Modeling of hydrogen sulphide removal from hot coal syngas in a coal-to-hydrogen pilot plant

Caterina Frau[a(*)],Giampaolo Mura[b] Alessandro Orsini[a], , Monica Caboni[a], Giovanni Raggio[a]

[a]*SOTACARBO S.p.A. – Grande Miniera Serbariu – 09013 Carbonia (CI), ITALY*

[b]*University of Cagliari -Department of Chemical Engineering and Materials–09100 Cagliari (CA), ITALY*

Abstract

Hydrogen production through coal gasification is becoming one of the most attractive options for energy production due to the remarkable advantages offered by this technology in pollution control and greenhouse gases-emissions monitoring. To this aim, Sotacarbo, together with Ansaldo Ricerche, ENEA and the University of Cagliari, is developing a research project to design, construct and test a pilot plant for hydrogen production from coal gasification (in particular from high-sulphur Sulcis coal). The project has been funded by the Italian Ministry of Education, University and Research (MIUR) and by the European Commission and the total cost has been estimated in about 12 million euros.

The pilot plant, which has been recently set up in the Sotacarbo Coal Research Centre located in Sardinia, includes two fixed-bed Wellman-Galusha gasifiers (a 700 kg/h pilot gasifier and a 35 kg/h laboratory-scale gasifier), fed up with high and low sulphur coals, and a syngas treating process, which is composed by a raw-gas cleaning section, an advanced integrated water-gas shift and CO_2 removal unit and the hydrogen separation unit. In particular, the raw gas cleaning section includes a hot- and a cold-gas desulphurization process, in order to compare their performances.

One of the most significant sections of the laboratory-scale plant is the hot gas desulphurization process, which includes two fixed-bed reactors. Hydrogen sulphide is the most abundant sulphur-containing compound in coal gas. Regenerable metal oxides sorbents are best candidates for the removal of hydrogen sulphide from hot coal gas. As part of sulphur removal process, a fixed-bed reactor simulating model has been developed using Fortran software, in order to evaluate the performances of this component.

This paper shows the process analysis and simulation model development and results. Because of demand to apply a simple and reliable correlation for the conversion rate of metal oxide or hydrogen sulphide in the sulphidation reaction, the unreacted shrinking core model is applied to this purpose. The sulphidation performance has been investigated in terms of breakthrough curves at different temperatures.

Introduction

Coal is widely available in the world and distributed more uniformly than other fossil fuels, otherwise oil and natural gas, which main fields are confined in a relatively small area [1]. This allows great price stability and represents a secure source from a strategic point of

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[*] Corresponding author:
Phone: +39 0781 670444 – Fax: +39 0781 670552
E.mail: c.frau@sotacarbo.it

view [2]. Moreover, the advanced in development of clean coal technologies, allows an environmental-friendly use of coal [3], in particular for power generation.

Among clean coal technologies, gasification is particularly interesting since it allows both power generation (mainly by using integrated gasification combined cycles power plants, IGCC) and clean fuels production, with a particular reference to hydrogen. Really, hydrogen production through coal gasification is becoming one of the most attractive options for energy production due to the remarkable advantages offered by this technology in pollution control and greenhouse gases-emissions monitoring.

To this end, Sotacarbo, together with Ansaldo Ricerche, ENEA and the University of Cagliari, is developing an integrated gasification process for combined production of hydrogen and electrical energy, to be used in medium and small-scale commercial plants. The research project, called Co.Hy.Gen. (COal to HYdrogen GENeration), concerns the development of gasification and syngas treatment pilot plant, which is located in the Sotacarbo Research Centre in Carbonia, in Sardinia island (Italy). The research project is co-funded by the Italian Ministry of Education, University and Scientific Research (MIUR) and the total cost is estimated in about 12 million euros. The plant includes a pilot-scale (700 kg/h) and a laboratory-scale (35 kg/h) coal-gasifiers; in particular, the latter is equipped with a syngas treatment process for hydrogen production. At the moment pilot plant is under assembling.

The treatment syngas line, being part of the laboratory-scale plant, is typical of the hot gas desulphurization process, which includes two fixed-bed reactors. Hydrogen sulphide is the most abundant sulphur-containing compound in coal gas. Regenerable metal oxides sorbents are best candidates for the removal of hydrogen sulphide from hot coal gas. As part of sulphur removal process, a fixed-bed reactor simulating model has been developed using Fortran software, in order to evaluate the performances of this component.

