circulations (represented as  $\text{CH}_3\text{COOH}$  in the model), the formation of dissolved organic material ( $\text{CO}_2(\text{aq})$ ,  $\text{CH}_3\text{COOH}$  and  $\text{HCOOH}$ ) in peroxide bleaching in drum pulping, and the formation of calcium oxalate in both TMP refining and peroxide bleaching (Terelius et al. 2001a; Terelius et al. 2001b). In addition, the release of gaseous  $\text{CO}_2$ , which mainly originated from dissolved  $\text{CaCO}_3$ , was taken into account at selected process points (e.g. the defoamer).

Special chemicals used in minor amounts in the process were excluded. These include retention aids, fixatives, antifoaming agents, biocides, gaseous air, and  $\text{NaBO}_2$  in dithionite liquor (the  $\text{NaBO}_2$  amount was replaced by  $\text{NaOH}$ ).

The dissolution kinetics of solid compounds such as  $\text{CaCO}_3$  was not considered in the model. Equilibrium state calculations were therefore applied to each multi-phase reactor module.

## Simulation

As described above, the process model was adjusted to the production of paper grades with low brightness target on both PM lines. The simulation of simultaneous production of high brightness grades on both PMs was conducted in steady state calculation mode. For the low brightness grades, the minimum dithionite dose of the six different bleaching stages was 0% and the maximum 0.38%. During the production of high brightness grades, the minimum was 0.12% and the maximum 0.80%. The share of DIP and TMP used in paper production varied according to the brightness target of the paper. In the simulation, their proportions were set according to the mill data.

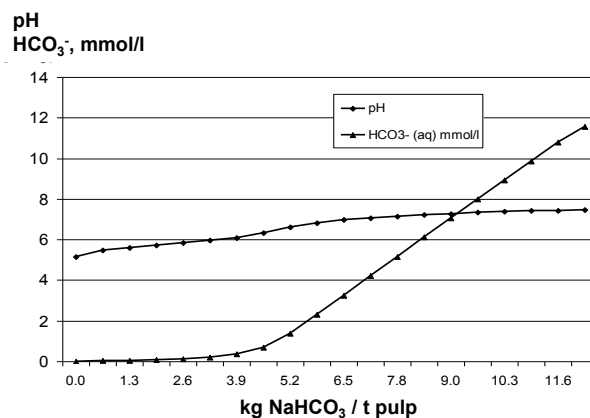


Fig 4. pH and buffering capacity ( $\text{HCO}_3^-$ ) of bleached kraft pulp as a function of dosed  $\text{NaHCO}_3$  (Weaver et al. 2002).

## Determination of solid calcium carbonate loss

Nine sub-processes of the overall process model were selected to study the loss of solid  $\text{CaCO}_3$ . The sub-processes (I-IX, Fig 1.) corresponded to the bleaching stages, broke circulations and short circulations of both PMs. In one of the sub-processes sequential dithionite bleaching was applied. The amount of solid  $\text{CaCO}_3$  entering and leaving each of the sub-process were computed. As a result, the amounts of dissolved  $\text{CaCO}_3$ , i.e. the pigment losses, were obtained. The quantities were calculated as kg/day. Fig 3 presents one of the sub-processes, PM B bleaching (VII).

## Results

### Unit operation models

ChemSheet models of single process stages were used to quantify chemical dosages for pH buffering test runs. Fig 4 presents the calculated values for pH and  $\text{HCO}_3^-$  ion concentration, used for determining the appropriate  $\text{NaHCO}_3$  dose for adjusting the pH of bleached kraft pulp (Weaver et al. 2002). Pulp acidification modelling has revealed that the use of carbon dioxide ( $\text{CO}_2$ ) is an effective choice for minimising  $\text{CaCO}_3$  dissolution in pulps containing high amounts of  $\text{CaCO}_3$ , such as deinked pulp (Pajarre et al. 2002; Weaver et al. 2002).

