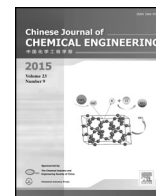




Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Process Systems Engineering and Process Safety

Equation oriented method for Rectisol wash modeling and analysis☆



Ning Gao, Chi Zhai, Wei Sun*, Xingyu Zhang

Beijing Key Lab of Membrane Science and Technology, College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, China

ARTICLE INFO

Article history:

Received 4 September 2014
 Received in revised form 19 January 2015
 Accepted 28 January 2015
 Available online 28 March 2015

Keywords:

Rectisol process simulation
 Modified statistical associated fluid theory
 Equation oriented
 Sequential quadratic programming

ABSTRACT

Rectisol process is more efficient in comparison with other physical or chemical absorption methods for gas purification. To implement a real time simulation of Rectisol process, thermodynamic model and simulation strategy are needed. In this paper, a method of modified statistical associated fluid theory with perturbation theory is used to predict thermodynamic behavior of process. As Rectisol process is a highly heat-integrated process with many loops, a method of equation oriented strategy, sequential quadratic programming, is used as the solver and the process converges perfectly. Then analyses are conducted with this simulator.

© 2015 The Chemical Industry and Engineering Society of China, and Chemical Industry Press. All rights reserved.

1. Introduction

The Rectisol wash technology with methanol as solvent is an economical and well-proven process for the removal of acid components from raw gases produced by partial oxidation of oil or coal [1], originally patented by Lugi [2] and Linde [3]. The two technologies remove contaminants and produce two streams, one with high purity CO₂ and the other rich in H₂S. CO₂ collection well follows current environmental protection trend and H₂S rich stream is a feed to the Claus plant for sulphur production. The two processes are different. Lugi uses a two-stage configuration for given absorption duty. Linde employs a more compact one column structure, in which CO₂ and H₂S are removed in sequence, giving a side draw free of H₂S that undergoes further flashing to give almost pure CO₂ byproduct and a bottom draw with almost all sulfide. Two-stage configuration is appropriate in the CO shift operation located next to the sulphur recovery for complete acid gas separation [4], but absorption and desorption units are needed with limited heat recovery. This study deals with stream right after CO shift unit, so one-stage configuration is chosen.

The solubility of methanol relative to CO₂ at −40 °C is 4.9 times larger than that of H₂S [5], and the quantity of CO₂ to be removed is much larger than that of H₂S. One-stage configuration is suitable and CO₂ and H₂S are separated in absorption and desorption columns. It also favors heat recovery [5], with more streams through heat exchangers, but

it is more sophisticated and difficult for operation and simulation. Although many simulations for Rectisol process are published, heat exchanger network is not integrated. Our current simulation is to incorporate a heat integration strategy into the absorption and desorption flow sheet, so that (1) the simulation fits practical situation better; (2) heat exchange results are determined by stream information and process configuration instead of adding or removing arbitrary quantity of heat; (3) more informative process analysis is possible by considering correlative relationships; and (4) novel heat integration strategies can be implemented.

In this study, one-stage configuration with the suggestion of Weiss [1] is the basis for our simulation (Fig. 1). A good simulator will reveal the physical and chemical nature of a process, namely, it should be able to predict when manipulated parameters change. Two levels of predictability are needed for the quality of a simulator, an accurate thermodynamic description for phase behavior and a proper mathematical representation for unit operations. In this paper, proper thermodynamic model is used and two categories of heat exchangers are mathematically distinguished. Convergence is a problem in this highly integrated process and equation oriented (EO) strategy with sequential quadratic programming (SQP) is the solver. This simulator is validated with designing data and used for analysis further.

2. Thermodynamic Model

As shown in Fig. 1, stream from shift CO unit is cooled and then goes to the Rectisol wash to remove CO₂, H₂S and COS for downstream usage.

☆ Supported by the National Basic Research Program of China (2013CB733600).

* Corresponding author.

E-mail address: sunwei@mail.buct.edu.cn (W. Sun).

