Energy and environmental analysis of an entire coke production plant using ECLIPSE

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SUMMARY

In the present work the sequential code ECLIPSE is used to perform an energy analysis of an entire industrial process—a coke production plant—aiming its characterization and optimization in terms of energy requirements and environmental impact. The code is validated by comparing its results against existing experimental data acquired at the above-referred plant, for the present operating conditions. Agreement is observed to be rather good, as the maximum relative errors between the ECLIPSE predictions and the actual values are 9.2, 9.7 and 8.7 per cent, respectively, for mass flows, temperatures and pressures. Moreover, those errors occur only once and at different streams, the vast majority of the relative errors for the remaining streams being below 1.0 per cent. In order to optimize the process both as far as energy and environmental aspects are concerned, alternative or new unit operations are suggested and are included in the production flow sheet or added to it and the entire new processes are simulated. More specifically, the better sealing of the coke ovens doors eliminating 80 per cent of the volatiles escape, the recovery of the lost sensible heat in the coke extinction operation and the restart of the 10 non-productive coke ovens would yield remarkable energy savings-losses would reduce from 46 440 to 9260 kW, apart from the environmental benefits emerging from the elimination of the volatiles escape to the atmosphere. In addition, for the coke gas cleansing sub-process, the substitution of the stripping process in the column distillation by a separation process, making recourse to a reverse osmosis installation, together with the operation setting of the ammonium destruction oven at a more convenient temperature, would allow both for energy savings of 66 per cent and a substantial reduction in both gaseous and liquid emissions, namely naphthalene, ammonia, nitric oxides and sulphur oxides. The improvements attained are noticeable and encouraging. Therefore, ECLIPSE proved to be an adequate tool for global industrial processes simulation, analysis and optimization, in spite of some limitations exhibited by the code in simulating detailed complex physical phenomena, such as combustion or coal distillation. Copyright © 2001 John Wiley & Sons, Ltd.

KEY WORDS: energy analysis; environmental analysis; coke production process; optimization; industrial process design; ECLIPSE code

1. INTRODUCTION

During the last two decades, the problem of energy consumption within industrial processes has called the attention of several researchers and industrial engineers, whose work has been directed

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Received 19 November 1999 Accepted 11 January 2000 towards its reduction without sacrificing the production, the product quality and, more recently, the environment. The reduction of the energy consumption in any industrial process requires the definition of its controlling parameters and of the process dependence on them, a task that may not be simple. Until a few years ago, this had been done by empirical methods, extrapolating data from similar equipments. However, it is presently recognized that this approach can lead to erroneous conclusions and new approaches have been developed.

Mathematical models able to quantify the effect of the various parameters on the global performance of the system have been lately developed and applied to actual industrial processes, this approach having not been possible until the development of digital high-speed computers due to the complexity of the phenomena occurring in general industrial processes. With the advent of such computers it is presently possible to simulate an industrial process and to obtain quantitative and qualitative indicators of its performance. After the simulation completion of the actual process it constitutes a simple task for researchers and industrial engineers to numerically experiment changes in the operating parameters of the process aiming possible improvements.

As a consequence of the latest developments in the area of process simulation, following the above-mentioned approach, several commercial computer codes have recently appeared in the market. For instance, Sundberg and Wene (1994) developed a non-linear model of analysis and optimization of flow systems. It was named MIMES and was successfully applied in the energy optimization of a paper mill. Bridgwater and Double (1994) developed the AMBLE program to technically and economically simulate a vast range of technologies to obtain liquid fuels from biomass. Bridgwater and Anders (1994) modelled several indirect coal liquefaction processes through computational sequential codes. Goldthorpe et al. (1994) presented the ACCESS code that permits the execution of parametric studies on the thermodynamic performance and on economic analysis of direct coal liquefaction processes. The ACCESS code was successfully tested in the initial stages of the coal liquefaction systems of the British Coal Corporation. Williams and McMullan (1994) reported the development of the package ECLIPSE. This package, which runs in an ordinary personal computer under the MS-DOS environment, allows for technical and economic simulations of industrial processes, and was tested and validated with the coal liquefaction systems of the British Coal Corporation, providing results in good agreement with those of ACCESS. Caldas et al. (1998) modelled and optimized, in terms of energy consumption and emissions, a coke gas cleansing process and a steel industry power plant using the ECLIPSE code. The authors obtained a set of results that were most encouraging to proceed with the use of ECLIPSE sequential code to analyse and improve industrial processes. Pinto et al. (1999) used the same code—ECLIPSE—to simulate in terms of energy requirements an industrial process of cement production. The results obtained with ECLIPSE were also encouraging as they were in good agreement with the actual consumption values obtained from the plant.

