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A SOFTWARE INTEGRATION STRATEGY FOR COMPREHENSIVE SIMULATION OF INTEGRATED GASIFICATION COMBINED CYCLES

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Abstract. *Given the current scenario of economic, environmental, and energy security constraints, Integrated Gasification Combined Cycle (IGCC) power plants are among the most attractive options for power generation. As a consequence, IGCC plants have attracted the attention of several studies regarding their physical and economic characteristics. In particular, from a thermal system engineering viewpoint, due to the coupling of complex equipment such as gasifiers and gas turbines, it is important to consider accurately the effects of operational changes of one piece of equipment onto the others. In this context, this paper presents a software integration strategy to enable the detailed analysis of specific phenomena in each of the main components of an IGCC system, without losing sight of the power plant behavior as a whole. For the gasification process, the software CeSFaMB™ has been selected, whereas the software NGGT is responsible for the gas turbine simulation. To interconnect the different equipment, include the other components related to the steam cycle, and perform the global system simulations, the professional process simulator IPSEpro has been chosen. It is shown through a simulation example, that the proposed software integration methodology results in a powerful platform for the analysis of complex engineering systems.*

Keywords: *Energy systems, IGCC power plants, gasification, process simulators, software integration*

1. INTRODUCTION

The relationship between sustainable development and the use of energy resources is fundamental for society (Dincer and Rosen, 2013). Thus, as far as energy is concerned, the achievement of a sustainable development – expression whose precision is discussed in Daly (1996) – should be connected to the use of sustainable resources (Dincer and Rosen, 2013). Based on this scenario, regarding the development of economically feasible energy conversion technologies, attention should be given to at least two relevant topics: energy security, and climate changes.

Generally speaking, climate changes are associated with the average temperature increase, variations in precipitation and seasonal patterns, variations in intensity and pattern of extreme weather events, and sea level rise in many regions (Mideksa and Kallbekken, 2010; IPCC, 2014). In Brazil, on the one hand, the national electricity matrix is now 74.6% based on renewable resources, against 88.1% in 2011 (MME, 2015). On the other hand, considering a sustainability path, it must be noted that hydroelectricity accounts for 65.2%. As presented by Lucena *et al*. (2009), an expected decrease in rivers' flows would cause draughts in hydroelectric power plants' reservoirs. Hence, one must consider that the Brazilian matrix is susceptible to climate changes and, consequently, not totally reliable concerning energy supply.

Given such a picture, in order to follow the sustainability path more dependably, a closer look at renewable energy resources other than hydroelectric must be taken. As examples of such resources, one can mention solar power, wind power, ocean power, and biomass. Hence, several studies are involved with the inclusion of such technologies in the Brazilian matrix, assessing their physical, technological, economic, and environmental characteristics.

In this work, due to their potential for low emissions, and for diversification of the energy matrix (Sahraei *et al.*, 2014), Integrated Gasification Combined Cycle (IGCC) power plants are assessed. Such plants are composed of complex equipment, such as gas turbines and gasifiers. The accurate simulation of the equipment behavior is of great importance to understand the plant performance under a variety of operational envelopes. Thus, this work presents a software integration strategy for the comprehensive simulation of an IGCC plant. The methodology enables the concomitant use of three different programs to address each piece of equipment in detail, while not letting aside the power plant behavior as a whole. Different professional softwares with an individual expertise can, with the suggested integration strategy, work together to improve the assessment of complex systems. In order to validate the methodology, the plant suggested by Souza-Santos and Beninca (2014) is simulated, and the results compared.

2. IGCC POWER PLANTS CHARACTERISTICS

Combined cycle power plants are those in which power generation is a consequence of the combination of two different thermodynamic cycles. Such structure allows a higher global thermal efficiency when compared to the isolated cycles. The thermal efficiencies of state-of-the-art combined cycles have crossed the 60% barrier (General Electric Company, 2011; Mitsubishi Heavy Industries Ltd., 2012; Siemens A. G., 2012). For the present study, the gas turbine *Brayton cycle* is coupled to a *Rankine cycle* with water as the working fluid. The usual choice for water is due to the fluid's availability, low environmental risks, and adequate behavior at low to medium temperatures. Other fluids should be considered, shall the Rankine cycle work at lower temperatures.

