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# Process simulation of a dual-stage Selexol unit for pre-combustion carbon capture at an IGCC power plant

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## Abstract

It is aimed to simulate a dual-stage Selexol process for removing $CO_2$ as well as $H_2S$ from the syngas typically found in the IGCC power plant with a dry-coal fed gasifier. Temperature-dependent Henry's law is employed in the process simulation to estimate the solubilities of gas components in Selexol. The operating conditions of dual-stage Selexol unit were found so as to meet simultaneously various specifications such as 99+% $H_2$ recovery, 90% or 95% $CO_2$ recovery and 99+% $H_2S$ recovery. The power consumptions for auxiliary units and $CO_2$ compression estimated by the simulation are in good agreement with those reported in the literature [1]. It is shown that the conventional, integrated dual-stage Selexol unit can achieve 95% carbon capture rate as well as 90% by simply changing the operating conditions.

*Keywords:* Selexol; Pre-combustion carbon capture; Dual-stage Selexol process; Process simulation; Integrated Gasification Combined Cycle

## 1. Introduction

Anthropogenic $CO_2$ emissions are being increasingly viewed as a major problem the humanity is facing. The Integrated Gasification Combined Cycle (IGCC) power plants have been gaining an attention due to their high electricity production efficiency and their ability to produce power with low environmental impact [2,3]. Since the 1990s there have been various researches on carbon capture from IGCC power plants. Doctor et al. [4] evaluated several commercially available $CO_2$ capture technologies that are incorporated into IGCC power plants for 90% carbon capture. Chiesa and Consonni [5] studied a Selexol process to recover 90% $CO_2$ from the shifted syngas and

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they concluded that the addition of the Selexol process for carbon capture would result in 5 to 7 % reduction in the LHV-based power efficiency and around 40% increase in the cost of electricity. DOE NETL [6] investigated $CO_2$ capture from oxygen-blown, Destec and Shell-based IGCC power plants at the scale of a net electrical output of 400 MW with which a dual-stage Selexol process was integrated for capturing $CO_2$ at an overall capture efficiency of 87%. O'Keefe et al. [7] studied a 900 MW IGCC power plant integrated with a Selexol process for recovering 75% of the carbon that the coal feed contains. Davison and Bressan [8] compared the performances of several chemical and physical solvents including Selexol solvent for recovering 85% $CO_2$ from a coal-based 750 MWe IGCC. Cormos and Agachi [9] performed various case studies on 400 - 500 MW scale IGCC plants integrated with acid gas removal processes with several physical solvents including Selexol for 90+% carbon capture rate.

According to literature review on this issue, it is obvious that dual-stage Selexol units have been recognised as the most conventional absorption process for recovering $H_2S$ and $CO_2$ simultaneously. This is because

1) The solvent loss by its evaporation at the process is almost negligible due to the very low vapour pressure.
2) The $CO_2$ and $H_2S$ contained in the syngas can be recovered separately thanks to Selexol owning a good selectivity of $H_2S$ over $CO_2$.
3) Selexol has a substantial $CO_2$ solubility and it also has very low $H_2$ solubility. Therefore the $H_2$ loss by AGR unit can be reduced.

Regarding the design of acid gas removal processes using Selexol, Kohl and Nielsen [10] exhibited a simple two-stage Selexol process where the 1st stage is for $H_2S$ removal and the 2nd stage is for $CO_2$ removal. The simple two-stage Selexol process was simulated by Robinson and Luyben [11]. Recently, Bhattacharyya et al. [12] presented the simulation results on a dual-stage Selexol process. Padurean et al. [13] reported an Aspen Plus simulation on a dual-stage Selexol unit at 70%, 80% and 90% $CO_2$ capture rate.

While most past researches have been made mainly on a basis of 90% carbon capture rate, this study shows the change of operating conditions to achieve up to 95% carbon capture rate.

## 2. Solubility model

It is essential that process simulations for gas absorption and stripping should be implemented on reliable solubility model. Very few experimental data on the solubility of syngas components in Selexol solvent have been reported so far and good solubility models for this system are not easily available either. This is because Selexol solvent is not a pure component solvent but a mixture of various dimethyl ether of polyethylene glycol, $CH_3O(C_2H_4O)_nCH_3$ where n changes in a range of 2 to 9.
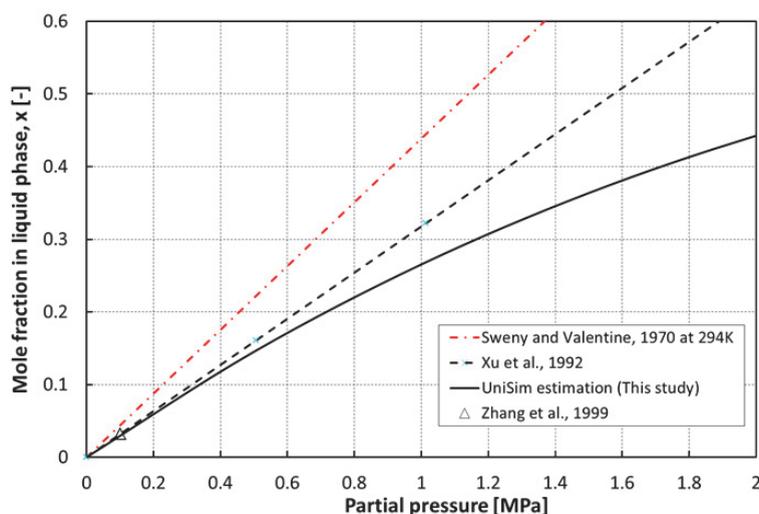


