THERMODYNAMIC MODELING OF A COGENERATION SYSTEM FOR A SUGARCANE MILL USING ASPEN -PLUS, DIFFICULTIES AND CHALLENGES

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Abstract. *The combined production of steam and power has become the norm in the sugar cane industry worldwide. Thus the utilization of cane bagasse as fuel for the cogeneration system allows sugarcane plants to be self sufficient of thermal and electrical energy despite using low efficiency systems. The simulation / analysis of this systems would contribute to its improvement. The aim of this work is to accomplish a thermodinacmic modelling of a cogeneration system using ASPEN -PLUS and compare the results of this simulation with results accomplish with THERMOFLEX which is a specialized software for analysis of cogeneration systems. The interest in an accurate modelling of the cogeneration system with ASPEN PLUS become from the fact that this software is rather adequate to modelling the entire plant. As case study , a cogeneration system with a boiler of 67 bar and condensing-extraction steam turbines is presented. This case correspond to a real Brazilian sugarcane mill. In the last part, a comparison of results is accomplished in order to evaluate possible differences between these softwares.*

Keywords*: cogeneration; efficiency; sugarcane mill; aspen plus; thermoflex*

1. INTRODUCTION

In sugarcane plants, the cogeneration using bagasse as fuel, has become the norm because it provides all plant energy demands (and even surplus electricity). In Brazil almost all sugarcane plants are self-sufficient in thermal, mechanical and electrical energy but generally these cogeneration systems have low efficiency as they are based on steam cycles with live steam at 22 bar and 300°C. (Macedo et al. 2001 cited by Ensinas et al. 2007)

In the last few years, electricity is becoming a new product in sugarcane plants and alcohol distilleries, due to rises in electricity price paid. According Kamate and Gangavati (2009) the sugar industry is moving towards substantially improved cogeneration systems, by adopting high pressure and temperature steam conditions and high efficiency steam turbines, so, it can export surplus power to grid when the prices are attractive, or otherwise can save (fuel) surplus bagasse, which can be utilized for many other productive purposes.

In this context the motivation to simulate the cogeneration plant in ASPEN PLUS is related to the intention of simulate the entire plant of ethanol production, due to ASPEN PLUS is an adequate software to simulate chemical process.

Then it is necessary to construct the cogeneration plant from the unit operations blocks available in ASPEN PLUS as well as to do the necessary considerations in order to obtain results close to real values.

To validate the results obtained with ASPEN PLUS, a comparison was made with the same systems simulated with the software THERMOFLEX. THERMOFLEX is a software specialized in modeling and simulation of thermal cycles that was developed by the company THERMOFLOW Inc (Thermoflow, 2008).

2. COGENERATION SYSTEM – STUDY OF CASE

The case of the cogeneration system studied in this work corresponds to a sugar cane mill in Sao Paulo State in Brazil. This cogeneration system has two condensing-extraction steam turbines and one boiler of 67 bar/510°C with steam production of 55.56 kg/s. In the first turbine, Turbine 1, the extraction is accomplished at 17 bar, to driving mills and other prime movers whilst in the second turbine, Turbine 2, the extraction is accomplished at 2.5 bar belonging to the conditions of the process. According to the turbine project data, the bleed flow for both turbines is 70% of the total flow. The steam after passing through the turbines continues to the condenser where it is cooled down and condensed to liquid water, which is recirculated.

The liquid water from the condenser joins to the condensed water from the process and goes to the deaerator which runs with steam at 2.5bar. After that the water is pumped to the boiler and desuperheaters. Figure 1 shows the diagram of the cogeneration system studied (sketch of THERMOFLEX^{TM}).