This paper shows the process analysis and simulation model development and results. Because of demand to apply a simple and reliable correlation for the conversion rate of metal oxide or hydrogen sulphide in the sulphidation reaction, the unreacted shrinking core model is applied to this purpose. The sulphidation performance has been investigated in terms of breakthrough curves at different temperatures. Looking forward to experimental data, this report attends the expected performances of sulphur removal system at high temperature, supplying information about design of small-scale industrial applications.

The Sotacarbo coal-to-hydrogen pilot plant

In order to test different plant solutions and different operating conditions, a very flexible and simple layout for the pilot plant has been considered. The experimental results obtained by means of this pilot plant will constitute the basis of the second phase of the research project, which will lead to the realization of the demonstrative unit of the Sotacarbo coal-to-hydrogen process.

The current layout of the Sotacarbo pilot plant includes two fixed-bed up-draft Wellman-Galusha gasifiers: a 700 kg/h pilot gasifier and a 35 kg/h laboratory-scale gasifier. The choice of this kind of gasification process is a consequence of the particular commercial interest in the field of small-scale industrial applications.

Whereas the main goal of the experimental tests on the 700 kg/h pilot gasifier is the optimization of the gasification process and the definition of start-up and shut-down procedures, the 35 kg/h laboratory-scale plant is used to develop the syngas treatment process for hydrogen production.

As a matter of fact, coal is primarily made of carbon and mixed with varying amounts of mineral matter and chemicals compounds. When coal is gasified and converted to fuel gas, chemical compounds are released as gaseous contaminants, and mineral matter is released as particulates. These contaminants must be removed to protect the equipment from corrosion and erosion, and simultaneously prevent environmental pollution.

Therefore, while the pilot plant is equipped with a wet scrubber (for syngas cooling, tar and dust removal) and a flare where the cold syngas is sent to, the laboratory-scale plant is equipped with a complete and flexible syngas treatment process for hydrogen production whose a schematic diagram is given below in figure 1.

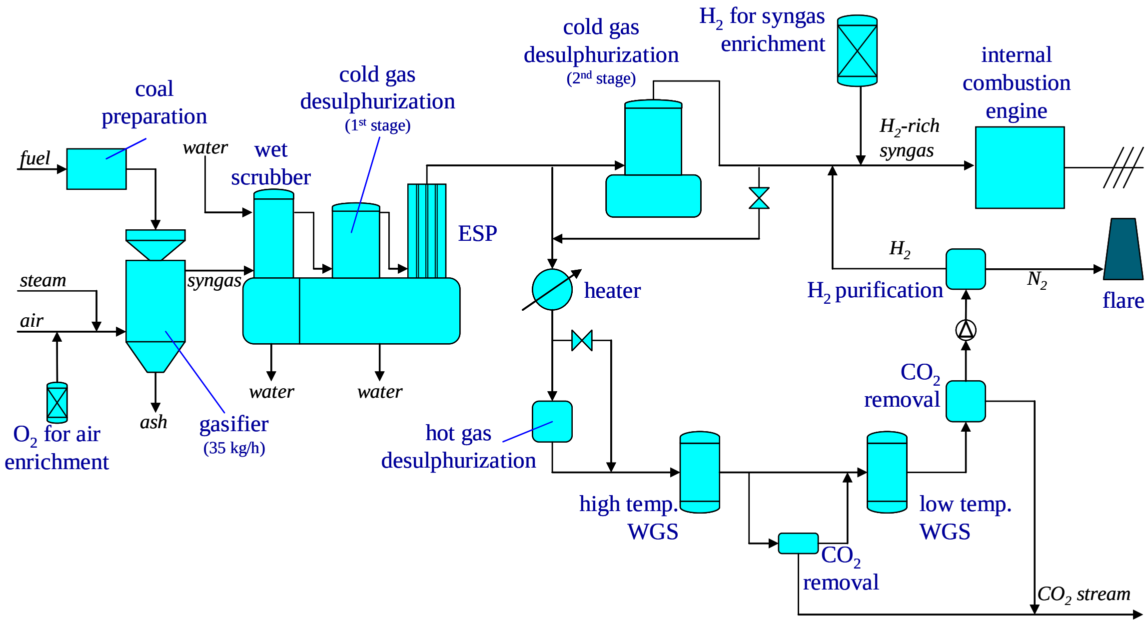

***Figure 1** – Simplified scheme of the Sotacarbo laboratory-scale experimental plant.*

	High sulphur coal Sulcis	Low sulphur coal SouthAfrican
Carbon	53.17	65.84
Hydrogen	3.89	3.71
Nitrogen	1.29	1.50
Sulphur	5.98	0.55
Oxygen	6.75	5.35
Chlorine	0.10	0.05
Moisture	11.51	8.00
Ash	17.31	15.00
LHV [MJ/kg]	20.83	24.79

***Table 1** – Sulcis and South African coal*

The laboratory-scale gasifier will be fuelled by several coals. In particular, a high-sulphur Sulcis coal and a low-sulphur South African coal (whose ultimate analyses are shown in table 1) have been selected for the experimental campaigns. When coal is gasified, reducing conditions are created and sulphur is mainly converted to H_2S and tar and dust are formed. Therefore coal syngas must be cleaned before it is used to obtain hydrogen.