Fig. 1. Solubility curve of $CO_2$ in Selexol at 25 °C.

The physical properties of Selexol solvent in the UniSim database were utilised without any modification in the process simulator except for the Henry constants. This is because the physical properties, such as molecular weight, density and heat capacity that UniSim contains are very close to what were reported in the references but the solubility data are not.

Sweny and Valentine [14] shows the Henry constants of $CO_2$, $H_2S$, $CH_4$, COS and $CH_3SH$ at 70 °F. Xu et al. [15] measured the solubility of $CO_2$ and $H_2S$ in a Selexol solvent at a very low partial pressure to obtain Henry constants at different temperatures. In Figure 1, the solubility data of $CO_2$ in Selexol are plotted given the Henry constants [14, 15]. The Henry constant by Xu et al. is in perfect agreement with the solubility data measured by Zhang et al. [16].

Compared to the corrected Henry constant, however, the Henry constants provided by UniSim database are too high to be used in the simulation without modification. Now that the Henry constants and their temperature dependency are known, it is possible to use them instead of the default values in UniSim database.

The Henry constants for $CH_4$, CO and $N_2$ are obtained based on their solubility relative to $CO_2$ reported in the reference [17, 18] assuming the selectivity is kept constant regardless of temperature.

Figure 1 also includes the solubility of $CO_2$ in Selexol estimated by UniSim using the modified coefficients. As expected, the estimated solubility data are in good agreement with those of the corrected Henry constants at a very low partial pressure. With increasing pressure, the estimated solubility deviates gradually from the straight line of Henry's Law due to non-ideal behaviour in the gas phase that is estimated by Peng-Robinson EOS.

## 3. Dual-stage Selexol process with 90% carbon capture

A conventional dual-stage Selexol process has been simulated using the newly estimated solubility data as discussed above. The temperature, pressure, gas composition and flowrate of a syngas feed to the dual-stage Selexol process are the same as those of the reference (DOE Case 6) [1]. The syngas properties reported in the reference has been confirmed to be correct by an independent process simulation [19]. It should be noted that the carbon capture rate include CO and $CH_4$ as well as $CO_2$ contained in the $CO_2$ product since Selexol is capable of capturing CO and $CH_4$ too despite their relatively lower solubilities in Selexol.

The process configuration of the conventional dual-stage Selexol unit is shown in Figure 2. In this simulation, a set of operating conditions was found with the following targets met at the same time.

- $H_2$ recovery : 99+ %
- Carbon capture rate : 90% or 95%
- $H_2S$ recovery :  99.99+%

The $CO_2$ product purity can be maintained as high as 97+ mol% easily if the above-mentioned targets for the $H_2$ and $H_2S$ recovery are met. Also the $H_2S$ content in the $CO_2$ product can be less than 20 ppmv with the 99.99+% $H_2S$ recovery.

A raw syngas is sent at 23.9°C to a $H_2S$ absorber where $H_2S$ that it contains is preferentially absorbed by Selexol solvent coming from a $CO_2$ absorber, hereinafter called $CO_2$-laden solvent. The $H_2S$ rich solvent leaving the $H_2S$ absorber flows to a $H_2S$ concentrator followed by a flash drum in order to desorb $CO_2$ out of the solvent and enrich $H_2S$ in the solvent. This is because the steam stripper for solvent regeneration makes the solvents free of the acid gases, i.e. $CO_2$ as well as $H_2S$ would be stripped off the solvent and included in the overhead sour gas stream. If a very high carbon capture rate is required or a $H_2S$ mole fraction in the sour gas needs to be maintained as high as possible, it is essential to desorb $CO_2$ out of the $H_2S$ rich solvent before the rich solvent is fed to a $H_2S$ stripper. As the recovered gas streams generated from the $H_2S$ enriching section also contain significant amount of $H_2S$ as well as $CO_2$, they cannot be sent directly to the $CO_2$ absorber but must be recycled to the $H_2S$ absorber.

