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Chemical process simulation for minimizing energy consumption in pulp mills

Marcelo Cardoso [a,*], Kátia Dionísio de Oliveira [a], George Alberto Avelar Costa [a], Maria Laura Passos [b]

[a] Department of Chemical Engineering/School of Engineering, Federal University of Minas Gerais (UFMG), Rua Espírito Santo, 35, 6° andar, 30160-030 Belo Horizonte/MG, Brazil
[b] Collaborator Researcher, Drying Center, Chemical Engineering Department, Federal University of São Carlos (UFSCar), Brazil

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ABSTRACT

Chemical process simulation has proven to be an effective tool for performing a systematic and global analysis of energy systems to identify routes for maximizing the process efficiency concerning to the heat recovery. This paper shows an application of computer simulations in a Brazilian pulp mill, using two strategies for minimizing the mill energy consumption. In the first one, the overall heat transfer coefficient has been predicted for each body of the multiple effect evaporators by using continuous on-line data from the industrial plant in the black liquor recover unit. By monitoring oscillations of this heat transfer coefficient, the suitable time for washing the evaporator heat transfer surfaces can be well determined, reducing the energy loss during black liquor evaporation. In the second strategy, the liquor combustion has been simulated as function of the black liquor solids concentration to analyze its effect on the recovery boiler efficiency improvement.

1. Introduction

Pulp and paper industries, one of the most important sectors in Brazil, require a high efficiency to produce the pulp. Therefore, one important goal of this sector is to minimize the energy consumption in the process. Note that there are several ways to find the most appropriate operating conditions for a specific pulp mill. One of them is the computer simulation, which is more economical and represents a useful tool for evaluating possible process alternatives (i.e. changes to new equipment and/or different operating conditions). Nowadays, there are several modeling and simulation software tools available. The most simulators used in pulp and paper industries are listed in Table 1 [1,2]. These software simulators are constituted of (i) modular units, representing the operations that occur in the pulp industry; (ii) executive program, responsible for administrating the modular units; and (iii) databases of physicochemical and thermodynamic properties of all components involved in the pulp process. In the present work, WinGEMS [3] has been chosen for predicting and simulating the specific changes in the overall process.

WinGEMS is a modular program designed to perform the mass and energy balance calculations. Calculations are grouped together in modules called blocks. The program has a wide selection of blocks, which perform specific process calculations. These blocks must be chosen and linked for creating the block diagram (flowchart), which should represent the specific industry.

Considering the complexity of the heat fluxes in the pulp industry plants, it is essential to evaluate different and specific operation condition alternatives to choose the best option for minimizing the energy consumption. This paper shows how to use this methodology as an efficient tool for industries.

To illustrate this use, two different scenarios have been tested as followed:

1.1. Case 1: Black liquor evaporation

The overall heat transfer coefficient has been predicted for each body of the multiple effect evaporators in the black liquor recovery unit, using continuous on-line data from the industrial plant [4]. With measurements on-line, the suitable time for washing the evaporator heat transfer surfaces can be well determined by monitoring continuously the predicted value of this heat transfer coefficient (including time oscillations).

1.2. Case 2: Black liquor boiler recovery

To analyze the effect of increasing the liquor solids concentration on the recovery boiler efficiency, the liquor combustion has been simulated as a function of the solids content in the liquor feeding this boiler [5].

2. Brief description of the pulp process

Pulp mills can be divided in two major processing lines: fiber and chemical recovery [6] (Fig. 1). The fiber processing line extends from the wood digester to the pulp bleaching section, passing by

* Corresponding author. Tel.: +55 31 3238 1789; fax: +55 31 3238 1789.
E-mail addresses: mcardoso@deq.ufmg.br (M. Cardoso), merilau@task.com.br (M.L. Passos).

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Table 1
Available simulators applied in the pulp and paper process [1,2]

Simulator	Institution or company
FlowCalc – flowsheet calculation	Simulation software
General energy material and balances system – GEMS;	Department of chemical engineering at university of Idaho and Pacific simulation
WinGEMS (GEMS version for Windows)	http://www.pacsim.com http://www.metsoautomation.com
Modulate analysis of pulp and paper systems – MAPPS	Institute of paper science and technology
Mass and energy balances – MASSBAL	SACDA Inc. (Systems analysis control and design activity) and Open Models Inc. http://www.openmodels.com
Advanced system goes process engineering – ASPEN PLUS	Aspen Technology, Inc. http://www.aspentech.com
CADSIM PLUS	Aurel Systems Inc. http://www.aurelsystems.com

the brown pulp washing step. The main goal of the fiber processing line is to remove lignin from wood and to achieve high brightness pulp in the end bleaching sequence. The chemical recovery cycle is necessary to make the pulping process economically feasible. The sub-product, extracted from pulping wood in the digester, called the black liquor, is concentrated by multi-effect evaporation system and burned in the recovery boiler where the combustion of organics provide energy to produce high pressure steam and to carry out the reduction reactions to recover Na_2S and Na_2CO_3. The inorganic product of the boiler recovery is used to regenerate the sodium hydroxide and sodium sulfide needed for pulping.