In the Sotacarbo laboratory-scale plant, the raw syngas from the gasification process is sent to a pre-treatment skid which incorporates a wet scrubber (which reduce syngas temperature from about 300 °C to 50 °C and operates a primary dust and tar separation), a first cold gas desulphurization stage (which uses a soda-based solvent) and an electrostatic precipitator (ESP), which allows to achieve a fine particulate and tar removal.

According to the design conditions, downstream the ESP, the syngas is split into two streams: the main stream, almost the 80%wt of the produced syngas, is sent to the cold-gas desulphurization unit (2° stage), whereas the remaining 20%wt is sent to the hot-gas desulphurization unit, followed by the hydrogen production section.

In particular, the cold gas desulphurization unit~~,~~ is based on an hydrogen sulphide (H_2S) absorption process (which uses a mixture of soda and sodium hypochlorite, diluted in water, as solvent), is directly followed by the power generation section, represented by internal combustion engine.

The secondary syngas treatment line includes a compressor, which increases the pressure to about 1.4 bars(a) in order to overcome the pressure drops of the treatment line. The compressor is followed by a dry hot gas desulphurization unit (which employs metal oxide-based sorbents), an integrated CO-shift and CO_2 absorption system and a hydrogen purification unit, based on PSA (Pressure Swing Adsorption) technology.

The concentration of H_2S at the inlet of the hot gas desulphurization unit (table 2), can change in the range 15000 - 1000 ppmv depending on the feed coal. In particular these limits are respectively expected during operations with 100% of Sulcis-coal and 100% of South African-coal.

Because the catalyst of the CO-Shift unit cannot tolerate a concentration of H_2S in the syngas higher than 10 ppm, the H_2S is removed under this limit in the hot gas sulphur removal system.

	Sulcis coal syngas	South African coal syngas
Temperature [°C]	300-450	
Pressure [mbarg]	239	
Molar flow [kmol/hr]	0.8156	1.1228
Volumetric flow [Nm^3/hr]	18.2809	25.1663
Molecular weight [kg/kmol]	24.458	22.840
H_2S [%vol]	1.49	0.10
COS [%vol]	0.08	0.01

***Table 2** –Inlet syngas to HT desulphurisation [5].*

High temperature hydrogen sulphide removal system

Studies about several hot gas desulphurization technologies performed by Sotacarbo have led to actual system design, whose schematic diagram is given below in figure 2. All components and devices are designed to ensure working and security, according to safety rules.

System is designed with aim to carry out a strong desulphurization of syngas and breakthrough during sulphidation runs are defined as 10 ppm H_2S in the effluent syngas. These strict conditions are dictated, as previously said, mainly to avoid poisoning of catalyst employed in the downstream CO-Shift section plant.

Desulphurization takes place in two stainless steel (AISI 321) fixed-bed reactors (*HySyTech*). Fixed-beds are made of suitable sorbent materials such as metal oxides. Adsorbers are identical, with 0.366-m inside diameter and 0.540-m channel length. The space velocity for the sulphidation runs is $3 \cdot 10^2$ hr $^{-1}$ for Sulcis coal-syngas and $4 \cdot 10^2$ hr $^{-1}$ for SA coal-syngas respectively. Hot gas desulphurization system operates at temperatures ranging from 300 to 450°C and a pressure of 1.4 bars. Maximum operating temperature is limited by physical strength of reactors material. To maintain temperature conditions required for good working of system, a suitable caulking must be realized on pipeline connection between reactors.

Main features of reactors and assumed operative parameters are resumed in table 3.