The present work extends that of Caldas *et al.* (1998) to the study of the entire coke production plant, including the coke gas cleansing plant. The ECLIPSE code is utilized herein to perform energy and environmental analysis of the above-mentioned industrial process and is evaluated as a tool for industrial processes analysis, characterization and optimization.

Notice should be given to the fact that such kind of sequential codes produce results based on global mass and energy balances and are, therefore, not appropriate for detailed design of equipments. The latter requires a totally different approach. Nevertheless, in an industrial process, both the replacement of a unit operation by another more efficient and the enlargement of a process achievable through the inclusion of new unit operations require a previous study and analysis of the energy, environmental and economic impacts on the process caused by such

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modifications. It is for this kind of study that sequential codes like ECLIPSE may constitute a very powerful tool.

2. THE ECLIPSE CODE

In order to perform the simulation of an industrial process with the ECLIPSE code it is first necessary to set the process boundaries and to establish its flow sheet. This is done in terms of modules—chemical engineering unit operations and reactors—connected together by streams: process flows. These streams are composed of a specified number of compounds, named the chemical components. These compounds must be previously defined in a compound database (see ECLIPSE, 1992). It should be noted that this database does not support radicals or ions, making difficult the simulation of detailed chemical reactions, such as combustion.

After the definition of the process flow diagram and the specification of the required technical data for each module, the program checks for consistency between the process technical data and the compound database. If no inconsistencies are found the equilibrium mass and energy balances are then automatically evaluated. For that, ECLIPSE has incorporated specific routines to calculate the necessary thermodynamic properties from the more fundamental data available at the compound database. When a convergent solution is attained the stream densities are calculated. It is then possible to calculate the process utilities requirements. The program matches the available utilities, as defined in the respective database, to the requirements of the process and then evaluates the differences that constitute the imported fuel usages. This concludes the technical evaluation of the process.

The conclusion of the technical evaluation allows for the economic calculations. To perform the economic analysis it is necessary to estimate the process and utilities capital cost. This estimation is based on the data obtained by the mass and energy balance, utilities usage calculations and on the operation and economic factors and indices specified on the cost database. Additional engineering cost data are also required which vary with module and equipment types. It is then necessary to calculate the process operating costs. These include the streams and fuel costs. As in the case of capital costs this evaluation is based on the data obtained by the mass and energy balances and utilities usage calculations, and on the operation and economic factors and indices specified in the cost database.

The previously described features make of ECLIPSE an appropriate tool to globally analyse a process and to perform process integration up to a certain level, that is, to characterize a process and to optimize it by identifying the less efficient unit operations and replacing them by more efficient ones. However, the code is hindered to perform detailed simulations of some particular equipments or by-processes, due to the way used by ECLIPSE to define them in terms of modules. Each module represents a unit operation and is usually restricted to some approximations, not always reliable to the case under study. For example, each chemical reaction module is either isothermal or adiabatic and only one equilibrium reaction is allowed to be defined within it. This makes it extremely difficult to perform a rigorous treatment of combustion systems or coal distillation ovens for coke production without resorting to a considerably high number of modules. Moreover, the sequential and iterative nature of ECLIPSE can make the optimisation of a process somehow lengthy, sometimes being necessary to resort to a trial and error approach. Indeed, due to some lack of flexibility of the input data allowed by the program, it becomes sometimes necessary to produce several outputs, adjusting the input data several times. For

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example, if a stream is to be defined with given temperature and quality, parameters that are frequently known *a priori*, an iterative procedure is required since temperatures and pressures are the only assignable thermodynamic variables. Therefore, it is necessary to establish the following routine procedure: estimation of the pressure of the stream, production of an output, check of the value of the stream quality and correction of the value of the pressure. This process has to be repeated until the quality output attains the required known value.

