

Model-based optimization of sulfur recovery units

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1. Introduction

The modeling and optimization of sulfur recovery units (SRUs) is an environmentally relevant and quite cumbersome problem since it involves different modeling scales such as the kinetic/molecular micro-scale, the reactor design meso-scale, and the chemical process macro-scale. This work is the extension to the total plant modeling and optimization of our previous contributions on the micro-scale and meso-scale modeling and industrial data fitting (Manenti, Grottoli, & Pierucci, 2011; Manenti, Papasidero, Cuoci, et al., 2012; Signor, Manenti, Grottoli, Fabbri, & Pierucci, 2010). This work illustrates the paramount benefits in production efficiency and steam generation coming from the use of an integrated multi-scale approach to optimize the SRU. Actually, the multi-scale modeling allows to take advantage of the specific detailed simulations for each scale as well as to account for the imposition of the correct boundaries for each scale involved, dealing with environmental laws, safety regulations, experience-driven decisions.

The present work takes advantage of the methodology for the simulation of chemical reactors with detailed kinetics developed in the past forty years by the chemical reaction engineering group of Politecnico di Milano. The works of professor Mario Dente (Dente, Ranzi, & Goossens, 1979), Eliseo Ranzi (Ranzi, 2006) and Sauro Pierucci (Klemes & Pierucci, 2002; Pierucci, Faravelli, & Brandani, 1994) have been pioneer in the field, and have been followed by

several others in the field of combustion modeling, process simulation, plant optimization, applied to several different processes. One of the highlight of the current approach is that of using detailed kinetics: this makes the difference with the simple use of actual process simulators (Pro/II, Aspen Hysys, Unisim), that are not able to easily manage simulations with large number of species. Simulations with detailed kinetics (as required for several combustion processes) need then specific tools like the one here used (or dedicated user added routines/unit operations) to manage that gap.

This approach to plant simulation has been joined to plant optimization with very robust and efficient solvers of the library BzzMath (Buzzi-Ferraris & Manenti, 2013), able to solve very complex systems.

The work of Manenti et al. (2011) demonstrated that online reconciliation poor redundancy systems can be feasible by adding some adaptive parameters with detailed process simulation. Claus process is one of these systems, since it is usually present in every refinery for sulfur recovery purposes, dealing more with environmental regulations than to effective economic appeal. This work's aim is to model and optimize that process to increase economical appeal, trying also to get the process energy integration. This latter solution is well known and discussed in literature, and has been proposed, for instance, in analyzing the effects of the impurities on Claus plants heat recovery (Haimour & El-Bishtawi, 2007), in the investigation of SRU-IGCC plant integration (Jones, Bhattacharyya, Turton, & Zitney, 2012), and evaluation and modeling of a whole gas treatment plant with heat recovery steam generator (HRSG) and a combined cycle (CC) (Perez-Fortes, Bojarski, Velo, Nougues, & Puigjaner, 2009). Optimizing different levels simultaneously, it is possible to further improve some solutions that are already considered optimal from the single-scale point of view. The optimization

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of elemental sulfur recovery and the integrated optimization of sulfur recovery and steam generation are then considered and compared in this work. A sensitivity analysis on the most effective variables on the process performance in terms of recovered sulfur and steam produced has been performed in order to identify the right optimization variables, avoiding to build a too big optimization problem.

2. Description of sulfur recovery unit

Task of the Claus process is to recover the elemental sulfur from the hydrogen sulfide and, more generally, from the by-product gases originated by physical and chemical gas and oil treatment units in refineries, natural gas processing, amine scrubbers, sour water strippers (SWS). It consists of a thermal reaction furnace, a waste heat boiler, and a series of catalytic (Claus) reactors and sulfur condensers (Fig. 1).

The overall reaction characterizing the process is $2\text{H}_2\text{S} + \text{O}_2 \rightarrow \text{S}_2 + 2\text{H}_2\text{O}$ and, behind it, certain complex kinetic mechanisms take place (Alzueta, Bilbao, & Glarborg, 2001; Glarborg, Kubel, Dam-Johansen, Chiang, & Bozzelli, 1996) in the thermal reactor furnace at high temperatures, in the waste heat boiler as recombination effects and in the catalytic reactors at low temperature. In the thermal furnace, one third of hydrogen sulfide is oxidized to sulfur dioxide using air. Temperatures are usually in the order of 1100–1400 °C. The oxidizing reaction (1) is exothermic and without any thermodynamic restriction.



The two thirds of the unreacted hydrogen sulfide react with the sulfur dioxide to produce elemental sulfur through the so-called Claus reaction:



This reaction takes place at high temperatures in the thermal furnace with an endothermic contribution or at low temperatures in the catalytic converters with an exothermic contribution. The off-gas leaving the thermal furnace enters the waste heat boiler, where it is quenched (by heat exchange with boiler feed water, BFW) to about 300 °C to prevent recombination reactions; then, before entering the catalytic region, the first separation of liquid elemental sulfur is carried out in the first condenser. The hydrogen sulfide conversion (3) goes on in the catalytic region.



