

Hydrogen sulphide to hydrogen via H₂S methane reformation: thermodynamics and process scheme assessment

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Abstract

Hydrogen Sulphide Methane Reformation (HSMR) represents a valid alternative for the simultaneous H₂S valorisation and hydrogen production at the industrial scale, without direct CO₂ emissions. The major concerns about the process commercialization are the possible coke formation in the reaction zone and the lack of active and selective catalysts. The study of the thermodynamics is the essential preliminary step for the reaction phenomena understanding. In this work, a deep thermodynamic analysis is performed to explore the system behaviour as a function of temperature, pressure, and inlet feed composition, using the Aspen Plus RGibbs module. In this way, the optimal process operating conditions to avoid carbon lay down can be identified.

Assessed the system's thermodynamics, a preliminary process scheme is developed and simulated in Aspen Plus V11.0[®], considering hydrogen production and its distribution in pipeline with methane. The process performances are discussed in terms of products' purity and process energy consumptions.

Keywords: methane reformation, H₂S valorisation, H₂ production, CO₂ emissions, H₂ gas-grid distribution

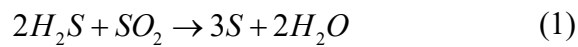
Abbreviations

GTI	Gas Technology Institute
HSMR	Hydrogen Sulphide Methane Reformation
IGT	Institute of Gas Technology
LNG	Liquefied Natural Gas
SMR	Steam Methane Reforming
SQNG	Sub-Quality Natural Gas
TRL	Technology Readiness Level

1. Introduction

As the global natural gas consumption is expected to increase in the next years [1], sour and ultra-sour natural gas reserves, that were previously considered economically unviable, are becoming fruitful. These kind of reserves are often defined as Sub-Quality Natural Gas (SQNG) ones, because of their high impurity content, that needs to be mitigated to meet pipeline or Liquefied Natural Gas (LNG) specifications.

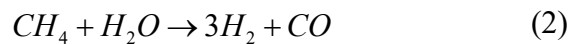
Typically, in natural gas processing, H₂S is a hazardous pollutant requiring deep removal and post-treating. To date, H₂S is generally separated from hydrocarbon gases by amine absorption and regeneration, producing a hydrogen sulphide rich gas. This gas is then sent to the traditional sulphur recovery unit, the Claus facility, to oxidize hydrogen sulphide to elemental sulphur (reaction (1)).



In reaction (1), the H₂S hydrogen content is converted into water vapour, to ensure the sulphur production. Sulphur is a key commodity: its large market volumes make it a low-value added product. It would be advantageous, in principle, to perform H₂S valorisation recovering its intrinsic hydrogen content, thus generating a high value-added product.

Nowadays, the benchmark process for hydrogen production is the catalytic Steam Methane Reforming (SMR). SMR is a very mature technology, with all process steps well developed, also accounting for a good process energetics. Nevertheless, in this process large quantities of natural gas, a valuable resource in itself, are required as both feedstock and combustion fuel.

The principal drawback of methane reforming are the large associated CO₂ direct and indirect emissions: for each mole of CH₄ reformed, more than one mole of CO₂ is released (see reactions (2) and (3) for direct emissions). For this reason, the production of H₂ as a clean burning fuel via steam reforming of methane does not make sense environmentally, since CO_x are generated in the process [2].



Several environmental-friendly technologies are reported in literature for the H₂S valorisation to H₂. Their complete review has been published in 2018 [3], where they have been classified according to their Technology Readiness Level (TRL) [4].

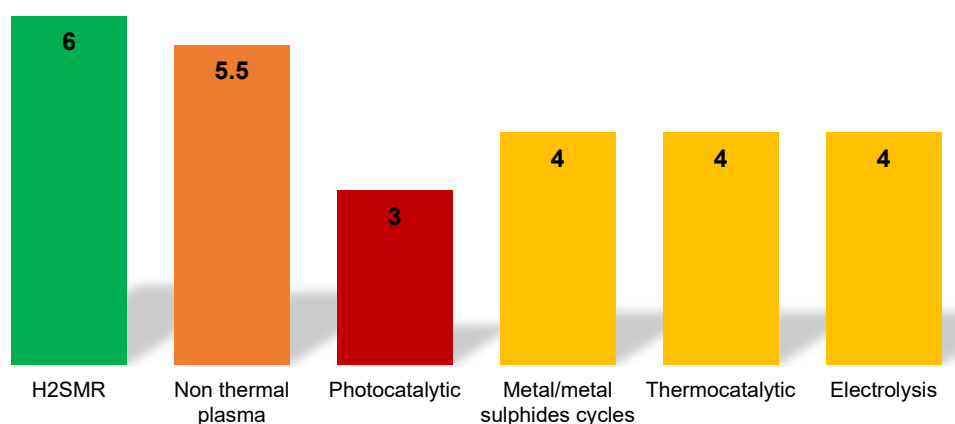
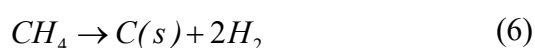
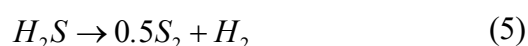
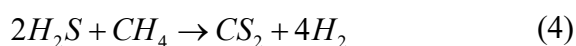


Figure 1. Available H₂S to H₂ valorisation technologies, classified according to their TRL.

As represented in Figure 1, among the available H₂S to H₂ valorisation technologies, the Hydrogen Sulphide Methane Reformation (HSMR) is the most ready to the commercial level scale up.

According to the hydrogen sulphide methane reformation, H₂S is converted into hydrogen and carbon disulphide through reaction (4). Carbon disulphide is generally employed in cellulose industry, rayon production, cellophane and tetrachloride. Other applications regard rubber chemicals, flotation agents and pesticides [5]. Reaction (4) is highly endothermic ($\Delta H_{298K}^0 = 232.4 \text{ kJ/mol}$): fuel combustion is needed to supply the duty necessary for the reaction to occur.

In the presence of H₂S and CH₄ at high temperature, also reactions (5) and (6) can take place.