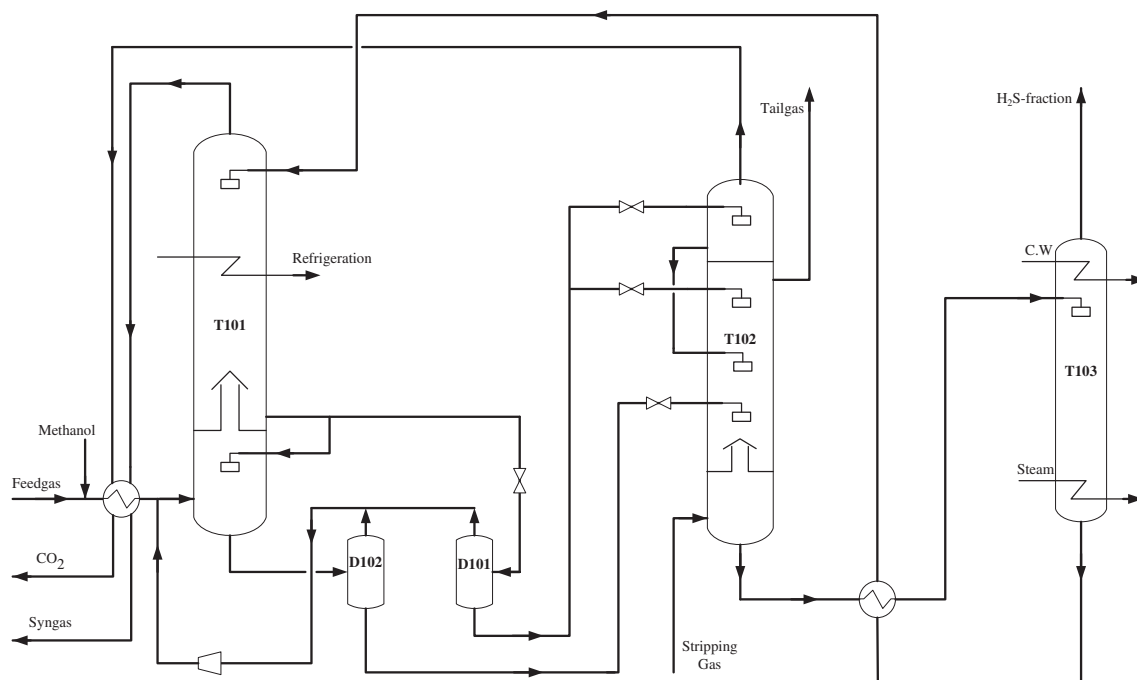


Fig. 1. The flow diagram of one-stage Rectisol wash unit.

A typical composition for the shift outlet is shown in Table 1. Chill methanol can dissolve CO_2 and $\text{H}_2\text{S}/\text{COS}$ selectively and the saturated liquid is desorbed for cyclic utilization, so the fluid package needs to cover a wide range of temperature and pressure for thermodynamic calculations. As Linde Company [6] claimed, their processes can operate in the temperature range of -20 to -60 °C and pressure range of 30 to 80 bar (1 bar = 10^5 Pa). Under the conditions, the presence of methanol and water, which are significantly polar, and H_2 , N_2 , CO_2 , CO , CH_4 , and AR, which are present as supercritical fluid, makes the system difficult to describe thermodynamically. Thus an appropriate thermodynamic model is vital for this simulation. Commonly used thermodynamic models for multiphase systems include vapor liquid equation (VLE) and equation of state (EOS).

Table 1
Feed gas components and composition

Feed gas mole composition/%								
CO_2	H_2	N_2	H_2S	H_2O	AR	CH_4	CO	COS
35.0044	43.6632	1.2596	0.2395	0.2439	0	0.01	19.5721	0.01

2.1. Vapor liquid equation model

Phase behavior for a mixture is commonly described by the VLE:

$$y_i \phi_i^V P = x_i \gamma_i f_i^0 \quad (1)$$

where ϕ_i^V denotes the vapor fugacity coefficient, γ_i denotes the liquid activity coefficient, and f_i^0 denotes the liquid reference fugacity, which is meaningless for Rectisol process since the working conditions for most components are supercritical. The activity coefficient is set to 1.0 at infinite dilution and Henry's law constant is the reference fugacity. Data are regressed in literature [7–10], but the amount of acid gas to be

absorbed is significant and multi-components limit the application of VLE model.

2.2. Equation of state model

R-K-Soave (RKS) equation of state for a system with highly polar components spurs the idea using a single equation of state for both vapor and liquid calculations. Boston and Mathias's pioneer work extrapolated RKS into supercritical region [11]. The earliest publication for Rectisol wash simulation is a thesis by an MIT graduate [12], using RKS method with data correlation for phase calculations. Li *et al.* [13] suggested PSRK [14] with practical data revision as a good model. Sun and Li [15] used RKSWs from Aspen Plus database to simulate the main wash column with small error, but the binary parameter in this method needs to be revised. These simulators are case oriented and corresponding thermo-parameters need to be rectified with practical data, so that their results lack universality. Since all the components are simple ones, a method strong in theoretical foundation would work in this dilemma.