A condenser is installed downstream each catalytic reactor to condensate and make feasible the separation of the elemental sulfur before entering the next catalytic reactor, with the twofold advantage of preventing the sulfur condensation into the downstream catalytic reactor and to shift the equilibrium of the Claus reaction toward the products side. In addition, the hydrolysis reactions of COS and CS₂ take place in the catalytic region according to the following reactions: $\text{COS} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2\text{S}$ and $\text{CS}_2 + 2\text{H}_2\text{O} \leftrightarrow \text{CO}_2 + 2\text{H}_2\text{S}$. It is important to reach high performances in the hydrolysis of COS and CS₂ because these species affect the global sulfur recovery. High sulfur recovery have to be obtained due to the increasingly strict environmental regulations. The most important key performance indicator is the molar ratio $\text{H}_2\text{S}/\text{SO}_2$ exiting the waste heat boiler. It should be as close as possible to the value of 2 in order to get the maximum conversion in sulfur (Karan, Mehrotra, & Behie, 1994; Monnery, Svrcek, & Behie, 1993; Nasato, Karan, Mehrotra, & Behie, 1994).

3. Multi-scale approach

Usually, commercial package for process simulation include global model of unit operations (UO) to be interconnected in order to obtain a numerical plant reproduction for the purpose of development, analysis, design and optimization of technical processes. Often, these UO models are not detailed enough to represent several aspects of the real UO, considering in particular the behavior of combustion processes that often needs detailed kinetic model to be developed. The multi-scale approach includes models at different scales to overcome possible limitations of conventional models. To do so, a full object-oriented model of the UOs dealing with SRU has been developed in this research activity and UOs have been interconnected in a multi-scale simulation. Specifically, the reaction scheme described in (Manenti, Papisidero, Cuoci, et al., 2012) is adopted. It consists of more than 2400 chemical reactions with 140 molecular and radical species involved (sulfur compounds, hydrocarbons, typical acid gas compounds). The scheme is the base for the reactor network analysis used to simulate the thermal reaction furnace with combustion flame accuracy. The same kinetic scheme is also adopted to account for the relevant recombination effects that take place in the first part of the waste heat boiler with consequent variation of the outlet molar fraction of the main compounds as well as of the steam generation (Manenti, Papisidero, Manenti, Bozzano, & Pierucci, 2012). At last, the catalytic converters are characterized by means of the kinetic model proposed by Abedini, Kooliv& Salooki, and Ghasemian (2010) with re-estimation of parameters using very robust algorithms and available data. Thanks to the high level of detail of models and the good agreement with the field data, it is possible to perform a reliable total plant optimization in terms of efficiency of the elemental sulfur recovery and generation of both the medium pressure steam generated at the waste heat boiler and the low pressure steam generated at the sulfur condensers. The resulting large-scale nonlinear programming problem is solved by means of nonlinear system solvers and optimizers belonging to BzzMath library and exploiting parallel computing and object-oriented philosophy (Buzzi-Ferraris & Manenti, 2012; Manenti, 2011).

4. Modeling

4.1. Thermal section

Thermal section consists of a burner, a reaction furnace (RF) and an associated waste heat boiler (WHB). In this section acid gases are partially oxidized at a temperature ranging from about 1000 to over 1400 °C, depending on the gas composition. Highest temperature is reached in the first part of the RF, close to the burner. Then, it slowly decreases along the RF for thermal losses and the flow enters the WHB where flow is quenched to 300–350 °C and medium pressure (MP, from 10 up to 40 bar) steam is produced. RF and WHB can be opportunely modeled using a non-ideal reactor network as discussed in our previous work (Manenti, Papisidero, Cuoci, et al., 2012). In this way burner could be represented by a perfectly stirred reactor and the RF and WHB as plug flow reactors. The acid gas stream entering the reactor network is characterized by high Reynolds and Peclet numbers, so diffusive terms can be neglected. The fluid-dynamics can be considered axial-symmetric due to the assumption of fully developed flow both in the RF and WHB with flat profiles across the sections. Due to the refractory covering it internally, the RF is characterized by very small heat exchange coefficient and can thus be modeled as a plug flow with constant thermal losses assumed to be in the order of 3 KW/m² (or adiabatic for some SRU). When the RF consists of two separate combustion chambers (split-flow configuration), each chamber can be represented by a plug flow reactor. This can be useful, for instance,

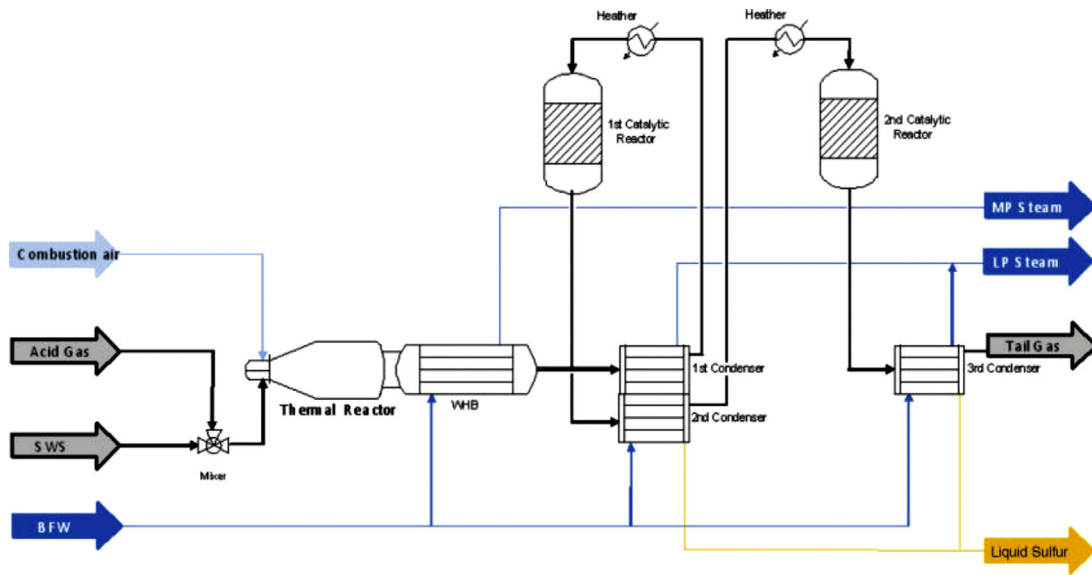


Fig. 1. Typical sulfur recovery unit.

when the ammonia content in the feed is more than 2%. In that case, the inlet stream from sour water stripper is feed to the thermal reactor with only a part of the other acid gases permitting to reach the high temperatures required to reduce the ammonia content according to the following reaction:



The other part of the acid gases is feed to the second chamber reaching the desired $\text{H}_2\text{S}/\text{SO}_2$ outlet ratio.

