EXERGETIC ANALYSIS OF COGENERATION PLANTS THROUGH INTEGRATION OF INTERNAL COMBUSTION ENGINE AND PROCESS SIMULATORS

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Abstract. Internal combustion engines (ICEs) have been used in industry and power generation much before they were massively employed for transportation. Their high reliability, excellent power-to-weight ratio, and thermal efficiency have made them a competitive choice as main energy converters in small to medium sized power plants. Process simulators can model ICE powered energy plants with limited depth, due to the highly simplified ICE models used. Usually a better understanding of the global effects of different engine parameters is desirable, since the combustion process within the ICE is typically the main cause of exergy destruction in systems which utilize them. Dedicated commercial ICE simulators have reached such a degree of maturity, that they can adequately model a wide spectrum of phenomena that occur in ICEs. However, ICE simulators are unable to incorporate the remaining of power plant equipment and processes in their models. This paper presents and exploits the integration of an internal combustion engine simulator with a process simulator, so as to evaluate the construction of a fully coupled simulation platform to analyze the performance of ICE-based power plants. A simulation model of an actual cogeneration plant is used as a vehicle for application of the proposed computational methodology. The results show that by manipulating the engine mapping parameters, the overall efficiency of the plant can be improved.

Keywords: internal combustion engine, exergy, energy systems, power plants, process simulator.

1. INTRODUCTION

Since the early days of the industrial revolution, power plant design and analysis have been important practical applications of thermodynamics. Both in energy producing facilities and energy demanding industries that generate their own power, the cost of power production can reach significant proportions of the overall operational costs. To build highly efficient power plants, the project of the thermal process usually grows in complexity to a point that the system solution depends on a large number of variables and equations. For steady-state calculations, the system is algebraic and nonlinear in mathematical nature. The practical solution of such systems depends indispensably on some kind of computational aid, usually provided by many process simulators commercially available. They all share basic characteristics, such as libraries of fluid properties and components, which model practical equipment such as heat exchangers and turbines. Exergetic analysis provides the preferred tool for power plant analysis, since it can precisely locate the processes which destroy most of the useful work of the system. The combination of this technique with economic evaluation has been studied by many authors, including El-Sayed (2003), Bejan *et al.* (1996), Kotas (1995), Lozano and Valero (1993), von Spakovsky (1986), and Frangopoulos (1983).

One of the common primary energy converters in power plants is the internal combustion engine (ICE). Since its introduction by the end of the 19th century, they have been used in industries and power plants for converting chemical energy from fuels into mechanical or electrical energy, much before being massively employed for transportation. Due to their high efficiency and excellent power-to-weight ratio, they quickly became an interesting alternative to steam engines, a position only menaced by steam and gas turbines in recent years. Nevertheless, ICEs are still used in many small to medium plants, where their cost and efficiency are very competitive. Although simple in design, the operation of internal combustion engines depends on a multitude of phenomena which are difficult to model with simple algebraic equations. The fuel vaporization, air and fuel mixing, and the combustion and expansion processes are examples of

phenomena that require more evolved modeling strategies. When modeling internal combustion engines, process simulators typically perform only an energy balance, and rely on user provided information to evaluate the properties of the engine fluids to solve this energy balance. Dedicated ICE simulators, on the other hand, can be fed with detailed engine data to calculate engine-process interface heat transfers and thermodynamic data of the cooling water, exhaust gas temperature, and heat loss to a particular power demand, thus solving the energy balance problem without coarse estimations.

The first law of thermodynamics is the most commonly used tool to perform engine simulation and analysis. However, as it shall be demonstrated, a second law analysis is desirable when engines are used as drivers in power plants. Rakopoulos and Giakoumis (2006) compiled the main publications regarding the application of second-law analysis to internal combustion engines. The authors report that those parameters whose control can increase the temperature and pressure levels in the cylinder, may lead to a reduction in combustion irreversibilities. Usually, however, this gain does not *necessarily* translate into higher power in the shaft. Instead, an increased availability appears in both exhaust gases and in the cooling fluid of the cylinder. While this increased availability would be considered waste in stand-alone engines, it may be beneficial in energy systems with cogeneration, to a point that it might be of interest to decrease the mechanical power output.