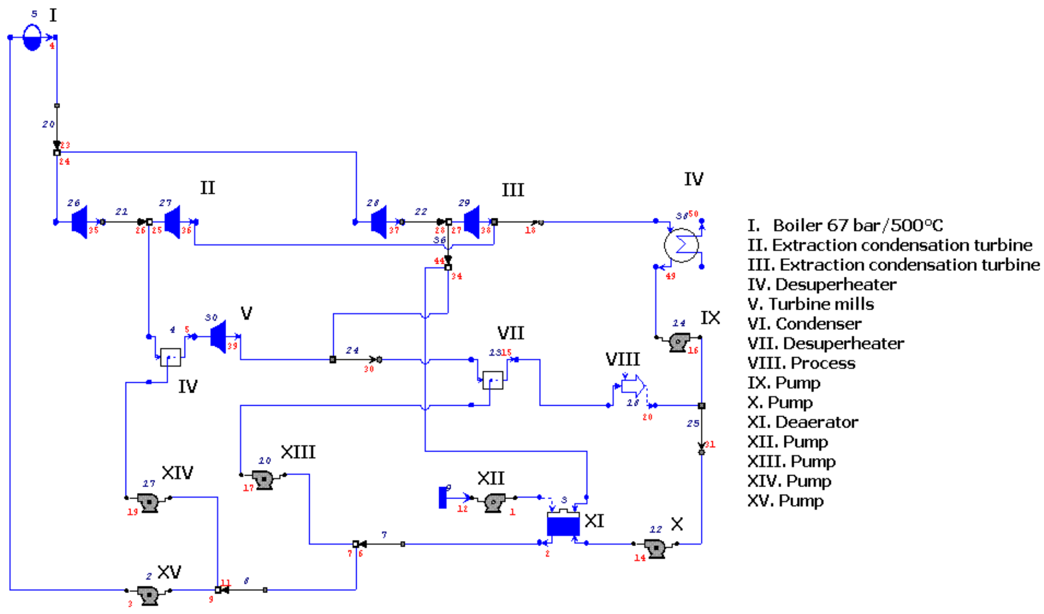

Figure 1. Diagram of the cogeneration system studied – Scheme of THERMOFLEX.

Table 1 shows isentropic efficiencies of the steam turbines. These values were supplied by the turbine manufacturer for the case of the condensing-extraction turbines. The isentropic efficiency of direct drive steam turbines was adopted from Ensinas (2008). It can be observed that direct drive turbines have lower efficiency than turbines for electricity generation due to they are, generally, single stage turbines. On the other hand, turbines for electricity generation are multistage type. For the condensing-extraction steam turbines, the manufacturer informs that the number of stages is 5 for the high pressure part and 3 for the low pressure part in Turbine 1, whilst for the Turbine 2 the number of stages is 5 and 8 respectively (Mari, 2008).

Table 1. Isentropic efficiency of steam turbines

Turbines of mills, shredders, cutters	55.0
Electricity Generation - Condensing-extracting Turbine 1[a] HP[b]	80.6
Electricity Generation - Condensing-extracting Turbine 1 LP[c]	86.2
Electricity Generation - Condensing-extracting Turbine 2[d] HP	87.2
Electricity Generation - Condensing-extracting Turbine 2 LP	79.2

[a] Turbine with extraction at 17bar
[b] HP: High pressure part
[c] LP: Low pressure part
[d] Turbine with extraction at 2.5bar

3. PROCESS SIMULATION IN ASPEN PLUS

The Aspen Plus is a chemical process simulation modeling software which was originally developed by the Massachusetts Institute of Technology for the U.S. Department of Energy to evaluate synthetic fuel technologies and in this work it is used to carry out the simulation of the cogeneration system of a sugar cane mill.

The Aspen Plus includes a library of standard unit operation blocks (e.g. reactors, mixers, splitters, heaters, pumps), which represent processes taking place in an actual chemical plant. The simulation of the plant is done by specifying configurations of the unit operations, properties and conditions of the material flows as well as heat and work streams. The program has also an extensive components database containing physical properties of a large number of pure components. Within the program there are mathematical routines (convergence algorithms) for solving different equations of material and energy balance (Magnusson, 2005).

3.1 Fuel

The fuel of the cogeneration system is the sugarcane bagasse. It is the fibrous residue of the cane stalk after crushing and extraction of the juice. The bagasse consists of water, fibers and relatively small quantities of soluble solids. Its composition varies according of the variety of cane, its maturity, method of harvesting and finally the efficiency of the milling plant (Paturau, 1982).