2.3. Thermodynamics of the Rectisol model

A modified statistical associated fluid theory (SAFT) equation by applying perturbation theory (PC-SAFT) to hard-chain reference fluid has been developed, which is a semi-empirical EOS based on mechanical statistical models and is widely used in polymerization process [16,17]. Sun and Smith [5] compared PC-SAFT with other methods in Rectisol process simulation and verified its superiority. Gatti *et al.* [4] also validated this model. PC-SAFT method fits experimental data well [18].

In this simulation, PC-SAFT is used, the unary parameters of methanol and water are revised by NIST [19] database, and a set of solute-solvent binary interaction parameters are regressed by experimental data. The computation is huge: every gas component has three parameters, while methanol and water need five, and the thermodynamic calculation subprogram is repeatedly called.

3. Process Modeling

3.1. Flow sheet description

A prototype flow sheet of Rectisol process is used for reference and the modeling strategy is shown in Fig. 1. T101 is the absorber with two sections: the lower part removes H_2S by CO_2 saturated solvent and the upper part is for CO_2 absorption by lean solvent from regeneration column (T103). A side-draw free of H_2S is sent to D101, $\text{H}_2\text{S}/\text{CO}_2$ rich methanol from the bottom of T101 is sent to D102, and both D101 and D102 under middle pressure flash out absorbed H_2/CO for synthesis gas recovery. T102 has three sections, part of the liquid from D101 at low pressure flashes out almost pure CO_2 , which is used as a solvent in the middle section to reabsorb H_2S ; the other part of liquid from D101 is used to reabsorb D102 low pressure gas and tail gas is drawn from the middle section containing mainly CO_2 and N_2 ; the bottom part strips CO_2 in the solvent by nitrogen. T103 is a steam stripper to collect H_2S for Claus plant and the liquid draw out is the lean solvent for cyclic utilization.

Usually two more small columns are used for methanol dehydration, the water washing tail gas from T102 middle section gas is drawn, and refrigerant recycling is an indispensable part of the unit. Our current work is focused on the three columns.

3.2. Heat integration design

The one-stage configuration has a more compact construction, which is more appreciable for heat recovery [5]. Since acid gas absorption operates at very low temperature achieved by refrigerant vaporization, when solvent regeneration works at quite high temperature and steam is needed as heat input, heat integration is important.

A flow sheet is set when different functional units are systematically connected by streams for process requirement. The Rectisol wash is used to separate contaminant components from a stream of gases, with columns for various separation tasks. Streams always need heating or cooling before entering next units. Stream specifications can be abstracted from this process and heat integration technique [20] is used for analyzing and improving the performance of heat exchanger network [21].

There are many heat integration design and optimization in Rectisol process [4,5,22], and some novel ideas have been embodied in industrial plants [23]. Fig. 2 presents a heat exchanger network design of a real

plant, but no process simulation with heat exchange integrated is presented. After heat integration design is finished, the geometry of each heat exchanger can be fixed accordingly, and the heat-integrated Rectisol simulation becomes an operational problem. Heat exchanger integration makes the simulation more complicated, but the relationship between variables is closer to that in real state, which can be used to test the feasibility and flexibility of novel heat integration strategies.

3.3. Heat-integrated process modeling

The heat integration design in Fig. 2 is implemented on the process modeling as shown in Fig. 3. Two categories of heat exchanger are distinguished. (1) Heat is removed by refrigerant. Ammonia is used as the refrigerant in this simulation, liquid ammonia vaporizes at 1 atm (1 atm = 101325 Pa) cools to around -34°C , and as long as liquid ammonia is sufficient, the hot stream outlet always has a temperature near -34°C if the deviation from designing point is not drastic. (2) Both cold and hot streams match for specific heat exchange to fulfill downstream specifications. For a real process, the geometry of this heat exchanger is set, any change on either side of the stream will have an interactive effect with each other, and eventually will influence the whole system. Therefore, the outlet temperature of the first kind is fixed and the heat exchange area of the second kind is fixed for the modeling.

Traditional approach of sequential modular method solves each block in sequence, and tearing and convergence technology is employed for process containing loops. Strong coupling and heat-integrated Rectisol process results in a large outside loop accompanied with many nested convergence loops (Fig. 3). Bad initial guesses and propagation of deviations make the process difficult to converge. Equation oriented (EO) strategy is an alternative approach for solving flow sheet simulation [24]. Instead of solving each block in sequence, EO gathers all the model equations and solves them simultaneously and a better convergence path will be found since the iteration direction is systematically determined. In this simulation, EO approach is used and all calculations converge well.