The Selexol solvent should contain a small amount of water in it so that the water can be boiled off and used as a stripping gas in the $H_2S$ steam stripper. In this study, the Selexol solvent contains 5 wt% water. It is reported that the water content in Selexol solvent is typically kept less than 5 wt% since the Selexol solvent has the low viscosity of around 7 cP at 20°C but the viscosity increases gradually as the solution temperature is lowered and it also increases slightly with the addition of water [20]. The $H_2S$ stripper driven by LP steam can regenerate the solvent completely, i.e. the lean solvent contains neither $CO_2$ nor $H_2S$.
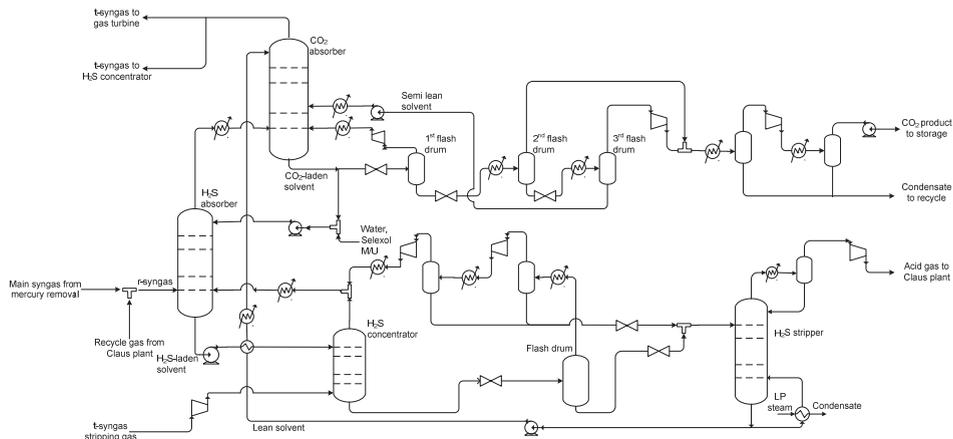
Fig. 2.Schematic diagram of a dual-stage Selexol unit with integrated solvent cycle.

The syngas leaving the $H_2S$ absorber is sent to the $CO_2$ absorber. There are two different solvents being used for capturing $CO_2$. One is a lean solvent coming from the $H_2S$ stripper and being sent to the top of the stripper and the other is a semi-lean solvent originating from the last stage of flash drum trains and entering the middle of the column.

## 4. 95% carbon capture rate
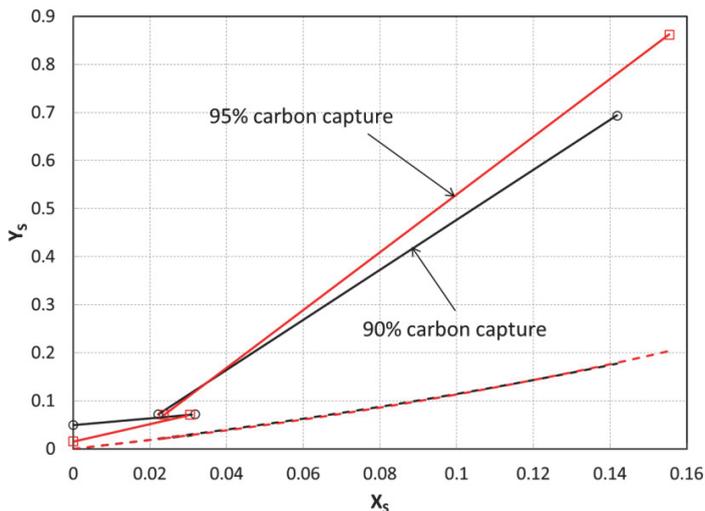


Fig. 3. Operating and equilibrium lines around $CO_2$ absorber of integrated dual-stage Selexol unit at 90% and 95% carbon capture rates (solid lines: operating lines, broken lines: equilibrium lines, symbols: UniSim simulation results).

While it is also possible to achieve 90% carbon capture rate with unintegrated dual-stage Selexol unit, it is hard to reach 95% carbon capture rate by increasing the circulating solvent flowrate due to a pinch point being formed at the top end of the $CO_2$ absorber. One obvious way of avoiding such a pinch point at the top end is to feed both a lean solvent, i.e. $CO_2$-free solvent, to the top end and a semi-lean solvent to the middle of the column just as implemented in the integrated dual-stage Selexol unit. The $CO_2$-free lean solvent flow gives rise to a discontinuity of operating line so that there are room for improving the carbon capture rate. Simply increasing the CO2-free, lean solvent flowrate makes it possible to improve the carbon capture rate up to 95%.

## 5. Conclusions

A dual-stage Selexol unit with integrated solvent cycle was simulated to find the operating conditions for $CO_2$ and $H_2S$ capture and estimate the energy penalty involved. Furthermore it was shown that the same dual-stage Selexol unit could achieve 95% carbon capture rate by simply changing the operating conditions.

## Acknowledgements

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