By definition, the fiber in bagasse is insoluble in water; it consists mainly of cellulose, hemicellulose and lignin. Table 2 present the average cane fiber composition according to Purchase (1995) appud Rein (2007). For the calculations in this work it is adopted a bagasse moisture of 50% and the cane fiber composition of Tab. 2.

Table 2. Cane fiber composition (in g/100g dry substance)

Component	%
Cellulose	40
Hemicelluloses	33
Lignin	22
Ash/other	5

Rein (2007)

In the simulation, the component ash of the bagasse is considered as SiO_2, due to this component is in larger quantity in the ash analysis (Rein, 2007). Other components of the bagasse such as sulfur, sucrose and other soluble solids were neglected.

3.2 Definition of Streams and Components

For the modeling it is necessary to define the nature of the streams that take part in the process. The stream class selected for the simulation is the MIXCISLD stream class, which allows two possible substreams: the CISOLID substream and the MIXED substream. The CISOLID substream (Conventional Inert Solid) is used for conventional components that appear in the solid phase but do not participate in phase equilibrium on the other hand the MIXED substream is used for conventional components that reach phase equilibrium whenever flash calculations are performed.

For specifying components, from the Aspen Plus database, the following components were selected: water (H_2O), carbon dioxide (CO_2), oxygen (O_2), nitrogen (N_2) as conventional components and the silicon oxide (SiO_2) as a solid component.

Physical property data for the sugarcane bagasse components are not available in the standard Aspen Plus database. Hence, physical properties for the cellulose, hemicelluloses and lignin were taken from the in-house “ASPEN PLUS DATABASE FOR BIOFUELS” developed by the National Renewable Energy Laboratory (NREL) of USA. It considers that cellulose, hemicelluloses and lignin are in solid phase.

3.3 Steam boiler

Figure 2 shows the process flow diagram for the steam boiler according Magnusson (2005). The boiler is composed by a reactor (BURNER), and four heat exchangers which represent the superheater (SUPRHEAT), evaporator (EVAPORAT), economizer (ECONO) and the air preheater (PHAIR).

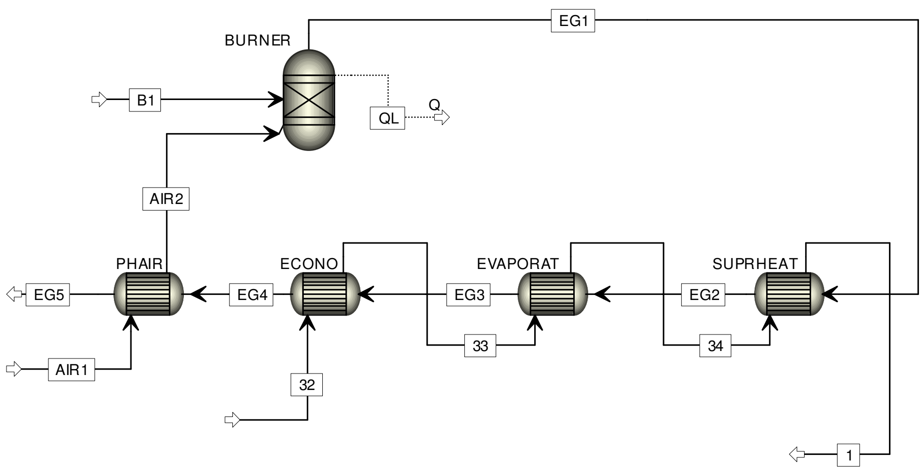

Figure 2. Scheme of the steam boiler in ASPEN PLUS

In Fig. 2 the streams of fuel (B1) and air (AIR2) get into the reactor and the water stream (32) get into the boiler in the economizer. The flue gases produced in the reactor (EG1) are used to preheat the incoming air (AIR1) as well as heating the water to superheating steam. In this modeling the heat exchangers are disposed in a counter-flow configuration.

It is considered that the bagasse is fed directly to the boiler and its temperature is 50°C according Lora and Zampieri (2008) and the temperature at the air preheater inlet is 29°C.