2.1. Evaporation

As shown in Fig. 2, the evaporation plant of a specific Brazilian mill, which has been chosen in this work, includes six effects, containing a total of eight falling film plate evaporators. In the first effect, which includes three evaporators (bodies), usually only two bodies are in normal operation while the other is being washed. This washing operation rotates regularly from body to body to provide the appropriate cleanness for all of them. From Fig. 2, it can be seen that the weak black liquor (with solids concentration about 15%) feeds the sixth, fifth and fourth effects. Then, the liquor flows countercurrently to vapor, finally leaving the first effect to expand in the flash tank where it attains the final solids concentration before entering into the storage tanks for strong liquor.

Scaling on black liquor evaporators is a serious problem, which must be overcame for improving the Kraft mill production [4]. This problem always occurs when the black liquor is concentrated at 48% of solids, above which the limit of solubility of sodium carbonate (Na_2CO_3) and sodium sulfate (Na_2SO_4) is attained. Then, Na_2CO_3 and Na_2SO_4 form the soluble double salt: burkeite ($2Na_2SO_4 \cdot Na_2CO_3$), which deposits on the equipment walls. The final evaporation stage occurs in the first effect and the liquor flow pattern in the first effect body is switched at regular intervals to ensure that the heating elements are continually washed with incoming weak black liquor. This should prevent the buildup of scaling on the heat transfer surfaces. However, the washing operation can become ineffective since it is normally carried out after fixed time periods, generally without any investigation on the real condition of evaporator surfaces. Thus, an excessive washing or a lack of washing may occur in such situation. This finding motivates the current work to analyze variations in the overall heat transfer coefficient (U) in order to define the time for washing. By specifying the washing time when the performance of the evaporator drops to a predetermined level (i.e. when the U-value decreases from a level stipulated by the statistical analysis), it is possible to minimize energy consumption and production losses.

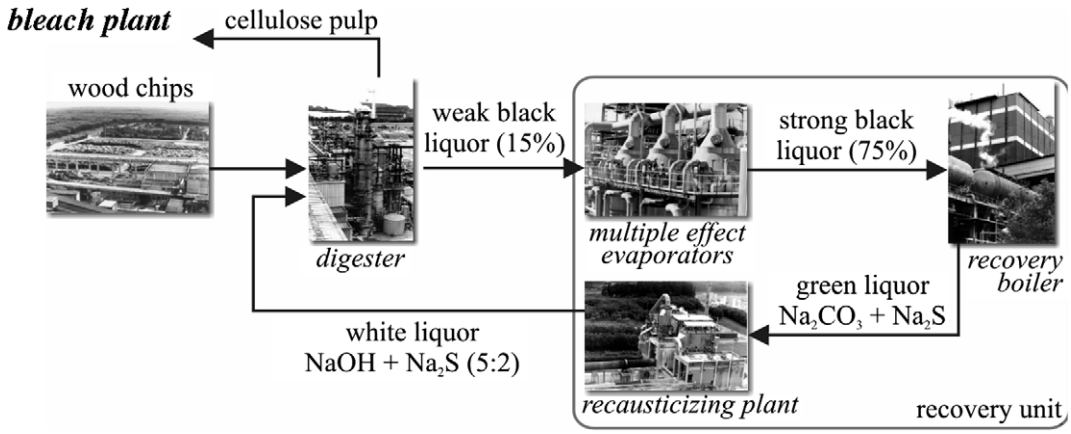

Fig. 1. Schematic representation of the pulp mill plant.