When related to gasification processes, combined cycle power plants, usually fed with natural gas, also take advantage of such fuels as coal, heavy oils, and biomass (Kehlhofer *et al*., 2009; Souza-Santos and Beninca, 2014). In spite of being more expensive than conventional plants, IGCC power plants have already been put in operation in some countries using coal. IGCC has had its concept proven, such that new projects, based on more mature technologies, may start commercial operation by 2020 (Kehlhofer *et al*., 2009; Sahraei *et al*., 2014).

Adopting the sustainability approach, biomass arises with excellent potential, with sugar cane bagasse being the main choice in Brazil, due to its abundance and its overall near zero greenhouse gases emissions (Souza-Santos and Beninca, 2014). With this solution, already proven from the technology point of view (Ståhl and Neergaard, 1998), the raw biomass is treated so as to be fed to the gasifier, where it is submitted to a partial oxidation process in the presence of an oxidizing agent, such as air, oxygen, steam, carbon dioxide, or a mixture of these (Ruiz *et al*., 2013). Onwards, the resulting gas, composed of CO, H_2, CO_2, CH_4, N_2, water vapor, and impurities such as tar, particulate matter, sulfur compounds, hydrochloric acid, ammonia and alkali metals, undergoes a cleaning process in order to meet the gas turbine inlet gas requirements (Asadullah, 2014). From this point on, the gas turbine generates power, and its exhaust gases are used to feed the bottoming Rankine cycle.

As stated by Asadullah (2014) and Kehlhofer *et al.* (2009), the IGCC technology using biomass needs to be better understood, and further developed. Hence, tools to aid the analysis of the behavior of IGCC plants are of great engineering relevance, and should consider the important aspects of these complex, but promising, systems.

3. INTEGRATED PLATFORM

The simulation platform developed in this work aims to integrate three different specialized softwares. Integration permits not only the detailed individual simulation of each equipment, but also the understanding of the effects of operational changes in one component onto the others and, consequently, onto the power plant. With an approach similar to the one undertaken by Carvalho *et al.* (2013), the platform performs accurate and comprehensive simulation of an IGCC power plant composed of a gasification process, a gas turbine, and a superheated Rankine cycle.

First, in order to simulate the gasification process, the CeSFaMB™ – *Comprehensive Simulator of Fluidized and Moving Bed Equipment* software (Souza-Santos, 1989) has been chosen. This program has already been used in several previous works (e.g., Moutsoglou, 2012; Souza-Santos and Beninca, 2014), and is capable of simulating equipment such as gasifiers, boilers, driers, and furnaces. The program deals comprehensively with the dynamics of the reaction flows in the equipment, and solves the non-linear equations derived from the mass and energy balances.

Second, the software NGGT – *Natural Gas Gas Turbine* (Ferreira, 2002) has been selected to simulate the gas turbine at steady state, operating both at design and off-design points. Several works have used NGGT to perform failure diagnostics and performance assessments of gas turbines (Barbosa and Ferreira, 2012; Celis *et al*., 2008).

Finally, the professional process simulator IPSEpro (SimTech, 2014) has been elected to simulate the superheated Rankine cycle, and, more importantly, to mediate communication amongst all the programs. The process simulator adopts a modular approach, allowing for the simulation of complex systems composed of several components chosen from a library. The plant components are represented by a set of mathematical equations, that are simultaneously solved for the whole system simulation. The software permits the creation of new component models, or the editing of existing models through the module Model Development Kit (MDK). This module allows for the communication with external functions through Dynamic Link Libraries (DLL), written in either Fortran or C++ (Carvalho, 2011).

3.1 Architecture overview

The structure adopted is such that the integration is entirely centralized in the IPSEpro program. Using MDK, models are created in order to represent the gasifier (or whichever equipment is to be handled by CeSFaMB™) and the gas turbine. In each model, the output (molar fractions, temperatures, pressures, other thermodynamic quantities) of the equipment is supplied by an external function, which is calculated by the external software, as illustrated in Fig. 1. Once the model is built, a library is compiled, and made available to the kernel *Process Simulation Environment* of IPSEpro, where the thermal system to be simulated is created.