For the simulation the streams of water (1; 32; 33 and 34) and air (21% O_2 and 79% N_2) are considered of type MIXED on the other hand the stream of fuel B1 has got substreams type CISOLID for the cellulose, hemicelluloses, lignin and SiO_2 and a substream MIXED for the water in the bagasse (moisture).

A stoichiometric reactor is adopted to represent the boiler burner. Due to the ashes is inert material it is considered that only the cellulose, hemicelluloses and lignin react. The combustion reactions are taken from Wooley and Putshe (1996):

Cellulose: $C_6H_{10}O_5 + 6O_2 \rightarrow 5H_2O + 6CO_2$
Hemicelluloses: $C_5H_8O_4 + 5O_2 \rightarrow 4H_2O + 5CO_2$
Lignin: $C_{7.3}H_{13.9}O_{1.3} + 10.125O_2 \rightarrow 6.95H_2O + 7.3CO_2$

In order to consider the losses by incomplete combustion due to mechanical causes it is assumed that the combustion efficiency is 98% for each reactant of the fuel. The excess air recommended for sugarcane bagasse boilers is 30% according Lora and Zampieri (2008). This value is considered for the simulation.

Heat losses due to incomplete chemical combustion are assumed in 2.51% and losses due to radiation and convection to ambient air is considered in 0.5% according Rein (2007). As well as in the standard ASME PTC 4, which considers carbon boilers, Rein (2007) indicates the Gross Heat Value (GHV) as calculation base for these losses.

In this simulation it is considered that the bagasse GHV is 9314 kJ/kg and the mass flow of bagasse fed in the boiler is 25.96kg/s. Thus, from these data, the losses due to incomplete chemical combustion joint to the losses due to radiation to ambient air represent 7277.9 kW. These losses are represented in the simulation as the heat stream Q_L in the burner (Fig. 2).

Table 3 shows the specifications for the components of the boiler. In this simulation the heat losses to ambient air in the heat exchangers are neglected due all these losses are considered into the stream Q_L. About the operation conditions in the heat exchangers, presented in Tab. 3, the temperature at the air preheater outlet is from (Magnusson 2005) whilst the others were obtained from the sugarcane mill.

Table 3. Specifications for the boiler components

Model name	**Description**	**Specifications**
BURNER	Combustion chamber	Pressure: 1.0325 bar Heavy duty: 7277.9kW
PHAIR	Air preheater	Cold stream outlet temperature: 250°C
ECONO	Economizer	Cold stream outlet temperature: 168°C
EVAPORAT	Evaporator	Cold stream outlet vapor fraction: 1 Cold side outlet pressure:70 bar
SUPRHEAT	Superheater	Cold stream outlet temperature: 510 °C Cold side outlet pressure: 67 bar

3.4 Steam Turbines

For the modeling of steam turbines in ASPEN PLUS it is used the unit operation model *Turbine,* type *Isentropic* which performs the calculations taking into account the isentropic efficiency, discharge pressure and the mechanical efficiency.

At figure 3 the condensing extraction Turbine 1 is represented by two blocks: TH1 and TL1 whilst the condensing extraction Turbine 2 is represented by the blocks TH2 and TL2. Direct driven turbines of mills cutters and shredders are represented by the block TM.

Isentropic efficiencies for each turbine are indicated at Tab.1. Mechanical efficiency of turbines was considered 98.2% (η_m) whilst the alternator efficiency was considered as 97.55% (η_a), according Mari (2008). In order to obtain directly the electric power it is informed to the software the product of these efficiencies (η_mx η_a) as a mechanical efficiency 95.74%.

3.5 Other Operations

The other components of the cogeneration system of the sugarcane mill should also be defined. There are the desuperheaters, the deaerator, the process, the condenser and the pumps. Table 4 presents the specifications for these components.

The process and the condenser are modeling using the unit operation model *Heat exchangers* whilst the desuperheaters and the deaerator are modeling using the unit operation model *Mixer* which accomplishes an energy and mass balance. About pumps it is assumed an efficiency of 70% according Magnusson (2005).