On the other hand, the modular and sequential structure of the program becomes most convenient to thoroughly simulate large processes, as the case studied herein. The possibility of calculating the utilities usage with minimum effort after the achievement of a convergent solution for the mass and energy balances becomes extremely convenient. In fact, it avoids the fastidious and repetitive non-automatic calculations usually performed when such type of codes is not available. Moreover, the integration of the economical and the technical calculations provides more reliable results than those that would be produced with independent calculations.

3. THE INDUSTRIAL PROCESS ANALYSED

This section presents the case selected to validate the ECLIPSE code—an entire coke production plant. The plant is thoroughly studied: from the coal preparation process collected at the coal yard up to the incandescent coke extinction operation, including all the sub processes, namely the coke gas cleansing. Owing to the size and complexity of the industrial process studied in this work only energy and environmental analysis are performed, that is, the economic study is not performed herein. Besides the validation of ECLIPSE by means of comparison of the predicted values against the corresponding experimental data acquired at the plant, the code is also used herein to optimize the process, as far as energy consumption and emissions are concerned.

As mentioned earlier, the process analysed in this work is that of an entire coke production plant of the Portuguese Steel Industry (Siderurgia Nacional, Empresa de Serviços SA). Coke, that may be regarded as the reduction element in a blast furnace process, is the main product obtained from the distillation of the metallurgic coal, operation that is performed in batteries of coke ovens. In the coke production process coal is submitted to a distillation process where it is heated up to a temperature of about 1300°C in an inert and temperature-controlled atmosphere to prevent combustion, that causes the release of all its volatile components. Therefore, additionally to coke, several high-energy content by-products are also extracted from this volatised elements, such as coke gas, coal tar and ammonia, that are usually obtained in a separated plant. Both above-mentioned plants are described below.

3.1. The coke production plant

The coke production process is a complex one as it involves a high number of different unit operations with an intricate network of process flows connecting them (see Figure 1). Moreover, the number of solid, liquid and gaseous compounds that constitute the huge amount of process flows is also high, which makes it a process difficult to be simulated.

The process under study is initiated by the coal preparation where the required blending is made ready in two steps, the first step comprising the coal collection from the yard and its transportation, milling and storage into the appropriate dosing granaries. The second step includes the blending and mixing of different coals in the mixer, after collecting them from the

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 $\begin{array}{l} AMV - Ammonium \ oven \ ; \ AW1 - Ammonia \ washer \ 1; \ AW2 - Ammonia \ washer \ 2; \ B1 \ to \ B13 - Pumps; \\ BAT1 - Battery \ of \ coke \ ovens \ 1 \ (28 \ ovens: \ 18 \ productive \ and \ 10 \ non \ productive); \\ BAT2 - Battery \ of \ coke \ ovens \ 2 \ (14 \ productive \ ovens); \\ CET - Coke \ extinction \ tower; \\ CGT - Coal \ granary \ tower; \\ CHIL - Coal \ mill; \ COYA - Coal \ yard; \\ CPRP - Coke \ preparation; \\ CT - Creosote \ tank; \ DC - Decanter; \\ DCLC - Decalcification; \ DCO - Distillation \ column; \ DGR - Dosing \ granaries; \\ ETP - Electrostatic \ tar \ precipitator; \ FCD - Final \ condenser; \\ FN - Fan \ (radial \ ventilator); \ GCO - Gas \ collector; \ HE1 - Heat \ exchanger \ 1; \\ HE2 - Heat \ exchanger \ 2; \ ITT - Intermediate \ tar \ tank; \\ MIX - Mixer / blender; \ MT - Mixture \ tank; \ NW - \\ Naphthalene \ washer; \ PC1 - Purge \ collector \ 1; \ PC2 - Purge \ collector \ 2; \ PCD - Primary \ condenser; \ SP - \\ Separator; \ STT - Small \ tar \ tank; \ TCH - \ Torch; \ TT - \ Tar \ tanks; \ WA1 - Ammonium \ water \ tank \ 1; \ WA2 - \\ Ammonium \ water \ tank \ 2; \ WRS - Water \ re-pumping \ station \ Fantary \ Ammonium \ tank \ 2; \ WRS - Water \ re-pumping \ station \ Fantary \ Sampling \ station \ Fantary \ Sampling \ station \ Fantary \ Sampling \ Sampling \ Sampling \ Sampling \ station \ Sampling \ Sampling$