In order to allow IPSEpro to deal with the variety of gaseous species present in the IGCC cycle, a module called *Perfect Gas* has been created (Fig. 1). Such module allocates to each gas a 28-component array. Following Ferreira (2002), each property is the result of an external function written in Fortran. Properties such as enthalpy, entropy, and specific heat are obtained from the polynomials suggested by McBride *et al*. (1993). As an example, the enthalpy of a gas with a given composition and at a specified thermodynamic state, defined by its pressure and temperature, is needed. The known data are sent by IPSEpro to the interface by means of an enthalpy function. The interface organizes the data, calls the enthalpy routine, and returns the calculated value to IPSEpro.

As the system simulation runs, the following tasks are executed for the communication between IPSEpro and the external softwares:

1. a specific function, with its input parameters properly prepared, is called by IPSEpro;
2. the respective interface first organizes the data, so that it is readable by the external program, be it CeSFaMB™, NGGT, or the Perfect Gas routine, and then calls the software;
3. after the software runs, it returns a set of output values that corresponds to the set of input parameters;
4. the interface draws the value corresponding to the function called, and sends it to IPSEpro.

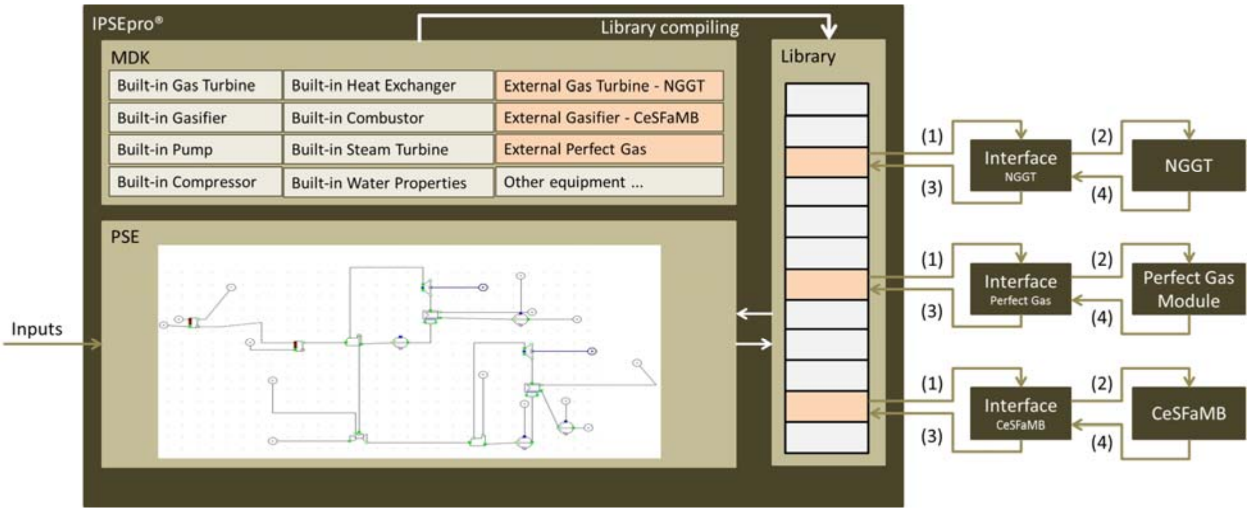

Figure 1. Information flow through IPSEpro, CeSFaMB™, and NGGT.

With this structure, each model runs independently of the others. The process simulator decides when or how many times to call each function. Hence, the external models behave, from IPSEpro's point of view, as built-in models.

3.2 Communication interfaces

The interface programs, or simply interfaces, are the core of the communication process. An interface main goal is to transfer data between IPSEpro and the respective external software. Data transfer between two interacting codes must ensure compatibility of format and unit through the two-way data flows, and be fast enough to not overly extend the simulation time.

In IPSEpro, a component model is composed of separate functions, which collectively determine its behavior. An interesting issue thus arises, when an external software – a complex specialized model that, given an array of input variables, solves a specific equipment behavior – needs to be called. In fact, as many calls as the number of output model variables are needed. From the system modeling point of view, such structure is not a problem, and works properly. However, depending on how long each call takes to run, the system simulation may become prohibitive.