Fouling in the WHB tubes is not considered. In practice, the acid gas partially oxides in the burner flame, then it reach the thermodynamic equilibrium in the remaining part of the RF, due to the high temperature and residence time (usually higher than 1.0s). The equilibrium and kinetics are shifted in the WHB because of the cooling. Fig. 2 shows this behavior. As example, taking into

consideration the H_2S pyrolysis/formation reaction, one can see that when changing the operating conditions from TR to WHB (considering the whole equipment, when reaching 6.5 m in Fig. 2) the composition of the three species involved in this global reaction is changed. The reaction equilibrium is then shifted due to the lower temperature, until it reaches a new plateau when the temperature gets constant.

Recombination reactions thus take place in the first part of the WHB (Manenti, Papasidero, Manenti, et al., 2012), before the quench is effective. The temperature profile regarding the TR and WHB is shown in Fig. 3. Comparing the charts in Figs. 2 and 3 it can be notice that the temperature at which the recombination reactions are quenched is about 910°C (1182 K).

MP steam production is calculated from the amount of heat exchanged in the boiler, directly extracted from the computational

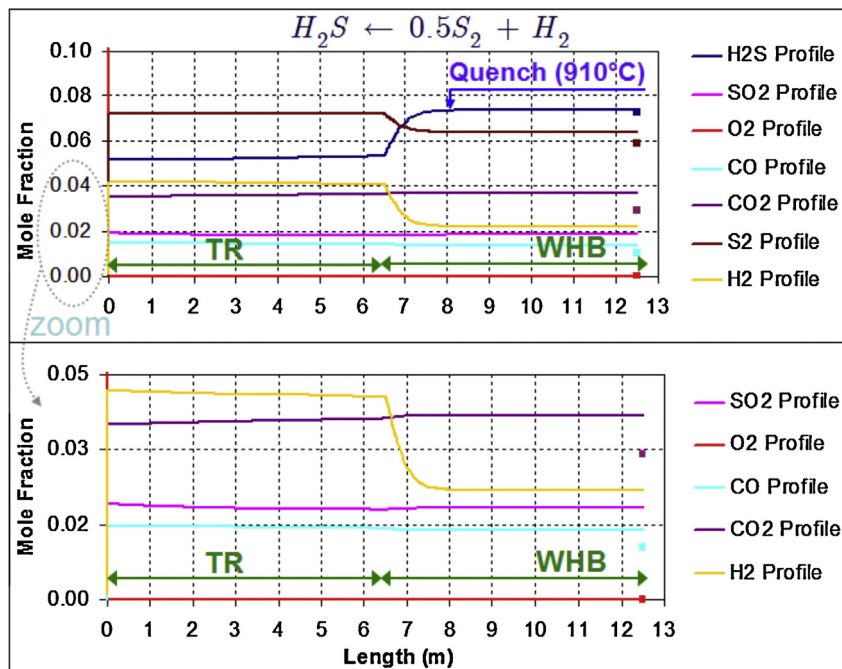


Fig. 2. Species profile in thermal furnace and WHB. Recombinations in WHB are taken into account.

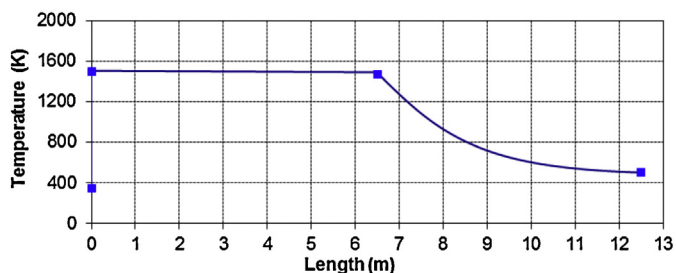


Fig. 3. Temperature profile in thermal furnace and WHB.

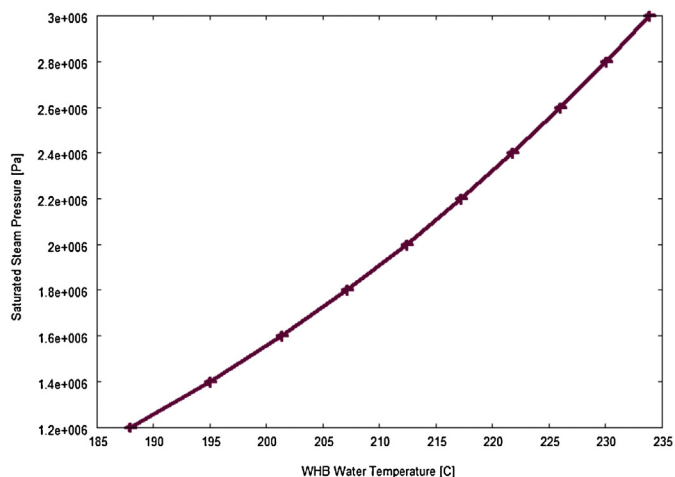


Fig. 4. Relation between water pressure and water temperature inside WHB.

tool used, taking account of changing in water latent heat of vaporization as a function of pressure (Figs. 4 and 5).