Fig 5 shows results from an example study of neutral conversion on a PM producing coated paper (Viitikko, Kalliola 2002). In this case, modelling was applied to define the share of coated broke of the machine chest pulp, which maintains neutral pH conditions in the short circulation. The results suggested that at a broke share of 10%, 15%, and 26% and a corresponding minimum of 40%, 27%, and 17%  $\text{CaCO}_3$  in the coating colour (mixture of different pigments), the machine chest pH is maintained slightly above 7. Usually, during efficient PM production, the coated broke share can be less than 10%. However, as long as solid  $\text{CaCO}_3$  or a buffering capacity ( $\text{HCO}_3^-$ ) exists in the circulation water, the pH in the PM process will not decrease sharply.

### Process integrate

The study focused on comparing the production of low to high brightness paper grades with respect to calcium chemistry. The major cations and anions were nevertheless also included in the model to provide the

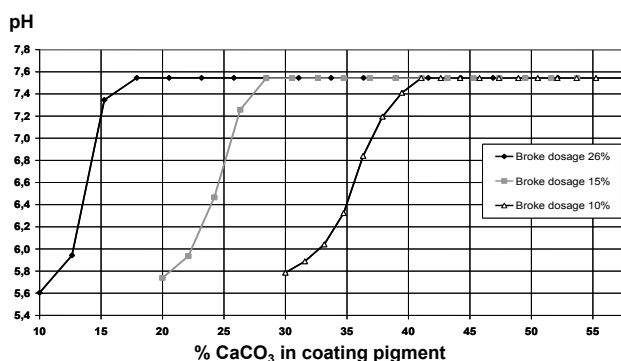


Fig 5. pH of machine chest pulp as a function of CaCO<sub>3</sub> content in coating colour (Viitikko, Kalliola 2002).

existing ionic conditions for the multi-phase calculation. The quantitative loss of solid CaCO<sub>3</sub> was computed for these production conditions. Fig 6 presents the modelled and measured values of dissolved calcium (Ca<sup>2+</sup>) and pH for the DIP, PM A, and TMP processes during the production of paper grades with a low brightness target. In general, the model validation gave satisfactory results as regards all cations and anions, with the exception of

sulphate ions, which appeared at a lower level than the measured values at almost every process point of the model.

Fig 7 presents the simulated values of dissolved calcium and pH during the production of paper grades with a high brightness target. Several measurements of dissolved calcium and pH are also presented in Fig 7.

The applicability of the model proved to be satisfactory in terms of its correspondence with the measured values of dissolved calcium and pH (Fig 6). In practice, it has been observed that the more dithionite is used the more CaCO<sub>3</sub> is dissolved and the higher the amount of free calcium ions in the process (Kalliola, Pakarinen 2002). The simulation was in line with these observations. However, at certain process points the measured values of dissolved calcium were more than double when compared to the simulated values (these points are marked with arrows in Fig 7). Increased dithionite dosing decreases the process pH. The simulated and measured pH values correlate closely for PM B, but are less closely correlated for the deinking and TMP 2 processes (Fig 7).