In order to overcome this difficulty, a database is created to store the input data and the associated results (output data) for each new call. Hence, every time IPSEpro calls an external function, the set of input parameters is compared to each of the sets in previous runs. If there is a match, the external software is not executed, and the corresponding results are read from the database. Otherwise, it is a new set, the external software is then called, and the output (i.e., all the variables calculated by the software, and not only the one demanded by the external function) is stored. The benefit of the database is illustrated by a simple example. An external software that runs in 5 minutes and has 12 output variables, would otherwise take 1 hour to run when called successively by IPSEpro.

3.2.1 IPSEpro–CeSFaMB™ interface

In spite of sharing a similar structure, the interfaces between the different software pairs are not identical, for they have to deal with different specificities. Regarding CeSFaMB™, it requires data in an input text file to run, and provides the user with the results in an output text file, subject to internal organization rules. In order to make the interaction between IPSEpro and CeSFaMB™ automatic during simulations, the input and output files must be manipulated by the interface to enable the appropriate data flows. The approach here undertaken is to use Fortran and Perl (*Practical Extraction and Reporting Language*) routines to execute the interface tasks.

Once an external function is summoned by IPSEpro, Fortran routines are called in sequence in order to organize the data flow. First, as shown in Fig. 2, the incoming data set is compared to those stored in previous calls. If it is a new set, it is stored in the database, and then written to an intermediate file. Perl routines then manipulate this file to appropriately input the correct data to the CeSFaMB™ program.

After CeSFaMB™ has executed, a Perl routine is called in order to extract the relevant data from the output file, and write them to another intermediate file in Fortran-friendly format. A Fortran routine, in turn, captures these data, and stores them in the database to be consulted in future calls. Finally, the particular variable related to the external function called by IPSEpro is returned. Had the incoming data set been not new, and used in a previous run, the associated output would have been retrieved from the database. As already mentioned, the construction of the database has a marked influence on the runtime, mainly when a large output data set is demanded.