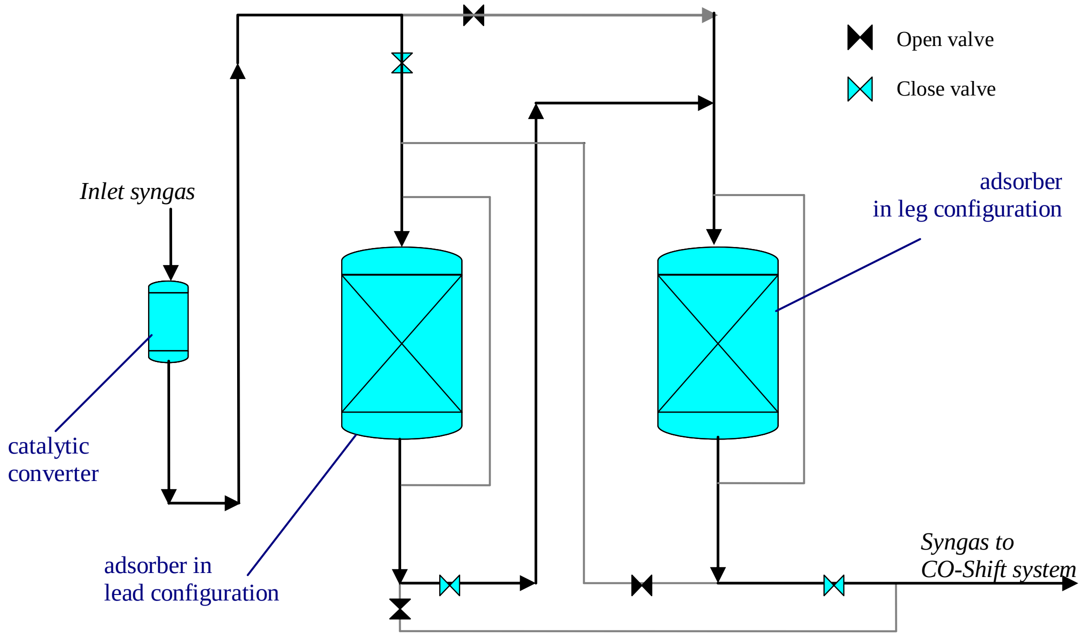

Figure 2 – Simplified scheme of hot gas desulphurization system

Operating Conditions / Mechanical Data	
Operating Temperature, Max/Norm/Min [°C]	450 / 375 / 300
Operating Pressure [barg]	0.40 / 0.30 / 0.20
Design Temperature [°C]	500
Design Pressure [barg]	0.48
External diameter [mm]	358
Thickness wall, minimum [mm]	0.5
Height [mm]	680
Filling	Metal oxide based sorbent
Cat. Volume [liters]	42
Channel diameter [mm]	356
Channel length [mm]	540
Void fraction	0.31

Table 3 *– Features of adsorbers in H_2S removal hot system*

The whole desulphurization system is designed to enable setting of flowing way of syngas by pipeline valves devices.

Reactors, working serial, are arranged in “Lead/Lag” configuration. In this way, when there is a breakthrough point in the first reactor (in lead configuration), the second absorber (in lag configuration), avoids CO-Shift catalyst poisoning. After breakthrough point, exhaust fixed-bed has to be replaced with fresh and piping valves configuration has to be setted to reverse syngas flowing. In this way, adsorbers change their position with respect to syngas flow and sorbent employment is optimized every desulphurization run.

Avoiding slip of organic sulphur compounds, before entering the reactors, syngas goes through a catalytic converter. This converter contains a catalytic matter which is able to get ready possible organic sulphur compounds to be adsorbed by downstream reactors. Moreover this component captures traces of lead, vanadium, arsenic and other heavy metals that can be attended in coal syngas.

In this removal sulphur system, sulphur compounds concentration in the outlet flowing syngas is maintained less than 10 ppm by a suitable fixed-bed material sorbent.

Hydrogen sulphide, in fact, can react easily with metal oxides.

The literature reports several studies on metal oxides as candidate desulphurization sorbents: pure oxides (e.g. ZnO, CuO, Cao, Fe_2O_3, SnO [6]-[9]), solid mixtures of metal oxides that react with H_2S (e.g. ZnO- Fe_2O_3, ZnO-MnO [6]-[8]) or mixtures of a inert oxide with a solid reactant (e.g. ZnO-TiO_2, Fe_2O_3-Al_2O_3 [6]-[8]) have been investigated as sorbents for the removal of H_2S, especially at high temperatures. The addiction of an inert solid in the pure metal oxide is expected to stabilize the metal oxide against its reduction to metal form and/or volatilization.

Among the different tested oxides, zinc oxide has the highest equilibrium constant for sulphidation, yielding H_2S removal down to even fractions of 1 ppm. Its principal limitation is that in the highly reducing atmosphere of syngas it is partially reduced to elemental zinc, volatile above 600°C, with consequent sorbent loss. In contrast, if the operating temperature is low, pure zinc oxide has been singled out as the sorbent of choice for desulphurization of coal syngas.

