CHEMAC Project Final Report

Process Chemistry in

FlowMac and KraftMac Simulator

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1.   Introduction

The CheMac library in Extend simulation platform is based on a thermodynamic routines and chemistry database. The target is to construct the pulp and paper making unit models with rigorous chemistry calculation.

CheMac uses Gibbs energy minimization library, ChemApp, for calculating equilibrium between vapour, water and fiber water phases. It also includes dissolution/precipitation of solid phases. Thermodynamic routines are in a separate dynamic link library (DLL) that is called from Extend models.

2.   Washing Model Theory

The modeling principle described in the following combines the modeling principles of dilution-dewatering and ideal displacement in such way that a washer model with adjustable washing efficiency can be created.

Washing by dilution-dewatering can be described by a single cstr unit; pulp is mixed with desired amount of washing water, and then pulp slurry is thickened by removal of excess water so that desired consistency is reached (Figure 1). In the model developed we have assumed that chemical equilibrium is reached during dilution-dewatering.

Dilution-dewatering describes poor-efficiency washing. Industrial washers take advantage of displacement phenomenon, i.e. washing water flows through immobilized pulp cake in such way that it pushes dirty liquor from the pulp cake like piston. Ideal displacement describes high efficiency washing.

Displacement washing can be described by a number of series-connected cstr units, where pulp to be washed flows counter-currently towards washing water flow (Figure 2). Concerning each cstr unit, we assume that chemical equilibrium is reached at each time step of calculation, i.e. there are no mass transfer limitations.

A real washer never operates ideally. More or less of the pulp is washed by displacement, while mixing effects decrease the overall washing efficiency. This nonideality can be accounted for by combining dilution-dewatering and displacement principles. In the model, dilution-dewatering and displacement units are connected in parallel. Washing efficiency of model can be simply adjusted by dividing the pulp and wash liquor flows into two fractions; one fraction goes into displacer unit, while another goes to dilution-dewatering unit (Figure 3). The division ratio of the pulp and washing liquor flows uniformly define the washing efficiency of the model. After the displacer and dilution-dewatering units the pulp and wash liquor flows are combined again.

This principle is new and has not been published before. The benefit of the model is that the model facilitates modeling of 'real' washing efficiencies of different components (sodium, calcium and potassium species, COD, SO4, etc.) without any artificial efficiency factors. The use of flow distribution ratio is a theoretically sound principle to account for washing with varying efficiency, because it reflects the direct reason of the nonideality of washing.
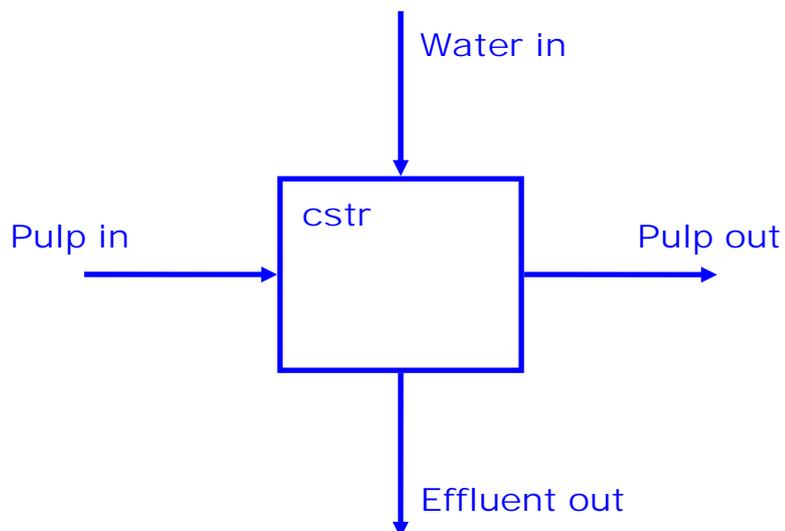
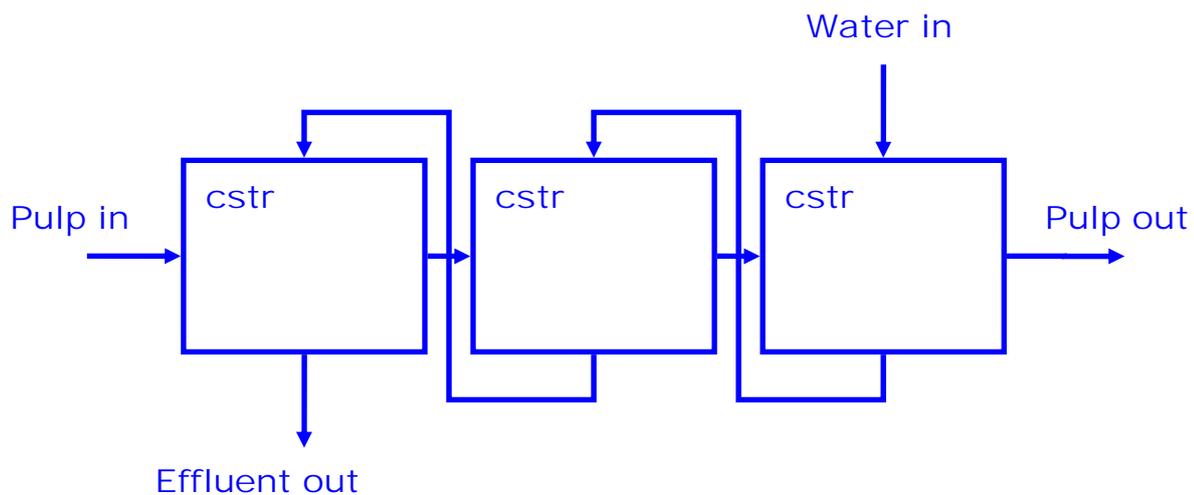**Figure 1 Dilution-dewatering unit comprising of a single cstr.**

Figure 2 Displacer unit comprising of a number of cstr units. Washing water runs countercurrently towards the pup stream
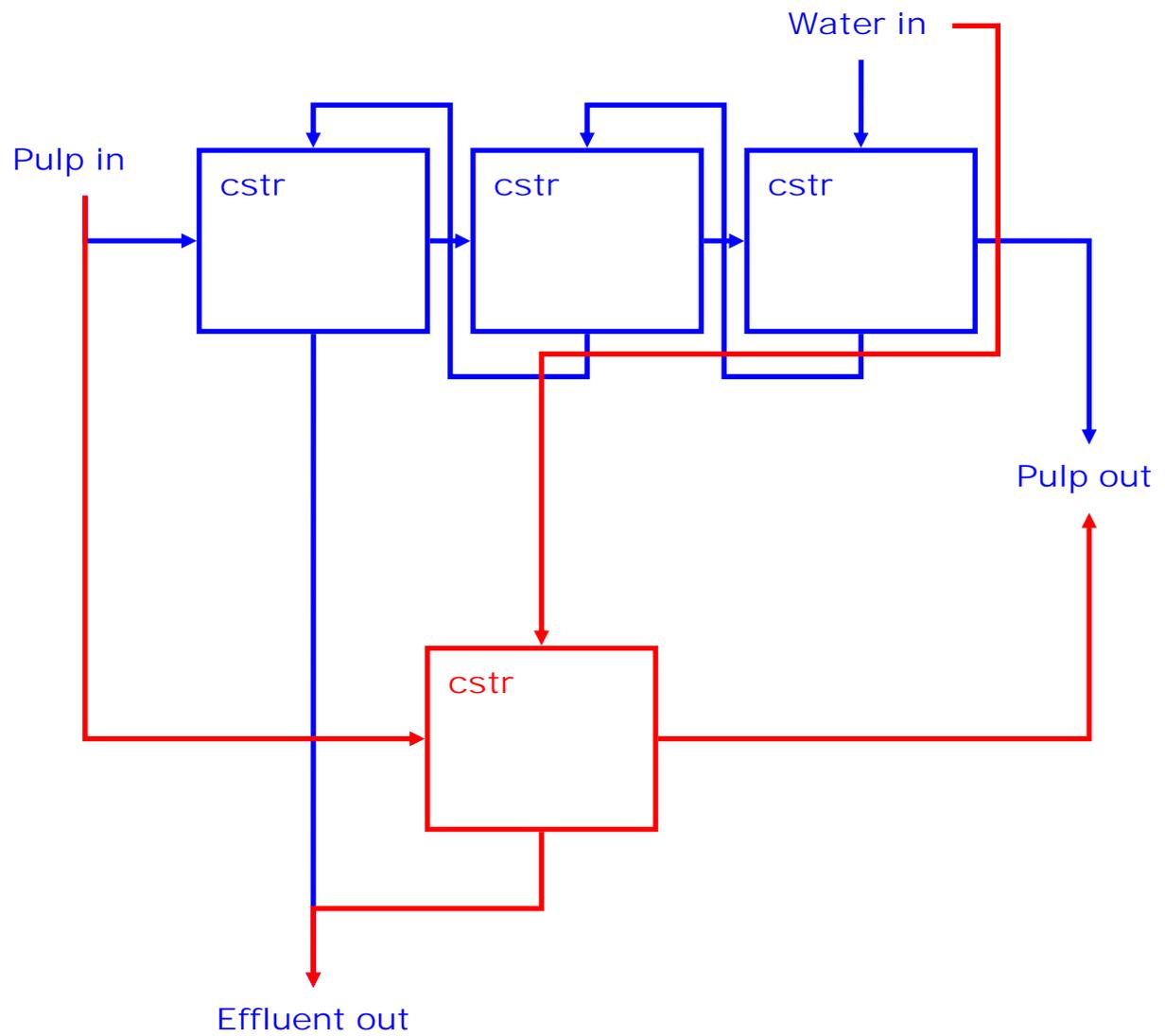
Figure 3 Washing model comprising of displacer (blue) and dilution-dewatering units (red) connected in parallel. The distribution ratio of wash water and pulp streams defines the washing efficiency of the washer unit.