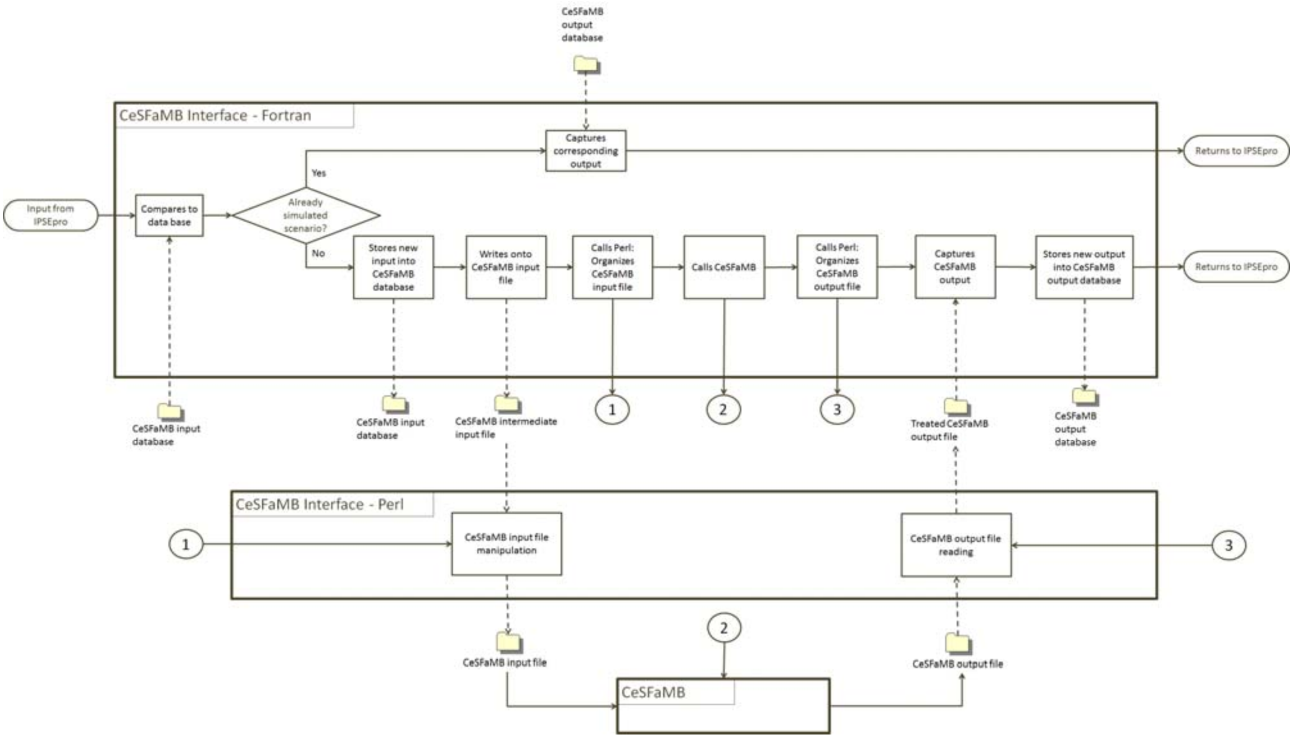

Figure 2. The IPSEpro–CeSFaMB™ interface.

3.2.2 IPSEpro–NGGT interface

On the NGGT side, the interface has a more straightforward scheme. There are two main differences between the IPSEpro–NGGT and the IPSEpro–CeSFaMB™ interfaces. First, it is not necessary to use Perl routines to manipulate the NGGT input and output data, for they are already read and written in a Fortran-friendly format. Second, NGGT is set up to distinguish between design-point simulations (NGGT.DP) and more complex off-design simulations (NGGT.OD). Thus, the necessary data sets are not the same, and the associated information flows are handled differently.

As depicted in Fig. 3, when the gas turbine is summoned by IPSEpro, the design point data, which comprise the gas turbine configuration and its design parameters, are stored. This information is relevant for both the design-point and the off-design simulations. Next, it is verified whether the requested run is for a design-point or an off-design simulation, a piece of information provided by the user in the IPSEpro environment. If it is a design-point, the NGGT.DP is called, and its output captured and returned to IPSEpro.

If the user demands an off-design simulation, the input data set is first compared to a database of previous runs. If the set has already been used in a previous run, the associated output is captured from the database, and returned to IPSEpro. If the set is new, the specific off-design data are stored in the database for future comparisons, and written to an input file. Next, the NGGT.OD is called. Once the run is complete, the model output is captured, stored, and the calculated data associated with the IPSEpro external function are returned.