Table 4. Specifications for the other unit operations

Model name	**Description**	**Specifications**
DES1	Desuperheater	Outlet pressure: 17 bar
DES2	Desuperheater	Outlet pressure: 2.5 bar
P	Process	Outlet pressure: 2.092 bar * Outlet temperature: 102°C *
CONDEN	Condensador	Hot stream outlet vapor fraction: 0
DEAERA	Deaerator	Outlet pressure: 2.246 bar
B1	Water Pump	Discharge pressure: 2.092 bar
B2	Water Pump	Discharge pressure: 2.246 bar
B3	Water Pump	Discharge pressure: 17 bar
B4	Water Pump	Discharge pressure: 2.5 bar
B5	Water Pump	Discharge pressure: 72 bar

(*) Data from Sanchez (2003)

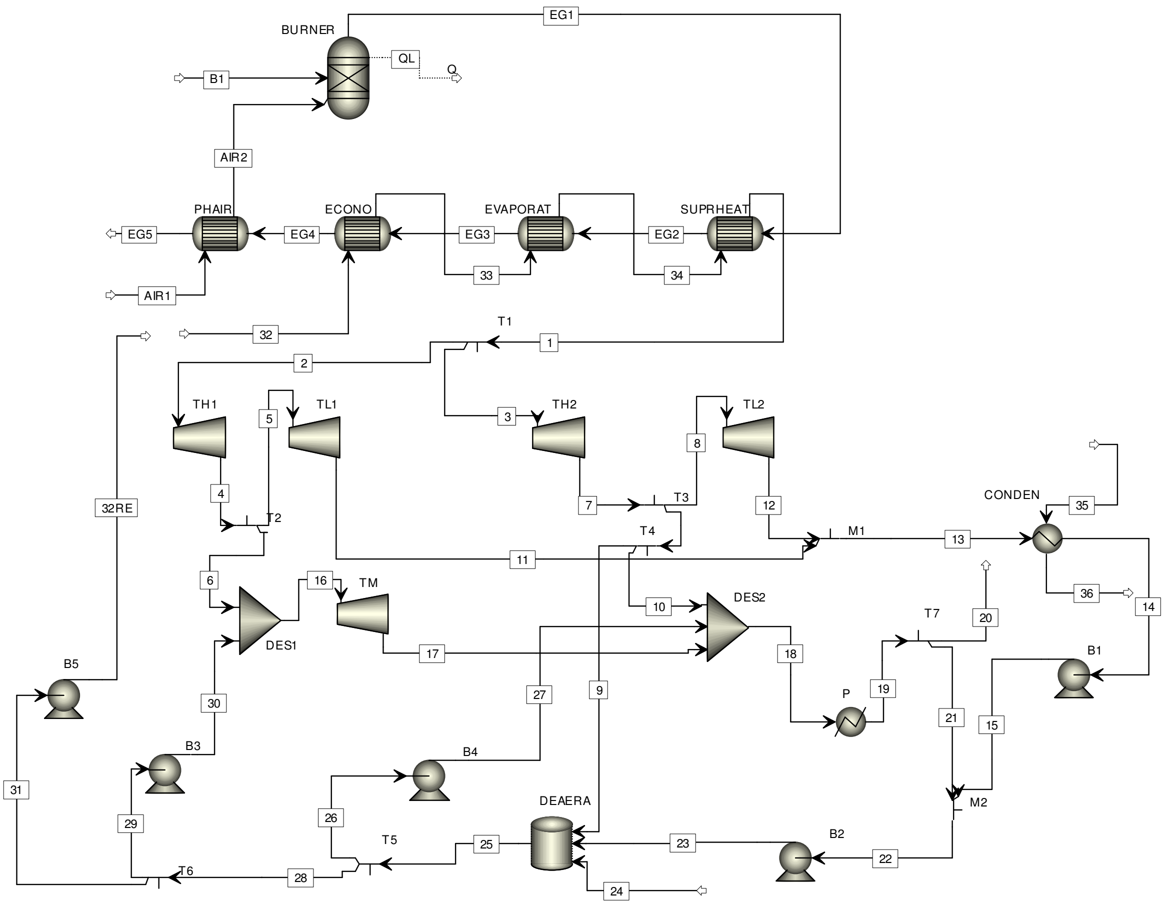

Figure 3. Scheme of the cogeneration system in ASPEN PLUS

Figure 3 shows the complete scheme of the cogeneration system. For the calculations it was specified as initial point the conditions of the stream 32 (water fed to the boiler) which is re-calculated at stream 32RE. Steam losses in the process were represented at stream 22 which are reposed at the deaerator (stream 24).