The methodology employed in the present work (Carvalho *et al.*, 2010) integrates a process simulator with an internal combustion engine simulator to construct a complete ICE-based power plant simulator, where the user can describe not only the power plant, but also intrinsic details of the engine. Engine mapping variations are taken into account by the ICE simulator. A subset of the results of the ICE simulator is then used as input to the process simulator. The purpose of this work is to investigate the effects of realistic variations of some engine mapping parameters on the power plant operation variables and global efficiency. The integration of the process simulator with the engine simulator is believed to be of great importance, since a significant source of irreversibility in an ICE-based power plant is the internal combustion engine itself. In fact, Kanoglu *et al.* (2005) identified that the combustion process may be responsible for up to 60% of the total exergy destruction in ICE-based power plants. It thus appears crucial to perform the engine simulation with greater care than would be allowed by process simulators models.

2. METHODOLOGY

2.1. Process Simulator

A wide variety of computational codes dedicated to process simulation is available, and in the comprehensive review by Silva *et al.* (2002) the main techniques employed in these codes are briefly presented. The review paper argues that the development of new process simulator codes from scratch is unnecessary, due to the extensive offer of commercial systems in the market. The choice of process simulator then becomes a matter of identifying the features of each candidate software that are desired or needed to solve the specific problem in hand. In the present study, the process simulator chosen for the integration task is the *IPSEpro* system (software version 4.0, Build 874; SimTech, 2003). A distinct feature of *IPSEpro* is that it enables users to create new component models, or to edit existing component models in the library. Other process simulators may be more complete when the number of components and representations are considered, but do not appear as flexible and robust as *IPSEpro*.

One complementary calculation implemented in the present work is the computation of exergy variables. The simulator already provides the usual thermodynamic properties of the working fluids at the various system points. Hence, the thermomechanical flow exergy e_{TM} may be directly calculated through the expression

$$e_{\rm TM} = (h - h_0) - T_0(s - s_0) \tag{1}$$

where T0 is the ambient reference temperature, h and h_0 are the fluid specific enthalpy at T and T_0 , respectively, and s and s_0 are the fluid specific entropy at T and T_0 , respectively. The chemical counterpart, however, requires the specification of the composition of each fluid stream. Therefore, a chemical exergy database has been implemented (Carvalho, 2011), so that the chemical exergy can be derived from it. The chemical exergy values assigned to the constituents encountered in this study follow the methodology proposed by Szargut *et al.* (1988). The full exergy content of the fluids is then the sum of both thermomechanical and chemical exergies, though in many cases one of these parts is sensibly predominant. Once all flow exergies are computed, one can calculate the exergetic efficiency of each equipment, as well as of the entire power plant (Bejan *et al.*, 1996).

The exergetic efficiencies defined in the literature (Rakopoulos and Giakoumis, 2006) express the ability of an equipment to convert an exergy input into desirable products,

$$\varepsilon = \frac{\text{exergy output in products}}{\text{exergy intake}}$$

For instance, for the mechanical engine exergetic efficiency, the expression becomes

$$\varepsilon_{\rm m} = \frac{\dot{W}}{\dot{m}_{\rm f} \, {\rm e_f}} \tag{3}$$

where e_f is the exergy of the fuel, which usually consists of the chemical exergy only, since the fuel is stored at ambient pressure and temperature. The mechanical engine efficiency does not take into account the exergy transfers to the cooling water or the exhaust gases. These can be accounted for by defining a global cogeneration plant exergetic efficiency, ε_g . In this case, the output products include the mechanical power and the exergy change of the utilities supplied by the cogeneration plant, and the exergy intake is still the fuel chemical exergy, such that

$$\varepsilon_{g} = \frac{\dot{W} + \sum_{i} (e_{i,out} - e_{i,in})}{\dot{m}_{e} e_{e}}$$
(4)

Another feature of the process simulator is the ability to perform plant optimizations. *IPSEpro* has an optimization module based on a genetic algorithm, where the user prescribes an objective function and defines the decision variables for the optimization problem. With the integration between the process and engine simulators, the optimization algorithm may employ engine mapping variables as decision variables. Several authors have solved optimization problems for power plants (Dimopoulos and Frangopoulos, 2008; Cordeiro, 2007; Mothci *et al.*, 2005; Manolas *et al.*, 1997), and showed that the genetic algorithm is able to reach satisfactory results, albeit sometimes at high computational costs.