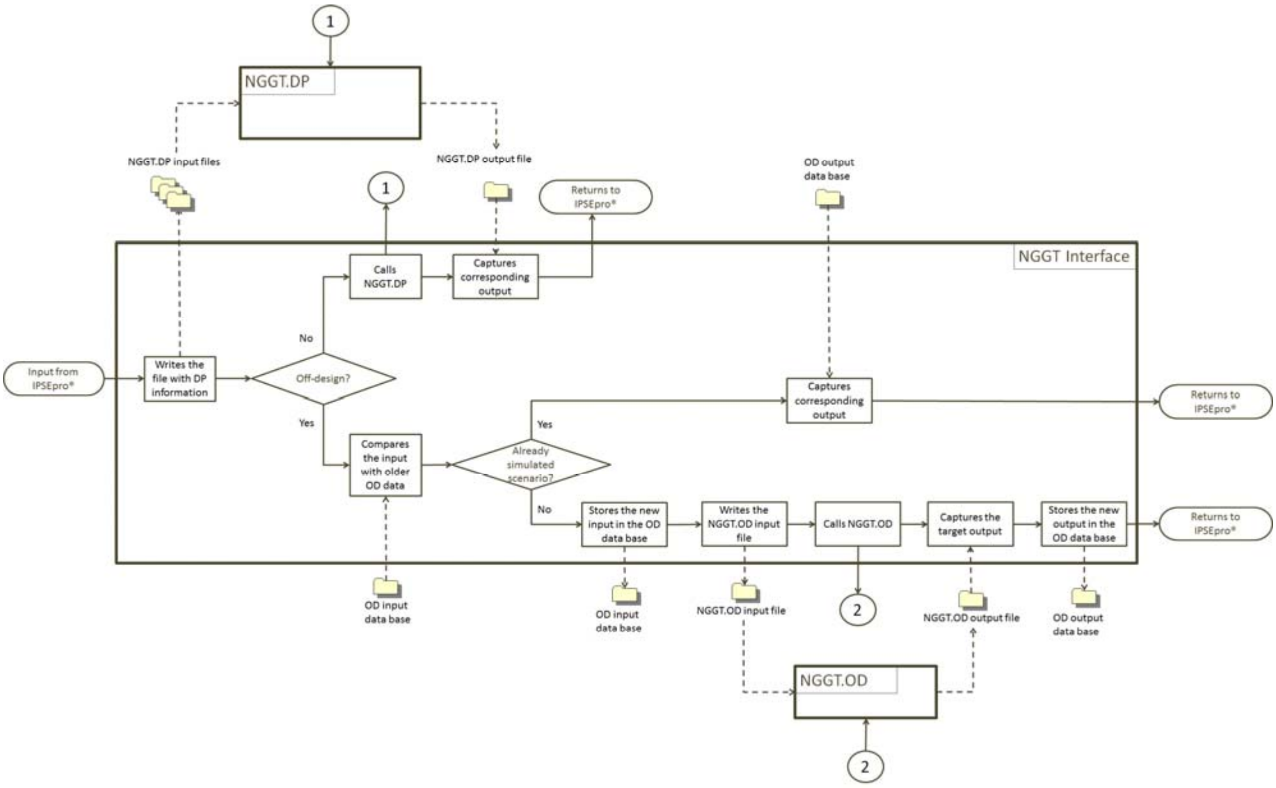

Figure 2. The IPSEpro–NGGT interface.

4. CASE STUDY

For validation of the software integration methodology described in the previous section, the IGCC power plant, configuration C, suggested by Souza-Santos and Beninca (2014) is chosen as the reference system. Figure 3 illustrates the configuration C, which includes several interesting features. The plant uses sugar cane bagasse slurry as fuel, such that the feeding process is easier. Air is used as the oxidizing agent in the gasifier, avoiding the need for an energy intensive air separation unit.

The bagasse, after undergoing the appropriate pre-treatment, is dried with the aid of the gas turbine exhaust gases, and subsequently fed to the gasifier. The resulting syngas has its temperature reduced to 800 K by a cooling system, which provides heat to a superheated Rankine cycle. The syngas is burnt in the gas turbine, and the exhaust gases provide energy to a second superheated Rankine cycle through a heat recovery steam generator (HRSG). A fraction of the gases is then compressed, and returned to the drier. The other fraction is discharged to the atmosphere.

According to the assumptions proposed by Souza-Santos and Beninca (2014), the fuel main characteristics are those shown in Tab. 1. It is also considered that the gasifier is a Bubbling Fluidized Bed equipment, due to its flexibility regarding the fuel variability, that operates at an average pressure of 2 MPa. The isentropic efficiency of both the air compressor and the gas turbine expander is estimated as 87%, and the steam turbine and pump isentropic efficiencies are assumed to be 80% and 90%, respectively. Due to the low concentration of alkaline species, it is also assumed that the energy consumption to clean the syngas is negligible. Finally, the expander inlet gas is considered to be at 1700 K, and the pinch point temperature in the HRSG downstream of the gas turbine output is set at 10 K.