Besides the indirect CO₂ emissions associated to the fuel combustion, no direct CO₂ emissions are produced in the reaction phase. However, reaction (6) is one of the major concerns about hydrogen sulphide methane reformation process. If this reaction takes hold in the reacting system, carbon lay down can damage the equipment and poison the catalyst, eventually. For this reason, a detailed knowledge of the system's thermodynamics is crucial to identify in which conditions carbon deposits are likely to occur. The chemical equilibrium at high temperatures of methane and hydrogen sulphide has been investigated since 1991[6]. More recently, Huang and T-Raissi [7] performed equilibria calculations to explore the system dependence on the inlet reactants ratio. After that, different numerical and experimental studies were conducted to characterize the system's kinetics and to identify the best reformation catalyst [8-16]. The search for such a catalyst has been conducted by the Institute of Gas Technology (IGT, now Gas Technology Institute, GTI) researchers firstly [17], to

find active bi-functional species capable of dissociating H₂S while holding activity toward reformation reaction. Results showed that Cr₂S₃ and SeS₂ catalysts present the highest activity for inhibiting carbon formation, as well as for the regeneration after carbon deposition. As a matter of fact, major efforts are devoted to define the operability ranges in which carbon deposition can be avoided. Thinking to the process scale up, the best possible operating conditions in terms of operating temperature, pressure and inlet feed composition have to be carefully identified. No information about the system dependence on the operating pressure and on the possible reactants impurities is available in the literature. To fill this gap, the chemical equilibrium composition of the examined system has been studied by minimizing the Gibbs free energy for given operating conditions (i.e., temperature and pressure) and inlet feed mixture. Considering the origin of H₂S and CH₄, the presence of CO₂, higher hydrocarbons and water in the feed stream has been also investigated.

Once assessed the system's thermodynamics, a preliminary process scheme has been developed. Its performances have been analysed in view of the process scale up to the industrial level, considering hydrogen production for pipeline distribution together with methane. Hydrogen distribution in pipelines was experimented in 2019 by Snam S.p.A. energy company, who introduced H₂NG, a hydrogen-gas mixture, into its transmission network with a H₂ content up to 10% by volume. The field trial revealed that, currently, about 70% of Snam's natural gas pipelines are compatible with hydrogen, so that carbon dioxide emissions could be reduced by 5 million tons [18].

2. Thermodynamic assessment

The assessment of the system's thermodynamics has been performed through the RGibbs module available in Aspen Plus V11.0[®] [19]. Fixed the inlet reactant mixture and specified the operating temperature and pressure, this tool evaluates the chemical equilibrium composition through the Gibbs free energy minimization, once all the possible existing equilibrium species have been defined by the user.

The system behaviour as a function of reaction temperature and at variable CH₄/H₂S inlet molar ratio has been analysed at atmospheric pressure, firstly. Temperature has been varied between 800 – 2000°C, while CH₄/H₂S inlet molar ratio ranges from 1:3 to 1:10.

Results are reported in Figure 2 in terms of H₂, CS₂, S₂ and C yields. Product yields are intended as percent yields and calculated according to eqs. (7) to (10).

$$Y_{H_2} = \frac{F_{H_2}^{out}}{F_{H_2S}^{in} + 2F_{CH_4}^{in}} \cdot 100 \quad (7)$$

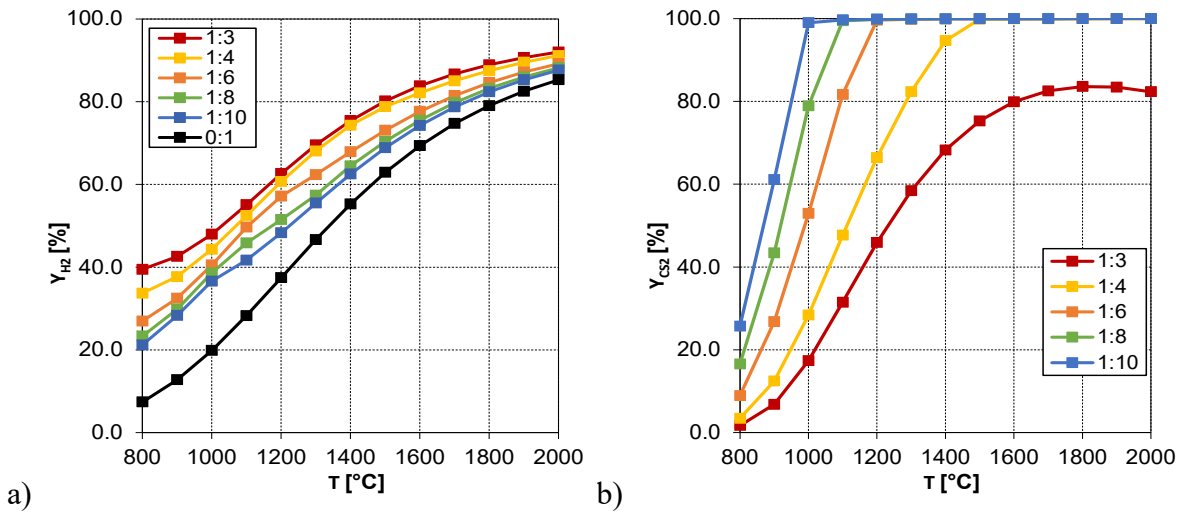
$$Y_{CS_2} = \frac{F_{CS_2}^{out}}{F_{CH_4}^{in}} \cdot 100 \quad (8)$$

$$Y_C = \frac{F_C^{out}}{F_{CH_4}^{in}} \cdot 100 \quad (9)$$

$$Y_{S_2} = \frac{2F_{S_2}^{out}}{F_{H_2S}^{in}} \cdot 100 \quad (10)$$

Results of Figure 2 are in line with the analysis conducted by Huang and T-Raissi [7] and confirm that hydrogen, carbon disulphide, sulphur and carbon are the thermodynamically favoured products at high temperatures. As stated by the authors, the coke yield decreases at increasing temperature for a specified CH_4/H_2S inlet molar ratio. The minimum temperature at which no coke formation occurs at a specific CH_4/H_2S inlet molar ratio is usually defined in literature as pinch point temperature. It is known that this temperature decreases at decreasing CH_4/H_2S inlet molar ratio.

Accordingly, from a thermodynamic point of view, it would be beneficial working with a large excess of hydrogen sulphide in the reaction zone. Nevertheless, this situation corresponds to a significant higher H_2S content in the process than the stoichiometric. The downstream separation of products from reactants would be much more difficult in this case: a sensitivity analysis is necessary to identify the best reactants inlet ratio in the process simulation phase.