On account of this, the initial experimental phase on hot syngas desulphurization system will be carried out with zinc oxide based sorbent. However testing several kinds of sorbents will be the target of further experimental runs.

Therefore, fixed-beds of adsorbers are made with a commercial spherical ZnO based pellets (*Katalco 32-5*) with 3.7-mm diameter. Physical properties and chemical composition are resumed in table 4.

Main sorbent performances expected are:

1. low and stable pressure drop due to high particle strength;
2. very high H_2S capacity due to high density coupled with high porosity giving a high accessible zinc oxide content per volume of adsorbent;
3. sulphur removal to very low levels;
4. realable performance and long predictable lives.

In the actual desulphurization system, sorbent regeneration is conducted outline to avoid stress on material reactors and operating troubles.

KATALCO 32-5 Hydrogen Sulphide Adsorbent	
General Description	High porosity spherical zinc oxide adsorbent
Physical Properties	
Form	Spherical granules
Size [mm]	2.8 - 4.75
Bulk density [kg/m^3]	1400
Surface area [m^2/g]	35
Pore volume [ml/g]	0.26
Chemical Composition	
ZnO	92 wt%
Binder	Balance (CaO/Al_2O_3)

Table 4 *– Features of material adsorbent [11]*

Modeling approach

In order to predict the performance of the hot gas sulphur removal system under different operation conditions, a one dimensional model has been developed.

The involved chemistry between the gas phase and the metal oxide particles has been represented according to the general reaction MyOx(s) + xH_2S(g) →MySx(s) +xH2O and the rate of the heterogeneous reaction has been evaluated according to an unreacted shrinking-core model.

Moreover, the followings assumptions have been done:

1. plug-flow pattern fluid dynamics
2. negligible axial-back mixing
3. no radial-mixing, [12]
4. constant pressure along the reactor
5. thermal equilibrium between solid-phase and gas-phase.

Based on previous assumptions the model developed in the present report consists of a set of the mass-balance equations for gas-phase reactants and the energy-balance equation. A further mass-balance equation is considered for remaining gas-phase compounds, collected as inert-phase. Therefore a set of four ordinary differential equations it is obtained. The H_2S equation mass-balance and energy-balance equation are:

$$\frac{d\dot{N}_{H2S}}{dz} = -S\rho_s(1-\vartheta)R_{H2S} \qquad (1)$$

$$\frac{dH}{dz} = R_{H2S}S\rho_s(1-\vartheta)(-\Delta H_r) - \pi D_r U(T - T_e) - S\rho_s(1-\vartheta)Cp_{sol}\frac{dT}{dt} \qquad (2)$$

Equations for mass-balance and energy-balance are coupled through the kinetic term R_{H2S}.

Because of demand to apply a simple and reliable correlation for the overall kinetics on sorbent pellet, the unreacted shrinking core model is applied to this purpose in this study. In fact, an essential characteristic of noncatalytic gas-solid reactions like sulphidation, where a solid product is produced, is that during conversion, a product layer gradually builds up, separating the solid reactant from the gas-phase. To reach the fresh sorbent core, the H_2S molecule must be transferred from the bulk of gas-phase to the particle external surface (external mass transport), then must diffuse across the internal pores (internal mass transfer), and finally undergo a chemical reaction with the core unreacted. It was evidence [13] that with fresh sorbent particles the transport resistance due to internal diffusion is relatively negligible. Under these conditions, the system is limited by reaction kinetics at low temperature (less than 50°C) and by external mass transport at higher temperature. The relative importance of internal mass transport increases as the sorbent particles are consumed. In particular, it could be observed already when the radius of the internal unreacted core reaches the 99-97% of the initial particles radius, the system operates in an internal mass transport. On account of this, contribution of reaction kinetic on overall resistance is considered negligible.

The R_{H2S} that appears in previous equations is the specific adsorption rate of H_2S, that can be expressed as

$$\rho_s R_{H2S} = -(Ka)_{oy} C_{H2S} \qquad (3)$$

The overall kinetic constant $(Ka)_{oy}$ of equation (3) is obtained by integration of transport equation. The following expression is accomplished:

$$\frac{1}{(Ka)_{oy}} = \frac{1}{4\pi r_e^2 K_{ext}} + \frac{r_e - r_i}{D_{eff}4\pi r_i r_e} \qquad (4)$$