3.   Bleaching Model Theory

Bleaching models available in literature are generally pseudo-kinetic models that have the following form:

$$\frac{dX}{dt} = -k[K]^{\alpha}[X]^{\beta}[OH^{-} / H^{+}]^{\gamma}$$ (1)

k	is a reaction rate coefficient ($k = A_0 \exp(-Ea/RT)$)
K	[K] is the "concentration" of kappa in pulp suspension
X	is the chemical concentration, or pressure of gaseous chemicals
OH^- / H^+	is the hydroxyl or hydronium ion concentration
α, β, γ	are empirical exponential factors

Usually the reaction rate coefficient k accounts for varying temperature dependency according to Arrhenius relationship, but it usually is strictly empirical; this parameter usually lumps together reaction rates, mass transfer relationships, consecutive reaction pathways & other kinetic relationships. The 'real' reaction rates of chemicals (with lignin & other reactive structures) should be separated from other kinetic relationships:

$$k = \bar{k} \cdot f(t)$$ (2)

$\bar{k}$	is the intrinsic reaction rate of a chemical with reactive structure in fibre
$f(t)$	if a function that describes the effect of eg. mass transfer on overall reaction rate.

The function *f(t)* can have different forms depending on the mechanistic details one wishes to include into model. The simplest way is to define a kinetic rate coefficient:

$$f(t) = k_{\phi}$$ (3)

k_{ϕ}	kinetic rate coefficient

The overall reaction rate coefficient is then a product $k = \bar{k} \cdot k_{\phi}$, where $\bar{k}$ describes the known chemical reaction rate (eg. ClO2 with phenolates) and k_{ϕ} relates the observed reaction rate to "unknown" time-dependent effects like mass transfer rates.

Kappa number describes how much structures that can be oxidized are present in fibres. These structures consist mainly of phenolic and non-phenolic lignin (approximately 20/80 weight ratios present in fibres) and hexenuronic acids. Thus there are at least three different groups of chemical structures that react differently with a bleaching chemical. Thus, the kinetic equation can be modified as:

$$\frac{dR_i}{dt} = -\overline{k_i} \cdot f(t)[R_i]^{\alpha}[X]^{\beta}[OH^- / H^+]^{\gamma} \tag{4}$$

R_i is a reactive structure (phenolic or non-phenolic structure or HexA group) present in fibre. Concentrations (or amounts) of X_i can be obtained from kappa number of pulp using oxidation-equivalents of different structures.

The bleaching reactions generally occur (with exception of radical reactions) via <u>dissociated form</u> of reactive structures R_i, or <u>protonated form</u> of chemical X. Thus the H+ or OH- concentration (or activity) term in eqs 1 and 3 can be replaced by a term f (pH) that depends on pH and is specific for a reaction mechanism:

$$f(pH) = 1 - K_{a,X} / \left(K_{a,X} + H^+\right) \tag{5a}$$

$$f(pH) = K_{a,X} / \left(K_{a,X} + H^+\right) \tag{5b}$$

$$f(pH) = K_{a,R_i} / \left(K_{a,R_i} + H^+\right) \tag{5b}$$

Eq (4a) is used, when a bleaching reaction occurs via protonated form of bleaching chemical. Should the chemical be in dissociated form, eq (5b) is used. Eq (5c) is used, when reaction involves dissociated form of reactive fibre structure. In specific cases, $f(pH)$ can be a product of any of equations 5a – 5c.

Now we can write a general form of a reaction of a reactive structure R_i with chemical X_i. We can ignore the exponential factors α and γ, since the equations 2 - 5b incorporate the specific pH and time dependencies into the kinetic model.

$$\frac{dR_i}{dt} = -\overline{k_i} \cdot f(t) \cdot f(pH)[R_i][X]^{\beta} \tag{5}$$

Integration of eq (5) over the desired reaction time yields the consumption of chemical and reactive structures, and formation of reaction products. The amounts of reaction products (from reactive fibre structures and chemicals) are obtained from mass balances:

$$R_{reacted}(t) = R_{initial} - R(t) \tag{6a}$$

$$X_{reacted}(t) = X_{initial} - X(t) \tag{6b}$$

Reaction products of lignin, for example, can remain attached to fibre. In some bleaching reactions (eg. lignin with ClO2) the chemical oxidizes lignin structures and lignin dissolves as small-molecular products and as macromolecular fragments as the degree of oxidation of lignin increases. This can be modelled by using the following relationship for lignin dissolution:

$$\frac{dX_{dissolved}}{dt} = k_{dissolution} X_{reacted} \tag{7}$$

In CheMac models the the equations 4 – 7 are used to model the chemistry of the following bleaching stages: A (hot acid stage), E, O, P and different different variants of alkaline stages (Eop, PO etc.). The D stage models (D0, D1 and D2) are based on equation 1 and contain stoichiometric coefficients after Mortha /1/.

4.   Thermodynamic System

Thermodynamic system consists of number phases. Phases contain one or more chemical species (also known as phase constituents). Species are composed of system components (like NaOH contains 1 mole Na, O, and H), which is same as stoichiometry of species. System components are normally elements but they can also be stoichiometric composition of elements.

The phases needed to model pulp bleaching reactions are vapour, free water, fiber bound water + fiber and solids phases.

Vapour phase consists mainly of common species like O2 and Cl2 and other various chemicals needed in bleaching (like O3, ClO2 and H2O2).

Free water phase contains dissolved non-organic solids and organic bleaching products as well as dissolved gaseous species. They can exist as neutral species and cations or anions depending their nature.

Fiber bound water phase contains same species as free water as well as fiber specific species that are used to describe reactive fiber structures (of which phenolic and non-phenolic groups and hexenuronic acid are the most common). Anionic groups in fiber contribute to the ion exchange between free and fiber bound water /2, 3/.
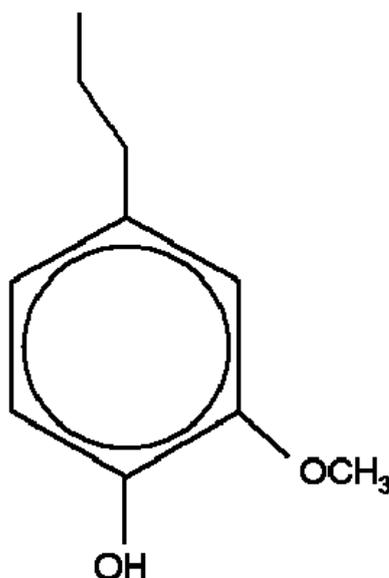
Figure 4 Phenyl propane monomer (Acid56 and Acid90 species use its stoichiometry).

Fiber   Fiber water   Free water

Fiber	Fiber water		Free water
	Acid56H		
	Acid56-		
	Acid90H		
	Acid90-		
	HexAH		
	HexA-		
	MegAH		
	MegA-		
	HCOOH		HCOOH
	HCOO-		HCOO-
	CH3COOH		CH3COOH
	CH3COO-		CH3COO-
	H2[Muconic]		H2[Muconic]
	H[Muconic]-		H[Muconic]-
	[Muconic]-2		[Muconic]-2
	H5[DTPA]		H5[DTPA]
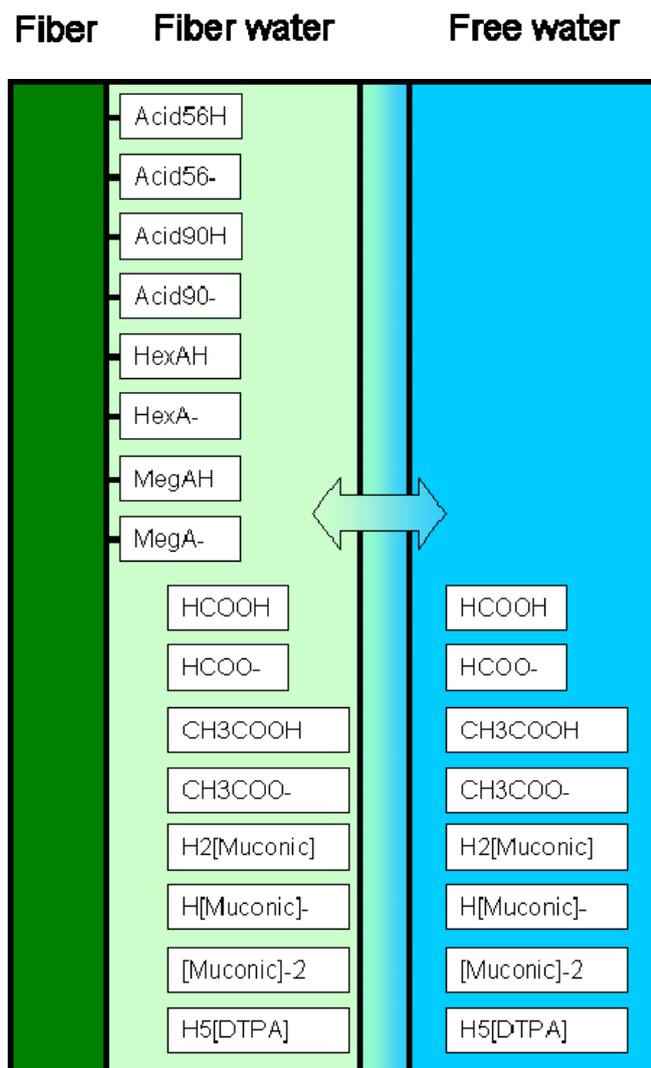
Figure 5 Some organic species in fiber (phenolic and non-phenolic groups in fiber lignin), fiber water and free water phases.

Table 1 shows the normal system components used in CheMac.

Table 1 System Components.

C	Carbon	Elementary component
H	Hydrogen	Elementary component
O	Ogygen	Elementary component
Cl	Chlorine	Elementary component
S	Sulfur	Elementary component
Ba	Barium	Elementary component
Ca	Calsium	Elementary component
K	Potassium	Elementary component
Mg	Magnesium	Elementary component
Mn	Manganese	Elementary component
Na	Sodium	Elementary component
ClO2(g)	Chlorine dioxide	Pseudo component
HOOH(g)	Hydrogen peroxide	Pseudo component
O3(g)	Ozone	Pseudo component
Formic(a)	Formic acid	Pseudo component
Acetic(a)	Acetic acid	Pseudo component
Muconic(a)	Muconic acid	Pseudo component
Oxalic(a)	Oxalic acid	Pseudo component
DTPA(a)	DTPA	Pseudo component
HexA(f)	Hexenuronic acid in fiber wall	Pseudo component
MeGlcA(f)	Methyl glucuronic acid in fiber wall	Pseudo component
Acid56(f)	Acid groups in fiber wall having pK 5.6	Pseudo component
Acid90(f)	Acid groups in fiber wall having pK 9.0	Pseudo component
Fiber(f)	Rest of fiber (cellulose, hemicellose, ...)	Pseudo component
e-	electron in free water	Needed for electro-neutrality in water
e-f	electron in fiber bound water	Needed for electro-neutrality in fiber water
H2O-f	fiber bound water	Needed to constrain fiber bound water

Pseudo components are needed to constrain reactions of organic species that are not stable with used thermodynamic system (they would normally react to CO2 and H2O in equilibrium calculation). Also many chemicals are not thermodynamically stable (but they also tend to decompose in real life easily).