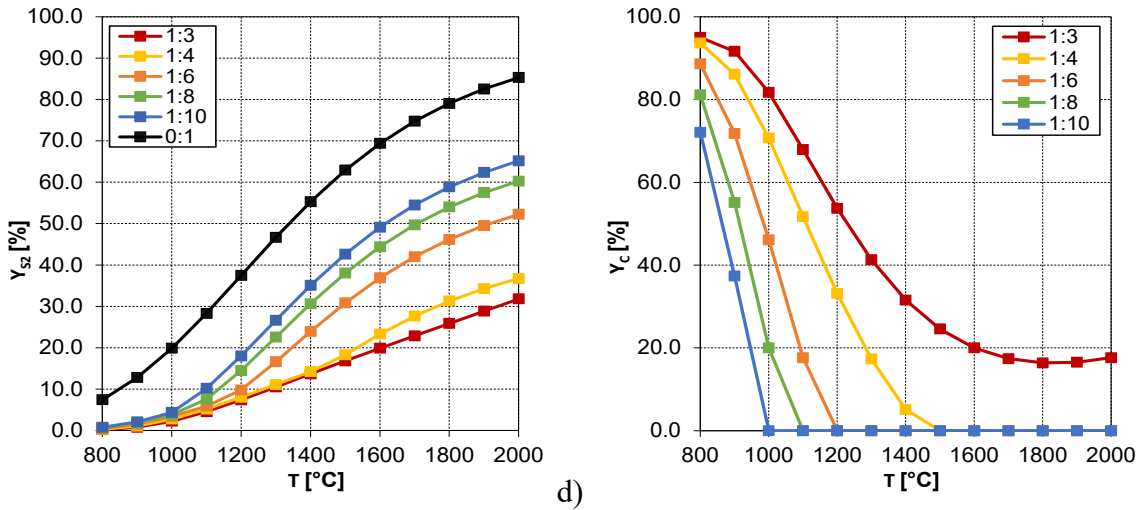
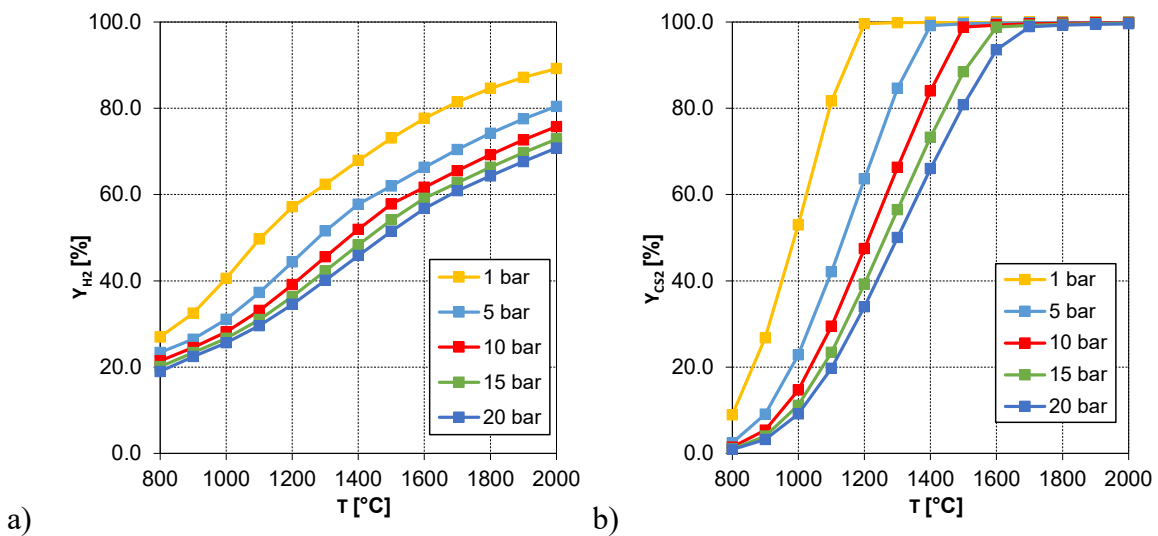


Figure 2. Yield of H_2S methane reformation products as a function of temperature T and at variable CH_4/H_2S inlet molar ratio. Pressure is fixed at $P = 1$ atm.

As for the traditional methane reforming, high pressures can be helpful from the kinetic point of view, to reduce the reactor volumes. For this reason, the effect of the operating pressure has been investigated on the system thermodynamics. Figure 3 reports the pressure effect on products yield as a function of temperature and at fixed CH_4/H_2S inlet molar ratio of 1:6. The pressure effect has been evaluated in the range 1 – 20 bar. The reformation reaction (reaction (4)) occurs with an increase in the number of moles: it is not favoured by an increasing of pressure, as can be observed in Figure 3a and 3b for the H_2 and CS_2 yields. The decreasing hydrogen production is accompanied by an increase in coke formation, as reported in Figure 3d. If increasing the pressure would be beneficial to reduce the reaction volume and to speed up the kinetics, on the other hand it has a negative effect on the system thermodynamics, determining an increase of the pinch point temperature for a given CH_4/H_2S inlet molar ratio.



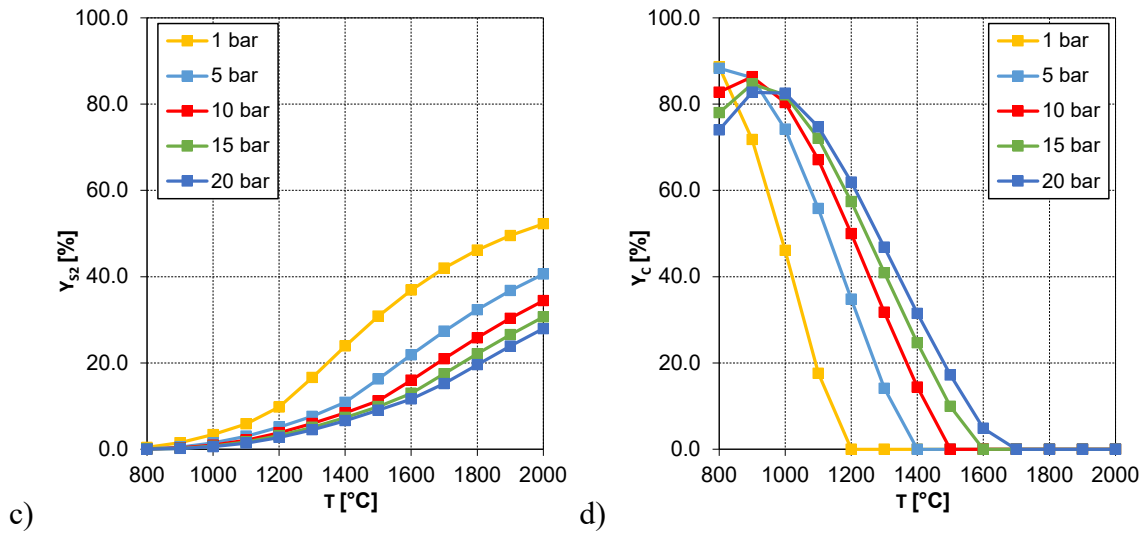
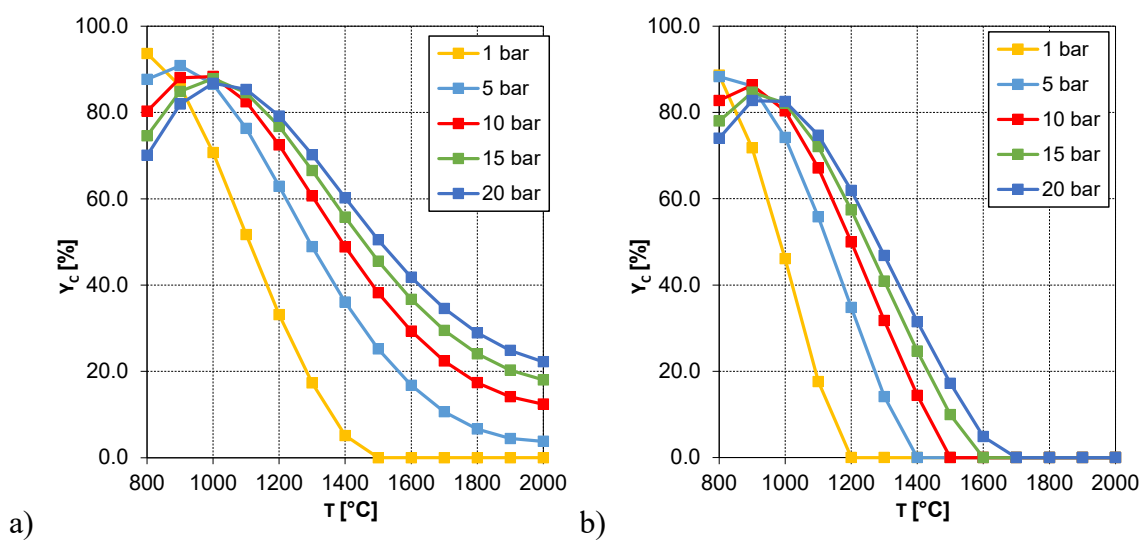