Figure 1. Detailed flow sheet of the coke production plant.

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Figure 2. Schematic view of the batteries ovens.

appropriate granaries, according to the properties of the type of coke required. After the achievement of the blending the coal is stored at the granary tower. The present study is referred to a coal blending with mass percentages of 45 per cent of Fording Coal, 25 per cent of Race Fork Coal and 30 per cent of Pinnacle Coal.

The blending of coals is then fed to both the existing coke ovens batteries: battery 1 with 28 ovens (10 of which are non-productive due to coke production restrictions) and battery 2 with 14 ovens.

Figure 2 shows a scheme of the batteries structure. As it can be observed, the distillation chambers or coke ovens (No. 5, Figure 2) are separated by dense silica walls, named *piedroit* (No. 4, Figure 2). Each distillation chamber, exhibiting 15 m length (L), 6.3 m height (h) and 0.4 m width (l), is adjacent to two neighbouring narrow combustion chambers where coke gas is used as fuel, energy of which released in the combustion process is used to heat up the *piedroits*. Heat is then conducted through the silica walls to heat up the coal at a defined slow and controlled rate, in order to ensure a correct distillation process. The efficiency of the batteries is improved by using the sensible heat of the exhausting combustion products to preheat the incoming air of combustion. This heat exchange is performed in the refractory blocks of regenerators that operate in a cyclic way in order to allow air and exhaust gases to commute their passage through the blocks. These blocks are either being heated up by the exhaust gases or being cooled down by the incoming air.

The coal feeding into the batteries is made by gravity through a feeding machine that circulates on the batteries ceiling. In turn, the coke extraction is made through the narrow coke ovens doors located at their front walls. The leaving coke is at a very high temperature (incandescent state) and has to be cooled down (extinguished) prior to its preparation. This operation is performed at the coke extinction tower (see Figure 1) using water as heat sink. After leaving the extinction

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tower the coke is reduced in size by mechanical preparation to be fed to the blast furnace or to be sold.

3.2. The coke gas cleansing plant

The volatile components released during the coal distillation are the constituents of raw coke gas and are collected in an adequate equipment: the gas collector. This coke gas is to be used as a gaseous fuel but, due to its high content of impurities, has to be previously cleansed. This fuel, as mentioned before, will be primarily used to heat up the distillation ovens and, as it is normally produced in excess, will be used elsewhere in the steel plant.

In the present application it is intended to optimize the energy consumption of the entire plant, keeping the coke and gas production and the gas quality standards, the latter established on the basis of its impurity contents at the process outlet. A serious problem existing in this kind of processes is the fouling of valves and burners due to the presence of naphthalene in the gas composition. It has been established that to prevent this from occurring a well-defined temperature profile must be observed, which will cause the majority of the naphthalene to condense in the appropriate locations inside the cleansing system.

In the gas collector (see Figure 1) the raw coke gas emerging from the batteries is cooled by water injection down to a temperature low enough to prevent damaging of subsequent equipments. In the electrostatic precipitator dust and tar particles in suspension are removed. Further downstream, in the naphthalene washer, a creosote shower, creosote being a solvent for naphthalene, removes some of the remaining naphthalene, after the ammonia removal in the two sequential ammonia washers. The mixture of water and ammonium, resulting from the washing operations and referred to as ammonium water from hereafter, is stripped in a distillation column and the resulting ammonia is burned in the ammonium oven. All the tar removed from the gas is stored in the tar tanks and is to be sold as fuel. Primary condensers and a final condenser are located in the upstream side of the coke gas cleansing plant to remove from it the tar and the water, by condensation. A detailed description of the entire process can be found in the work of Magrinho (1999).