4.2. Sulfur condensers

Exiting the WHB, the cooled stream achieves the first condenser where its temperature lowers to 180 °C. After each catalytic reactor (two or three, depending on the SRU layout) there is a sulfur condenser operating at about 160 °C. In these unit operations, low pressure (LP) steam is produced (3–10 bar). Sulfur produced in the catalytic steps is assumed to be ideally removed in the condensers. The other compounds are assumed incondensable. Steam production is calculated on the basis of the enthalpy difference for sulfur

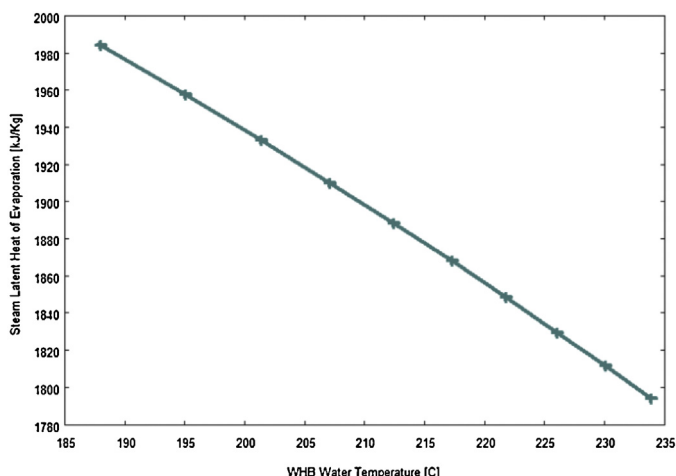


Fig. 5. Latent heat of evaporation as a function of water temperature.

in the two phases. Equilibria among the allotropic forms of sulfur is not implemented in the model.

4.3. Catalytic reactors

Claus converters (CC) are modeled as isothermal plug-flow reactors according to [Abedini et al. \(2010\)](#) with simplified kinetics. The CC catalytic stages are equilibrium-limited and for this reason more than one reactor is required to reach the desired conversion.

4.4. Computational environment

The whole process is developed in MicroSoft Visual C++ 2008. Numerical calculations and optimizations are performed by means of specific algorithms of BzzMath library ([Buzzi-Ferraris & Manenti, 2012](#)), a numerical tool for scientific computing. It includes several performing and robust solvers for many numerical problems. Reactor models are solved using DSmoke/OpenSMOKE suites, conceived to manage large kinetic schemes basing on the above numerical library. Parallel computing has been implemented by the BzzNonLinearSystem class of BzzMath libraries, that take advantage of OpenMP libraries with Shared Memory. The parallel approach is applied to the solution of the Linear System and to the Jacobian Matrix calculations. The BzzNonLinearSystem class ([Buzzi-Ferraris & Manenti, 2013](#)) is aimed at solving nonlinear problems and exploits the Quasi-Newton method, combined with other algorithm, such as the Gradient method or 2D searches in order to give the appropriate efficiency and robustness in the solution of the nonlinear systems.

5. Optimization

5.1. Mathematical problem description

The mathematical problem considers about 2000 reactions, with 142 species (radicals included) and a network of 4 ideal reactors for the thermal section of the SRU, while the catalytic section of the process have 2 reactors with 2 reactions. For each reactor, one global mass balance, 141 species mass balances and one thermal balance are solved. The optimization problem has 3 optimization variables (Furnace Pressure, AG/Air ratio, WHB water temperature). These variables have upper and lower boundaries in order not to reach values too far from the validated case. Equations for the used ideal reactors can be found in literature ([Levenspiel, 1999](#)).

5.2. Process and economic data

The objective function is to maximize the production of sulfur, MP and LP steam. Liquid sulfur has market price of 190–210 \$/ton ($C_{\text{sulfur}} = 155 \text{ €/ton}$). Steam cost is estimated from the electric energy potentially obtained from the derived production of electric energy. The efficiency of the energy conversion is assumed to be 30%. The chosen price for the electric energy is 0.10 €/KWh (equal to $C_{\text{energy}} = 27.8 \text{ €/}10^9 \text{ J}$). The simulation is good agreement with the data (plant data are reported in [Table 1](#)) and the error in fitting COS in the catalytic region is due to the assumption of negligible hydrolysis reactions into the CC. Scatter diagrams for the furnace and the process gas outlet are presented below. The first of the two ([Fig. 6](#)) seems to be good when comparing industrial and simulation data. The second ([Fig. 7](#)) shows a reasonable agreement, considering the assumptions for the catalytic part (e.g. all sulfur condenses).

5.3. Sensitivity analysis on the optimization parameters

Before choosing an objective function, it is necessary to investigate which parameters of those available can bring to a sensible

Table 1
Flow compositions and properties.