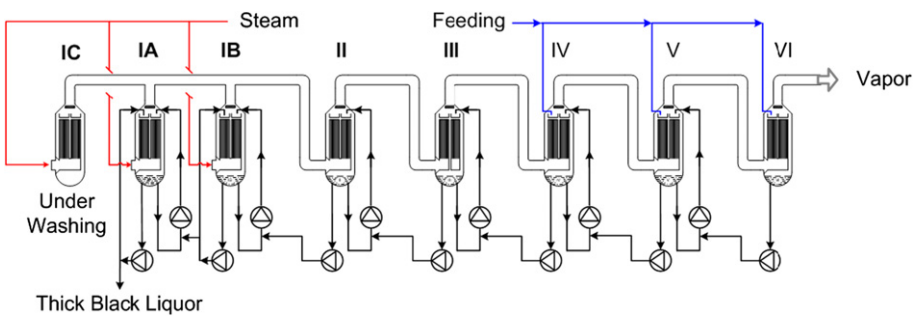

Fig. 2. Flowchart of the industrial evaporation unit of the Brazilian mill.

2.2. Recovery boiler

The boiler is formed by the furnace, where the black liquor combustion occurs, and auxiliary equipment, where the superheated steam used in the plant is generated, Fig. 3. Among auxiliary equipment, economizers, boiler bank, and superheaters are noteworthy. The residual black liquor from the wood cooking is concentrated and then burned in the furnace. Heat of black liquor combustion is used to produce superheat steam, and chemicals are also recovered. This generated steam is used by the mill as a hot fluid in heat transfer operations and as a producer of electrical energy. Chemicals regenerated along the recovery unit are recycled to the wood cooking digester. A detailed description of this equipment is found in the literature [5].

In the Brazilian mill analyzed here, about 13,500–15,400 kJ/kg dry solids are liberated during the black liquor combustion. Besides the usual thermal losses in the boiler, this heat rate supplies the necessary energy for: (i) evaporating water from the fed liquor; (ii) reducing sodium sulfate to sodium sulfide; (iii) melting inorganic compounds and (iv) producing superheated steam (5.4–6.4 kg per 1.0 kg of processed pulp). Steam is used in several process stages, generating, for instance, the electric power for the plant operation. The overall energy efficiency of the recovery boiler is relatively low (about 60%), but this efficiency can be improved by firing black liquor at higher solids contents.

3. Methodology

The methodology used in the simulation has been divided in the following four basic steps:

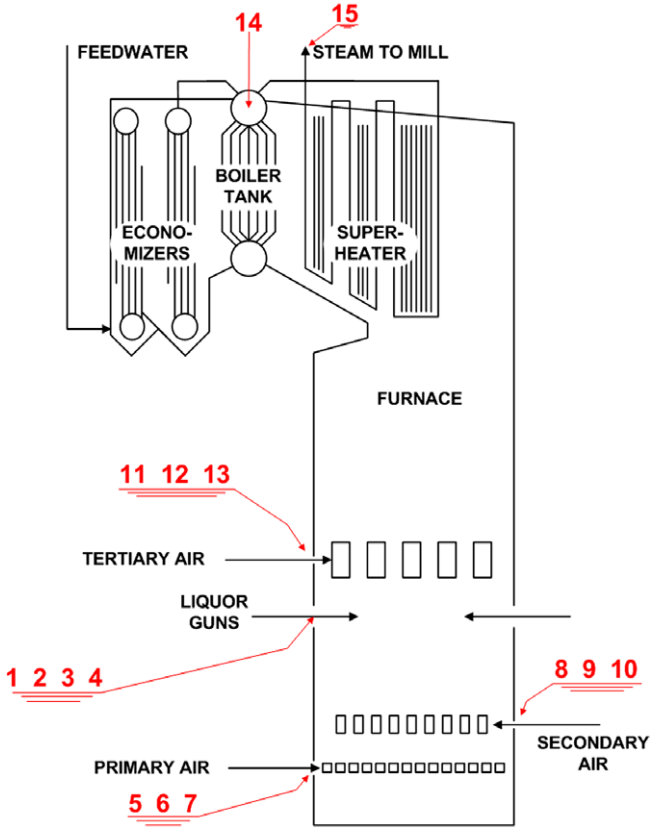

Fig. 3. Sampling points in the recovery boiler for variables shown in Table 3 (boiler diagram after Adams et al. [5]).

(1) acquisiting data from the Brazilian mill (including samplings and measurements);
(2) elaborating the block diagram that describes the process, using the basic modular units existed in WinGEMS, as shown in Table 2;
(3) evaluating and describing the required input data in the simulator;
(4) simulating the black liquor evaporation and combustion stages.