Figure 3. Yield of H₂S methane reformation products as a function of temperature T and at variable pressure. CH₄/H₂S inlet molar ratio is fixed at 1:6.

Results are obviously independent from the selected CH₄/H₂S inlet ratio, as observed in Figure 4.



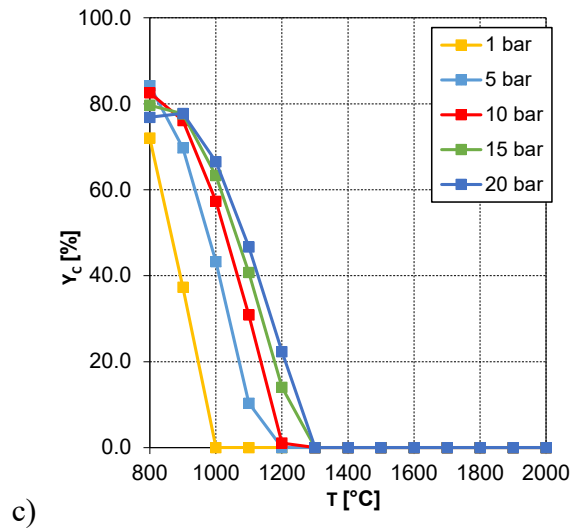


Figure 4. Pressure effect on carbon yield for: a) $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio = 1:4; b) $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio = 1:6; c) $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio = 1:10.

2.1 H₂O effect

Considering the origin of H_2S and methane streams, the effect of small water contents on the system's thermodynamics has been investigated, assuming a H_2O variable molar fraction in the feed stream in the range 0 – 7 mol %. For the sake of clarity, results are reported in Figure 5 in terms of carbon and carbon monoxide yields. As can be noticed, the water presence is responsible for a decreasing in the pinch point temperature, at fixed pressure and for a given $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio. If this is beneficial for the process operability, since carbon lay down can be more easily avoided, on the other hand carbon monoxide is produced and it has to be separated from the reacting mixture downstream the reaction section, if pure hydrogen is the desired product.

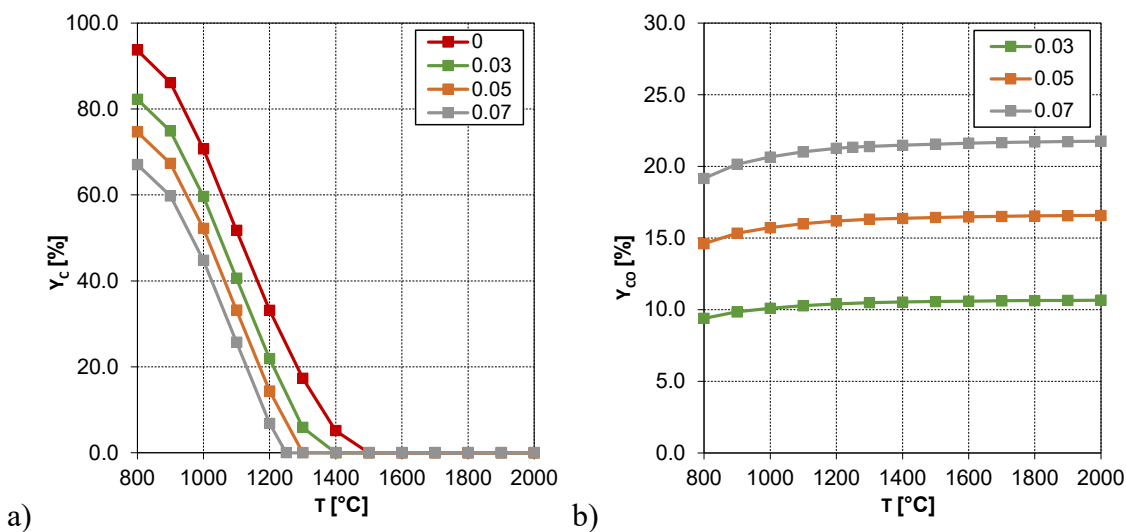
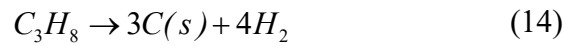
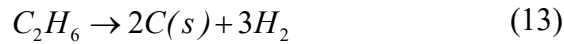
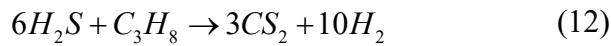
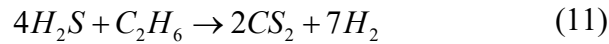