4. RESULTS AND DISCUSSION

In order to characterize and quantify the energy consumption of the process, data referring to the three-month period from October to December 1998 was measured and collected. With this data, and after a statistical treatment, the process was analysed and quantified with resort to non-automatic calculations, in order to allow for the validation of the ECLIPSE code. It should be mentioned that during the period under analysis the required temperature profile for the gas cleansing process mentioned earlier was not observed and, therefore, the simulation was performed with the actual temperature profile.

4.1. The actual process

As both mass flow rates of the produced raw coke gas and of the volatile losses through the ovens doors were unknown, the simulation of the coke production process and that of the coke gas cleansing process had to be performed separately (see different boundaries in Figure 1). The agreement observed between the non-automatic calculations based on measurements and the

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| | Maximum mass flow error (%) | Maximum temperature error (%) | Maximum pressure error (%) |
|-----------------------|-----------------------------|----------------------------------|-------------------------------|
| Batteries process | 9.2 | 3.6 | 1.6 |
| Gas cleansing process | 4.3 | 9.7 | 8.7 |

Table I. Maximum relative errors between non-automatic calculations and predictions using ECLIPSE.

Table II. Energy rate consumption in the batteries process.

| Energy flux | | | | | | |
|-------------|---------|------|---------------------------------|---|------|-----|
| Inlet | | | Outlet | lan an a | | |
| Stream | (kW) | (%) | Stream | (kW) | (%) | |
| Coal | 398 943 | 90.1 | Coke | 295 863 | 67.2 | 1.1 |
| Coke gas | 389 501 | 8.8 | Raw coke gas | 99726 | 22.7 | |
| Air | 4983 | 1.1 | Volatile escape losses | 22 2 5 3 | 5.1 | |
| | | | Exhaust gas losses | 9538 | 2.2 | |
| | | | Convection and radiation losses | 12908 | 2.9 | |
| Total | 442 877 | 100 | Total | 440 288 | 100 | |

corresponding predicted values with ECLIPSE is fairly good as it can be seen from Table I, where the displayed maximum errors occur only once and at different streams for each property. Moreover, the vast majority of the errors for the remaining streams is below 1 per cent.

The errors presented in Table I were calculated according to Equation (1), where measurements refer to measured and non-automatically calculated values.

$$Error = \frac{|ECLIPSE \text{ predictions} - \text{measurements}|}{\text{measurements}} \times 100 \tag{1}$$

The maximum errors obtained are acceptable given the uncertainties of measurements and the simplifying assumptions used in the non-automatic calculations. Moreover, it must be stressed that due to the number representation used by ECLIPSE, which is of the form xxxx,xxx, the smallest possible mass flow representable by ECLIPSE is limited to 1 g s^{-1} . In the studied process there are small gaseous fluxes, the smallest being around 5 g s^{-1} , that suffer severe rounding errors. On the other hand, the errors have also the origin in the simplifying assumption, used in the non-automatic calculations, of disregarding the interaction between water vapour and other gas constituents, that is taken into account by the ECLIPSE algorithm.

The energy rate consumptions of the actual processes, both for the batteries plant and for the gas cleansing plant are shown in Tables II and III. As it can be observed from Table II, the energy balance to the batteries process exhibits a relative closing error of 0.5 per cent (an inlet energy flux of 442 877 kW to an outlet energy flux of 440 288 kW), that is extremely good. For the gas cleansing process Table III contains also a comparison between the non-automatic calculated