These metastable species react or decompose (relatively) slowly following specific kinetics that is usually result of various mass transfer limitations.

Gibbs energy of many organic acids that are used are not known but their pK values can be measured. Measured values can be used to give necessary thermodynamic data to include their dissociation reactions (for example for $H_2[MuconicA](a) = H[MuconicA](-a) + H(+a)$ and $H[MuconicA](-a) = [MuconicA](-2a) + H(+a)$).

4.1.   Bleaching chemicals

Bleaching chemicals are:

ClO2	Chlorine dioxide	(D-stage)
HOOH	Hydrogen peroxide	(P-stage)
O3	Ozone	(Z-stage)
O2	Ogygen	(O-stage)
NaOH	Sodium hydroxide	(E-stage (with OP-stages))

Reactions of bleaching chemicals are constraint (excluding O2 and NaOH) so that they are not allowed to go to equilibrium with other species in the system (but their distribution to gasous and aqueous forms are calculated, i.e. their solubility to water). The reason being that their decomposition and reaction with pulp is kinetically constraint and happens in a "relatively" long period of time. In equilibrium calculation they normally would more or less decompose to elementary species (ClO2 to Cl and O2, HOOH to H2 and O2 and O3 to 1.5O2).

Chlorine dioxide and hydrogen peroxide are relatively soluble to water but oxygen and ozone would be present mainly as gaseous species and their reaction rate with pulp is also constrained with mass transfer from gas side to the pulp fiber.

In CheMac model sodium hydroxide is allowed to react according to equilibrium - mainly to Na(+aq) and OH(-aq) thus increasing the pH.

Bleaching chemicals are entered to flowsheet using Demanded Chemical block (where they can be mixed with appropriate amount of water). They would not decompose or react with pulp in Mixer.

4.2.   Gibbs Energy Minimization

CheMac uses thermodynamic programming library, ChemApp, to calculate equilibrium of vapour/water/fiber/solids systems.

ChemApp uses Gibbs energy minimization approach to solve the equilibrium composition of the system. In order to calculate the chemical equilibrium, the chemical potential of each phase constituent must be known. The standard Gibbs energy of species is normally given as one or more temperature dependent equation. Chemical potentials of species depend also on excess Gibbs energy, which is a result of interactions between species in phase. Pitzer's activity model is used for aqueous phases to calculate the excess energies /4/. Gas phase and pure condensed solids are normally modelled as ideal.

5.   CheMac Library

The CheMac library built in Extend is based on thermodynamic routines and chemistry database. The target is to construct the pulp and paper making unit models with rigorous chemistry calculation.

CheMac uses Gibbs energy minimization library, ChemApp, for calculating equilibrium between vapour, water and fiber water phases. It also includes dissolution/precipitation of solid phases. Thermodynamic routines are in a separate dynamic link library (DLL) that is called from Extend models.

Figure 6 Blocks CheMac library.

This block is used to initialize the thermodynamic system:

- Thermodynamic data

These blocks are used for defining various feed flows:

- Pushed Pulp
- Pushed Water
- Demanded Water
- Pushed Vapor
- Pushed Steam
- Demanded Steam
- Demanded Chemical

These blocks are used for various processes:

- Distributor
- Mixer
- Chemical Mixer
- Demanded mixer
- Splitter
- Washer
- Dilution
- Filtrate Tank
- Retention Tower

These two blocks are used to convert flows between FlowMac (another Extend model) and CheMac:

- FlowMac to CheMac
- CheMac to FlowMac

This block are used to control simulation:

- Convergence

6.   CheMac Models/Blocks

CheMac consists of a library of models (blocks) in Extend, DLL library containing thermodynamic routines and thermodynamic data file containing definitions and data for the needed phases and species.
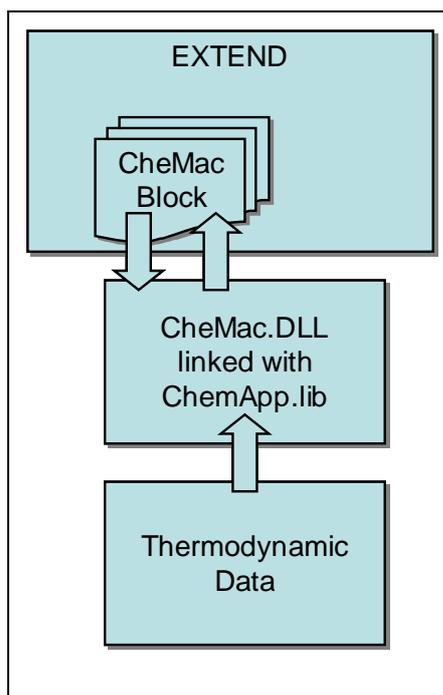
Figure 7 Flowchart of CheMac calculation.

Extend is a general simulation platform. Extend has an interactive and graphical architecture that is combined with a robust development environment /5/.

Figure 8 Extend platform.

Blocks are the basic model-building components in Extend. Each block represents some part of the process being modelled. A block's icon shows its meaning in the model, and double-clicking the icon reveals a dialog for entering data. Blocks contain unique procedural information and are stored in a library. Each library contains set of blocks with similar characteristics such as Discrete Event, Plotter and Electronics (these are Extend's build-in libraries).

Extend model is created by dragging blocks from a library onto a worksheet, connecting them, and then entering the appropriate data in the dialog.

During and after the simulation run, the results of the simulation are reported within the blocks, displayed on plotters, sent to reports, and exported to other applications. Double clicking on each block reveals the information collected from the simulation run.

The block development environment is one of Extend's most powerful features. Pre-built blocks provide basic functionality for normal operations, but the block development environment provides a way to program specific routines like mixers and splitters in chemical processing. By opening the block structure, the icon, dialog, help text, and programming code of the block can be edited. Extend includes a full featured programming language, ModL, similar to C programming language.
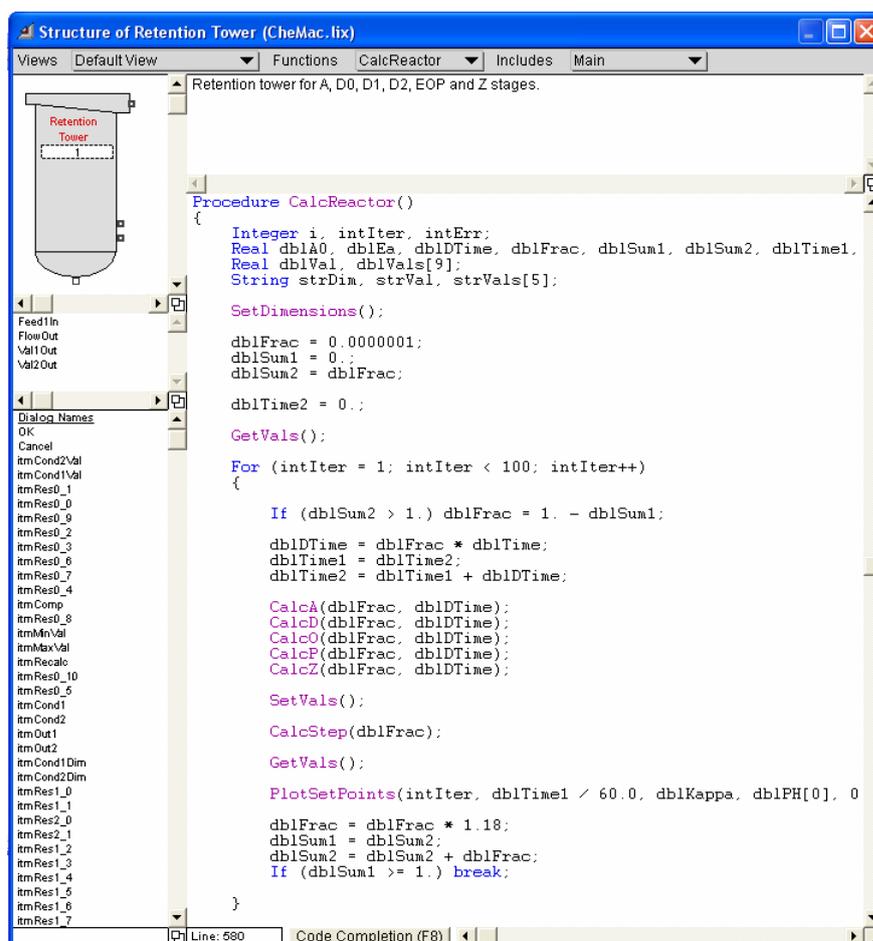
Figure 9 The block development environment.

Functionality in CheMac-blocks has been programmed with ModL language. Thermodynamic calculation and also many common routines have been included to CheMac.DLL, which can be called from Extend blocks.

6.1.   Thermo Data
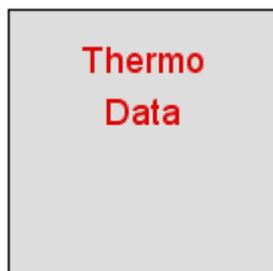
This block is used to initialize the thermodynamic routines and read the thermodynamic data from a given file. The data-file contains definitions and data of the thermodynamic system, which consists of phases and species. The phases are "Vapour"-phase, "Water"-phase, "Fiber"-phase (consists of fiber bound water and fiber specific species like lignin monomers) and "Solid"-phase (consists of a number of solid species like $CaCO_3$ and NaOH).

Thermo Data block must be the first block that is added to a new CheMac-model.