The external mass transport coefficient K_{ext} of H_2S in a fixed-bed system is evaluated by the equations:

$$\begin{cases} J_d = 0.91 Re^{-0.51}\psi & 0.01 \le Re \le 50 \\ J_d = 0.61 Re^{-0.41}\psi & 50 \le Re \le 1000 \end{cases} \qquad (5)$$

where [14]:

$$Re = \frac{Gdp}{6\mu(-\vartheta)} \qquad (6)$$

$$J_d = \frac{Sh}{Re\,Sc^{0.33}} \qquad (7)$$

$$Sh = \frac{K_{ext}\,dp}{D_r} \qquad (8)$$

$$Sc = \frac{\mu}{\rho D} \qquad (9)$$

To calculate the diffusion coefficient D_{eff} it is accounted both molecular diffusivity and Knudsen mechanism, by:

$$\frac{1}{D_{eff}} = \frac{1}{D_{H2S}} + \frac{1}{D_k} \qquad (10)$$

The molecular diffusivity D_{H2S} value is calculated by the Chapman-Enskog equation [15]. The Knudsen diffusivity is calculated with the following expression [16]:

$$D_k = 9700\,re\sqrt{\frac{T}{PM_{H2S}}} \qquad (11)$$

Results and discussion

The mathematical model has been implemented on a Fortran-code. Because of critical sulphur contained in Sulcis-coal derived syngas, tests are conducted based on 100% Sulcis-coal feed.

The sulphidation performances of adsorber are described in terms of breakthrough curves. Moreover thermal profile of syngas at different instants of adsorption process is obtained.

Figure 3 shows the breakthrough curves for an operating temperature of 375°C. The reaction front advancing in the fixed-bed reactor can be observed. The profile for all curves is the same. At the beginning the H_2S concentration in the outlet syngas is very low (less than 1 ppmv) because spatial velocity is very low and no axial dispersion is accounted. After a certain elapsed time, the breakthrough takes place and H_2S concentration increases steeply and tends to reach the H_2S concentration at the inlet gas of the reactor.

Advancing of reaction front is observable also in thermal profiles diagram showed in figure 4, where the temperature hot spot is identifiable due to reaction.

The breakthrough time, defined arbitrarily in this study as a time which the H_2S concentration in the outlet gas is 10 ppmv, differs for different operating temperatures. A comparison test is showed in figure 5. Based on these results, best performance of desulphurization reactor is expected at operating temperature of 450°C.

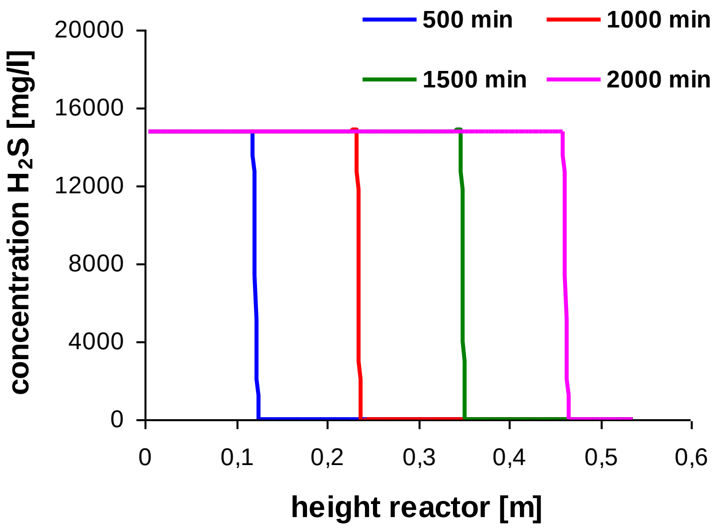

Figure 3 –Breakthrough curves for Sulcis-coal derived syngas (T=375°)

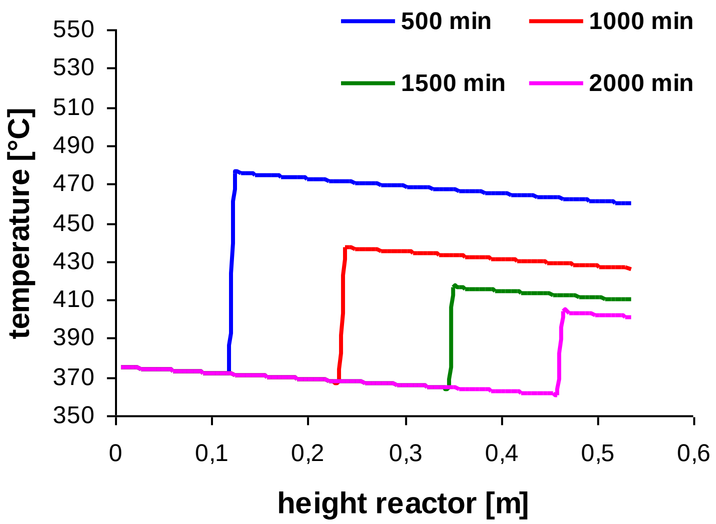

Figure 4 - Thermal profile curves for Sulcis-coal derived syngas (T=375°)