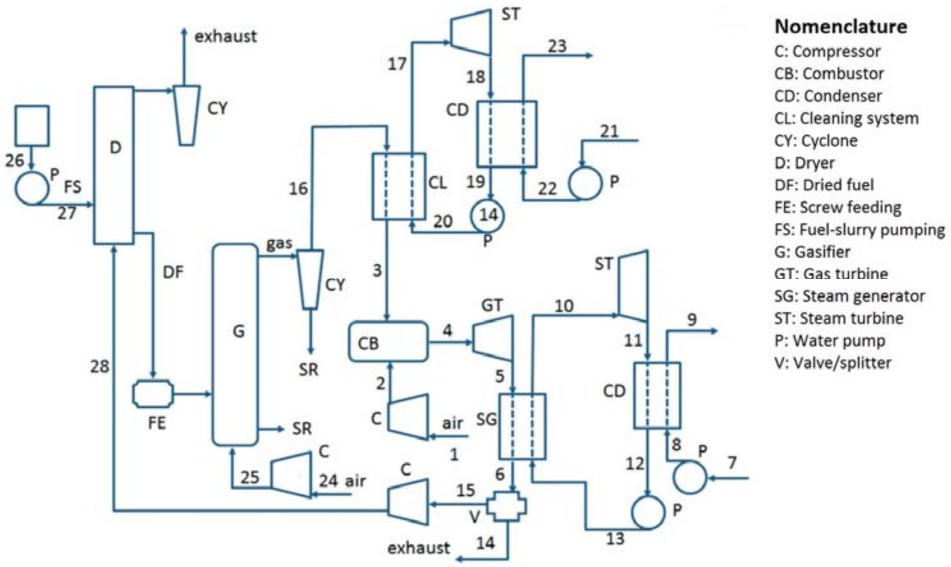

Figure 3. Reference IGCC power plant (adapted from Souza-Santos and Beninca, 2014).

Table 1. Fuel properties (adapted from Souza-Santos and Beninca, 2014).

Property	Value
Higher heating value (dry basis)	19.14 MJ/kg
Proximate analysis (wet basis)	
Moisture	50.00%
Volatile	40.78%
Fixed carbon	7.57%
Ash	1.65%
Ultimate analysis (dry basis)	
C	49.66%
H	5.71%
N	0.21%
O	41.08%
S	0.03%
Ash	3.31%

4.1 Results

Given the aforementioned integration scheme, both the drier and the gasifier are simulated by CeSFaMB™, whereas the gas turbine, which includes the compressor, the combustion chamber and the expander, is simulated by NGGT. The other system components are simulated by IPSEpro without the aid of external functions. The present results are compared to those presented by Souza-Santos and Beninca (2014). The pressures are considered input quantities, so no comparisons are made for this property. The air, gas turbine exhaust gases, and the syngas are treated as perfect gases.

It can be observed from Tab. 2, that the temperature values obtained with the integrated platform are generally quite similar to the reference results. It is first noted that the thermodynamic properties for water (streams from 7 to 13, and from 17 to 23) result from IPSEpro calculations, and have been validated against the literature (Borgnakke and Sonntag, 2013). IPSEpro uses a different enthalpy reference with respect to that adopted by Souza-Santos and Beninca (2014). Hence, an offset correction has been applied to the water enthalpy values shown in Tab. 2. The largest deviation, 31.6%, occurs with stream 18. However, the enthalpy difference for this same stream is not prominent. Because the syngas temperature in stream 16 is 1.8% higher than the reference, relatively more energy is transferred from the syngas to the water in stream 17. Such a discrepancy is then felt in stream 18.

Table 2. Comparison of integrated platform and reference results.