"Thermodynamic System" tab page lists the elements and species in the selected data-file.
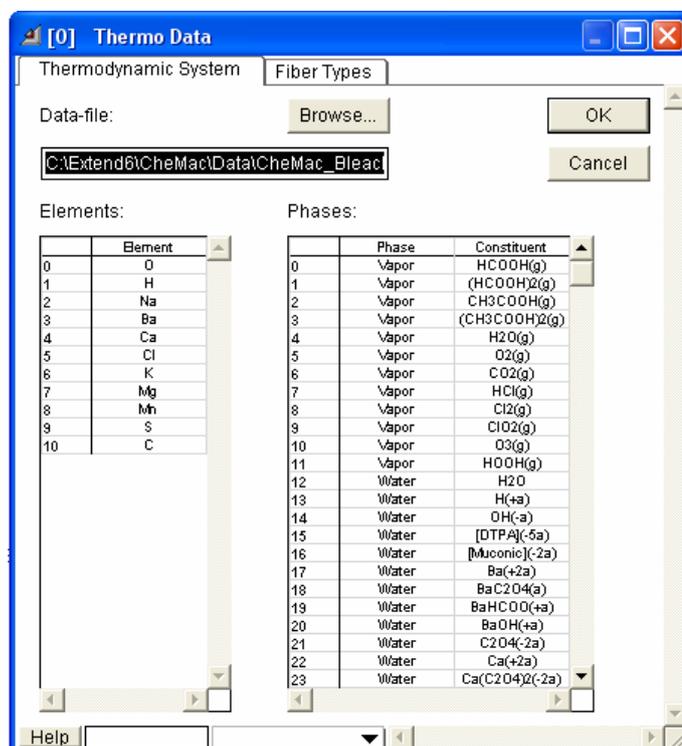
Figure 10 Thermodynamic System tab page in Thermo data dialog.

"Fiber types" tab page shows fiber properties for different fiber types. There are four predefined example types. User can give HexA and MeGlcA concentrations and Lignin pKa 5.6 and pKa 9.0 mass fractions (defines fiber charge that can be determined with a titration).

Elements table shows only elementary system components. Phases table shows all species that are defined in the data-file. There are over 200 species depending on the number of elements.
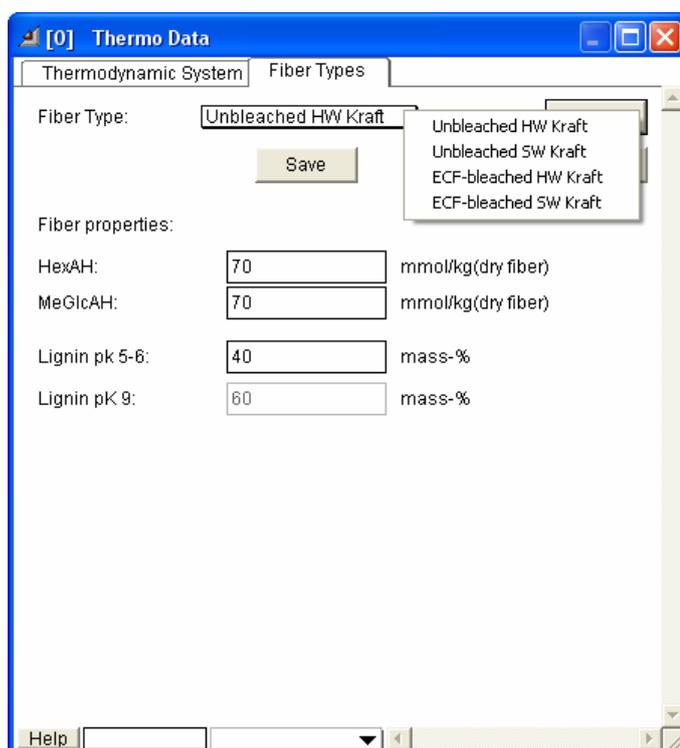
Figure 11 Fiber Types tab page.

The actual acid group masses are automatically calculated using these values when a new pulp feed and its kappa number is defined (see Pushed Pulp Block).

6.2.   Pushed Pulp
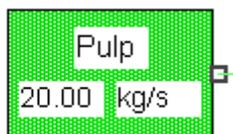
In Pushed Pulp block, the temperature, pressure, total flow, consistency, water retention and kappa number can be given for the selected fiber.

Figure 12 Pushed Pulp dialog.

HexA, MeGlcA and acid group amounts are set automatically based on the fiber type.

Flow rate can be given as Total flow, as ADFiber or BDFiber.

Figure 13 Selecting base for flow rate.

In all cases flow rates of free water, fiber bound water and dry fiber are calculated automatically. ADFiber contains 10% water and BDFiber 0 %.

Also amounts for several trace components can be given. Their amounts can be given as g/kg(dry fiber) or mol/kg(dry fiber).

If the "In equilibrium"-option is checked then the equilibrium composition of the flow is automatically calculated and its pH values are returned for reference (pH is calculated for free water and fiber bound water).

6.3.   Pushed Water
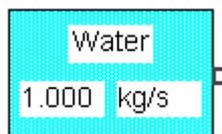
In this block the temperature, pressure, total flow and composition of the water feed is given.
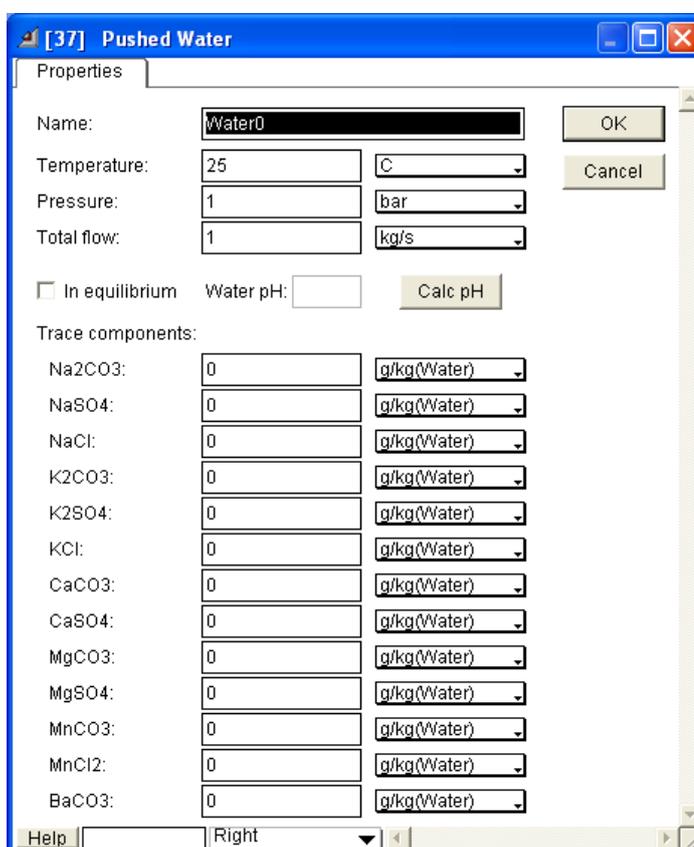
Figure 14 Pushed Water dialog

Also amounts for several trace components can be given. Their amounts can be given as g/kg(water) or mol/kg(water).

If the "In equilibrium"-option is checked then the equilibrium composition of the flow is automatically calculated and its pH values are returned for.

6.4.   Demanded Water
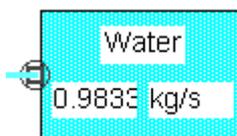
In this block the temperature, pressure and composition of the demanded water feed is given. The actual flow rate is set during the simulation as demanded in a block where the flow is connected to.
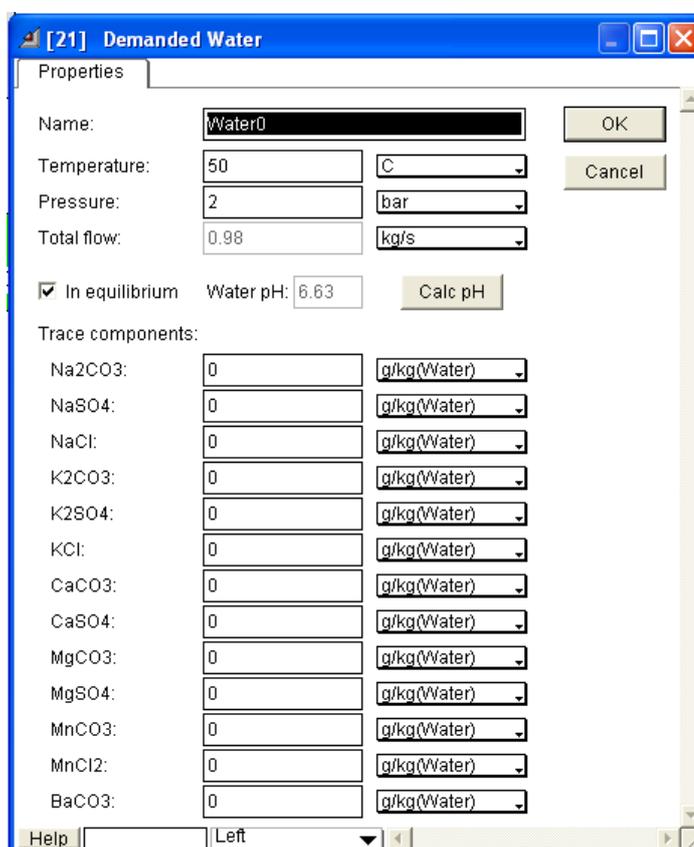
Figure 15 Demanded Water dialog

Also amounts for several trace components can be given. Their amounts can be given as g/kg(water) or mol/kg(water).

If the "In equilibrium"-option is checked then the equilibrium composition of the flow is automatically calculated and its pH values are returned for.

6.5.   Pushed Vapor

Here the temperature, pressure, total flow and composition of the pushed vapour feed is given
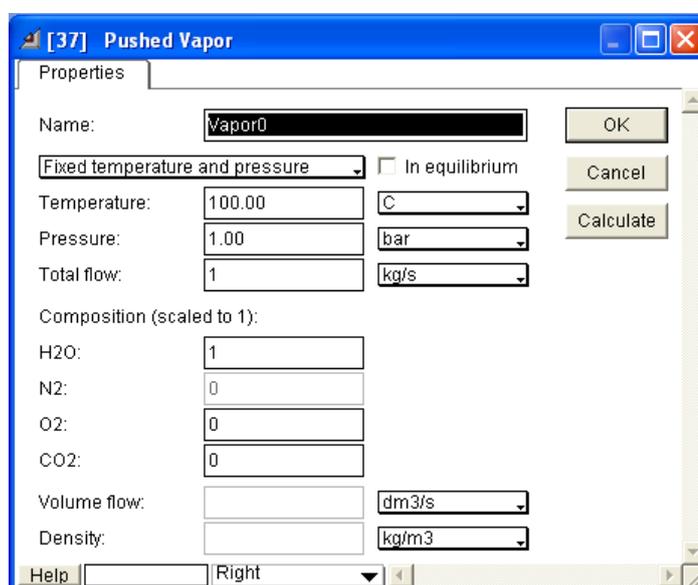
Figure 16 Pushed Vapor dialog

Component amounts are given as fractions (of total flow). Their values are automatically scaled to one.