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100

| Er | nergy rate consumption (kW) | | |
|--------------------------------|--------------------------------|-------------------|-----------|
| Equipment | Non-automatic values | ECLIPSE values | Error (%) |
| Gas collector | 30.1 | 32.9 | 9.3 |
| Separator | 0.0 | 0.0 | 0.0 |
| Primary condenser | 99.9 | 96.9 | 3.0 |
| Fan | 141.6 | 135.7 | 4.2 |
| Electrostatic tar precipitator | 4.1 | 4.2 | 2.4 |
| Final condenser | 21.9 | 20.8 | 5.0 |
| Ammonia washer 1 | 2.9 | 2.9 | 0.0 |
| Ammonia washer 2 | 4.0 | 4.0 | 0.0 |
| Naphtalene washer | 2.1 | 1.9 | 9.5 |
| Small tar tank | 3.0 | 3.0 | 0.0 |
| Intermediate tar tank | 7.8 | 7.9 | 1.3 |
| Tar tanks | 18.9 | 18.8 | 0.5 |
| Mixture tank | 0.0 | 0.0 | 0.0 |
| Distillation column (NH3) | 1381.3 | 1384.4 | 0.2 |
| Pumps | 366.2 | 366.2 | 0.0 |
| Total | 2083.8 | 2079.4 | 0.2 |

Table III. Energy rate consumption in the gas cleansing process.

energy rate consumptions and the corresponding ones predicted by ECLIPSE, revealing a very good agreement—0.2 per cent of error in the total energy flux. The major differences are referred to the gas collector and to the naphtalene washer with relative errors of, respectively, 9.3 and 9.5 per cent. However, both equipments have a pale contribution to the total energy consumption. Indeed, as it can be seen from Table III, the major energy consumer in the gas cleansing plant is the distillation column, representing 68 per cent of the total coke gas cleansing plant consumption. It should be noted that this unit operation exists only for environmental purposes, since the resulting ammonium is burned further downstream in the ammonium oven, which consumes cleansed coke gas. Moreover, the distillated water is not pure, but contains naphtalene and ammonium and is discharged into the river. These are the reasons why the distillation column requires a detailed analysis, including the possibility of its substitution in the process, in order to make it more environmental acceptable and less energy consumer, that is, more efficient. Another environmental flaw of the process is the NO_x emissions emerging from the ammonium oven, a point to be also dealt with in this work.

Table IV shows the comparison between the non-automatic values of the energy rate consumptions for the batteries and the corresponding ones predicted by ECLIPSE. As it can be observed, the code predicts very acceptably the process under study as the maximum relative error—7.5 per cent—is referred to the losses in the exhaust gases, which are originated by temperature errors in the ECLIPSE calculations.

Table V contains both the specific coke gas consumption for the batteries reported to the unit of coke production and the specific energy consumption per equipment in the cleansing gas plant reported to unit of cleansed coke gas produced. Comparison of those values against the

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| Energy flux | Batteries | | | |
|--|------------------------------------|------------------------|--------------|--|
| | Non-automatic calculations (kW) | ECLIPSE values (kW) | Error (%) | |
| Energy for coal distillation | 22736 | 23 1 39 | 1.8 | |
| Convection and radiation heat losses | 12908 | 13169 | 2.0 | |
| Sensible heat exhaust gases losses | 9538 | 8823 | 7.5 | |
| Auxiliary equipment energy consumption | 92 | 92 | 0.0 | |
| Losses from coke extinction | 10406 | 10 505 | 1.0 | |
| Volatile escape losses | 22 253 | 22 555 | 1.4 | |

Table IV. Comparison of energy rate consumptions in the batteries process between nonautomatic calculations and ECLIPSE predicted values.

Table V. Specific coke gas consumption in the batteries and specific energy consumption in the gas cleansing process.