Table 2
Basic modular units from the WinGEMS simulator used in elaborating the block diagrams for describing the evaporation system and the recovery boiler [3,7,8]

Modular unit and its function	Assumptions and basic calculations
Evaporation system	
Block reference [3]	
LTV – describing the mass and energy balances in any evaporator body	Heat transfer coefficient, U, calculated by $U = (A/Q)\,\Delta T$, considering Q equals the condensation heat of all input steam, A the heat transfer area supplied by evaporator design, ΔT the difference between the inlet vapor saturated temperature and the outlet vapor temperature.
FLASH – describing the partial liquid evaporation at low pressure, into two phases	Mass and energy balances for the two phases (the liquid phase and the vapor phase of volatile components) in equilibrium at low known pressure
Recovery boiler	
Modular units of PCFURN block in the simulator WinGEMS [7]	
DMIX – simulating the mixing of dust (coming from the electrostatic precipitator) into the black liquor, before it feeds the boiler	Mass and energy balances correlating the input flows (mass flow rate and temperature) to the output flows (mass flow rate and temperature), without any chemical reaction or energy source.
ENTN – describing the spraying of black liquor into the furnace, taking into account the carrying out of small droplets to the boiler top by gas flow.	The Grooved-Core atomizer type is the injector considered and the average diameter of the liquor droplet is obtained by the correlation proposed by Bennington and Kerekes [7]. Gas-droplet mass and momentum balances are developed to specify the liquor amount carried by gas.
SPLIT and MIX – simulating the splitting or the mixing of flow streams	Mass and energy balances correlating the input flows (mass flow rate, temperature, pressure) to the output flows (mass flow rate, temperature, pressure), without any chemical reaction or energy source.
COMB – describing the black liquor combustion, including the steps of oxidation, drying and pyrolysis.	Equilibrium concentrations of the final combustion products (gases and solids), obtained by the Gibbs energy minimization method (see more details and equations in [7]).
FURN – simulating the heat transfer between gases and furnace waterwall, as well as the heat rate used to vaporize water.	Temperature of exit gases and the rate of heat transferred are obtained from integral and differential energy balances in the considered area, assuming plug flow for gases and radiation heat transfer between gases and furnace walls [8]. When necessary, corrections in the temperature are made due to the accumulation of dust on the walls of the furnace.
HSMEL – describing the heat transferred rate at the lower furnace in the region of smelt spouts.	Outlet mass flow rates and the heat transfer rate from the char bed to furnace waterwall are calculated based on mass and energy balances in the lower furnace, considering reactions that occur in the char bed.
CBED – describing the char bed (reaction of sodium sulfate with carbon in the Kraft char and its reduction to sodium sulfide).	Temperature and concentration profiles for compound-products are determined based on the first order differential equations of Zhitlov's kinetic model [9].

Data acquisition from the Brazilian mill comprises projects and design data of equipment used [9] for identifying the fixed parameters defined in the industrial plant as well as data of operational variables (i.e. the flow rate, pressure, temperature or composition of gases, water or steam). These variables are measured continuously at different points or locations in the industrial plant, during a period of five months. Part of these data is used for running the simulator (input data for simulating), while the other part for validating the model and simulation methods (data for simulation validating). Note that both data (input and validating data) can be obtained simultaneously from the mill, since the WinGEMS performs the simulation of evaporating and recovery boiler units without needs of any adjustable parameter for solving its model equations.

After acquisition, all data obtained should be treated statistically to eliminate those that are time-dependent due to the process oscillation. Note that, during one-day operation, input variable values can oscillate, changing little or greatly. These changes induce a transient process operation (time-dependent) until new variable values are stabilized. This transient behavior in the variable values must be withdrawn from all data sets because all process simulations require a continuous process operation. The statistical data treatment consists of averaging each measured variable (during one-hour operation), computing the standard deviation from this mean value and analyzing their residuals as a function of time. Consecutive data strongly dependent on time or those with residual higher than three times the standard deviation are considerate outliners and eliminated from data sets.

Having eliminated outliners, data are organized into an electronic Excel spreadsheet for being transmitted to the WinGEMS simulator by an executable routine programmed in Visual Basic computer language. Receiving the input data, WinGEMS simulator starts running to solve by iterative calculations the mass and energy balances together with the model equations. The iterations stop when the convergence criterion is reached. Results from WinGEMS simulations include the operational variables of each equipment and current. Simulated results are available in another Excel spreadsheet for being compared to actual industrial data.