4. Algorithms

Since a steady state operation is considered in this simulation, EO approach treats the whole process as a system of algebraic equations. The equations consist of two parts: unit operation descriptions and

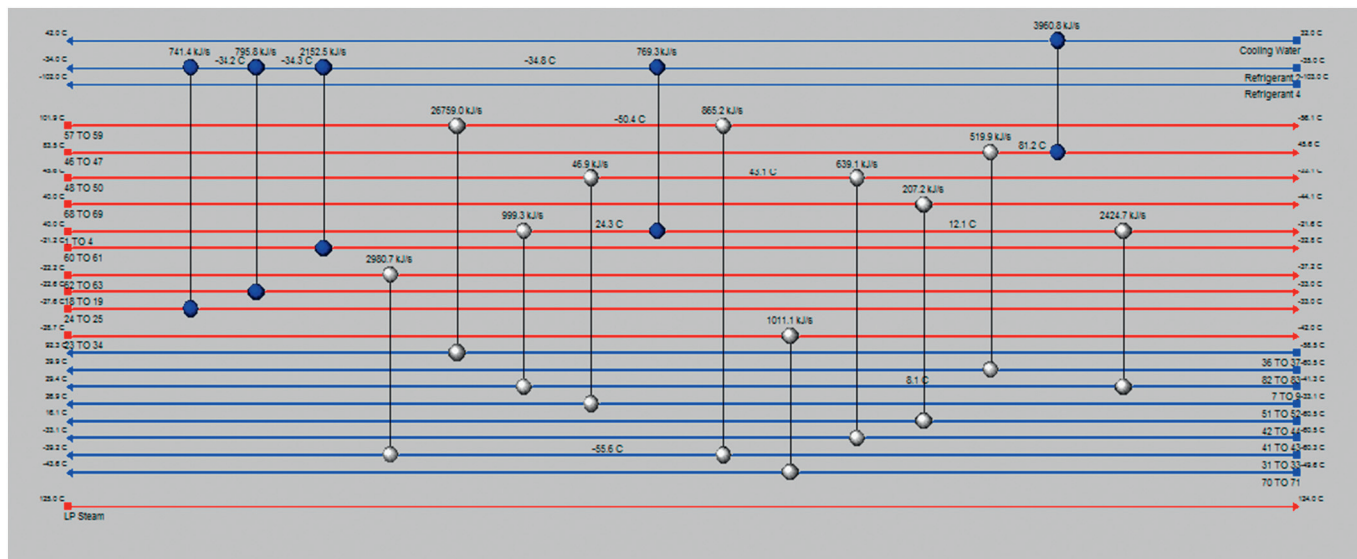


Fig. 2. The heat integration diagram of the Rectisol wash unit.