If the "In equilibrium"-option is checked then the equilibrium composition of flow is automatically calculated. This can be useful if enthalpy balance calculation is required in a mixer or splitter block to which this feed is connected

6.6. Pushed Steam

Here the temperature, pressure, total flow and composition of the pushed Steam feed are given.
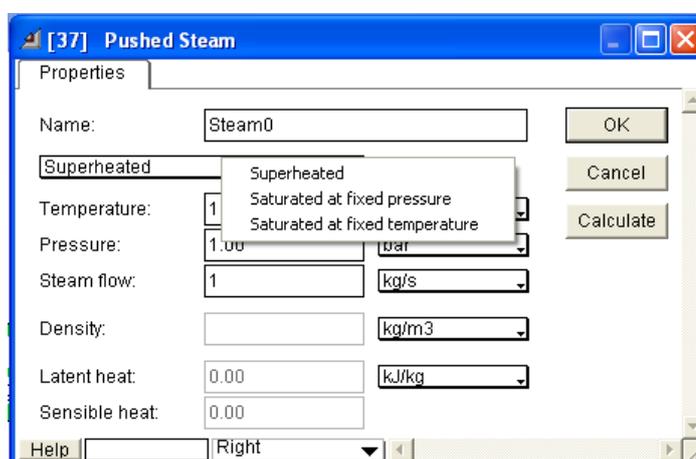
Figure 17 Pushed Steam dialog

Steam type can be given as superheated when its temperature and pressure must be given. If selected temperature is less than saturation temperature at given pressure then temperature is changed automatically. Or steam type can be saturated at fixed pressure or fixed temperature.

Latent heat is enthalpy difference between steam and liquid water at saturation. Sensible heat is enthalpy that is used to "superheat" steam (if it is superheated).

Density is calculated from ideal gas law so it is not accurate at elevated pressures. But gas phase uses correlation to virial equation to calculate enthalpies of gas species so steam enthalpy is calculated accurately up to several MPa.

6.7.   Demanded Steam
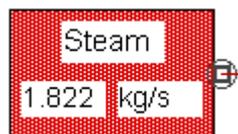
Here the temperature, pressure and composition of the demanded Steam are given. The actual flow rate is set during the simulation as demanded in a block where the flow is connected to.
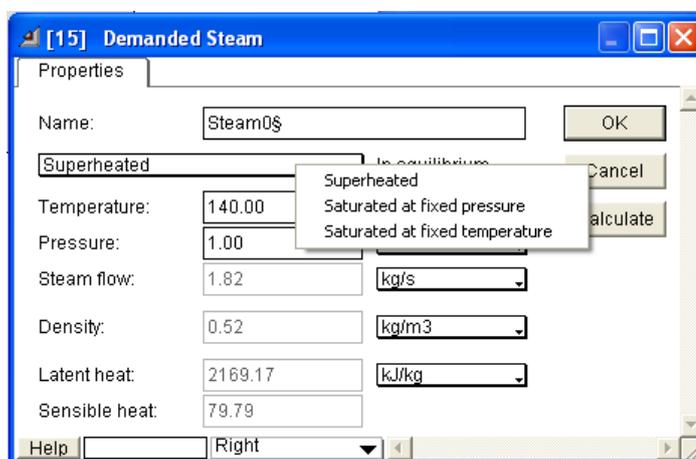
Figure 18 Demanded Steam dialog

Steam type can be given as superheated when its temperature and pressure must be given. If selected temperature is less than saturation temperature at given pressure then temperature is changed automatically. Or steam type can be saturated at fixed pressure or fixed temperature.

Latent heat is enthalpy difference between steam and liquid water at saturation. Sensible heat is enthalpy that is used to "superheat" steam (if it is superheated).

Density is calculated from ideal gas law so it is not accurate at elevated pressures. But gas phase uses correlation to virial equation to calculate enthalpies of gas species so steam enthalpy is calculated accurately up to several MPa.

6.8.   Demanded Chemical
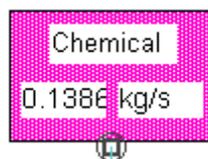
Here the temperature, pressure and composition of the demanded chemical species are given. Chemicals can also include water if needed. The actual flow rates of the chemicals are based on the dry fiber flow rate in **Chemical Mixer**.

Chemicals are used in bleaching stages. They are mixed with pulp flow in **Chemical Mixer** block before entering the retention tower where the bleaching takes place.

Figure 19 Demanded Chemical dialog.

6.9. Distributor

This block is used to take one demanded input flow and divide it into 1 to 8 demanded output flows. This way for example all demanded water or steam flows can be collected to one place where their flow rates can be seen tabulated.
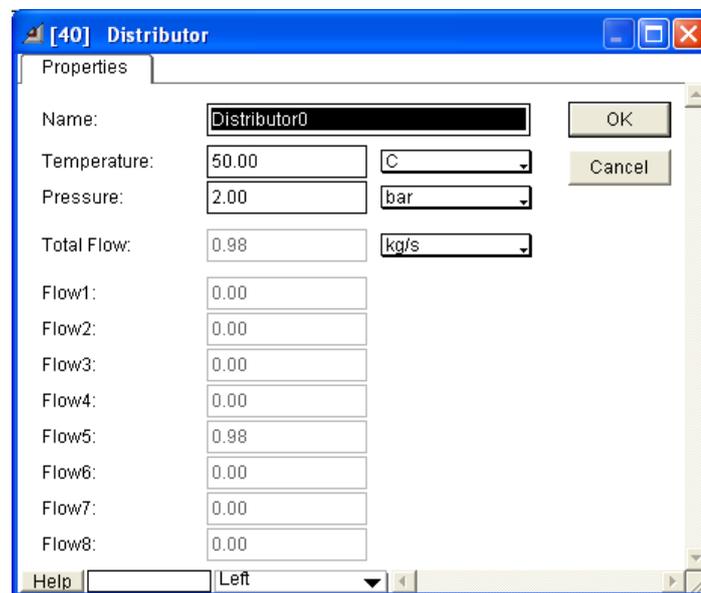
Figure 20 Properties tab page in Distributor dialog.

6.10. Mixer
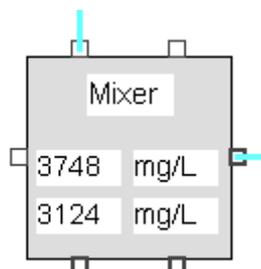
This block is used to mix two or three inlet flows together. There can also be only one inlet flow in which case flow's temperature and pressure can be changed (which can also change its phase composition).

When the "Calculate equilibrium"-option is checked, the equilibrium composition of outlet flow is calculated. Otherwise mixing takes place without any chemical reaction and some flow properties (like pH) are not calculated.
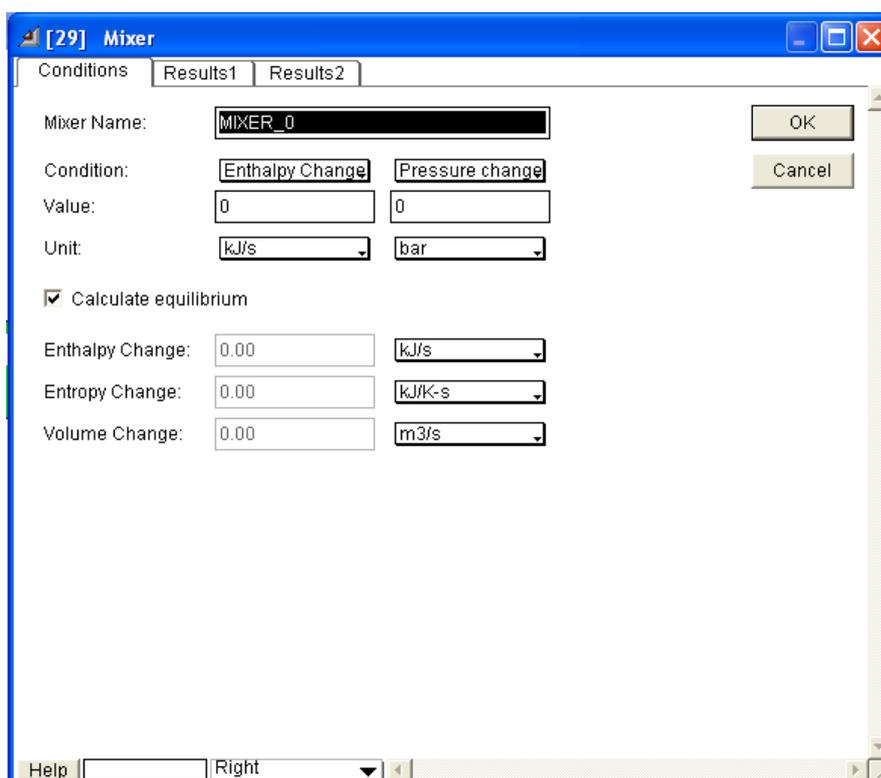
Figure 21 Conditions tab page in Mixer dialog.

Two conditions are needed to define the initial conditions for the equilibrium calculation:

- Fixed temperature and pressure.
- Fixed temperature and volume change.
- Enthalpy change and fixed pressure.
- Entropy change and fixed pressure.
- Volume change and fixed pressure.

The changes refer to difference between calculated equilibrium flow and inlet flows. For example enthalpy change 0 (J/s) and pressure 1 (bar) calculates equilibrium at fixed pressure so that the temperature is searched at which equilibrium enthalpy equals that of sum of enthalpies of inlets.

Instead of fixed pressure also pressure change can be used. In this case given value is added to minimum pressure of inlet flows and then used as pressure of outlet flow. In case of a loop one must make sure that not all process blocks in the loop contain pressure change definition as then pressure may decrease until it becomes negative.