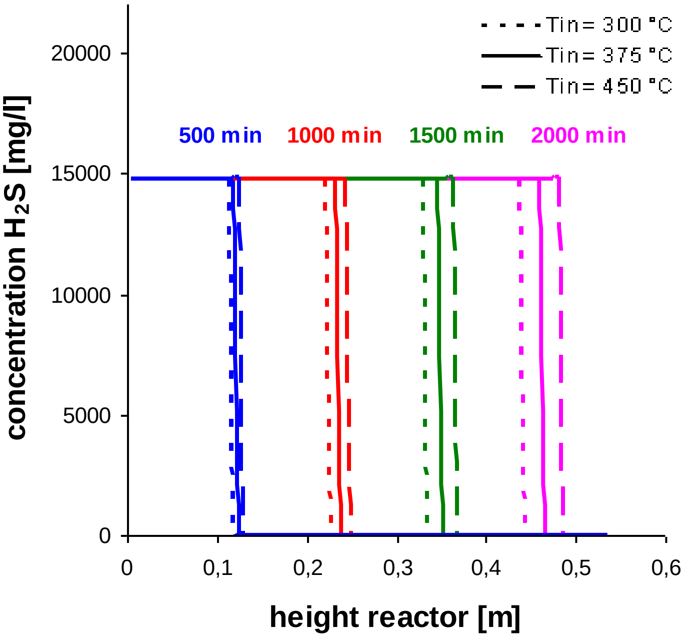

Figure 5 – Desulphurization performance test comparison among different operating temperatures of Sulcis-coal derived syngas

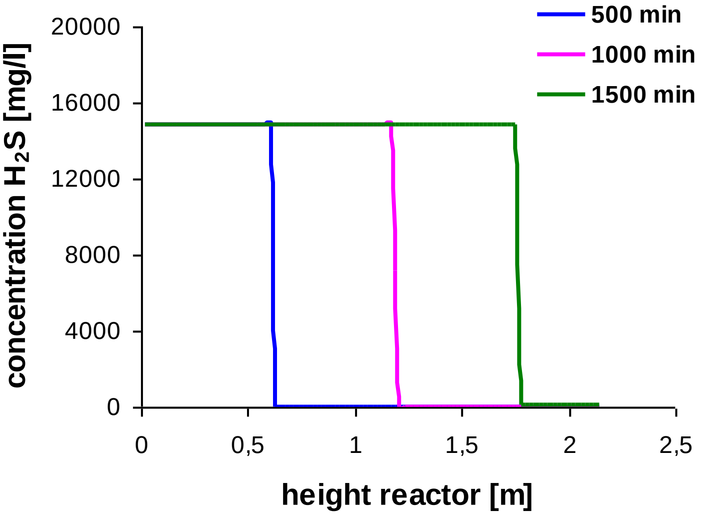

Figure 6 – Breakthrough curves for a fixed-bed reactor with same volume and D_1=0.5 D (Sulcis-coal derived syngas and T=375°)

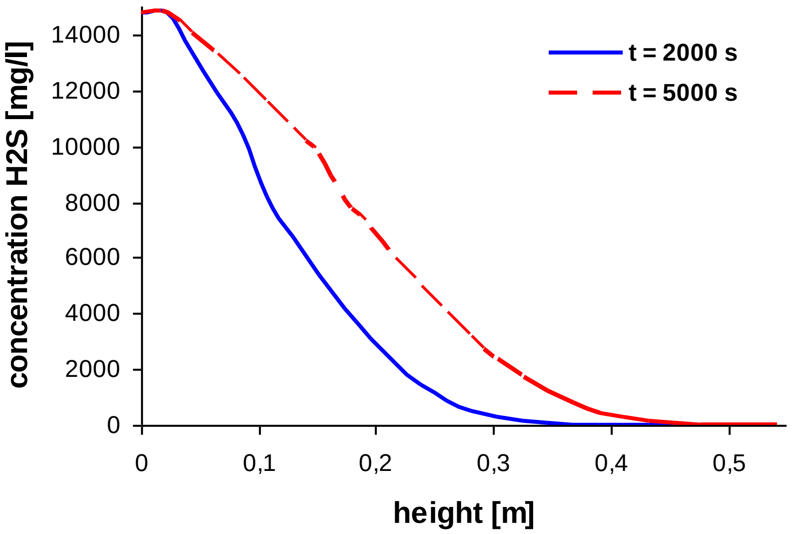

Figure 7 – Breakthrough curves - contribution of axial back-mixing is accounted

Runs carried out on mathematical code have pointed out some problems that have caused unstable computations. These problems arrive by comparing model assumptions to real process in the laboratory-scale plant.