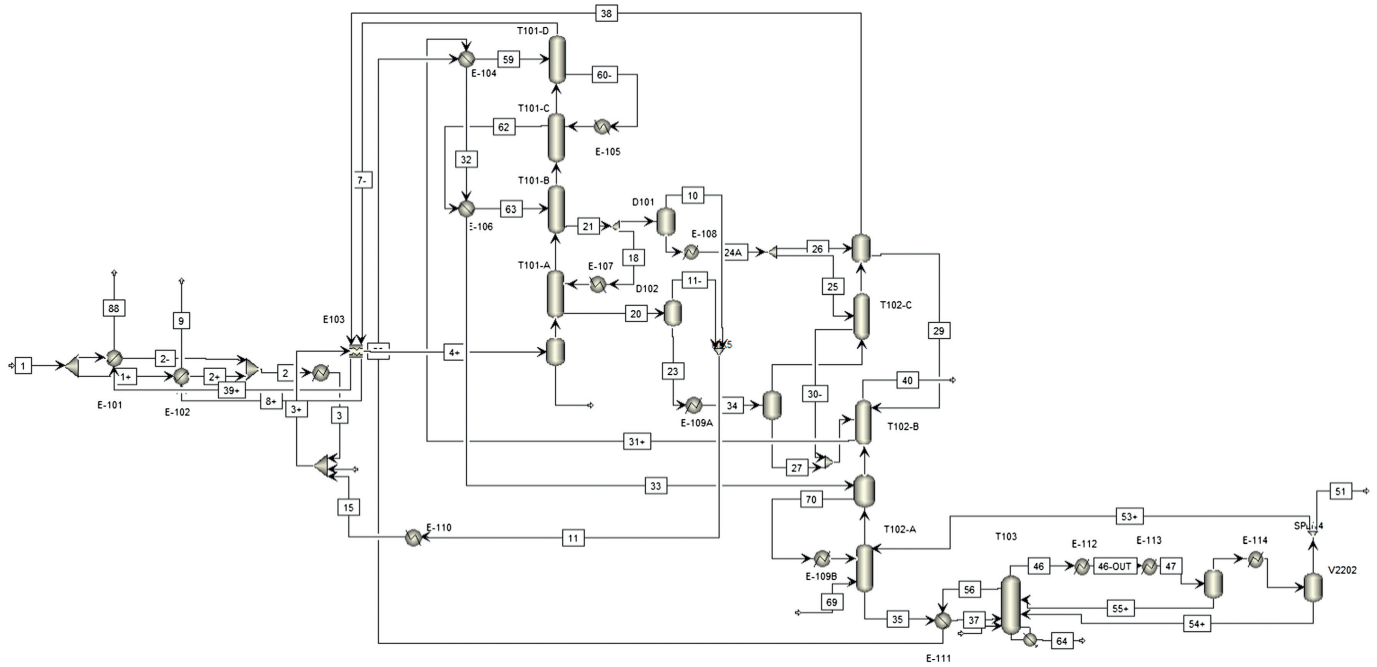


Fig. 3. Heat-integrated Rectisol simulation in Aspen Plus.

unit connection description. Thermodynamic calculations are always performed in subprograms and do not count as system equations. In essence, sequential modular and EO work on the same group of equations, which are physical and chemical descriptions of the process. However, EO method needs to solve the problem simultaneously, so a good solver is needed. In this simulation, SQP method is used to solve these highly nonlinear equations with 6423 variables, in which the solution of nonlinear equations is transformed into a constrained nonlinear programming problem at each searching step, then solved by SQP algorithm with a linear searching strategy. The algorithm is presented as follows.

Original equation group:

$$c_i(\mathbf{x}) = 0 \quad i = 1, 2, \dots, m \quad (2)$$

where $\mathbf{x} \in R^n$, $x_{\min} \leq x_i \leq x_{\max}$, and $c_i: R^n \rightarrow R$ for $i = 1, 2, \dots, m$ representing equation i . Eq. (2) can be equally posed as a minimization problem

$$\min : f(\mathbf{x}) = \mathbf{c}(\mathbf{x})^T \mathbf{c}(\mathbf{x}). \quad (3)$$

If initial point $\mathbf{x}_k$ at k th searching step is substituted into the set $\{1, 2, \dots, m\}$ of equations, subsets S_2 and S_1 are distinguished, where S_2 denotes the complements $\{1, 2, \dots, m\}/S_1$. Nie [25] defines the sets as

$$S_1 = \{i | c_i(\mathbf{x}_k) \neq 0, \dots, i_m\}$$

$$S_2 = \{i | c_i(\mathbf{x}_k) = 0, \dots, i_m\}.$$

Then Eq. (3) is transformed to

$$\begin{cases} \min : f(\mathbf{x}) = \sum_{i \in S_1} c_i^2(\mathbf{x}) \\ \text{s.t.} : \mathbf{c}_{S_2}(\mathbf{x}) = \mathbf{0} \\ \mathbf{x}_{\min} \leq \mathbf{x} \leq \mathbf{x}_{\max} \end{cases} \quad (4)$$

and the Lagrange function is further presented.

$$\min : f(\mathbf{x}) + \sum_{i \in S_2} \lambda_i c_i(\mathbf{x}) \quad (5)$$

where λ_i is a weighting factor, which is practically significant since the equalities have different properties to a great degree. Eq. (5) is the objective function and a linear search SQP algorithm is used for each searching step.

The objective function is replaced by a quadratic approximation and constrains are linearized as

$$\begin{cases} \min : \nabla f(\mathbf{x}_k)^T \mathbf{d} + \frac{1}{2} \mathbf{d}^T \mathbf{H}_k \mathbf{d} \\ \text{s.t.} : \mathbf{c}_{S_2}(\mathbf{x}_k) + \nabla \mathbf{c}_{S_2}(\mathbf{x}_k)^T \mathbf{d} = 0 \end{cases} \quad (6)$$

where $\mathbf{H}_k$ is the Hessian matrix of $f(\mathbf{x})$. In solving the SQP subprogram, search direction $\mathbf{d}_k$ is determined, performing a linear search to get step α_k , and $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$ is the new iteration. Merit function (7) can be utilized as the criterion for each iteration trial, but the actual reduction of merit function (8) draws more attention:

$$\mathbf{m}_k(\mathbf{x}) = \sum_{i \in S_1} c_i^2(\mathbf{x}) + \left\| \lambda_i \mathbf{c}_{S_2}(\mathbf{x}_k) \right\|^2 \quad (7)$$

$$\Delta \mathbf{m} = -(\mathbf{m}_k(\mathbf{x}_k + \alpha_k \mathbf{d}_k) - \mathbf{m}_k(\mathbf{x}_k)). \quad (8)$$