Table 3
Evaporation system, 38 variables per set

Measured variables/type of data used in simulation	Number of variables
Weak black liquor inlet temperature and concentration – INPUT DATA	2
Temperature in the first effect – INPUT DATA	1
Live steam, pressure and outflow in the first effect – data for simulation validating	2
Liquor solids content at the exit of the second effect – data for simulation validating	1
Weak black liquor outflow split among 4th, 5th and 6th effects – INPUT DATA	3
Liquor temperature, vapor temperature in each evaporating body – INPUT DATA	14
pressure in each evaporation body – data for simulation validating	7
Concentrated black liquor outlet temperature and flowrate – data for simulation validating	2
Concentrated black liquor outlet concentration – data for simulation validating	1
Outflow of low pressure steam and condensate in the stripping column – INPUT DATA	2
Pressure in the stripping column – INPUT DATA	1
Cooling water temperature and outflow in the condenser – INPUT DATA	2
Variables per set	38

3.1. Evaporation

For describing the evaporation system, 30,323 data sets are collected from the Brazilian mill, containing per set 38 variables, as shown in Table 3. In this table, one can see the variables used as input data for simulating and those used for simulation validating (i.e. outlet liquor and vapor temperature, pressure and flow rate, as well as the liquor solids concentration, at the second effect and at the evaporating system).

After applying the statistical treatment, 231 sets (7.6% of total data sets) are eliminated as outliners. The 2792 data sets remained are averaged over one hour of measurement [4] and used as input data in the simulation.

Mean values of the basic input variables are: vapor outflow = 74,600 kg h^{-1}; liquor outflow = 483,600 m^3 h^{-1}; vapor temperature = 151.7 °C; liquor temperature = 86.1 °C; steam pressure = 3.6 kgf cm^{-2}; liquor solids content = 15.4%; heat loss in the 1° and the 2° effects = 1.0% of the total heat transfer in each one effect and from the 3° to the 6° effects = 0.5% of the total heat transfer in each one effect.

3.2. Recovery boiler

For describing the recovery boiler unit of the Brazilian mill, 630 data sets are acquired from its plant, containing per set 14 variables, listed in Table 4. In this table, one can see the variables used as input data for simulating the liquor combustion operation and those used for simulation validating. Another variable used for validating models and simulation methods is the boiler temperature (upper furnace region). However, in this validation, only one data set is used since measured data obtained at boiler region are not precise as the other variable used in validation (generated steam flowrate, shown in Table 4).

After applying the statistical treatment, 58 sets (9.2% of total data sets) are eliminated as outliners. The 572 data sets remained are averaged over one hour of measurement and used as input data in the step simulation.

Block diagram of the recovery boiler, composed by interconnected modular units from the WinGEMS simulator, representing the recovery boiler type used in the industrial plant unit of the Brazilian mill. Each block in this diagram consists of theoretical or empirical equations that describe a phenomenon and/or an operation occurred during the stage of the liquor combustion along the boiler regions. More details about these blocks can be found in the earlier work [9] or in the specific literature [7,8,10].

Table 4
Variables for the recovery boiler

Boiler operational variable	Sampling point[a]
Input data for simulating	
Black liquor: flow rate, t/h	1
Black liquor temperature, °C	2
Black liquor pressure, mm H_2O	3
Solids concentration in liquor, %	4
Primary air: flow rate, t/h	5
Primary air temperature, °C	6
Primary air pressure, mm H_2O	7
Secondary air: flow rate, t/h	8
Secondary air temperature, °C	9
Secondary air pressure, mm H_2O	10
Tertiary air: flow rate, t/h	11
Tertiary air temperature, °C	12
Tertiary air pressure, mm H_2O	13
Steam drum pressure, kg_f/cm^2	14
Output data for simulation validating	
Steam flow rate, t/h	15

[a] Sampling points in the boiler for these variables are shown in Fig. 3.

Note that, in the Brazilian mill analyzed, the recovery boiler is built with three-level air system; four black liquor guns; three super-heaters (primary, secondary and tertiary); two drums generating bank and two economizers. The total airflow injects into this boiler is 294,800 kg/h, being 135,000 kg/h as air primary, 124,600 kg/h as air secondary and 35,200 kg/h as air tertiary. Original steam condition is 240,000 kg/h at 450 °C and 63 kg/spcm. The inlet current of the black liquor is characterized by the total flow rate = 75,130 kg/h; the dry solid flow rate = 54,094 kg/h; the solids content = 72% and the elemental composition: C = 34%, N = 0%, H = 3.7%, Cl = 1.5%, Na = 21.4%, S = 2.4% and K = 2.0%.