Component		Acid gas	Recycle	Air	Furnace	1st cond	1st react	2nd cond	2nd react	3rd cond
H ₂	Mole fract	0.00000	0.00005	0.00000	0.01737	0.01920	0.01947	0.01963	0.01976	0.01983
H ₂ O	Mole fract	0.05000	0.05582	0.05401	0.26131	0.28883	0.33536	0.33799	0.35685	0.35815
CO	Mole fract	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
N ₂	Mole fract	0.00000	0.00099	0.74781	0.51283	0.56683	0.57503	0.57955	0.58353	0.58565
O ₂	Mole fract	0.00000	0.00000	0.19818	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
CO ₂	Mole fract	0.05000	0.19301	0.00000	0.01769	0.01955	0.02095	0.02111	0.02125	0.02133
H ₂ S	Mole fract	0.90000	0.75012	0.00000	0.06062	0.06694	0.02556	0.02574	0.00938	0.00940
SO ₂	Mole fract	0.00000	0.00000	0.00000	0.03103	0.03429	0.01281	0.01291	0.00472	0.00473
COS	Mole fract	0.00000	0.00000	0.00000	0.00060	0.00066	0.00008	0.00008	0.00005	0.00005
CS ₂	Mole fract	0.00000	0.00000	0.00000	0.00053	0.00059	0.00010	0.00010	0.00010	0.00011
Equivalent S ₂	Mole fract	0.00000	0.00000	0.00000	0.09805	0.01219	0.03763	0.01137	0.01609	0.00292
Total flow	kmole/h	133.00	7.89	290.45	434.16	392.80	387.20	384.18	381.56	380.17
Pressure	MPa (g)	0.099	0.110	0.069	0.064	0.058	0.048	0.044	0.035	0.031
Temperature	°C	40	47	135	1261	182	300	174	229	134

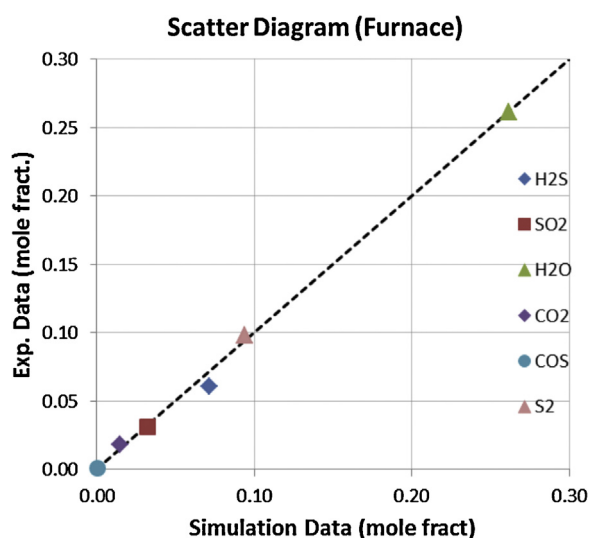


Fig. 6. Scatter diagram – furnace.

variation in the process macro-scale targets. It is important to underline that the aim of this analysis is not to find the mono-dimensional minima, but to analyze the sensitivity of the system to the operating parameters. The ones that have been considered are:

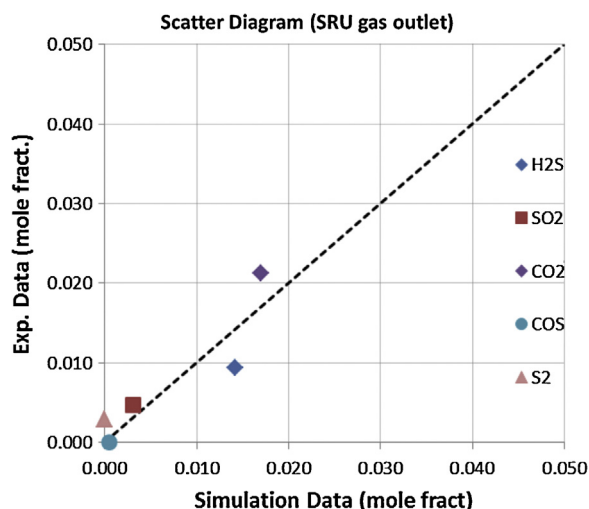


Fig. 7. Scatter diagram – gas outlet.

- Inlet acid gas/combustion air flow ratio,
- TR pressure,
- WHB boiling water temperature and related steam pressure.

As told before, the ratio between acid gas and combustion air is an important parameter for getting the right conversion of H₂S into SO₂ in the TR. It has also importance in the production of steam, because the more oxygen available, the higher temperature reached therefore increasing the steam production in the WHB. The original plant works with an air/acid gas ratio of 0.485. This ratio has been varied through the modification of inlet combustion air, in order to maintain a constant value of the sulfur to be potentially recovered (i.e. the total sulfur content in the inlet flow). The ratio has then been varied from 0.32 to 0.77. The sulfur recovery is shown in Fig. 8 where there is a maximum that lies between 0.45 and 0.50. One can notice that the value corresponding to the base case is close to the maximum.

Considering the vapor production, both that at medium pressure and that at low pressure have a decrease when air is low (Figs. 9 and 10). This happens because of the less combustion happening in the TR, with a consequent less heat recovered in the WHB.

Generally, inside the furnace there is a pressure between 1.3 and 2.0 Bar. Varying this parameter we encountered a scarce variability in the sulfur production (Fig. 11).

For what concerns steam generation, there is a variability in the production of medium pressure steam (Fig. 12), whereas a constant trend for low pressure steam generated after the catalytic reactors (Fig. 13).