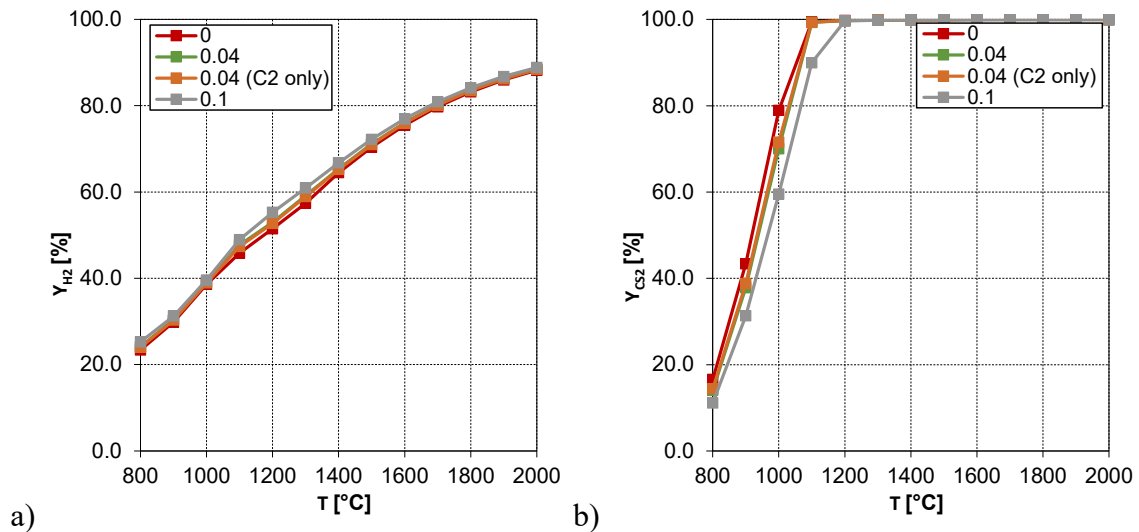
Figure 5. Yield of C and CO for H_2S methane reformation as a function of temperature T and at variable H_2O inlet molar fraction. Pressure is fixed at $P = 1$ atm and $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio is fixed at 1:4.

2.2 Higher hydrocarbons effect

As the inlet methane is likely derived from a natural gas stream, traces of higher hydrocarbons (e.g. C₂₊) can be also present in the feed stream. To analyse their effect on the system's thermodynamics, ethane and propane were selected as representative species. Their inlet content has been varied with respect to the methane inlet content in the range 0 – 10 mol %. Results show that C₂₊ are not only responsible for an increase in the pinch temperature, due to reactions (13) and (14), but also for a small increase in H₂ and CS₂ production, due to the reformation reactions (11) and (12), as confirmed in part by Megalofonos and Papayannakos [6].



The influence of the hydrocarbon distribution in the inlet feed mixture was also evaluated considering the possible presence of ethane only (see the orange curves in Figure 6). No appreciable differences are detected with respect to the effect of an equal quantity of ethane and propane in the inlet feed (green curve in Figure 6), probably because of the small molar concentrations considered, too.



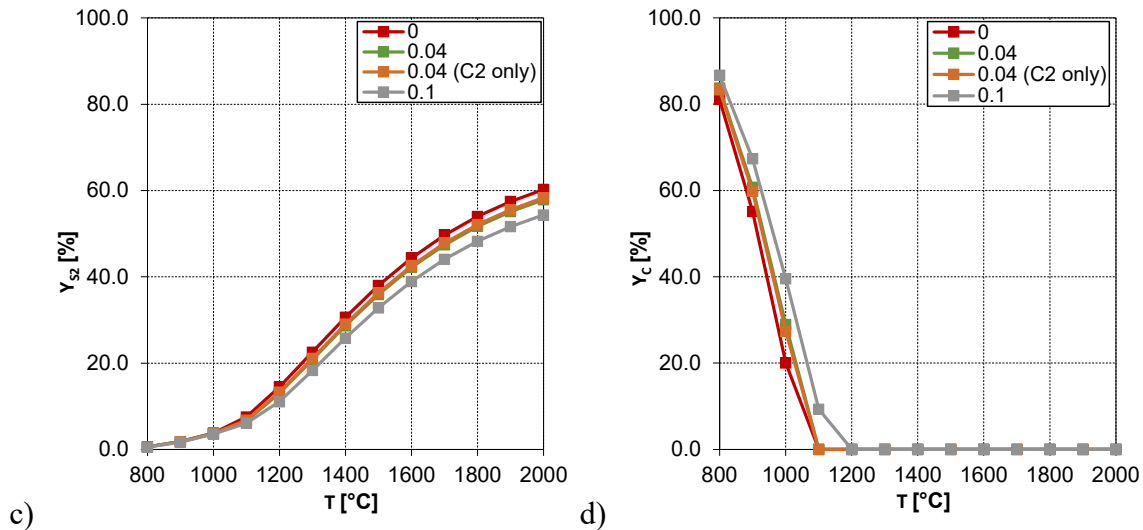


Figure 6. Yield of H₂S methane reformation products as a function of temperature T and at variable C₂₊ inlet content. CH₄/H₂S inlet molar ratio is fixed at 1:8.

The effect of C₂₊ on the pinch temperature is clearly visible in Figure 7, where the pinch temperature is represented as a function of the ratio between the inlet carbon atoms and the inlet hydrogen sulphide. An almost linear trend is observed in this case, stressing the influence of the feed hydrocarbon content on the pinch point temperature.