A remarkable facet concerns fixed-bed fluid-dynamics and, in particular, the assumption of plug-flow patterns adopted in this study. In reactor of lab-scale plant, diameter and height have the same magnitude order, whereas PFR assumption can be accounted as satisfactory for low values of fixed-bed diameters or, generally, if the ratio between fixed-bed height and diameter is very high.

To analyze the effect of plug flow pattern assumption on model results, runs are carried out with same fixed-bed volume but different diameter (in particular Dnew=0.5 D). Results showed in figure 6, are not remarkable, but unstable computations are removed.

Further important facet originates by scale-up. Noticeably, laboratory-scale plant equipment has very reduced dimensions despite of normal-scale plant equipment. As matter of fact, design equations, referring to industrial equipment, are used in model setting together with mass-balance and energy-balance equations.

The scale-up problem appears when heat exchange trough a surface is considered. In the energy-balance equation appears term related to heat exchange trough reactor lateral surface. This surface, referred to volume unit, increases proportionately with diameter decreasing. The obvious effect is that in low-dimensions reactors, like in this case, rate of heat exchange is higher of generated reaction heat. This problem is noted especially in tubular reactors, since in this kind of reactors internal temperature is high because of reaction and then thermal flows are very high. Because of this, in thermal profile showed in figure 3 the temperature reaction decreases while reaction advances in the reactor.

Finally, in order to investigate the effect of dispersion parameter on model results, fluid-dynamics assumptions are changed and model is adjusted. This part of study is still in progress. Preliminary results, obtained for operating time of about 1.5 hr, are showed in figure 7. The breakthrough curves slope more gradually, in according to a real behavior. A first remark can be made at this point: if real dispersion and supposed dispersion in fluiddynamic of reactor have the same order of magnitude, laboratory –scale reactors management could be hang-up.

Model results have to be validated by data from experimental runs accomplished in laboratory-scale plant.

Conclusions

In this work, analysis of the hot gas desulphurization system adopted in Sotacarbo laboratory-scale plant, where the sulphur removal is performed by two fixed-bed reactors was conducted. A fixed-bed reactor simulating model has been developed based on ideal assumptions, in order to evaluate the performances of this section. The model was implemented on Fortran code.

The sulphidation performances have been investigated in terms of breakthrough curves at different temperatures. Moreover thermal profiles were obtained.

Main limits of this model were pointed out and optimizations are still in progress. Further results will be object of elaboration.

Nomenclature

C_{H2S} = molar concentration of H_2S in the gas phase [kmol/m^3]

Cp = specific heat at constant pressure [kjoule/kg]

d_p = diameter of sorbent particle [m]

d_r = diameter of reactor [m]

D_{eff} = effective diffusivity [m^2/s]

D_{H2S} = molecular diffusivity [m^2/s]

D_K = Knudsen diffusivity [m^2/s]

G = specific flow rate [kg/m$^2 \cdot$ s]

H = heat flow rate [kj/s]

ΔH = reaction heat [kj/kmol]

D_{H2S} = molecular diffusivity [m^2/s]

De_{ff} = effective diffusivity [m^2/s]

D_k = Knudsen diffusivity [m^2/s]

J_d = mass – transfer factor

K_{ext} = kinetic constant of gas – phase transport [m/s]

$(Ka)_{ov}$ = overall kinetic constant multiplied by a mean exchange area [m^3/s]

$\dot{N}$ = molar flow rate [kmol/s]

PM = molecular weight [kg/kmol]

re = mean pore radius

r_e = initial radius of the sorbent particle [m]

r_i = radius of the internal unreacted core of sorbent particle [m]

Re = Reynolds number

R_{H2S} = specific adsorpion rate [kmol$_{H2S}$/kg$_s \cdot$ s]

S = reactor cross section [m^2]

Sc = Schmidt number

Sh = Sherwood number

t = time [s]

T = temperature [K]

U = heat – transfer overall factor [W/m$^2 \cdot$ K]

z = reactor axial coordinate [m]

ϑ = void fraction

μ = gas viscosity [kg/m $\cdot$ s]

ρ = mass density [kg/m^3]

ρ_s = sorbent mass density [kg/m^3]

ψ = shape factor

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