| | Specific mass consumption $(kg_{gas}kg_{coke}^{-1})$ | | | |
|--|--|-------------------------|-------------------|--|
| Equipment | Non-automatic calculations | ECLIPSE values | Error (%) | |
| Battery 1 (28 furnaces, 10 non-productive) Battery 2 (14 furnaces) Total | 0.108 0.091 0.100 | 0.108 0.091 0.100 | 0.0 0.0 0.0 | |
| | Specific energy consumption $(kJ kg_{eas}^{-1})$ | | | |
| Equipment | Non-automatic calculations | ECLIPSE values | Error (%) | |
| Gas collector | 15.5 | 17.0 | 9.7 | |
| Separator | 0.0 | 0.0 | 0.0 | |
| Frimary condenser | 51.5 | 50.0 | 2.9 | |
| Fan Electrostatic ter precipitator | /3.0 | /0.0 | 4.1 | |
| Electrostatic tar precipitator | 2.1 | 2.1 | 0.0 | |
| Ammonia washer 1 | 11.5 | 10.7 | 5.5 | |
| Ammonia washer 2 | 2.1 | 1.5 | 0.0 | |
| Nanhtalene washer | 1 1 | 2.1 | 9.1 | |
| Small tar tank | 1.5 | 1.0 | 1.3 | |
| Intermediate tar tank | 4.0 | 4.1 | 2.5 | |
| Tar tanks | 9.8 | 9.7 | 0.9 | |
| Mixture tank | 0.0 | 0.0 | 0.0 | |
| Distillation column (NH3) | 712.0 | 714.0 | 0.3 | |
| Pumps | 188.7 | 188.7 | 0.0 | |
| Total | 1074.1 | 1072.5 | 0.2 | |

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corresponding ones predicted by ECLIPSE is also displayed in Table V. Once again, as it can be seen from that table, the results do agree quite well.

4.2. The process optimisation

As mentioned before, in the coke gas cleansing plant the distillation column is the main energy consumer and its replacement is studied herein. Membrane separation process appears to be the best alternative to the distillation operation. However, it is not an easy task to separate NH_3 from H_2O through a membrane process, since the two molecules are very similar, as it can be inferred from their molecular weight, respectively, 17 and 18. Therefore, the finest membrane process (reverse osmosis) will be required (Marr & Koncar, 1993). Ho and Sirkar (1992) showed that separation efficiencies of 90 per cent can be attained through reverse osmosis using pressures up to 105 bar. For the present process higher efficiencies are requested, being therefore necessary to resort to two reverse osmosis separation units installed in sequence, allowing the accomplishment of a separation efficiency of 99 per cent, which is satisfactory for the present application.

The water resulting from the above-mentioned separation process will be almost pure water and can, therefore, be recycled and re-used in the ammonium washers, avoiding the need for such large amounts of fresh water in the process, as that required by the actual plant. The concentrate resulting from the reverse osmosis process is unattractive to recover since it consists of an aqueous solution of several gases, which is very difficult to separate into its constituents. So, as before, it will continue to be burnt in the ammonium oven.

Another problem in the coke gas cleansing process refers to the pollutants emissions from the ammonium oven. This oven usually operates at about 800°C. At this temperature the only significant reaction involving ammonium is its oxidation, producing NO. According to Miller *et al.* (1981), in the temperature range between 1000 and 1500°C another reaction becomes important, in which NH_3 is combined with NO removing it. It seems environmentally profitable to operate the ammonium oven at temperatures above 1000°C. For this, the excess air coefficient was adjusted to ensure a temperature around 1250°C inside the oven.

A gas cleansing process including both the above proposed modifications and obeying to the earlier mentioned temperature profile for the naphtalene condensation was simulated using ECLIPSE, and the results are presented in Table VI. As it can be seen, the pollutants emissions are expected to be substantially reduced, as already predicted by Caldas *et al.* (1998) using a similar procedure. Moreover, the substitution of the distillation column by the reverse osmosis separation system allowed for a reduction in the specific energy consumption of 66 per cent—from 1072.5 to 360 kJ kg^{-1} .

As far as the batteries plant is concerned, both losses from the coke extinction $(10\,460\,kW)$ and from the volatiles escape from the ovens doors $(22\,253\,kW)$ represent a considerable amount of wasted energy, respectively, 2.6 and 5.6 per cent of the inlet coal energy flux. Another flaw in the coke production process is the existence of 10 ovens in battery 1 that are non-productive for coke throughput restrictions, although they consume coke gas in order to both avoid the deterioration of the refractory walls and to maintain the battery energy in balance.