2.2. Engine Simulator

As with process simulators, there are many internal combustion engine simulators available, ranging from first-law balance calculators, to two-zone models and full three-dimensional computational fluid dynamics codes (Heywood, 1988). Among the notable differences between these modeling approaches is the required computational time, which can range from minutes and hours in 0D and 1D simulations to hours and days in 3D CFD calculations. While 3D models can serve primarily to understand details of the charge mixture flow and burning characteristics inside the combustion chambers, 0D models are prone when global efficiency and energy balance variables are being analyzed. Due to the computational time requisite, and also because several ICE simulator calls are anticipated in a single power plant integrated simulation, a 0D-model software is chosen as the engine simulator for the present work.

AVL (Anstalt für Verbrennungskraftmaschinen List, Austria) is one of the companies that provide 0D- and 3Dmodel programs. *AVL Boost* (version 2009.1, Build 2009-02:04:18; AVL, 2009) is the 0D engine simulator chosen for this study. AVL also commercializes the software *AVL Fire*, which is a 3D CFD solver with chemical reactions. A typical *AVL Fire* model computation takes hours or even days to be completed. Clearly, such computational times are unrealistic for an ICE-based power plant simulation or optimization, where the number of ICE simulator calls may be in the 10¹-10³ range. Although *AVL Boost* constitutes a simplification relative to its 3D CFD counterpart, it is still much more complete than the simple ICE model embedded in *IPSEpro*.

In *AVL Boost*, the engine geometry must be described, with engine in-cylinder dimensions, and also with temperature profiles and valve timings. It is important to remark that an exact and comprehensive representation of the engine may be difficult to obtain. Within the scope of the present work, despite efforts to obtain all the engine data precisely, a small number of engine geometrical parameters has had to be estimated. Still, as it is demonstrated by the obtained results, an acceptable quantitative analysis of the cogeneration plant and engine behavior is reported.

2.3. Integration of the Two Simulators

The integration of the ICE and process simulators requires the development of several tools to promote appropriate data transfer between the different codes. A schematic diagram of the integration procedure developed in the present work is depicted in Fig.1.

IPSEpro supports the introduction of external functions by using a DLL (Dynamic Link Library) interface, so that the user can implement thermodynamic tables or more complex component calculations through C++ or Pascal codes. The DLL arguments, *i.e.*, the list of variables that are exported as function parameters as well as the expected return values, can be defined in *IPSEpro* through its Module Development Kit (MDK). A new component model called *Engine External* has been developed, in which some of the variables that participate in the mass and energy balances for the engine are calculated in *AVL Boost*, rather than defined by the user. As an example, the exhaust temperature can be implemented as a function of inlet air temperature, pressure, spark advance, air-to-fuel ratio, and compressor pressure ratio. Not all of the engine parameters have to be in the *IPSEpro* model, only those whose effects on the plant are of

concern. The engine detailed specification is fed to *AVL Boost* through a .BST input file, which can be edited using *AVL Boost* Guided User Interface (GUI).

To realize this external calculation through *AVL Boost*, the DLL receives the engine input parameters from *IPSEpro* via function calls, and writes this information into the *AVL Boost* model files. A Perl script has been embebbed into the DLL in order to reliably and efficiently manipulate the data in string-type variables within these model files. The Perl script also sets the necessary environment variables, so that the *AVL Boost* kernel can be called and perform the ICE 0D model calculations. The Perl script, executing inside the DLL, runs *AVL Boost* and checks for possible errors. Once the engine simulation is successfully completed, the results are extracted from the output files by the Perl script, which relays an appropriate subset of variables from the obtained results back to the ICE-DLL, and therefrom to *IPSEpro*. The whole procedure runs under *IPSEpro* without interruption or user intervention.



Figure 1. Schematic diagram of the IPSEpro-AVL Boost integration procedure.

In the next section, the integrated *IPSEpro-AVL Boost* simulation platform is applied to an actual cogeneration plant model to demonstrate the capabilities of the proposed methodology.

2.4. The Energy Plant

The present methodology has been applied to the analysis of a real ICE driven cogeneration plant, in order to validate the simulated results against measured data. In fact, for this plant, the thermodynamic properties of the working fluids and performance data of the equipment are available (Leite, 2008). The system, illustrated in Fig. 2, produces 3240 kW of electrical power, as well as cold water for a distributed air conditioning system with absorption chillers. In turn, these chillers run on hot water and steam, both generated using the heat transfers from cylinder walls and exhaust gases leaving the engine.

The engines have been manufactured by Caterpillar, model 3532 LE Tandem. Each 3532 engine corresponds to two 3516 engines connected by their crankshafts and to the generator. The spark ignition engines run on natural gas provided by the local city supplier, and are turbocharged to improve the volumetric efficiency. By utilizing the engine manuals and other information provided by the manufacturer representative, a faithful representation of the ICE may be constructed in the engine simulator. Some geometrical approximations have had to be made, by visiting the power plant and measuring pipe dimensions and other parts.