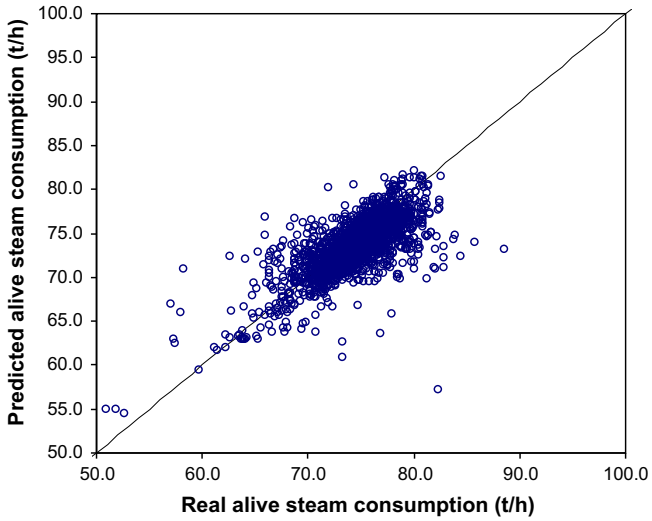

Fig. 4. Comparison between measured and simulated values for the steam consumption in the evaporation system.

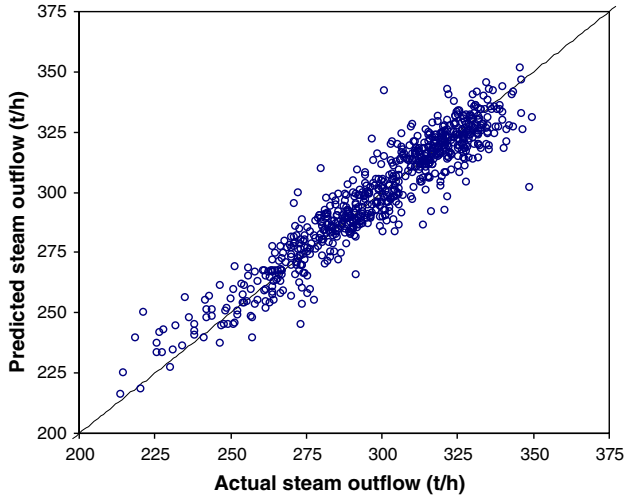

Fig. 5. Comparison between measured and simulated values of the outflow of steam generated in the boiler recovery.

4. Results and discussion

For testing the methodology used for simulating, comparisons between measured and simulated values of several variables are performed in the two industrial units studied. Examples of these comparisons are presented in Figs. 4 and 5 for the black liquor evaporation and the recovery boiler, respectively. As observed in these figures, the majority of data is lined up or even overlapping the 45° diagonal line, indicating that simulated values are close to measured ones. To quantify this result, the relative average error (RAE) is calculated using Eq. (1), being equal to 2.4% for the steam consumption in evaporation and 1.7% for the outflow of steam generated in the recovery boiler.

$$\mathrm{RAE} = \frac{1}{N}\sum_{N}^{1}\frac{|y_{\mathrm{measured}} - y_{\mathrm{simulated}}|}{y_{\mathrm{measured}}} \tag{1}$$

4.1. Evaporation

Simulated values of the overall heat transfer coefficient, *U*, during the three days operation of the evaporation body A in the first effect (IA) are shown in Fig. 6. Note that these values have been obtained by solving the mass and energy balance equations from the WinGEMS and using the traditional washing time cycle adopted by industrial mils (eight hours of operation and 4 h of washing each body). Although there are wide oscillations of *U*-value, a notary trend in decreasing the *U*-value are observed in the end of each 8 h of operating. This indicates the actual necessity of washing the 1A body. Then, as shown in Fig. 6, each washing cycle extends for 4 h before starting again the operation. The most appropriated time to start washing the body effect can be obtained by decreasing *U* up to an ideal value stipulated from the statistical analysis and criteria. Therefore, using WinGEMS, the *U* monitoring can be performing continuously and online to optimize the washing cycle in each effect body. Work is in development to define the statistical criteria for monitoring the *U*-value during the body operation, since the decrease in *U* up to an ideal value must be related to an inefficient heat exchange (and not to an suddenly change in operational condition of the process).

4.2. Recovery boiler

To study the effect of increasing solids concentration on the performance of the recovery boiler, the combustion of the liquor has

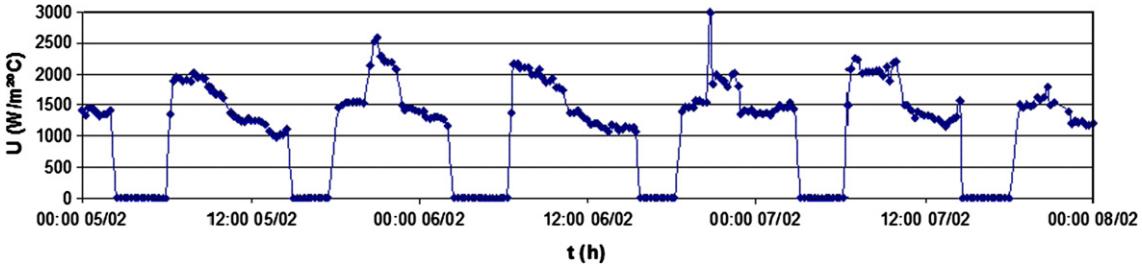

Fig. 6. Simulation of the overall heat transfer coefficient during 4 days of traditional cycle time operation in the evaporation A body (8 h of continuous operation and 4 h of washing).