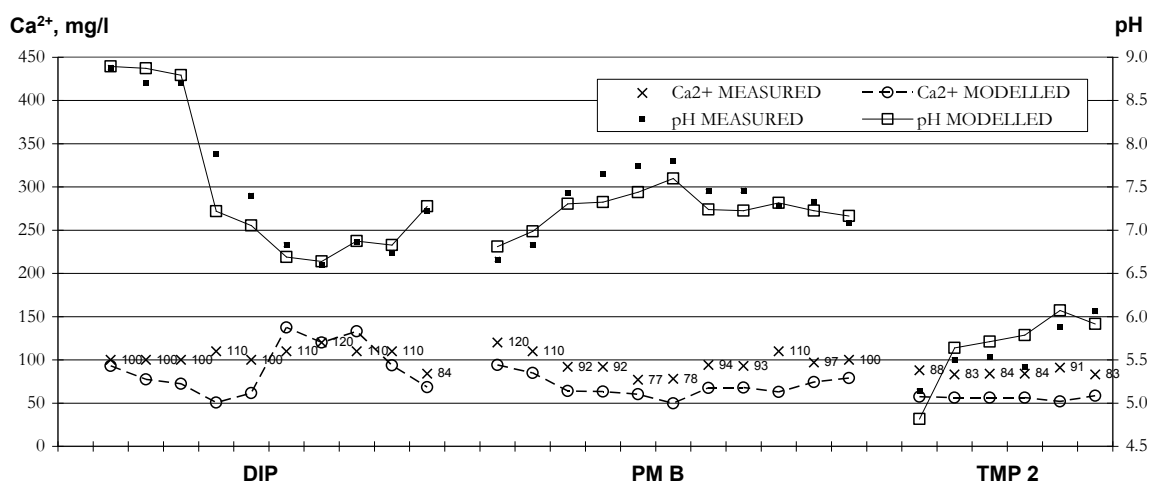


Fig 6. Production of low brightness paper grades: Modelled and measured values of dissolved calcium (Ca<sup>2+</sup>) and pH at the PM B line (x-axis corresponds to the process points in the DIP, PM B and TMP 2 processes).

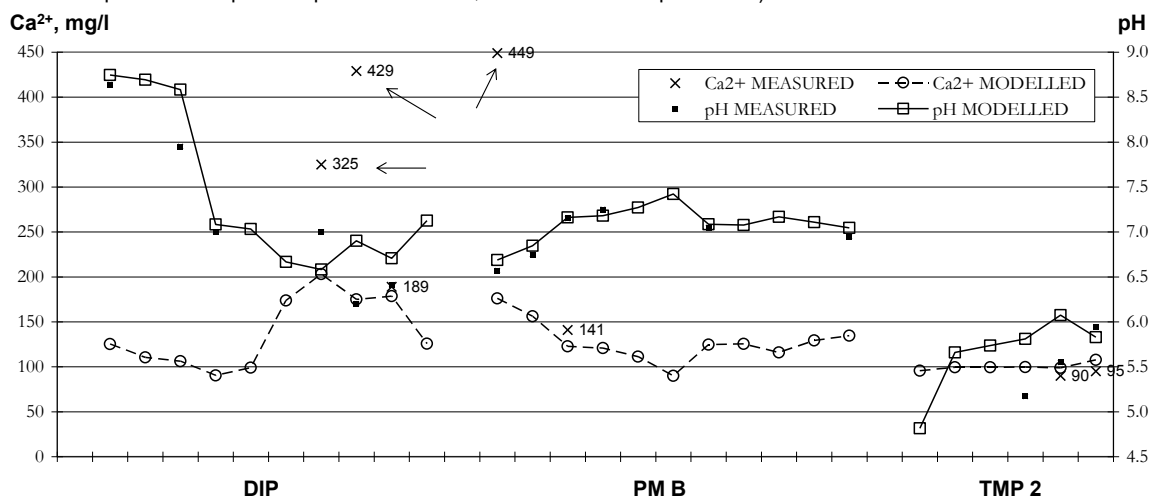


Fig 7. Production of high brightness paper grades: Simulated and measured (single point) values of dissolved calcium (Ca<sup>2+</sup>) and pH at the PM B line (x-axis corresponds to the process points in the DIP, PM B and TMP 2 processes). Highly deviating simulated values vs. measured values are marked with arrows.

Table 2. Solid CaCO<sub>3</sub> losses in the selected sub-processes of the papermaking integrate.