The engines not only provide electrical power for the site, but also supply the rest of the power plant with exergyrich material currents. High temperature exhaust gases feed boilers that generate saturated steam at 8 kgf/cm². The steam is used in an absorption chiller (Thermax EW 690 sx), which then generates cold water for air conditioning. The exhaust gases also preheat water in the economizer sections of the boilers. After leaving the boilers, the exhaust gases further heat water from the cooling water circuit. This water flow, together with the ones coming from both engines, feed another chiller (Thermax MT55s), to generate more cold water for the air conditioning system. The configuration of the described ICE-driven cogeneration plant is very common in practice, such that it is used in the present work as an appropriate typical system to demonstrate the usefulness of the integration methodology.



Figure 2. Flow diagram of the test-case cogeneration plant.

3. RESULTS

The power plant is modeled with *IPSEpro*, while *AVL Boost* is used for the engine model. The *IPSEpro* cogeneration plant and the *AVL BOOST* engine representations are shown in Figs.1-2, respectively. The total simulation time for one case is approximately 10 minutes, and convergence of the integration procedure is met after a maximum of five calls of *AVL boost*. As a starting point for the proposed analysis, the model is compared to a real plant operational data, in order to evaluate whether a base-case model of the power plant is consistent with the real case scenario. Basecase results and operational data are shown in Tab. 1 indicating a maximum deviation of 4.19%. Therefore, considering the assumptions behind models used in the simulations and on the obtained results, one can state that the model is able represent the power plant with appropriate accuracy, such that both the power plant model and the engine model appear representative of the involved engine-plant phenomena and interactions.

It is important to mention that the AVL Boost output variables may contain small uncertainties, such that the solution of the engine model energy and mass balance equations by *IPSEpro* may become impossible. In order to overcome this difficulty, one variable calculated by AVL Boost is made available for *IPSEpro* modification, lending some degree of freedom to the resulting system of algebraic equations being solved. In the present work, the chosen variable is the overall engine heat loss as understood by *IPSEpro*.



Figure 3. Engine model in AVL Boost (only one side of the tandem configuration is shown).

Table 1.	Comparison	between e	xperimental	data and	simulated	power	plant resul	ts

	\dot{m}_a (kg/s)	$\dot{m}_f~({\rm kg/s})$	\dot{E}_{e} (kW)	$\dot{E}_{_{W}}$ (kW)	\dot{E}_l (kW)	\mathcal{E}_{g}
original power plant	2.5658	0.09806	708.83	209.9	2520.8	0.3471
IPSEpro-Boost	2.5851	0.09912	705.42	201.1	2513.9	0.3589
	+0.75%	+1.08%	-0.48%	-4.19%	-0.27%	+3.40%

With respect to the base configuration, the sensitivity of power plant data to specific engine mapping parameters are analyzed. The influence of several engine parameters available for variation within *AVL Boost* may be evaluated, such as the influence of cylinder wall temperature, compressor output pressure. For the current initial analysis, the influences of the spark ignition timing (ζ) and on the equivalence ratio (λ) are studied. These parameters can be readily manipulated in the real plant engine, and sensible variations in the engine, power output, and heat transfers are expected.

Initially, variation on the spark advance ($\Delta \zeta$) from -5° to 10° from TDC are imposed from the engine nominal value, and the impacts on the exergetic efficiency, the exhaust gas exergy, and the exergy transfered to the engine cooling water in the cylinder walls are shown in Fig. 4. As spark ignition advances, the fuel heat release occurs earlier in the combustion cycle so that in-cylinder temperatures and heat transfer rate to the cooling water both increase, but the exhaust temperature drops. Figure 4a indicates that the exergetic efficiency may reach a maximum with some spark advance from TDC. From Fig.4b, one observes that by advancing the spark timing from its original value, some of the heat that would be transferred to the exhaust is otherwise transferred to the cooling water. The power plant still benefits from the new temperature conditions, since higher exergy is available to the water chillers.

The equivalence ratio influence on the plant and engine parameters have also been analyzed. As shown in Fig. 5, as the air-fuel mixture becomes richer in fuel, the global exergetic efficiency improves, reaches a maximum and then decreases. The rich mixture provides more exhaust exergy and cooling water exergy for the chillers, up to a point where the additional fuel being used overcomes the benefit of the excess exergy provided.