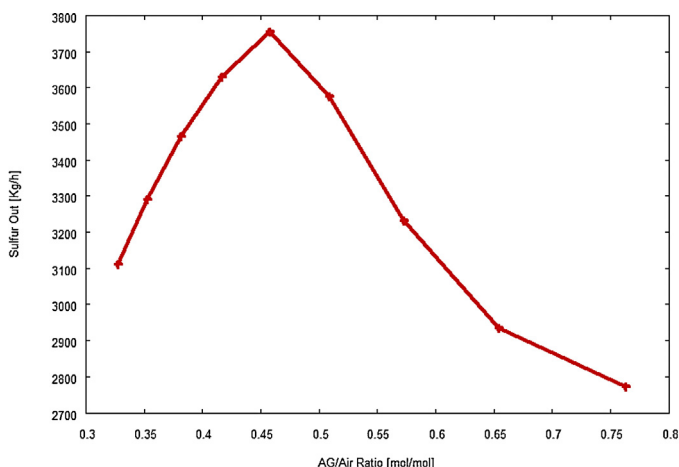


Fig. 8. Sulfur production as a function of acid gas/combustion air ratio.

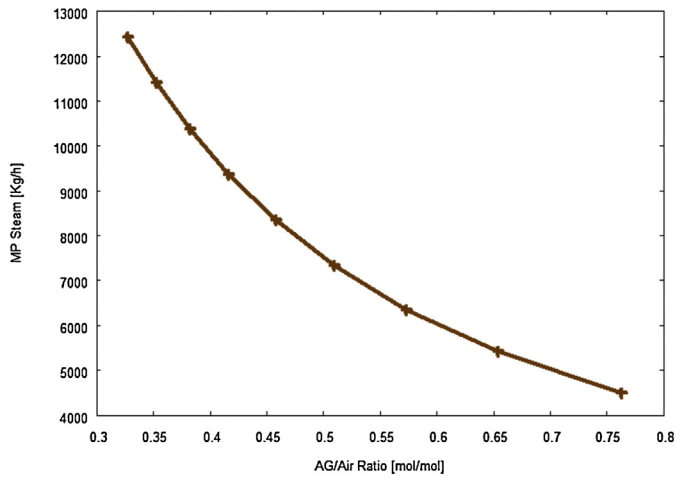


Fig. 9. MP steam production as a function of AG/air ratio.

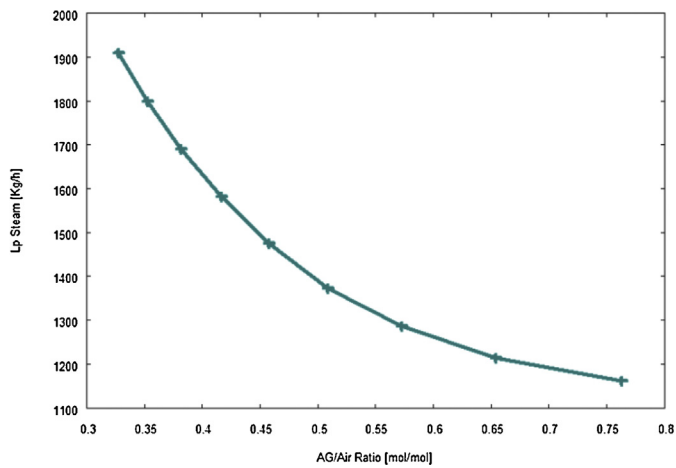


Fig. 10. LP steam production as a function of AG/air ratio.

The shell side pressure is a fundamental parameter for the temperature control in heat exchangers and multi-tubular reactors. It is directly related to the water boiling temperature, and a pressure increase brings to higher pressure steam generation, generally wanted for higher energy production in a steam turbine. It also influences the abovementioned recombination reactions in the

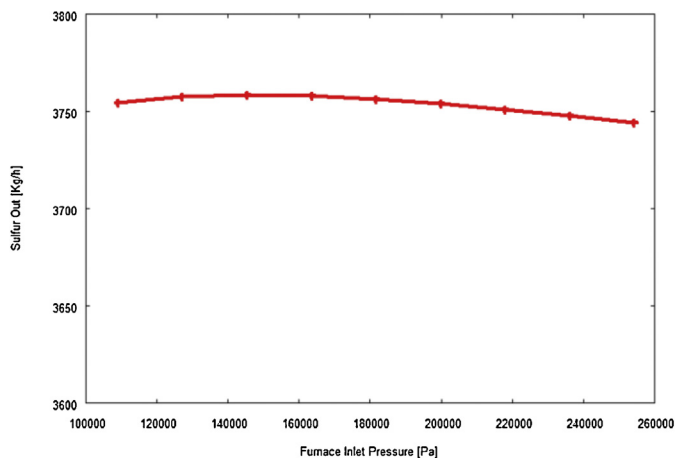


Fig. 11. Recovered sulfur as a function of the TR pressure.

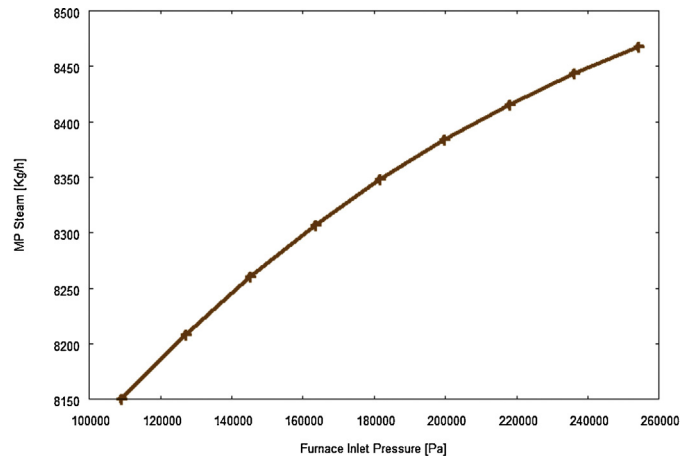


Fig. 12. Medium pressure steam generation as a function of the pressure in the TR.