been simulated for each increase in the solids concentration from 72% to 99.9%. In this simulation, the amount of dry solids in the liquor flow rate has been maintained constant (= 54,094 kg/h), as well as all other variables. The solids concentration has been varied by changing the liquor water content and, consequently, the liquor mass flow rate fed into the boiler. Then, for 72%, the liquor flow rate corresponds to 75,130 kg/h; for 80% to 67,617 kg/h; for 90% to 60,104 kg/h and 99.9% to 54,094 kg/h).

Results obtained in this simulation show the effects of the liquor solids concentration on the steam production (Fig. 7); the boiler thermal efficiency (Fig. 8); the gas boiler temperature at the oxidation and reduction zones (Fig. 9) and the overall boiler temperature (Figs. 10a and 10b). From Fig. 7, it can be noted that there is an increase of approximately 10% in the steam production as the liquor solids concentration increases from 72% to 99.9%. Such increase in the liquor solids concentration does not alter the reduction efficiency, i.e. the mass ratio of sodium sulfide to the total mass of sodium sulfide and sulfate. This assures an appropriate chemical composition for reforming the white liquor in subsequent stages of the process. Fig. 8 indicates an increment in the boiler efficiency as a result of increasing the liquor solids concentration. Note that the 10% increase in the superheated steam production does not represent a net improvement in the global process since

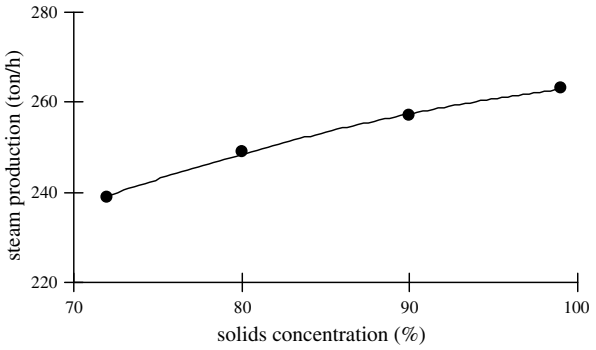

Fig. 7. Simulated value of the superheated steam production rate as a function of the solids concentration in the black liquor feeding the recovery boiler.

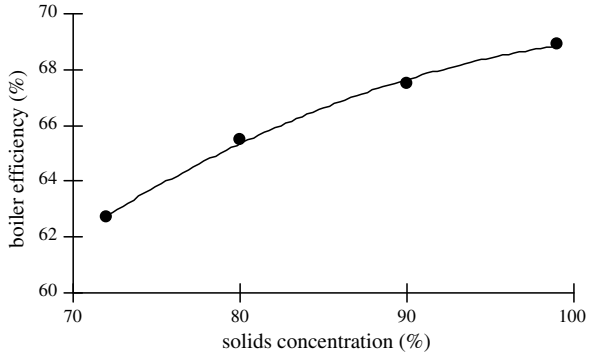

Fig. 8. Simulated value of the boiler thermal efficiency as a function of the solids content in the black liquor feeding the recovery boiler.

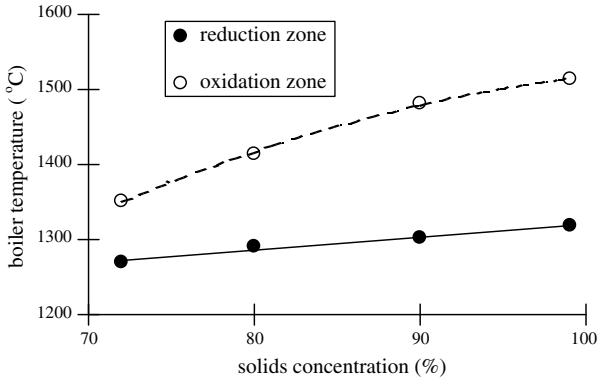

Fig. 9. Simulated value of the operational boiler temperature in the oxidation and reduction zones as a function of the solids content in the liquor feeding the recovery boiler.