At flow divisors T4, T5 and T6 the streams 9; 26 and 29 were specified in 1.699kg/s; 1.049kg/s and 0.58kg/s respectively (data from the simulation in THERMOFLEX) in order to reach suitable temperatures at desaerator outlet, inlet of the turbine block TM, and process inlet.

4. RESULTS

Table 5 shows the temperature, pressure and mass flow of the bagasse boiler streams obtained from the simulation in ASPEN PLUS. A complete table with all the streams of the cogeneration system is presented at the annex.

In Tab. 5 it is interesting to note that the temperature of the combustion gases at the boiler exit is 175.3°C (EG5). According Sosa-Arnao (2008) the mean boiler manufacturers in Brazil; Equipalcool, Dedini, Caldema and Sermateq, design their boilers with temperatures of combustion gases at the boiler exit in this range of temperatures (155 – 165°C) however several bagasse boilers operate with higher temperatures of the combustion gases exit.

Although THERMOFLEX performs calculations with several models of boilers for this paper it was used the simplest model, called package boiler, which supplies the steam at pressure and temperature specified without taking into account combustion calculations; for this reason comparisons between two programs were not done in this part of the work.

Table 5. Results of the simulation - Bagasse boiler streams

Stream	Nature	Temperature [°C]	Pressure [bar]	Mass flow [kg/s]
B1	Bagasse	50.0	1.033	25.96
AIR1	Air	29.0	1.033	105.5
AIR2	Air	250.0	1.033	105.5
32	Water	102.2	72	55.56
33	Water	168.0	70	55.56
34	Steam	285.8	70	55.56
1	Steam	510.0	67	55.56
EG1	Exhaust gases	1249.0	1.033	131.46
EG2	Exhaust gases	1058.8	1.033	131.46
EG3	Exhaust gases	421.7	1.033	131.46
EG4	Exhaust gases	326.3	1.033	131.46
EG5	Exhaust gases	175.3	1.033	131.46

Table 6 shows the results of the simulation for the steam turbines. This table presents the mass flow of steam in each turbine block as well as the inlet and outlet conditions of temperature and pressure in each turbine block. The indicated power ($W_{indicated}$) and the net power (W_{net}) produced in each turbine block also are presented in this table. The results of net power in each turbine obtained with ASPEN PLUS were compared with results obtained from THERMOFLEX considering the same conditions in each turbine and the same considerations of efficiency. The error obtained resulted very low in all cases which indicates that ASPEN PLUS is very suitable for these type of applications (error < 0,3%).

Table 6. Results of the simulation - Operation conditions and power produced in Turbines

	TH1 Aspen/Thermoflex	TL1 Aspen/Thermoflex	TH2 Aspen/Thermoflex	TL2 Aspen/Thermoflex	TM Aspen/Thermoflex
m_{steam} [kg/s]	27.78	8.33	27.78	8.33	20.03
T_{inlet} [°C]	510	334.8	510	138.2	300
P_{inlet} [bar]	67	17	67	2.5	17
T_{outlet} [°C]	334.8	45.83	138.2	45.8	174.6
P_{outlet} [bar]	17	0.1	2.5	0.1	2.5
x_{outlet}	-	0.896	-	0.903	-
$W_{indicated}$ [kW]	9085.0 / 9088.2	6471.6 / 6452.9	19409.6 / 19406.7	3215.1 / 3223.0	4359.3 / 4249.42
Losses [kW]	387.0 / 387.2	274.7 / 274.9	826.8 / 826.7	137 / 137	185.7 / 78.42
W_{net} [kW]	8698.0 / 8701	6173.4 / 6178	18582.7 / 18580.0	3078.1 / 3086.0	4173.6 / 4171
error W_{net} % (*)	0.04	0.07	0.01	0.26	0.06

(*) error W_{net}% indicates the difference between the value of the W_{net} calculated with ASPEN PLUS in relation to the value calculated with THERMOFLEX

About the Mixer blocks which represented the desuperheaters and the deaerator the temperatures obtained at the outlet of these components were: 300.4°C, 127.42 °C and 100.99°C for the desuperheater DES1, the desuperheater DES2 and the deaerator DEAERA respectively. These results presented errors lower than 0.2% in relation to the values calculated with THERMOFLEX.