In this simulation, SQP method in Aspen Plus is used to solve the system of equations and Kuhn–Tucker error is used as the convergence criterion. The simulation and analysis in this process all converge and satisfy the Kuhn–Tucker error of 0.001.

5. Results and Discussion

In a stream of crude synthesis gas ($7.056 \times 10^6 \text{ mol} \cdot \text{h}^{-1}$, 40 °C, with the mole composition as shown in Table 1) through Rectisol wash, $\text{H}_2\text{S}/\text{COS}$ are almost removed, CO_2 reduces to 2.967%, CO/H_2 recovery is 99.8%, 35.1% of CO_2 is collected as byproduct, the rest mixing with N_2 and other inert gases (stream 40) is discharged as tail gas, H_2S is concentrated to 25.1% for Claus plant, and the methanol recycling is $7.606 \times 10^6 \text{ mol} \cdot \text{h}^{-1}$.

Table 2 lists product stream simulation results and comparisons to the design data. Almost all simulation results match the process design

Table 2
Comparison of streams leaving the process

Stream ID	9		88		51		40	
	Simulation	Error	Simulation	Error	Simulation	Error	Simulation	Error
Temperature/°C	34.53	−0.176	26.69	−0.089	−33.15	0	−63.88	−0.062
Pressure/bar	31.8		2.3		2.8		1.35	
Mole flow/kmol·h ^{−1}	4682.94	0.0009	868.16	−0.007	65.34	0.053	1728.95	−0.003
Mole fraction/%								
CH ₃ OH	0.004	0.759	0.017	−0.303	0.091	0.092	0.011	0.858
CO ₂	2.967	0.019	99.086	−0.001	73.292	−0.027	81.974	−0.001
H ₂	65.776	−0.001	0.106	−0.350	0.001	−0.028	0	0.217
N ₂	1.889	−0.005	0.026	−0.603	1.505	0.493	17.99	0.000
H ₂ S	0		0		25.072	−0.023	0.019	
H ₂ O	0		0.001		0.03		0.001	
Ar	0		0		0		0	
CH ₄	0.015	0.005	0.002	0.128	0		0	0.369
CO	29.349	0.000	0.759	0.378	0.009	−0.059	0.006	−0.648
COS	0		0		0	1.000	0	

data except trace components. Therefore, the simulator can represent the real plant and can be used in further analysis.

5.1. H₂S removal analysis

Synthesis gas should meet rigorous specification of sulfide content for downstream usage, especially for catalytic reactions [26]. The effect of Rectisol relies heavily on sulfide removal, and because of CO shift feed change or other disturbances, sulfide content in Rectisol feed may vary significantly. A process for eliminating source sulfide disturbance will be preferred. In some plants auxiliary column section is added under the main wash column. When large disturbances of upstream sulfide content occur, the auxiliary part will cope with the situation.

In this process, a change of sulfide content in the feed gas will have a direct impact on T101 side draw (stream 21), so sulfide change in T101-A gas outlet and CO₂ product stream are detected. Fig. 4 reveals the change corresponding to feed disturbance. H₂S composition <0.63% does not change sulfide content in streams 9 and 88 significantly, so the process is well designed to deal with source sulfide disturbance. For H₂S content of 0.63%, T101-A solvent increasing to 110% in stream 18 by decreasing side draw will cut down a quart of T101-A gas outlet sulfide content, with refrigerant usage of E-107 added in equal proportion. Therefore, when feed gas sulfide content changes and objective stream (stream 9) is detected with high sulfide content, solvents should be added to the upper limit of their operational range, and if it fails, auxiliary equipment shall be used.