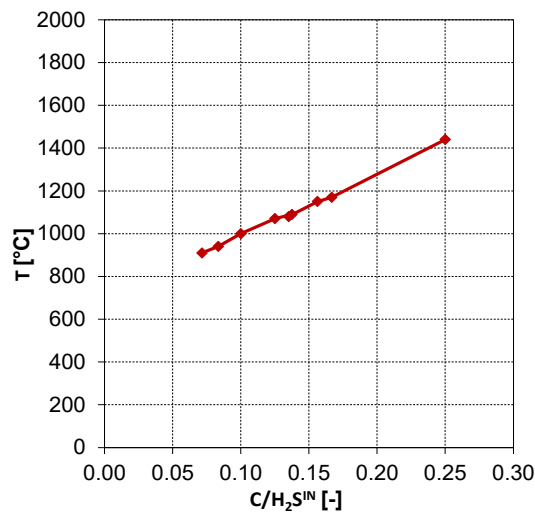


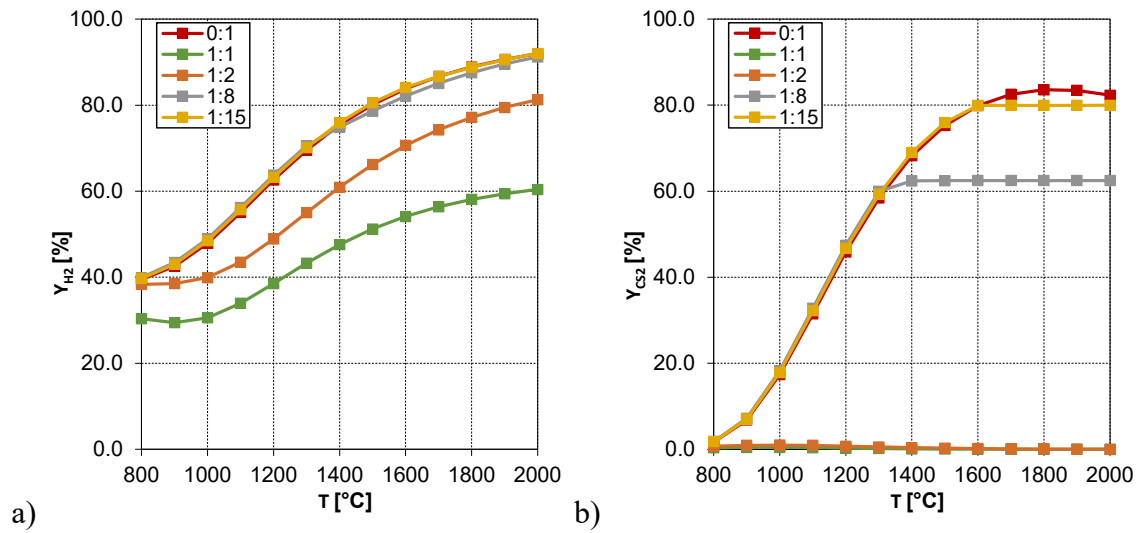
Figure 7. Pinch temperature T as a function of C/H₂S inlet ratio. Pressure is fixed at $P = 1$ atm.

2.3 CO₂ effect

Hydrogen sulphide content in natural gas is typically associated with a not negligible carbon dioxide content. Thereby, the effect of this acid gas on the system's thermodynamics has also been investigated. Results for this case prove that the system behaviour is function not only of the CO₂/H₂S inlet molar ratio but also on the CO₂/CH₄ molar feed ratio. Figure 8 reports the yield of H₂S

reformation products as a function of temperature T and at variable $\text{CO}_2/\text{H}_2\text{S}$ inlet molar ratio. Pressure is fixed at 1 atm and $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio is fixed at 1:3.

Figure 8 plots reveal two different trends: one for 1:8 and 1:15 $\text{CO}_2/\text{H}_2\text{S}$ inlet molar ratio (grey and yellow curves, respectively), which corresponds to CO_2/CH_4 inlet molar ratio lower than 1 and one for 1:1 and 1:2 $\text{CO}_2/\text{H}_2\text{S}$ inlet molar ratio (green and orange curves, respectively), which corresponds to CO_2/CH_4 inlet molar ratio higher than 1 (see Table 1 for the sake of clarity).



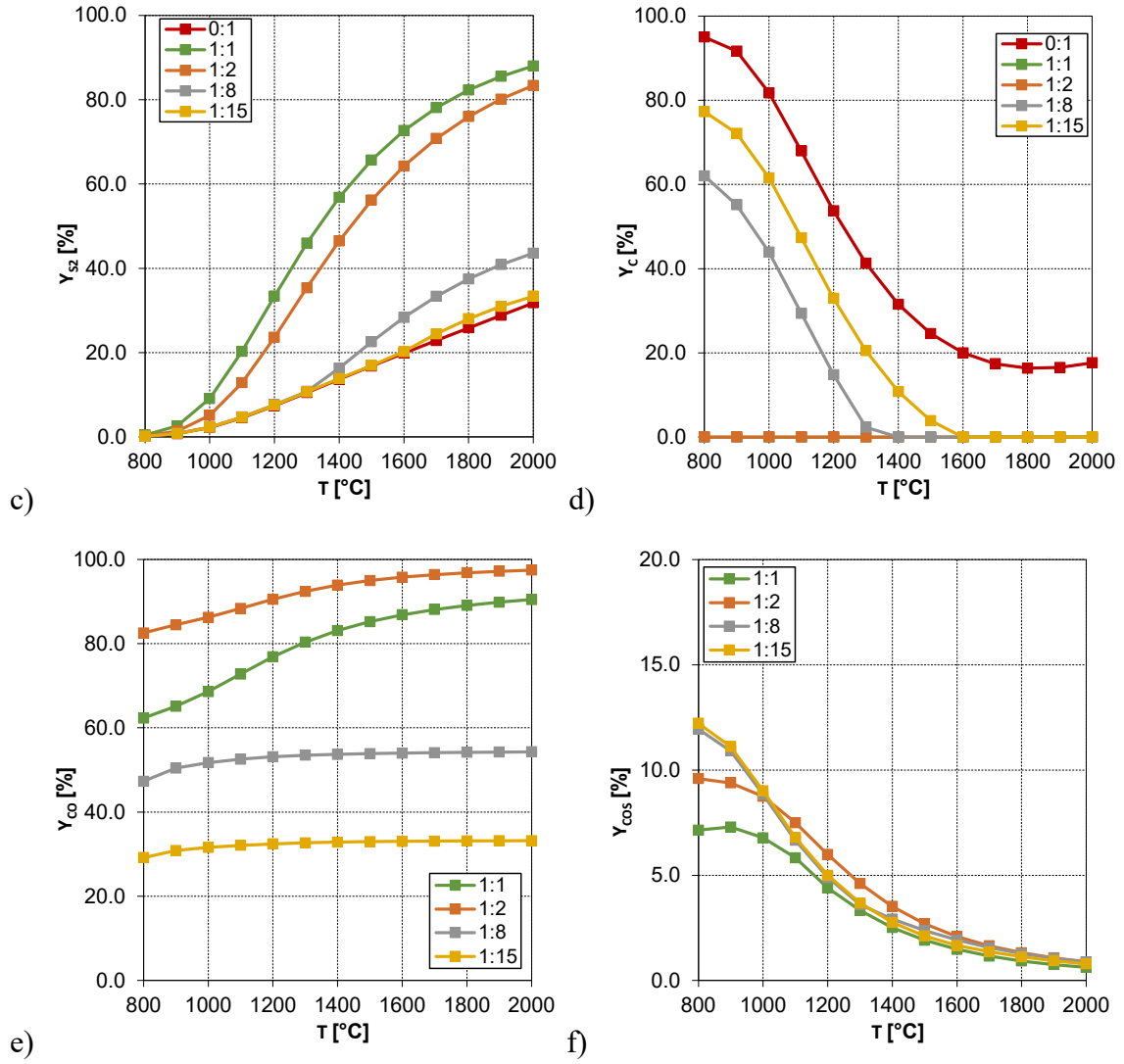


Figure 8. Yield of H_2S methane reformation products and carbon monoxide as a function of temperature T and at variable $\text{CO}_2/\text{H}_2\text{S}$ inlet molar ratio. Pressure is fixed at $P = 1$ atm and $\text{CH}_4/\text{H}_2\text{S}$ inlet molar ratio is fixed at 1:3.