Figure 4. Influence of spark advance on the exergetic efficiency (a) an on the exhaust gas exergy, and exergy transfer to the engine cooling water at the cylinder walls (b).



Figure 5. Influence of the air to fuel ratio variation on the exergetic efficiency (a) and on the exhaust gas exergy, and exergy transfer to the engine cooling water at the cylinder walls (b).

In view of the plant evaluation based on the chosen engine mapping parameters, it becomes clear that the engine will benefit from both a greater ignition advance and a richer mixture. It is thus of interest to formulate an optimization problem for the plant with the engine mapping parameters as decision variables. The objective function chosen here is the global exergetic efficiency of the plant,

$$\mathcal{E}_{g} = \frac{\sum_{i} \dot{W}_{i} / \dot{m}_{f,i} + \sum_{j} (e_{j,2} - e_{j,1})}{e_{ch}}$$
(5)

where in this case $W_i / \dot{m}_{f,i}$ are the specific power for both engines and $(e_{j,2} - e_{j,1})$ the difference between the output and input of the air conditioning water passing both chillers. The decision variables are the equivalence ratio (λ) and and spark advance deviation from the engine's nominal value ($\Delta \zeta$).

As mentioned earlier, the process simulator has a built-in genetic-algorithm optimizer (SimTech, 2003). A careful selection of the genetic algorithm parameters is required, because each simulation takes several minutes to converge. Thus, the population size is minimized, whereas the number of generations is increased. It should be noted that, instead of the optimization procedure carried out in the present work, a response surface could have been obtained for the engine response with respect to different spark advance and mixture formation settings. However, because the present methodology can be applied to several other engine mapping parameters, such as cooling water temperature and fuel properties, the several input dimensions would render a response surface solution strategy relatively difficult to obtain.



Figure 6. Objective function results along several generations of the genetic algorithm.

The evolution of the exergetic efficiency within the optimization processes is depicted in Fig.6. The optimized spark advance and mixture composition are presented in Tab. 2. As detected in the individual sensitivity analysis (Figs.4-5), the power plant exergetic efficiency benefits from a greater spark advance and leaner mixture. The results obtained with the developed methodology indicate that by changing the mapping parameters, the original chemical exergy of the fuel gets redirected to different destinations. As illustrated in Fig. 7, the engine acts as an exergy router which can change the percentage shares of shaft power, cooling water heat transfer and exhaust exergy content as its parameters are manipulated.

Table 2. Optimum engine mapping parameters, obtained with the genetic algorithm optimization.

λ	$\Delta \zeta$	\dot{m}_a	$\dot{m}_{_f}$	\dot{E}_{e} (kW)	\dot{E}_w (kW)	\dot{E}_l (kW)	\mathcal{E}_{g}
1.4989	+3.2	2.5934	0.09983	703.27	207.8	2489.0	0.3615



Figure 7. Illustration of the engine as an exergy router for the chemical exergy of the fuel.

It is important to remark that uncertainties in the internal combustion engine geometrical description can lead to numerical difficulties and even prevent convergence of the engine simulator. This issue is specially critical for calculation involving optimization. Despite efforts to obtain all the engine data precisely, a small number of engine geometrical parameters has had to be estimated for the present work. Comparison between plant measured and simulated results indicates that the estimated values fall within the precision of the calculations. Nevertheless, an ongoing effort to obtain complete and precise engine geometrical data remains.

4. CONCLUSIONS

A new methodology, which integrates an engine and a process simulators, able to analyze the impact of engine mapping parameters on the global exergetic efficiency of the energy system has been proposed and implemented. The insights of the results point to a promising strategy for improvement of ICE driven power plants.

An ICE driven power plant is analyzed in the light of this methodology, supplying new insights on how to increase overall efficiency. The manipulation of spark advance and mixture composition provides a different balance between mechanical power output, cooling water exergy transfer, and exhaust gas exergy. Thus, in the context of the power plant analyzed, exergetic efficiency is increased.

The genetic algorithm native to the process simulator has been employed. The optimum operating point of the engine has been identified for the power plant configuration. As the objective function gradient appears smooth, a high number of generations with small population size have been able to reach the optimum target.

Other considerations shall be made for the application of this technique, such as full emissions consideration, metallurgical limits of the engine materials, and combustion knocking, that can limit the amount of spark advance or impose a leaning limit for proper ignition.

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