About water pumps Tab.7 presents the operational conditions and the power required in each pump. Results in pump calculations do not present differences in comparison to the results obtained with THERMOFLEX (errors < 1% in relation to the power pump).

Table 7. Results of the simulation - Operation conditions and power requirements for water pumps

	B1	**B2**	**B3**	**B4**	**B5**
m_{water} [kg/s]	16.7	54.71	0.58	1.05	55.56
T_{inlet} [°C]	45.8	85	101	101	101
P_{inlet} [bar]	0.1	2.092	2.246	2.246	2.246
T_{outlet} [°C]	45.9	85.0	101.3	101.0	102.2
P_{outlet} [bar]	2.092	2.246	17	2.5	72
W_{hid} [kW]	4.791	1.243	1.277	0.04	578.2
W_{el} [kW]	5.010	1.298	1.334	0.04	604

Table 8 shows the heat exchanger of the system. About the boiler components it can be observed that the evaporator is the component with higher rate of heat exchanged whilst the economizer is the component with lower heat exchanged in the boiler. An important value in this table is the heat exchanged in P (process) due to it is necessary for the calculation of indicators of efficiency of the system.

Table 8. Results of the simulation – Heat exchanged

Component	Description	Q [kW]
PHAIR	Air preheater	23880
ECONO	Economiser	15543
EVAPORAT	Evaporator	114415
SUPRHEAT	Superheater	36934
CONDEN	Condenser	35882
P	Process	88813

5. CONCLUSIONS

It was presented a detailed methodology to the modeling of a cogeneration system of a sugarcane mill in ASPEN PLUS.

The accuracy of the ASPEN PLUS results, in comparison with the specialized software THERMOFLEX, indicates that ASPEN PLUS is suitable in a good level to perform this type of calculations.

In order to obtain reliable results it is important to be careful to define the fluid property method in ASPEN PLUS; a wrong choose of the fluid property method could result in large deviations from the right values.

There are also some limitations of the modeling in ASPEN PLUS. For example at the boiler modeling it was used a stoichiometric reactor to simulate the boiler furnace, in terms of energy balance there is not so much difference in relation to other models, as equilibrium model, but this consideration does not work if the focus is an emission evaluation . An equilibrium model was not utilized in the present work due to the combustion of solids materials is a complex process and due to there are not available data of the free Gibbs energy of solid formation for the elements: cellulose, hemicelluloses and lignin of the bagasse. Moreover, the gas exhaust temperatures at the inlet and outlet of each heat exchanger of the boiler are not real and correspond only to energy balance, due to all heat losses for convection and radiation of the boiler were considered previously, at the burner. In fact, this last aspect can be improved in future works, simulating the heat loss for each one of the components.

In general terms it can be affirmed that ASPEN PLUS is good enough to perform simulations of cogeneration systems presenting results with high accuracy and reliability.

6. ACKNOWLEDGEMENTS

The authors wish to thank to Adriano Viana Ensinas, Marina Dias and Tassia Lopes Junqueira, for the valuable information given and discussions, to CNPq (PQ 10 - 307068/2006-4), CAPES for the PhD fellowship and FINEP (Contract FINEP – FUNCAMP Nr. 01/06/004700) for the financial support.

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8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.