The "Results1" tab contains common values of the inlet flows and the calculated outlet flow. This tab page is common to all CheMac-blocks.

Figure 22 Results1 tab page.

Table 2 shows the properties of flows:

Table 2 Flow properties

Temperature	Temperature of flow	C, K, ..
Pressure	Pressure of flow	bar, Pa, …
Water pH	pH of free water	
Fiber pH	pH of fiber bound water	
Total flow	Total flow rate	kg/s, kg/h, …
Total vapour	Flow rate of vapour phase	kg/s, kg/h, …
Total water	Total flow rate of water	kg/s, kg/h, …
Total fiber	Flow rate of dry fiber	kg/s, kg/h, …
Consistency	dry fiber / (water + dry fiber)	%
Kappa number	Kappa number	
COD	Chemical oxygen demand (of dissolved organics)	g(O)/dm3, mg(O)/dm3
Brightness	Brightness of flow	%
Dissolved solids	Total dissolved solids	g/dm3, mg/dm3
TOC	Total organic carbon (of dissolved organics)	g(C)/dm3, mg(C)/dm3
Alkali	Alkali content as equivalent N2O	g/dm3, mg/dm3

Using "Outlet Scalar1"- and "Outlet Scalar2"-popup menus the user can define current values for two scalar outputs in the block. These output values can for example be connected to plotters to visually observe them during model simulation.

Composition table in Results2 tab page shows either composition of species or elements in the outlet flow. As the number of species in the thermodynamic system is quite large, there is an easy way to limit the number of species in the table depending on their values.

Figure 23 Results2 tab page with composition of species.

Mass flow can be mass or mole flow based (mol/s, kg/s, ...).

Minimum and maximum can be used to skip species, which amounts are less than the minimum or more than the maximum.

Number format is used to alter the numeric format of values in the table (General, Scientific, Fixed).

"Value" field in table is the flow rate of species or element, "% in Phase" field is its fraction in phase scaled by 100 and "% of Total" is its fraction in whole flow scaled by 100. Phases are "Vapour", "Water", "Fiber" and "Solid". Last row in each phase shows the flow rate of phase and its fraction in whole flow.
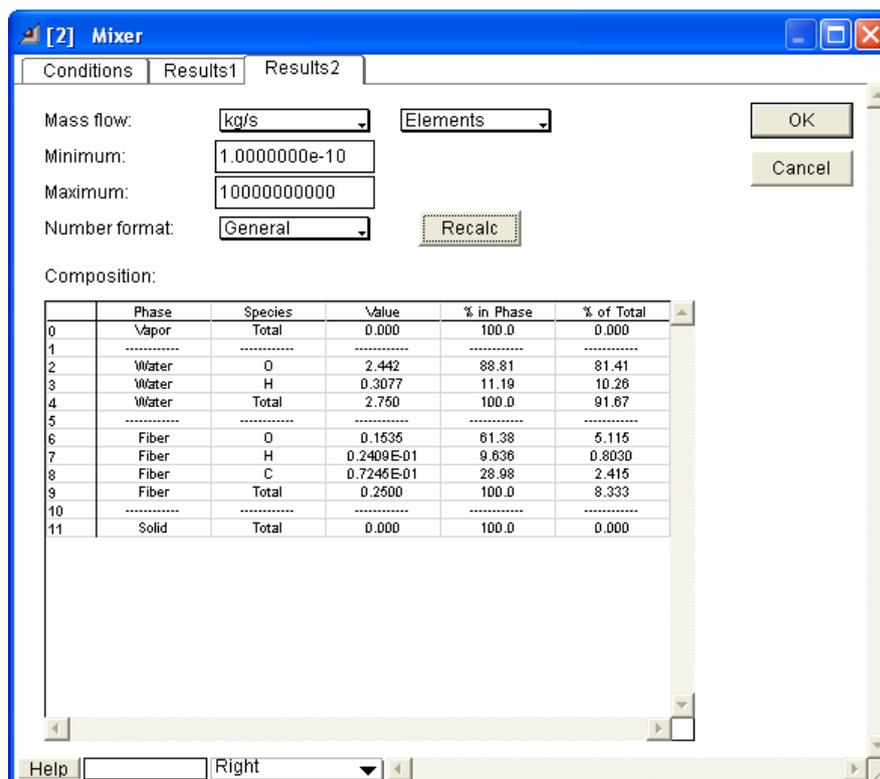
Figure 24 Results2 tab page with composition of elements.

6.11. Demanded Mixer
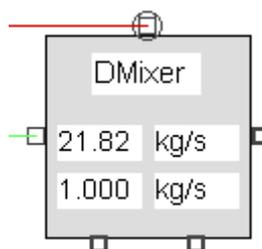
This block is used to mix one pushed flow and one demanded flow together. Flow rate of demanded flow is solved from energy balance so that output flow has given temperature and pressure.

This block calculates the equilibrium.
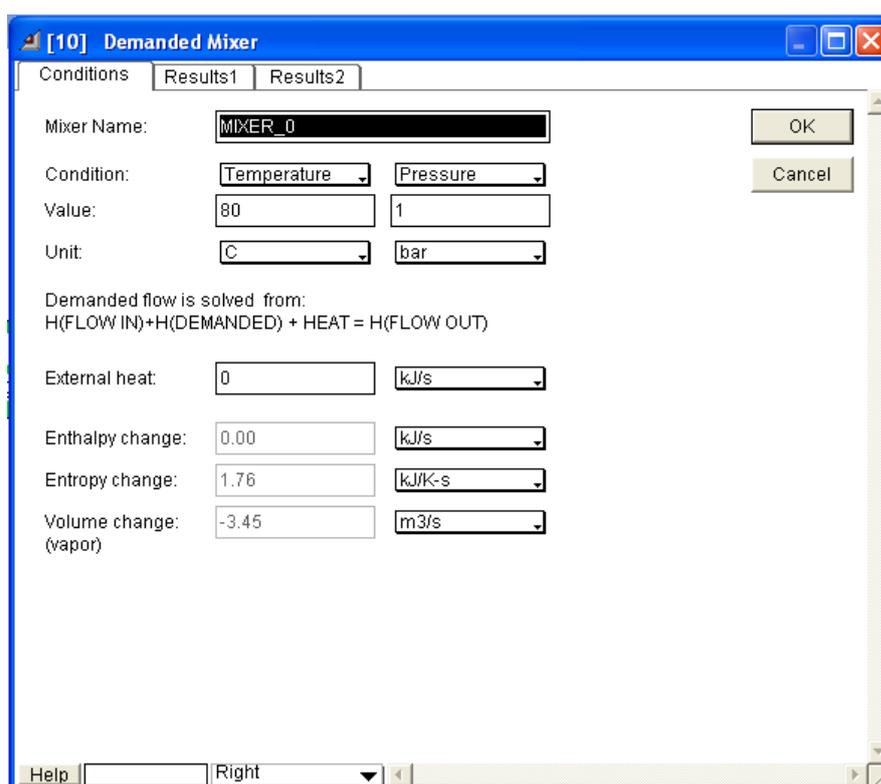
Figure 25 Conditions tab page in Demanded Mixer dialog.

6.12.   Chemical Mixer
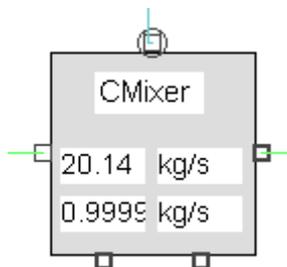
This block is used to mix demanded Chemical flow with pushed pulp flow. Chemical flow has fixed temperature, pressure and composition, but its flow rate is scaled with dry fiber flow rate in pulp flow..

When the "Calculate equilibrium"-option is checked, the equilibrium composition of outlet flow is calculated. Otherwise mixing takes place without any chemical reaction and some flow properties (like pH) are not calculated.
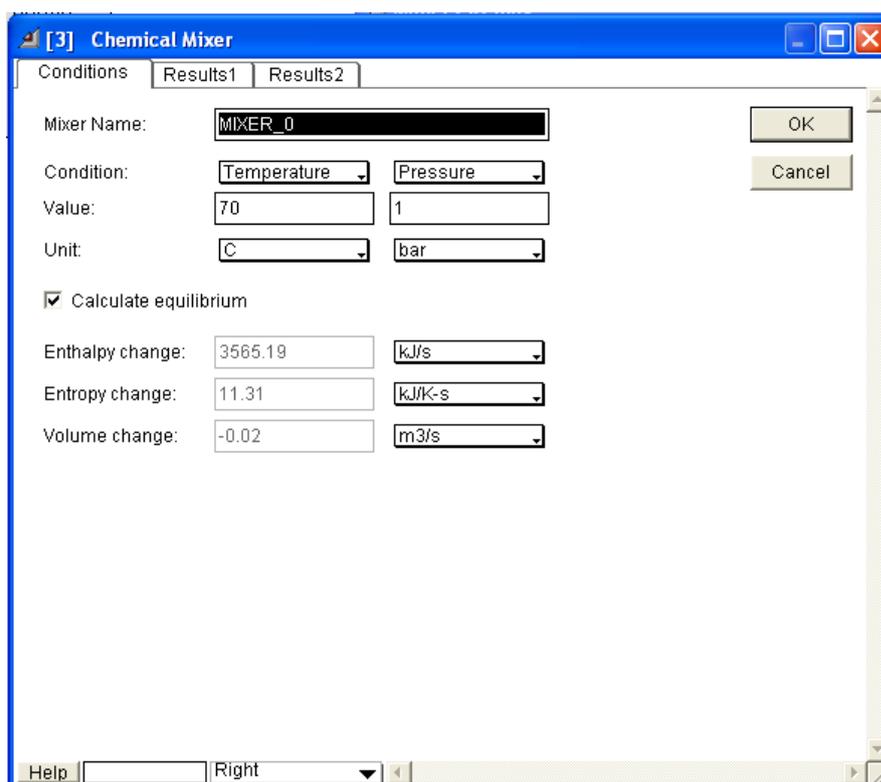
Figure 26 Conditions tab page in Chemical Mixer dialog.