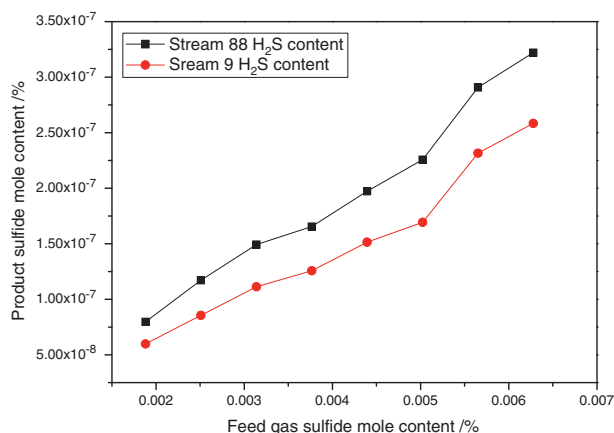


Fig. 4. Simulation results with respect to feed gas sulfide content.

5.2. CO₂ removal and collection

This Rectisol wash specifies the cleaned gas to CO₂ content of 3.0%–5.0%, with the simulation result slightly less than 3.0%, as shown in Table 2. Solvent recycling will affect the CO₂ content of cleaned gas, while the amount of methanol used in the process affects hot and cold utilities greatly. Fig. 5 shows CO₂ content and T101 ammonia usage with respect to solvent recycling change. Two exchangers behave differently: refrigerant consumption of T101 does not decrease proportionally. The reason is that T101-D liquid draw out conditions are affected not only by solvent recycling quantity, but also by the rest of the integration, which jointly determine E105 refrigerant consumption since the stream cools to a temperature near −34 °C before entering T101-C. The same goes to E107. Proper adjustments of solvent recycling will have a direct reward of utility reduction, while satisfying product specifications. For example, solvent recycling downsize to 95% of its designing amount will still satisfy relative specifications, but cuts down 2.8% of cold utility usage.

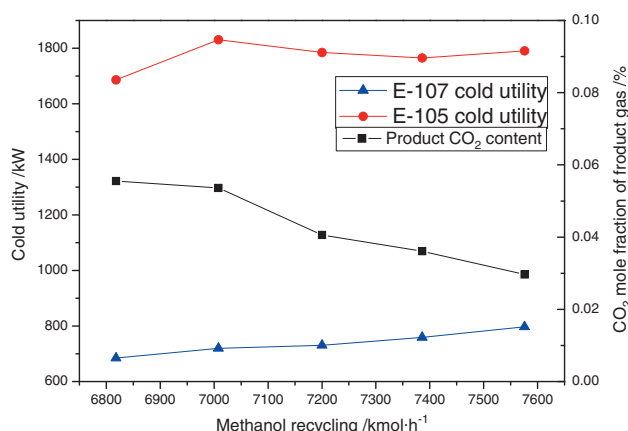


Fig. 5. Simulation results with respect to methanol recycling change.

All CO₂ washed from crude feed gas needs to be desorbed, here only 35.1% of CO₂ is collected as product. T101 side draw out (stream 24A) contains 1.373×10^6 mol·h^{−1} of CO₂, which is H₂S free. When it flashes at 1.5 bar, only 7.392×10^5 mol·h^{−1} of CO₂ product will be produced. Splitting a part to reabsorb D102 low pressure gas outlet (stream 34) will increase CO₂ product to 8.682×10^5 mol·h^{−1}, which means that 1.290×10^5 mol·h^{−1} of pure CO₂ is re-captured from T101-A bottom

draw out (stream 34) and this stream is not H₂S free. Intuitively, decreasing reabsorb amount to 50% (design operability of T102-C) will not increase CO₂ production ($8.556 \times 10^5 \text{ mol} \cdot \text{h}^{-1}$), but has to venture the increase of H₂S content in CO₂ product.

This scheme restricts CO₂ collection not because the side-draw of main wash column is split to H₂S re-absorption, on the contrary, it promotes CO₂ collection by 17.4%. The obstacle for CO₂ collection and storage is the use of N₂ as the H₂S stripping medium and 57.4% of feed CO₂ discharges as tail gas since this stream contains N₂, leading to a low CO₂ collection. Concerning the environmental effect, Gatti *et al.* [4] suggested using steam instead of nitrogen, because the stripping medium will promote CO₂ collection, and corresponding design strategy was proposed.

6. Conclusions

In this work, PC-SAFT method is used for phase behavior. Rectisol simulation with heat integration is built for a real plant and EO algorithm with SQP is used to solve this highly integrated process. An analysis on the Rectisol schemes previously proposed is used, focusing on one-stage configuration and characteristic analysis. The PC-SAFT EOS method can predict phase behavior and good results are obtained. EO algorithms are studied to obtain convergence. A simulator for the reference scheme is built and the simulation is satisfactory. This simulation can further be used as a guidance for industrial application and optimization purpose.