Sub-process	Production of low brightness grades			Production of high brightness grades		
	Solid CaCO <sub>3</sub> IN kg/day	CaCO <sub>3</sub> Dissolved (-) / precipitated (+) kg/day	Solid CaCO <sub>3</sub> loss (-) / gain (+) %	Solid CaCO <sub>3</sub> IN kg/day	CaCO <sub>3</sub> Dissolved (-) / precipitated (+) kg/day	Solid CaCO <sub>3</sub> loss (-) / gain (+) %
I TMP 1 bleaching	2	-2	-100	0	0	0
II PM A broke circulation	597	-48	-8.1	47	-47	-100
III PM A short circulation	12902	638	4.9	1535	-358	-23.3
IV TMP 2 bleaching	11	-11	-100	9	-9	-100
V DIP 1&2 bleaching	15464	-603	-3.9	17402	-1525	-8.8
VI DIP 3 bleaching	8677	-700	-8.1	3541	-215	-6.1
VII PM B bleaching	14847	-711	-4.8	15862	-777	-4.9
VIII PM B broke circulation	5130	-234	-4.6	5453	-222	2.2
IX PM B short circulation	28045	514	1.8	29820	582	2.0

Table 2 summarizes the solid CaCO<sub>3</sub> losses in the selected sub-processes of the process integrate. In the production of high brightness grades, a high rate of CaCO<sub>3</sub> loss (kg/day) occurs in sub-process DIP 1&2 bleaching (V). On the other hand, the quantities of solid CaCO<sub>3</sub> entering sub-processes TMP 1 (I) and TMP 2 bleaching (IV) are relatively minor, even though dissolving totally. In PM A (III) and PM B short circulations (IX), the precipitated quantity of CaCO<sub>3</sub> may not be fully reliable due to the equilibrium calculation in sub-processes being conducted with a very short delay.

## Discussion

The chemistry model of the process integrate included approximately 200 multi-phase reactor modules in total. With such an extensive model, the chemical system needs to be kept concise as any additional constituent is a new variable, and the computational load increases respectively.

Deviation from the measurements is interpreted as inaccuracy of the model data, i.e. the input data for an extensive process is not comprehensive in terms of chemical inputs. Another obvious source of disagreement is the systematic use of the basic assumption of chemical equilibria in the chemistry units of the model. The simulation nevertheless shows quantitative agreement with respect to the expected pH as well as the vast majority of concentration values.

Discrepancies between the model and measurement can be used to interpret unexpected operational practices as well as to detect unknown 'chemistry sources'. For example, one may conclude that both calcium and sulphur (e.g. in the form of gypsum pigment) are entering the process with recycled paper to some extent, which cannot be quantified as a model input. Furthermore, sulphate anions tend to concentrate in the process circuits and metal cations in the fibres in order of increasing valence. When troubleshooting a process, model/measurement deviations can serve as valuable clues for recognising unwanted chemical behaviour, or, as explained above and shown in Fig 7, for identifying previously unknown sources of surplus ionic strength affecting the process.

Improved pH and calcium control has led to savings, e.g. as a remedy for CaCO<sub>3</sub> losses. A further advantage is the explanation of process chemistry variations when different grades are produced. However, such a large-scale process simulation also entails some drawbacks. While the agreement between the model and mill data

remains satisfactory, the model validation still requires extensive measurements at the mill. The model can then be used for predictions as long as no major changes emerge in the process flowsheet. Updating the model after optional process changes may become an arduous task during the course of active renovation. The substantial computation time (several hours) required by a multi-reactor system may also be a retarding factor with respect to development work.

Nonetheless, the outcomes of applying multi-phase thermodynamics combining the Donnan effect in modelling unit operations or whole processes have been beneficial. Such calculations unite basic research and mill applications. Furthermore, they are likely to come under increasing interest in the current strive towards further reductions in mill water usage and filtrate discharge, which will raise the need for metal management and scale control in order to maintain process efficiency. The method also offers new possibilities to develop energy saving process concepts in the dryer section, as the Donnan model also allows estimation of chemically bound water in different salinity conditions.

## Conclusions

The unit operation models have been useful in comparing different chemicals in pulp acidification and have supported, for example, the replacement of H<sub>2</sub>SO<sub>4</sub> with CO<sub>2</sub>. The models' quantification of pH buffering aid dosage has enabled the number of test runs to be minimized. Additionally, the models have enabled a deeper understanding of the chemistry involved in each neutral conversion. Usually, simplified small-scale models containing only the most important chemical phenomena are sufficient enough to support thought and can be used for control or decision-making processes.