6.13. Splitter
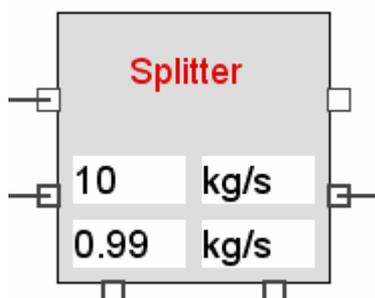
This block is used to split one (or two flows) to two separate flows.

When the "Calculate equilibrium"-option is checked, the equilibrium composition of inlet flow or of mixture between two inlet flows is calculated for the output flow before splitting.

Two conditions are used to define the initial conditions for the equilibrium calculation:

- Fixed temperature and pressure.
- Fixed temperature and volume change.
- Enthalpy change and fixed pressure.
- Entropy change and fixed pressure.
- Volume change and fixed pressure.

The changes refer to difference between calculated equilibrium flow and inlet flows. For example enthalpy change 0 (J/s) and pressure 1 (bar) calculates equilibrium at fixed pressure so that the temperature is searched at which equilibrium enthalpy equals that of sum of enthalpies of inlets.

Instead of fixed pressure also pressure change can be used. In this case given value is added to minimum pressure of inlet flows and then used as pressure of outlet flow.

The fractions for separated phases (and phase constituents) are defined in "Composition of 2. outlet"-table.

Figure 27 Conditions tab page in Splitter dialog.

Results1 and Results2 tab pages are similar to the ones in the mixer block.

6.14.   Washer
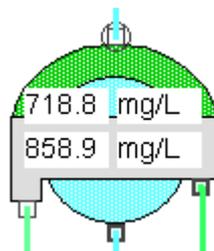
Washer is used to for washing the dissolved solids from the pulp flow using displacement. It contains optional dilution using circulated filtrate, thickening, displacement and optional pressing stages. The displacement stage contains one to four counter-current washing stages.

Because of circulated filtrate and counter-current nature of displacement, the washing block uses iteration to solve the composition of its output flows (washed pulp and non-circulated part of wash filtrate).

Figure 28 Conditions tab page in Washer dialog.

Minimum dilution factor is used for adding required amount of fresh water to washing if inlet wash water amount is not enough for the given dilution.

Simulated dilution factor can be higher than minimum if there is more than required amount of water in inlet wash. Added water shows the added fresh water.

Results1 and Results2 tab pages are similar to the ones in the mixer block.

6.15.   Dilution
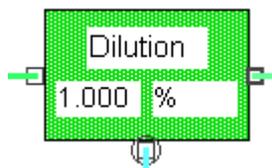
Dilution block is used to dilute pushed pulp flow to given consistency by setting the flow rate of demanded water flow.
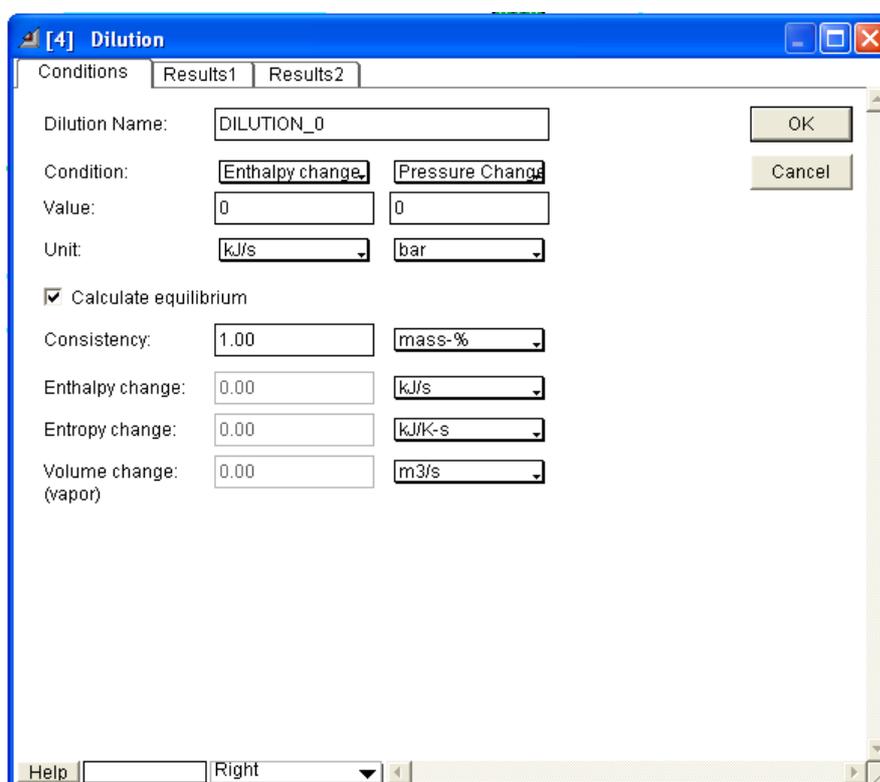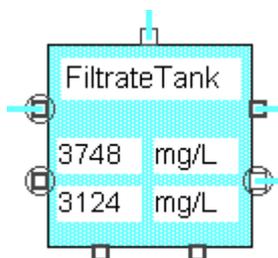

Figure 29 Conditions tab page in Dilution dialog.

6.16.   Filtrate Tank

Filtrate Tank takes one pushed input flow (from washer) and one demanded input flow and it has two demanded output flows and pushed overflow.
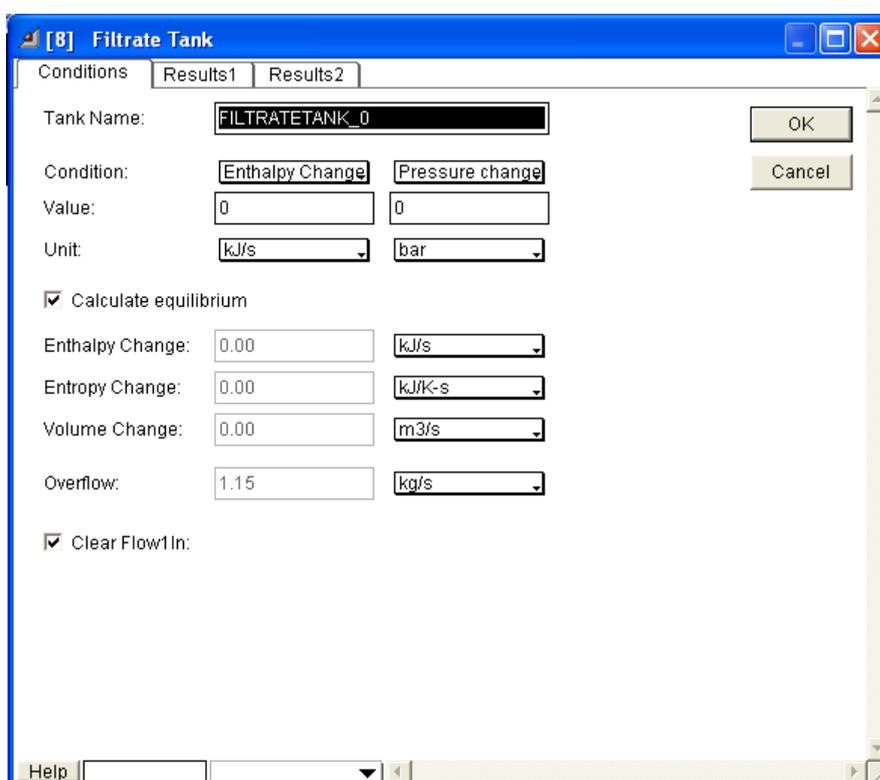
Figure 30 Conditions tab page in Filtrate Tank dialog.

If Clear Flow1In is not checked then values from previous simulation are used for the flow from Washer Block (Flow1In). This makes convergence of the model faster if there is a loop back to Washer (via Dilution block).

6.17.   Retention Tower
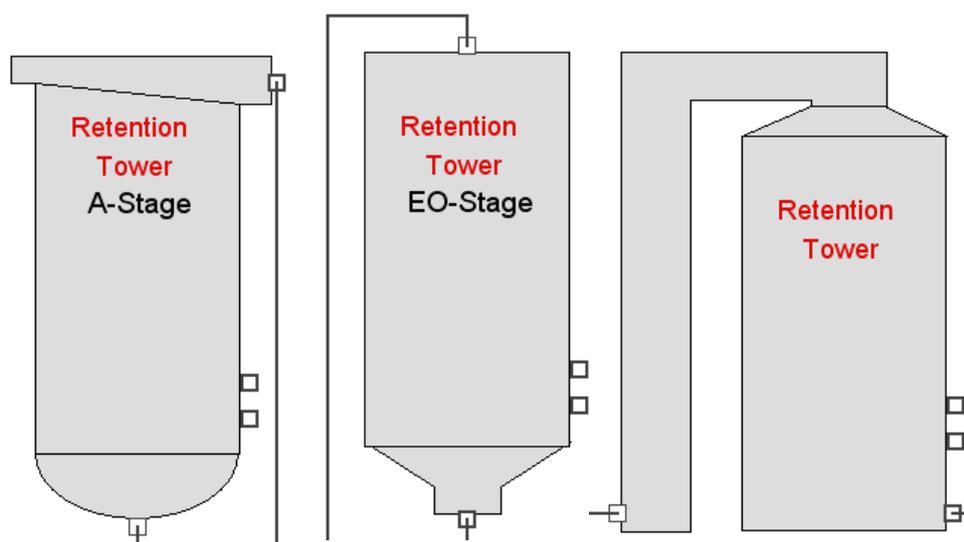
Retention tower block is used for various bleaching stages. There are three separate views: up-flow, down-flow and up-down-flow. Only difference between these is that the visual looks and inlet and outlet port positions are different (according to flow direction).

Retention tower contains routines to calculate A, D, E, O, P stage kinetics for lignin dissolution (and any reasonable combination of them).

The set of stages that are actually calculated depends on the chemicals that have been added to inlet pulp flow.

- A-stage kinetics (HexA hydrolysis) is calculated always (if there is any HexA remaining in fiber)
- D-stage kinetics is calculated if there is ClO2 present in the pulp feed
- O-stage kinetics is calculated if there is O2 present in the pulp feed
- P-stage kinetics is calculated if there is H2O2 present in the pulp feed
- E-stage (NaOH) is usually combined with O- and P-stages.

Figure 31 Conditions tab page in Retention Tower dialog.