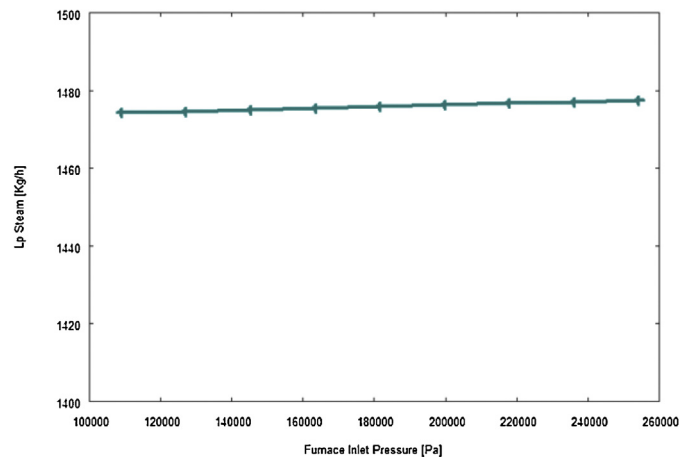


Fig. 13. Medium pressure steam generation as a function of the pressure in the TR.

WHB due to the fact that it affects the rapid cooling of the furnace outlet gases.

Evaluating the influence of this parameter on the sulfur production, we can see that there is apparently no effect on that (Fig. 14). This happens probably because the recombination reactions stop at higher temperature (about 850–900 °C) and then a little difference in the shell-side water temperature is not relevant for the outlet

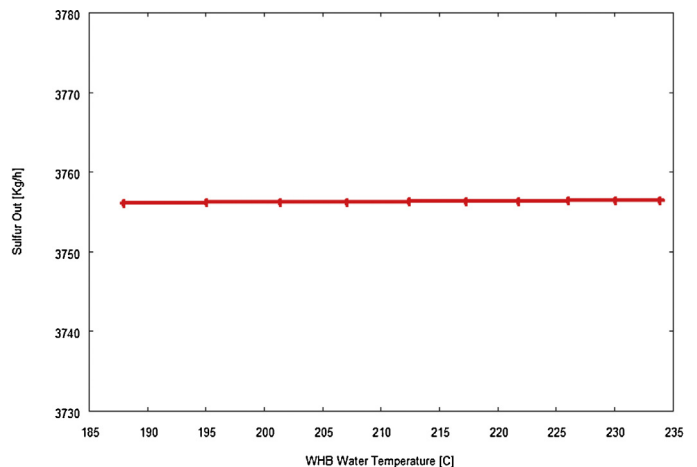


Fig. 14. Sulfur production as a function of WHB water temperature (an related pressure).

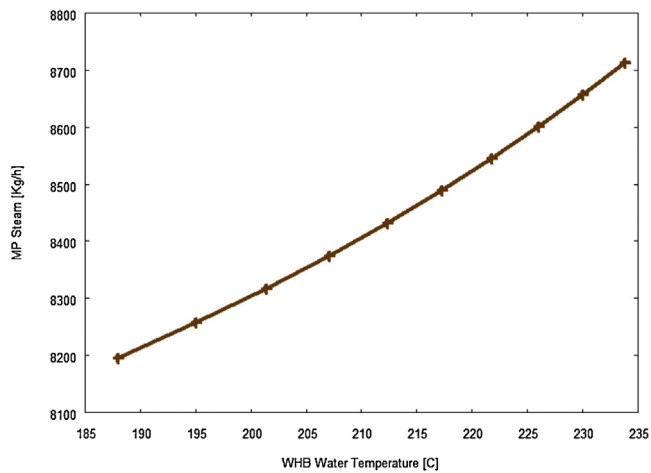


Fig. 15. MP steam production as a function of WHB water temperature (and related pressure).

composition (and then, for H_2S and SO_2 content). For this reason this parameter has not been included in the objective function for the only sulfur production.

On the contrary, it has great influence, as expected, on steam generation (Figs. 15 and 16). With higher pressure latent heat of evaporation of water is lower, then a higher quantity of water is evaporated with respect to the same heat exchanged. For this reason this parameter has been considered for the integrated optimization of both sulfur and steam. Modest effects on quenching time and heat exchanged can be expected, but the results seem to indicate that these effects are not relevant for the results of this analysis.

Further sensitivity analyses have been performed on the variation of H_2S content in the feed stream, of the total flow rate and on the losses in the TR. The first analysis shows that with a less “clean” acid gas (with a higher content of CO_2 instead of H_2S) in the feed, the plant reaches lower temperatures in the furnace, bringing to less heat recovered in the WHB and a lower quantity of recovered sulfur, being then a sensitive parameter for the optimization purpose. Anyway, since it is not a direct operating parameter to be varied, it has not been included in the objective functions. For what concerns the total flow rate, obviously, when increasing it, both the sulfur and steam production increases. But a too high flow rate can bring to problems with the capacity of the plant, as well as for low residence time in the furnace, bringing to a non-optimized H_2S/SO_2 outlet ratio.