The extension of the multi-phase chemistry model within the calculation framework of a process simulator has enabled the monitoring of the chemistry of large process integrates. In the present study, the solid CaCO<sub>3</sub> losses at selected sub-processes of the papermaking integrate were quantified. The information obtained could be used to modify certain bleaching practices.

Multi-phase chemistry modelling thus offers a valid means of supporting the reduction of mill water usage and maintaining process efficiency.

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## Appendix 1. Multi-phase calculation in process simulation

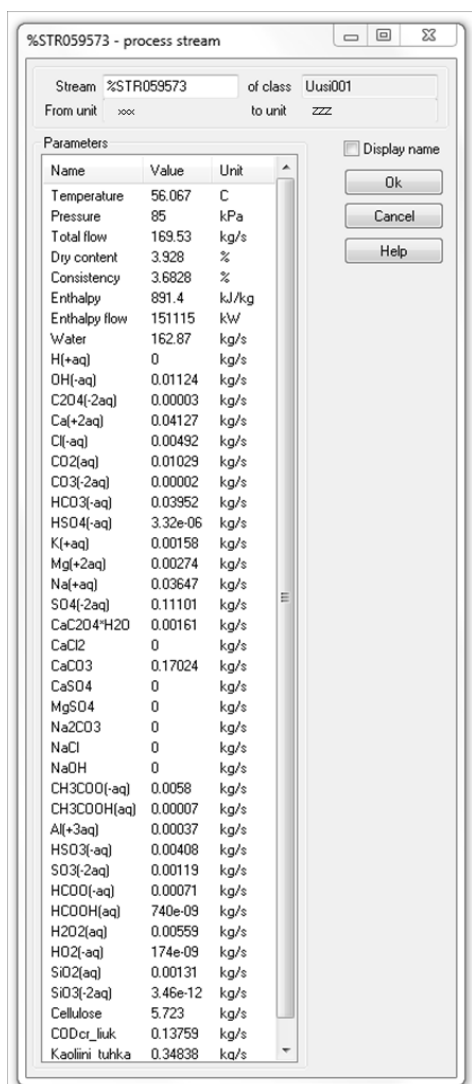


Fig A1. An example of a process stream with a given conditions and constituents in BALAS process simulator extended with multi-phase equilibrium calculation.

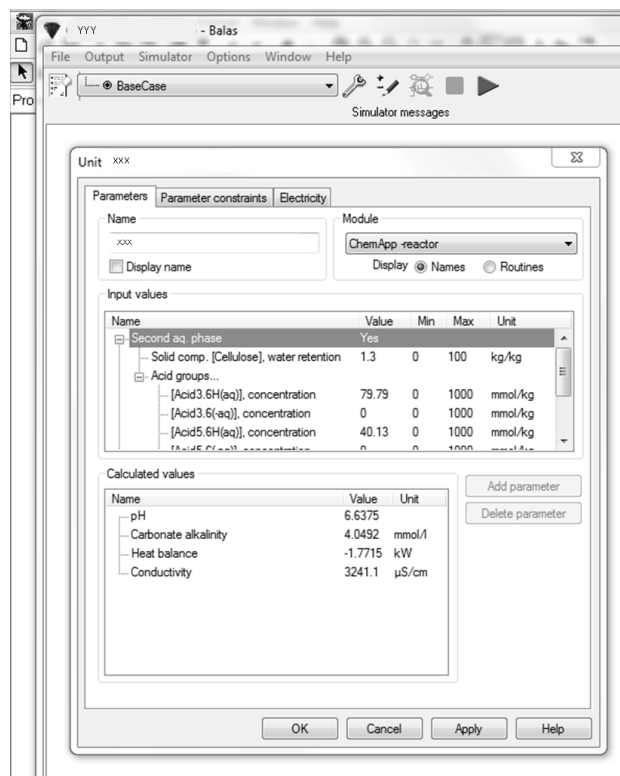


Fig A2. An editing window of the equilibrium module (ChemApp reactor) in BALAS process simulator.