Temperature [K]														
Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Reference	298.0	763.4	800.0	1700.0	1046.7	350.0	298.0	298.0	350.6	999.8	386.6	330.0	330.3	350.0
Integrated platform	298.2	764.9	800.0	1730.1	1025.4	368.9	298.2	298.2	350.5	949.5	367.7	330.0	330.7	368.9
Rel. Deviation [%]	0.1	0.2	0.0	1.8	-2.0	5.4	0.1	0.1	0.0	-5.0	-4.9	0.0	0.1	5.4
Stream	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**
Reference	350.0	1070.0	854.0	407.2	317.0	317.3	298.0	298.0	308.6	298.0	766.4	298.0	298.1	864.9
Integrated platform	368.9	1089.3	1001.5	535.9	317.4	318.0	298.2	298.2	309.9	298.2	760.1	298.2	298.2	844.0
Rel. Deviation [%]	5.4	1.8	17.3	31.6	0.1	0.2	0.1	0.1	0.4	0.1	-0.8	0.1	0.0	-2.4
Enthalpy [kJ/kg]														
Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Reference	-0.21	488.3	-2848.7	38.0	-809.7	-1599.3	-15906.0	-15906.0	-15685.0	-12043.0	-13268.0	-15772.0	-15760.0	-1599.3
Integrated platform	0.00	488.5	-2865.8	82.7	-814.5	-1556.7	-15906.0	-15906.0	-15687.1	-12199.0	-13340.7	-15773.1	-15761.7	-1556.7
Rel. Deviation [%]	-100.0	0.0	0.6	117.8	0.6	-2.7	0.0	0.0	0.0	1.3	0.5	0.0	0.0	-2.7
Abs. Deviation [kJ/kg]	0.21	0.2	-17.1	44.7	-4.8	42.6	0.0	0.0	-2.1	-156.0	-72.7	-1.1	-1.7	42.6
Stream	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**
Reference	-1599.3	-2406.3	-12393.0	-13233.0	-15826.0	-15815.0	-15906.0	-15861.0	-15861.0	-0.23	491.7	-15906.0	-15904.0	-1028.0
Integrated platform	-1556.7	-2393.3	-12071.4	-13014.3	-15825.6	-15814.6	-15906.0	-15906.0	-15856.8	0.00	483.3	--	--	-1031.3
Rel. Deviation [%]	-2.7	-0.5	-2.6	-1.7	0.0	0.0	0.0	0.3	0.0	-100.0	-1.7	--	--	0.3
Abs. Deviation [kJ/kg]	42.6	13.0	321.6	218.7	0.4	0.4	0.0	-45.0	4.2	0.23	-8.4	--	--	-3.3

The compositions of the gas turbine exhaust gases and air are not given in the reference, and quite likely are a source of deviation. Differences in the exhaust gases fed to the drier and in the air fed to the gasifier can bring about discrepancies in the resulting drying and gasification processes. Regarding the enthalpy results for air (stream 1) and gases (stream 4), while the percentage deviations observed when they are near the respective reference enthalpies are large, the absolute differences are not at all significant for the cycle. In fact, for example, as the air is compressed from stream 1 to stream 2, while the absolute deviation is the same for both streams, the relative deviation falls dramatically.

In Tab. 3 the obtained syngas composition is compared to the reference. Generally, the deviations lie within a 2% margin. The largest relative deviation occurs with the ammonia content. The former is judged irrelevant because of the low absolute value of the latter.

Table 3. Comparison of syngas composition results.

Syngas composition [%mol]																				
Component	H_2	H_2O	H_2S	NH_3	NO	NO_2	N_2	N_2O	O_2	SO_2	CO	CO_2	HCN	CH_4	C_2H_4	C_2H_6	C_3H_6	C_3H_8	C_6H_6	tar
Reference	25.19	4.07	0.01	0.22	0.00	0.00	23.57	0.00	0.00	0.00	36.51	6.24	0.019	3.78	0.18	0.14	0.01	0.01	0.06	0.00
Integrated platform	24.61	4.23	0.01	0.20	0.00	0.00	23.62	0.00	0.00	0.00	36.82	6.25	0.018	3.86	0.17	0.14	0.01	0.01	0.06	0.00
Rel. Deviation [%]	-2.3	3.7	2.9	-11.1	--	--	0.2	--	--	0.0	0.9	0.2	-5.3	2.0	-0.2	-0.2	0.0	0.0	-0.2	--

5. CONCLUSIONS

In this work a strategy has been proposed to integrate three different specialized softwares. The resulting platform allows for the detailed simulation of complex IGCC power plant configurations, accurately assessing the mutual effects of the various pieces of equipment. This powerful capability is of great interest to both academia and industry, due to the growing concerns regarding sustainable and clean power generation. To this end, the comprehensive analysis of different power plant configurations is a desirable, perhaps obligatory, engineering task.

With the present integrated platform, it is suggested that future simulation studies investigate the effects of low calorific value fuels on the gas turbine performance, the influence of the biomass variability on the whole plant, and the consequence of changing the gasifier type on the power plant efficiency. These are issues, that should be addressed for the proper operation of IGCC plants run with biomass, and that can only be suitably resolved when dedicated models are employed.

6. ACKNOWLEDGEMENTS

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