References

- [1] H. Weiss, Rectisol wash for purification of partial oxidation gases, *Gas Sep. Purif.* 2 (1988) 171–176.
- [2] W. Herbert, H.U. Kohrt, R. Becker, F. Danulat, US patent number 2,863,527 (1958).
- [3] G., Ranke, H. Weiss, Separation of gaseous components from a gaseous mixture by physical scrubbing, US patent number 4,324,567 (1982).
- [4] G. Manuele, M. Emanuele, M. François, C. Stefano, Review, modelling, heat integration, and improved schemes of rectisol-based processes for CO₂ capture, *Appl. Therm. Eng.* 70 (2) (2014) 1–18.
- [5] L. Sun, R. Smith, Rectisol wash process simulation and analysis, *J. Clean. Prod.* 39 (1) (2013).
- [6] B. Munder, S. Grob, P.M. Fritz, Selection of wash systems for sour gas removal, 4th International Freiberg Conference on IGCC & Xtl Technology, 2010.
- [7] Y.G. Pi, The calculation of vapor–liquid equilibrium and phase equilibrium model for methanol washing at low temperature(1), *Hunan Chem Ind.* 4 (27) (1997).
- [8] Y.G. Pi, The calculation of vapor–liquid equilibrium and phase equilibrium model for methanol washing at low temperature(2), *Hunan Chem. Ind.* 1 (28) (1998).
- [9] G. Niu, Y.h. Huang, J. Wang, The calculation of vapor liquid equilibrium for the Rectisol wash technology in natural gas purification process, *Nat. Gas Chem. Ind.* 2 (2004).
- [10] Z.P. Xiao, D.Y. Fei, W.Y. Ying, S. Liu, J. Chen, Thermodynamic model and process simulation for CO₂ removal with low temperature methanol, *Chem. Eng. China* 7 (39) (2011).
- [11] J.F. Boston, P.M. Mathias, Phase equilibrium in a third generation process simulator, 2nd International Conference on Phase Equilibria and Fluid Properties in the Chemical Industries, West Berlin, 1980.
- [12] A.P. Rosalyn, A Computer Model of the Rectisol Process Using the Aspen Plus, [D].MIT, 1981.
- [13] Q.H. Li, S.W. Zhang, Y. Li, Simulation of Rectisol process based on non-equilibrium model, *Chem. Ind. Eng. Prog.* (2012) S1.
- [14] T. Holderbaum, J. Gmehling, PSRK: a group contribution equation of state based on UNIFAC, *Fluid Phase Equilib.* 70 (1991) 251–265.
- [15] J.H. Sun, Y. Li, Process simulation for Rectisol simulation for methanol wash column, *J. Gansu Sci.* 2 (19) (2007).
- [16] J. Gross, G. Sadowski, Modeling polymer systems using the perturbed-chain statistical associating fluid theory equation of state, *Ind. Eng. Chem. Res.* 41 (2002) 1084–1093.
- [17] J. Gross, G. Sadowski, Application of the perturbed-chain SAFT equation of state to associating systems, *Ind. Eng. Chem. Res.* 41 (2002) 5510–5515.
- [18] Aspen Technology Inc., Rate-based Model of the CO₂ Capture Process by Methanol Using Aspen Plus, Aspen Technology, Inc., US, 2008.
- [19] <http://webbook.nist.gov/chemistry/fluid/>.
- [20] R. Smith, Chemical Process Design and Integration, John Wiley & Sons Ltd, Chichester, England, 2005.
- [21] Aspen Technology Inc., Aspen Energy Analyzer Reference Guide, Aspen Technology, Inc., US, 2009.
- [22] L. Liu, F. Cai, J. Sun, W. Han, Simulation and optimization of rectisol using revised thermodynamic methods, 2012 Spring Meeting & 8th Global Congress on Process Safety, AIChE, 2012.
- [23] M. Nilesch, Acid gas removal by the rectisol wash process, *Chem. Ind. Dig.* 8 (2013) 61–63.
- [24] Aspen Technology Inc., Getting Started Using Equation Oriented Modeling, Aspen Technology, Inc., US, 2004.
- [25] P. Nie, An SQP approach with line search for a system of nonlinear equations, *Math. Comput. Model.* 43 (2006) 368–373.
- [26] Y. Feng, Requirements and analysis methods of sulfides content in ammonia synthesis feed gas, *J. Chem. Ind. Eng. China* 1 (24) (2003).