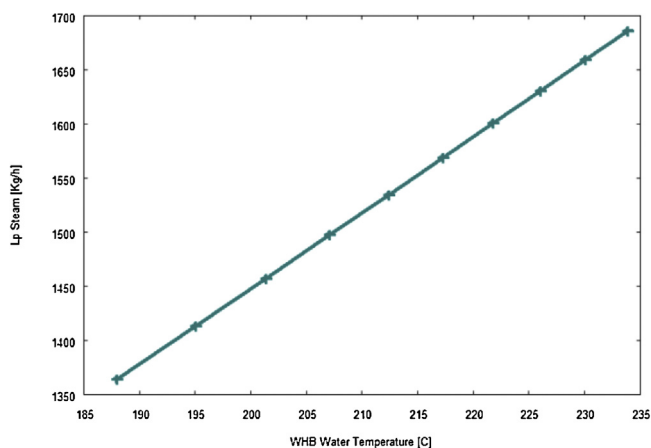


Fig. 16. LP steam production as a function of WHB water temperature (and related pressure).

Moreover, considering the losses in the TR as a parameter to be optimized during the design phase (and, of course, not an operating parameter for the plant), this parameter seems not to affect the sulfur production (very low impact on the equilibrium of the outlet species), while it obviously affects the MP steam production. In fact, higher losses bring to a lower temperature for the TR outlet stream, with the consequent lower heat to recover in the WHB. This analysis is useful, however, for design purposes, highlighting the importance of choosing the right construction materials and the level of cohibentation for losses control.

5.4. Definition of the objective function and optimization objectives

The following process values have been considered as degrees of freedom of the total plant optimization problem:

- Inlet combustion air/acid gas flow ratio (ranging from 0.6 to 1.4),
- TR pressure (ranging from 1.35 to 2.02 atm),
- WHB boiling water temperature and related steam pressure (temperature range is from 185 to 250 °C).

The first target is to maximize the sulfur production, as it usually happens for the SRU. The second target of the optimization is to re-estimate the degrees of freedom in order to simultaneously maximize the elemental sulfur production and the steam generation, according to the abovementioned economic and process data.

For the first purpose, the objective function to be minimized considered only the sulfur production:

$$\Phi_{\text{sulfur}} = E_{\text{sulfur}}(P_{\text{furnace}}, F_{\text{air}}) \quad (5)$$

As written before, the sensitivity analysis indicated us to vary the pressure in the furnace and the acid gas/air ratio, here varied changing the air flow rate.

In particular, the E_{sulfur} term means:

$$E_{\text{sulfur}} = C_{\text{sulfur}} \cdot \sum_j F_{j,\text{sulfur}} \quad (6)$$

where C_{sulfur} is the abovementioned Sulfur price and $F_{j,\text{sulfur}}$ represents the flowrates of the recovered sulfur.

For the integrated sulfur-steam optimization, two contributes have been inserted in the objective function, taking into account the income from the sulfur production and the energy generated with the produced steam. This function takes the following form:

$$\Phi_{\text{sulfur+steam}} = E_{\text{sulfur}}(P_{\text{furnace}}, F_{\text{air}}) + E_{\text{steam}}(P_{\text{furnace}}, F_{\text{air}}, P_{\text{water,WHB}}) \quad (7)$$

As said before, steam generation is sensitive to the pressure (and then temperature) in the WHB, so the relating part of the objective function is dependent to that parameter.

Here we have E_{steam} term as:

$$E_{\text{steam}} = C_{\text{energy}} \cdot \eta_{\text{conversion}} \cdot \sum_j (H_{j,\text{steam}} - H_{j,\text{liquid}}) \quad (8)$$

where C_{energy} is the abovementioned industrial cost for energy, $\eta_{\text{conversion}}$ is the efficiency in the energy production from steam, $H_{j,\text{steam}}$ and $H_{j,\text{liquid}}$ represent the enthalpies of the streams involved in the energy production.

5.5. Optimization results

Results for the first and the second optimization are reported in Table 2, along with the original data of the industrial case. Sulfur

Table 2
Industrial data and optimization results.

Industrial data				
Ratio air/AG	TR pressure [atm]	Water temperature WHB [°C]	Sulfur prod [kg/s]	Energy prod [kW]
1.0	1.690	204.0	1.03999200853	1605.28837858
<i>Sulfur production optimization</i>				
0.97892425477	1.72245682424	204.0	1.05177137767	1568.79331349
<i>Sulfur production and energy production optimization</i>				
1.0548564781	2.02782646175	190.4224	1.03891575600	1712.71592478

production is in kg/s; steam production is in equivalent electric power produced (kW).

As we can see from the results, the optimum for the elemental sulfur production optimization leads to a little increase of the pressure in the TR with an air/acid gas ratio lower than that of the industrial data. The difference is mainly due to the robustness of optimizers adopted in this work and on the real plant from which we acquired the data. This testifies that the industrial case is already optimized to maximize the sulfur production. In this way, the equivalent energy produced as steam is decreased and this is due to the reduced combustion air entering the burner that leads to lower temperatures in the TR and then to less heat recovered in the WHB. Dealing with the sulfur and energy production optimization, it is relevant that the optimum is achieved with a lower sulfur production despite an enhancement of energy production, considering the economic balance between the two aspects. This optimum is reached at a TR pressure of 2.02 atm that is the upper bound in the range of variation settled. The combustion air is increased, inducing higher temperature in the TR and the heat exchanged in the WHB grows consequently.

6. Conclusions

The work has presented an integrated total plant optimization based on the multi-scale modeling of sulfur recovery units. The use of multi-scale approach has allowed to combine the maximization of elemental sulfur production with the steam generation, directly basing on the complex combustion mechanisms occurring at the kinetic scale. The optimization shows that the power (steam) generation can be improved of more than 6% by preserving the amount of recovered sulfur with respect to operating conditions that are optimized with traditional techniques.

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