Geometry of tower with volume flow of inlet defines the retention time of pulp in the tower. Retention time can be given as input and tower diameter and height is then set automatically during the simulation (if height and diameter are also given then the diameter/height-ratio is kept constant when their values are updated).

The actual chemicals in input and output pulp flows are shown in the lower part of dialog (values are set during the simulation).

To better visualize the calculated composition and other important process parameters during the reaction time in a retention tower, there is an option to open plotter window after simulation that shows values in the tower. Below is an example of Kappa number and water pH given as a function of retention time.
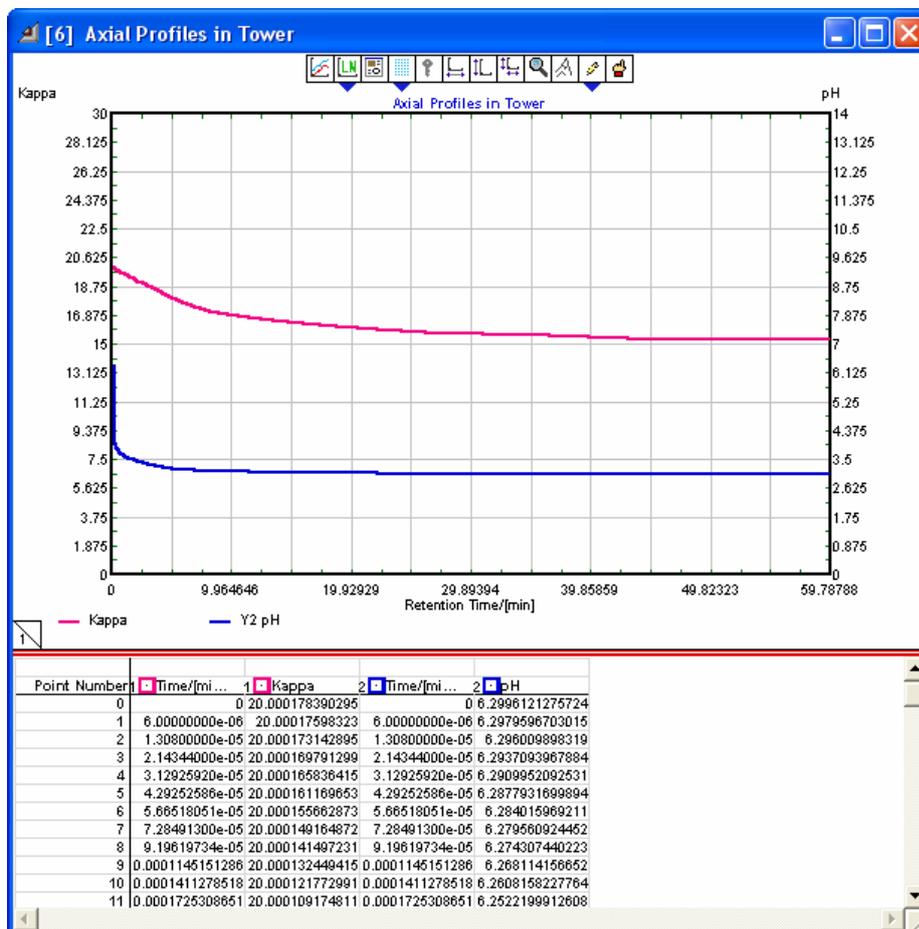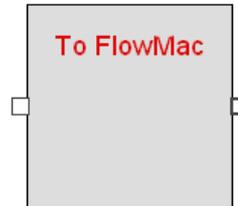
Figure 32 Plot showing axial profiles in tower.
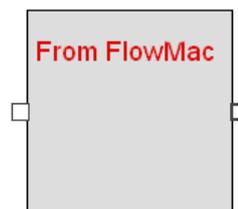
6.18.   CheMac to FlowMac

This block is used to convert CheMac flows to FlowMac flows, which then can be used as input to any FlowMac block. The conversion is necessary as the flow types are not compatible with each.
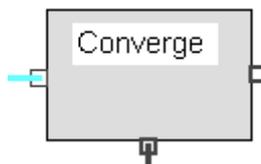
6.19.   FlowMac to CheMac

This block is used to convert FlowMac flows to CheMac flows, which then can be used as input to any CheMac block. The conversion is necessary as the flow types are not compatible with each other.

6.20.   Convergence

This block is used to monitor convergence of the model. It follows relative change of total flow rate and dissolved solids in input flow. When change becomes less than the given tolerance the simulation has converged.
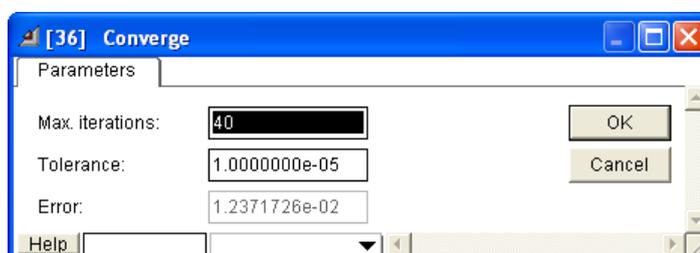

Figure 33 Convergence Dialog.

7.   CheMac FlowSheet

7.1.   Bleaching Model

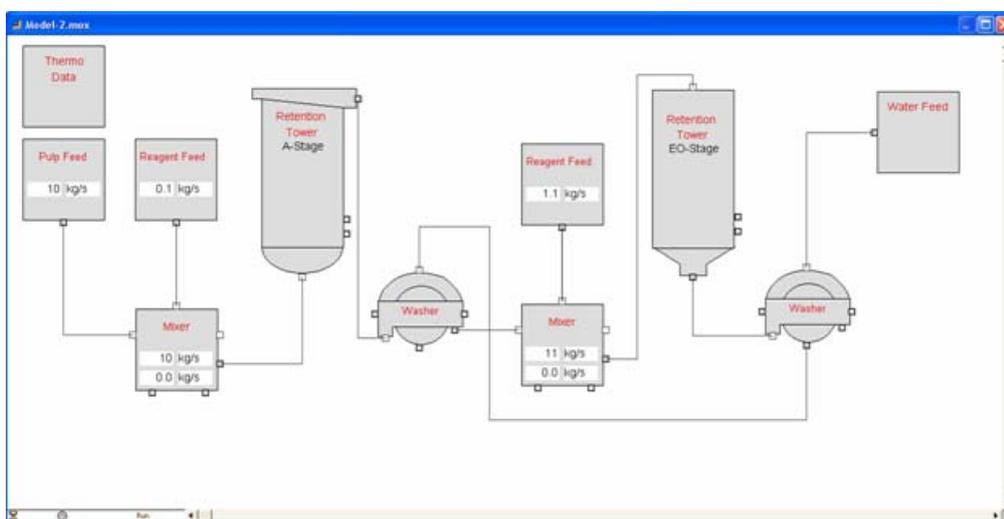Figure 34 shows simple 2-stage bleaching (with D and EO stages).

Figure 34 Simple bleaching line example.

7.2. Washing Model

Figure 35 shows washing model that uses mixer and splitters for various washing stages. The separate washer block contains basically the same functionality than this model but it is more easier to use.
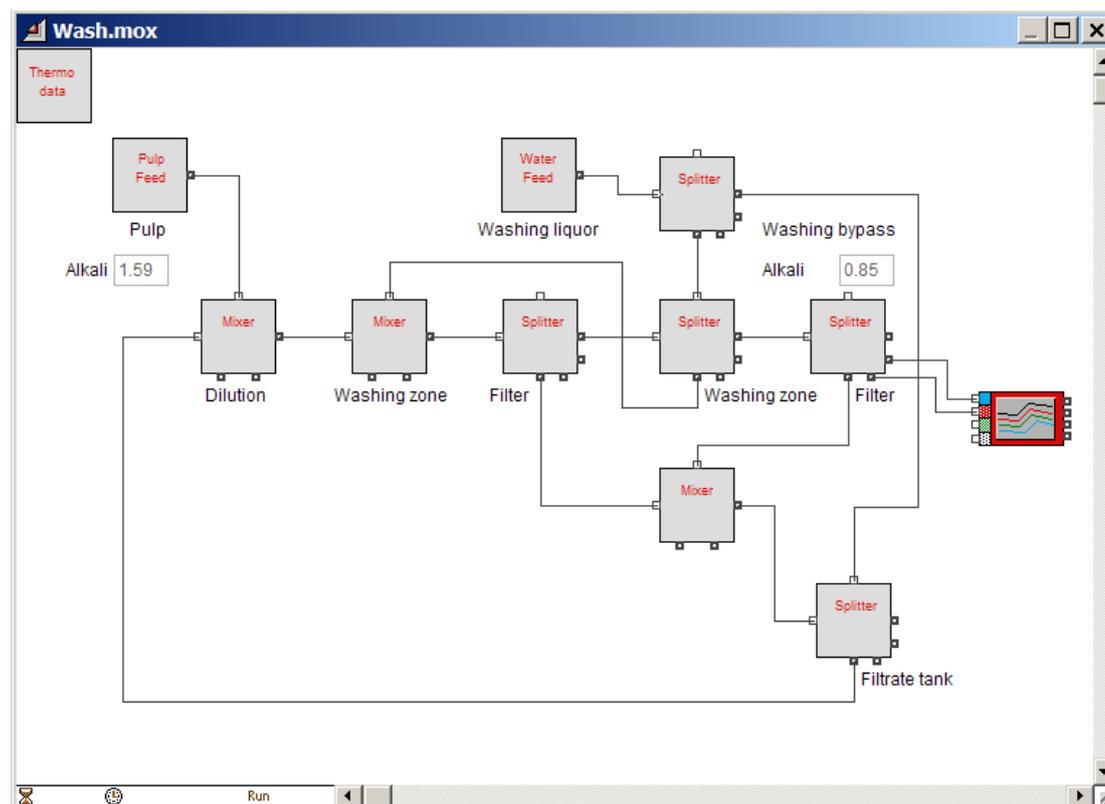

Figure 35 Washing model.

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[4] Pitzer, K.S. (1991): Activity Coefficients in Electrolyte Solutions. 542.

[5] Yücesan, E., Chen, C.-H., Snowdon, J. L., and Charnes, J. M., THE EXTEND SIMULATION ENVIRONMENT, Proceedings of the 2002 Winter Simulation Conference.