Table 1. Inlet reactants ratio for the different cases analysed for H_2S methane reformation with CO_2 .

#case no.	$\text{CO}_2/\text{H}_2\text{S}$	CO_2/CH_4
1	1:1	3:1
2	1:2	3:2
3	1:8	3:8
4	1:15	1:5

At higher CO_2 contents, H_2 and CS_2 production decreases as well as coke formation, which is reduced in favour of CO and COS production.

For this reason, if small CO₂ traces can be beneficial to avoid carbon lay down, at higher acid gas contents in the feed stream other gaseous compounds are coproduced which can hinder the hydrogen separation and purification downstream the reaction section.

As a general remark, impurity content has to be carefully tuned depending on the nature of the desired product. If hydrogen has to be obtained, low H₂O, C₂₊ and CO₂ contents are admissible. On the other hand, if syngas (H₂-CO mixture) has to be produced, higher impurity contents can be tolerated.

3. Process scheme development

Analysed the system's thermodynamic behaviour, a methane reformation process scheme has been set up for hydrogen production to be distributed in pipeline together with methane.

Two different process schemes have been proposed in literature considering hydrogen production through H₂S methane reformation. Huang and T-Raissi [7] presented three alternatives for liquid hydrogen production, considering liquid hydrogen separation from the product mixture through liquefaction or membranes. Due to the preliminary nature of these flowsheets, specific details about equipment consumptions or operating conditions were not provided.

Martínez-Salazar and co-workers [20] performed a techno-economic analysis of hydrogen production via methane reformation. The reaction section was simulated considering a tubular reactor, where a kinetic scheme derived elsewhere [12] was implemented. The flowsheet set up was not deeply discussed and basic assumptions for the economic analysis were not presented.

Based on the thermodynamic analyses reported in section 2, a process scheme (Figure 9) has been developed in Aspen Plus V11.0[®] for the gaseous hydrogen production. This process diagram has to be intended as a preliminary feasibility analysis of H₂S valorisation to H₂ through the reformation reaction. For this reason, the feed mixture is assumed as composed of H₂S and CH₄ only, while the inlet reactants molar ratio CH₄/H₂S is set at 1:4, the minimum to avoid carbon lay down in the temperature range 800 – 2000°C.

The effect of other impurities in the feed, as well as a sensitivity analysis as a function of the inlet feed ratio, will be part of future development of the present study.

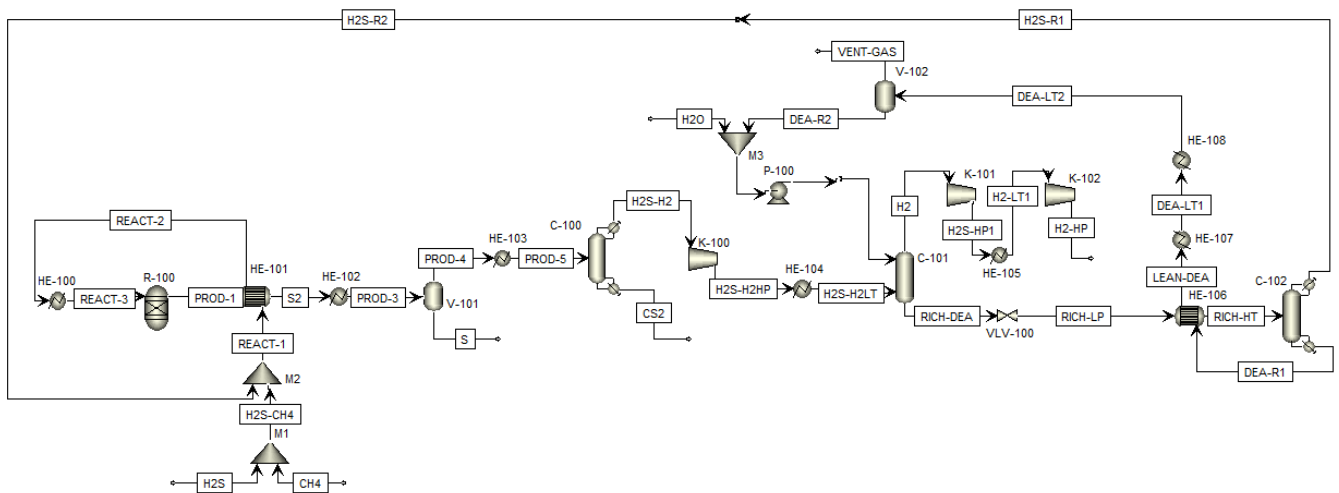


Figure 9. Process scheme simulation in Aspen Plus V11.0[®].

The process flow diagram presented in Figure 9 can be subdivided into different subsections, each one discussed in the following.

- Reaction section, essentially consisting of the reformation reactor (R-100 in Figure 9). This reactor was simulated using the RGibbs module available in Aspen Plus. The conversion of the reagents under the specified operating conditions (reaction temperature = T_{pinch} at the fixed CH₄/H₂S inlet molar ratio = 1:4 and pressure P slightly above the atmospheric one, $P = 1.7$ bar), therefore, is that of thermodynamic equilibrium. The reaction section receives the fresh H₂S and CH₄ streams as feed (H₂S and CH₄ streams, respectively, in Figure 9), together with the recycled H₂S. The reactant mixture is preheated by heat exchange with the reaction products, to recover the high enthalpy contribution associated with them.
- S₂ separation section, consisting of the phase separator V-101, operating at temperature $T = 135^{\circ}\text{C}$, as in both the Claus and the Frasch process [21], which allows to recover a sulphur stream, S in Figure 9, in the liquid phase whose purity is in line with commercial standards (> 99.5 mol %).
- CS₂ separation section, in which CS₂ is separated from the remaining components (mainly, H₂, H₂S and traces of CH₄) by distillation in the C-100 column. The CS₂ product (stream CS2 in Figure 9) whose purity is > 99.5 mol %, is recovered from the bottom of the column, while the mixture leaving the overhead condenser is sent to the H₂ separation section.
- H₂ separation section, consisting of the absorption column C-101, which uses diethanolamine at 20 wt.% as solvent, followed by the regeneration column of the solvent C-102. This section is aimed at the separation of the hydrogen produced from unconverted H₂S: H₂ leaving the absorption column is sent to compression, while the amine solution rich in H₂S is recovered from the bottom of the same column and sent for regeneration to column C -102. The column

allows the separation of H₂S, which is recovered at the top, from the diethanolamine solution which, after cooling, is pumped and sent back to the C-101 column. The overhead stream, composed of H₂S and a small amount of water (around 2.5 mol %) to ensure a temperature at the C-102 condenser that can use water as a cooling medium, is recycled to the reaction section.