9. ANNEX

Table 9. Streams of the cogeneration system

	T	P	M	H	Components flow [kmol/h]						
	[°C]	[bar]	[kg/s]	[MMkcal/h]	H2O	N2	O2	SiO2	Celulose	Lignin	Hemice-lulose
AIR1	29	1.03	105.5	0.3	0	10399.9	2764.5	0	0	0	0
AIR2	250	1.03	105.5	20.9	0	10399.9	2764.5	0	0	0	0
B1	50	1.03	26.0	-274.9	2593.8	0	0	38.89	115.28	125.89	77.81
EG1	1249.0	1.03	131.5	-260.3	4321.1	10399.9	456.3	38.89	2.31	2.52	1.56
EG2	1058.8	1.03	131.5	-292.1	4321.1	10399.9	456.3	38.89	2.31	2.52	1.56
EG3	421.7	1.03	131.5	-390.5	4321.1	10399.9	456.3	38.89	2.31	2.52	1.56
EG4	326.8	1.03	131.5	-403.8	4321.1	10399.9	456.3	38.89	2.31	2.52	1.56
EG5	175.8	1.03	131.5	-424.4	4321.1	10399.9	456.3	38.89	2.31	2.52	1.56
1	510	67	55.6	-598.8	11102.6	0	0	0	0	0	0
2	510	67	27.8	-299.4	5551.3	0	0	0	0	0	0
3	510	67	27.8	-299.4	5551.3	0	0	0	0	0	0
4	334.8	17	27.8	-307.2	5551.3	0	0	0	0	0	0
5	334.8	17	8.3	-92.2	1665.4	0	0	0	0	0	0
6	334.8	17	19.4	-215.0	3885.9	0	0	0	0	0	0
7	138.2	2.5	27.8	-316.1	5551.3	0	0	0	0	0	0
8	138.2	2.5	8.3	-94.8	1665.4	0	0	0	0	0	0
9	138.2	2.5	1.7	-19.3	339.5	0	0	0	0	0	0
10	138.2	2.5	17.7	-201.9	3546.4	0	0	0	0	0	0
11	45.8	0.1	8.3	-97.7	1665.4	0	0	0	0	0	0
12	45.8	0.1	8.3	-97.6	1665.4	0	0	0	0	0	0
13	45.8	0.1	16.7	-195.3	3330.8	0	0	0	0	0	0
14	45.8	0.1	16.7	-226.1	3330.8	0	0	0	0	0	0
15	45.9	2.092	16.7	-226.1	3330.8	0	0	0	0	0	0
16	300.0	17	20.0	-222.8	4001.8	0	0	0	0	0	0
17	174.6	2.5	20.0	-226.5	4001.8	0	0	0	0	0	0
18	127.4	2.5	38.8	-442.5	7757.8	0	0	0	0	0	0
19	102	2.092	38.8	-518.9	7757.8	0	0	0	0	0	0
20	102	2.092	0.8	-10.4	155.3	0	0	0	0	0	0
21	102	2.092	38.0	-508.5	7602.5	0	0	0	0	0	0
22	85.0	2.092	54.7	-734.6	10933.3	0	0	0	0	0	0
23	85.0	2.246	54.7	-734.6	10933.3	0	0	0	0	0	0
24	25	1.03	0.8	-10.6	155.3	0	0	0	0	0	0
25	101.0	2.246	57.2	-764.5	11428.1	0	0	0	0	0	0
26	101.0	2.246	1.0	-14.0	209.6	0	0	0	0	0	0
27	101.0	2.5	1.0	-14.0	209.6	0	0	0	0	0	0
28	101.0	2.246	56.1	-750.5	11218.5	0	0	0	0	0	0
29	101.0	2.246	0.6	-7.8	115.9	0	0	0	0	0	0
30	101.3	17	0.6	-7.8	115.9	0	0	0	0	0	0
31	101.0	2.246	55.6	-742.8	11102.6	0	0	0	0	0	0
32	102.2	72	55.6	-742.3	11102.6	0	0	0	0	0	0
33	168.0	70	55.6	-728.9	11102.6	0	0	0	0	0	0
34	285.8	70	55.6	-630.5	11102.6	0	0	0	0	0	0
35	28.0	1.013	1179.7	-16080.9	235739	0	0	0	0	0	0
36	35.2	1.013	1179.7	-16050.1	235739	0	0	0	0	0	0