Escape of volatiles is mostly due to the sealing degradation of the ovens doors originated by ageing and thermal stresses. A possible solution to this problem is the doors fixing or replacement by new ones, a measure that could reduce the volatiles escape losses up to 80 per cent.

As far as the coke extinction losses are concerned, Sazanov and Sumas (1990) proposed a recovery system that is already being used presently in some coke production plants. The

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| Process | Species | Actual | Optimized |
|-----------------------------|--|--------|-----------|
| Emissions to the river | Tar | 0.0 | 0.0 |
| | Naphtalene (C ₁₀ H ₈) | 0.31 | 0.0 |
| | Ammonia (NH ₃) | 0.08 | 0.005 |
| Emissions to the atmosphere | Nitric oxides (NO_x) | 40.0 | 0.42 |
| | Sulphur Oxides (SO_x) | 1.37 | 1.37 |

Table VI. Pollutant emissions in $g kg^{-1}$ of cleansed coke gas for the actual and for the optimized processes.



1 – Incandescent coke (900 °C – 1000 °C) ; 2 - Extinguished coke (200 °C – 250 °C) ; 3 – Water ; 4 – Steam ; 5 – Inert gas (180 °C – 200 °C) ; 6 – Inert gas (750 °C – 800 °C)

Figure 3. Recovery system of incandescent coke sensible heat (after Sazanov and Sumas, 1990).

system consists of the use of the incandescent coke sensible heat to produce steam at low pressure, as sketched in Figure 3.

The incandescent coke is cooled from 950 down to 250°C by a gaseous inert fluid (e.g., argon or nitrogen) capable of absorbing the coke sensible heat. This fluid carries the energy to a heat exchanger where water extracts it to be heated up and to produce steam at low pressure.

Assuming a new sealing system for the ovens doors with a reduction of 80 per cent in the volatiles escape, the above-described recovery system for the coke extinction was added to the coke plant flow sheet, together with the restart of the 10 non-productive ovens, and the entire new process was simulated again making recourse to ECLIPSE. In this way, the code predicts the global effect from all the modifications performed in the process. This value differs considerably from the summation of the individual effects in the process caused by each modification, as modifications interact between them. A total energy recovery of 37 180—out of 46 440 kW of losses in the original process—would be accomplished, from which 23 450 kW would emerge from the volatiles escape reduction.

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Figure 4. Comparison of energy consumption (coke gas and coal) and throughputs (coke, tar, raw coke gas and steam) between original and optimised processes.

The restart of the 10 non-productive furnaces into normal operation, measure that is not presently executable for governmental restrictive measures, would yield an energy recovery of 2810 kW just as a consequence of the losses elimination—burnt coke gas without throughput. Additionally, there would be an increase in the production of coke, coke gas and other energy by-products, shown in Figure 4, as a consequence of the increase in coal consumption. From the coke extinction recovery, the energy rate loss was reduced by 84 per cent—from 13 037 to 2117 kW, where an amount of 10.8 ton hr^{-1} of steam would be produced as a result of this energy saving. This production would also reduce the amount of utilities—steam—imported from the outside.

5. CONCLUSIONS

The ECLIPSE code has proved to be a suitable tool for global industrial process simulation. In spite of the difficulties arising in the detailed simulation of equipments such as combustors or distillation ovens, the agreement between the predicted and the experimental values is rather satisfactory, suggesting that, for the present kind of purposes, a thorough and detailed simulation of all the physical processes is not essential.

The improvements suggested to the studied processes were evaluated based on predictions obtained making resort to ECLIPSE simulations. Without using ECLIPSE, the quantification or even a realistic estimate of the benefits resulting from the alternatives presented herein would be very difficult to perform.

Although some features of ECLIPSE were not tested, namely the economic analysis and the maintenance program, as the aim of the study was purely technical, the results have shown that energy and environmental benefits are important and technically achievable. Obviously, an economical analysis would complement the scenario and would provide a more funded decision. Nevertheless, the use of ECLIPSE code is undoubtedly a powerful and useful tool to perform the optimization of industrial processes.

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