- H₂ compression section, comprising two stage compression with intermediate cooling, which has the purpose of compressing the hydrogen produced for its distribution into the pipeline together with methane (stream H2-HP in Figure 9).

All sections operate at approximately atmospheric pressure, except for the H₂ separation section, which is operated at 10 bar. The pressure of 10 bar is to be considered as a first attempt value: it is one of the degrees of freedom of this analysis, to be optimized at a later stage of the study.

As for the CS₂ separation section, it is placed upstream of the H₂ separation section to reduce energy consumption of the K-100 compressor. However, this choice results in cryogenic temperatures of the C-100 column condenser, which operates at atmospheric pressure. Therefore, also in this case a sensitivity study would be necessary to identify the optimal process configuration in terms of performances.

4. Preliminary process performances

The performances of the process scheme described in section 3 are reported in the following. The CH₄/H₂S inlet molar ratio is fixed at 1:4 at the reactor entrance. Due to the inlet feed ratio imposed, methane is the limiting reactant, so its equilibrium conversion is close to 1 ($\chi_{CH_4}^{EQ} = 0.9970$). On the other hand, hydrogen sulphide conversion results $\chi_{H_2S}^{EQ} = 0.6298$, since it is fed in excess at the process unit battery limits.

Table 2 reports the inlet streams conditions specified in the Aspen Plus simulation, while Table 3 summarizes the conditions of the streams exiting the battery limits.

Hydrogen product (H2-HP) has to be distributed via natural gas pipeline: its pressure is in line with the gas grid distribution pressure, while its molar purity results equal to 98.54%. If its impurity content would be not acceptable, an eventual post-treating can be considered for this stream.

Carbon dioxide and sulphur by-products present a purity higher than 99.5%, so that they can be distributed on market as valuable chemicals.

Table 2. Inlet streams conditions in the Aspen Plus V11.0® simulation.

Reactants		H2S	CH4
T	°C	44.3	40
P	bara	1.8	1.8
Molar fractions			
H2O		-	-
H2S		1	-
CH4		-	1
F_{TOT}	kmol/h	82.3076	32.6617

Table 3. Outlet streams conditions in the Aspen Plus V11.0[®] simulation.

Products		H2-HP	CS2	S
T	°C		61.13	135
P	bara	75	1.6	1.7
Molar fractions				
H2O		0.0056	19ppm	1ppm
H2S		1ppm	0.0003	0.0009
CH4		0.0006	-	-
CO2		-	-	-
CO		0.0083	-	-
H2		0.9854	-	-
CS2		-	0.9991	0.0052
S2		-	0.0005	0.9939
CH4S		-	10ppm	-
COS		0.0001	1ppm	-
C		-	-	-
F_{TOT}	kmol/h	150.8875	31.2746	9.8832

Table 4 reports the heating and cooling requirements for the analysed process scheme.

As can be observed, the major contributions in the process energy balance are the reaction section heating requirements, which must be supplied through fuel combustion, C-100 cooling requirements, to be provided through an ad-hoc refrigeration cycle, and C-102 reboiler heating requirements, which needs low pressure steam.

The diethanolamine choice as absorbing agent is motivated by the presence of sulphur compounds such as COS and mercaptans in the gas stream to be purified: since the secondary amines are less reactive towards these species, their presence does not hinder the absorption of hydrogen sulphide [22]. However, the discussed process scheme has to be intended as a preliminary methane reformation feasibility analysis, for the process scale-up to the industrial level. A further process optimization following the GPSA [23] design guidelines is needed to reduce the associated energy consumption and will be part of future developments of the present work.

Table 4. Heating and cooling requirements in the Aspen Plus simulations, together with the corresponding working fluid.

equipment	T_{IN} [°C]	T_{OUT} [°C]	Q [kW]	<i>working fluid</i>
HE-100	1301.15	1500	550.84	fuel
R-100	1500	1500	2841.96	fuel
HE-102	400	135	-811.57	cooling water
HE-103	135	50	-180.12	cooling water
C-100 reboiler	56.69	61.13	4569.43	LP steam
C-100 condenser	-53.88	-77.47	-5007.16	refrigeration cycle needed
HE-104	85.55	50	-60.09	cooling water
C-102 reboiler	119.75	120.17	7684.81	LP steam
C-102 condenser	115.40	31.85	-4451.63	refrigerated water
HE-107	100.49	50	-2509.39	cooling water
HE-108	50	35	-739.37	refrigerated water
HE-105	163.87	70	-115.18	cooling water

Consumptions for compressors and pumps are not so impactful in the process energy balance, as reported in Table 5.

Table 5. Compression power requirements in the Aspen Plus process simulation.

equipment	P_{IN} [bara]	P_{OUT} [bara]	Power [kW]
K-100	1.6	10	282.88
P-100	1	10	16.09
K-101	10	34	166.52
K-102	34	75	187.36

5. Conclusions

The methane reformation process has been analysed for the simultaneous H₂S valorisation and H₂ production. For the system behaviour's understanding and in view of the process scale up at the industrial level, a deep thermodynamic analysis has been performed. The thermochemical equilibrium calculations show that temperature and pressure can significantly affect the carbon deposition in the reaction phase, which is more likely to occur at high pressure and low temperature. Feed composition, also, is responsible of pushing or avoiding coke formation. As a matter of fact, H₂O and CO₂ presence can be beneficial to avoid carbon lay down while C₂₊ traces in the feed stream are undesired in this respect. However, if hydrogen is the desired product, impurities content in the reactants mixture has to be carefully managed because of the eventual production of CO, COS and other sulphur based compounds. The thermodynamic assessment of the reacting system is the essential step for selecting the optimal operating conditions in terms of temperature, pressure and feed compositions for the process simulation phase. In the process simulation, a preliminary process scheme has been set up through the Aspen Plus V11.0[®] simulation software. Its performances have been analysed in terms of energy and material balances, to build up the starting point for a future sensitivity study and optimization.

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