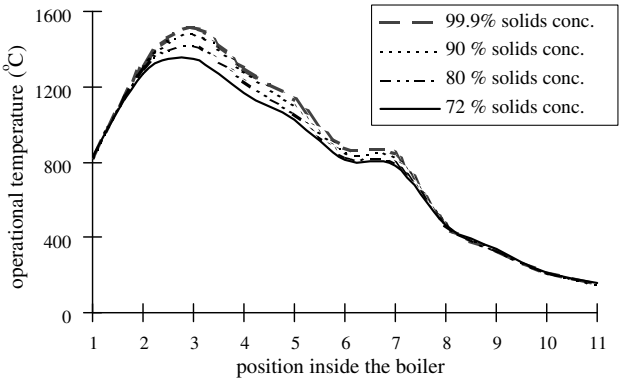

Fig. 10a. Simulated profile of the recovery boiler operational temperature as a function of the solids content in the liquor feed (positions identified in Fig. 10b).

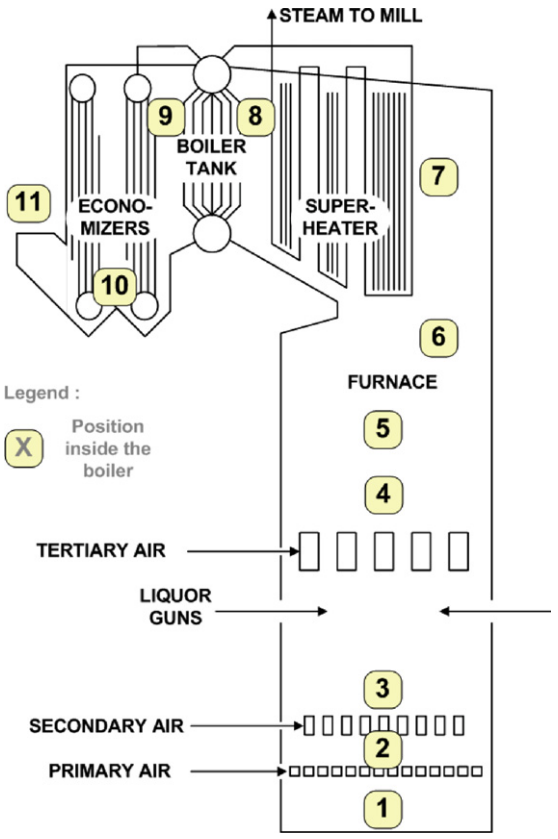

Fig. 10b. Positions inside the boiler at which the operation temperature has been simulated by WinGEMS (shown in Fig. 10a).

the liquor must be concentrated before being injected in the boiler. However, results presented in Fig. 9 and Fig. 10 show that there is a real increment in the operational temperature of the boiler, mainly in the furnace where the liquor combustion occurs. According to the simulated data in Fig. 9, the increase in the liquor solids concentration from 72% to 99.9% results in an increment in the gas boiler temperature of 50 °C at the reduction zone and of 160 °C at the oxidation region. This promotes a greater stability of the combustion reactions, avoiding problems related to the explosion or the extinction of the char bed. Moreover, there is an increase in the amount of the combustion products, as well as dusts or ashes, which tend to incorporate sulfur, avoiding its release to atmosphere.

By this simulation, one can conclude that any increase in the solids concentration ($C_{ss} > 72\%$) of the black liquor feeding the boiler improves the combustion reaction stability and avoids the boiler explosion problems and releases dust to environment. Then, research for new process methodologies to concentrate the inlet black liquor of the boiler ($C_{ss} > 72\%$) is feasible and required from industries. Moreover, as the black liquor is concentrated over 50% of solids, its rheological behavior changes from a Newtonian to a pseudoplastic fluid. This results in higher liquor viscosity as the solids concentration increases over 72%. Because of this viscosity increase, any methodology to concentrate the black liquor should also incorporate techniques to reduce the liquor viscosity as the solids concentration rises.

5. Conclusion

As shown in this work, application of the simulation methodology to *find Energy Recovery opportunities* must contribute to significant savings in energy use.

As shown by results obtained, the burning of liquors with a higher solids concentration (above 80%) leads to an increase in the boiler efficiency and stability, releasing dust to environment. Presently, the limitation for obtaining such liquors lies in the difficulty to concentrate them since the viscosity increases as the concentration of the solids rises. Therefore, changes into the traditional Kraft pulping process for feasible energy savings should be associated to new advanced technologies. These must include techniques for reducing the black liquor viscosity at higher solids concentrations.

Finally, this simulation methodology associated to computational methods for process integration must be applied to the overall industrial process since all units are linked together and any change in one operation affects the others.

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