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CALCULATION OF THERMODYNAMIC PARAMETERS OF CHEMICAL REACTIONS IN THE PROCESS OF CLEANING EXPANDER GASES FROM ACID COMPONENTS

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ABSTRACT
Today, calculation of thermodynamic parameters of any processes provides an opportunity to determine the direction of chemical reactionsTaking this into account, this article calculated the thermodynamic parameters of substances formed during the cleaning of expander gases. As a result, the mechanisms of formation of substances and directions of reaction were determined. Entropy (ΔS) and Gibbs energies (ΔG) of reactions were calculated to determine the direction and realization of the reaction.

KEYWORDS: ***cleaning, acid components, hydrogen sulfide, carbon dioxide, absorption, thermodynamics, entropy (ΔS), enthalpy (ΔH), activation energy (E_a), solubility product (SP)***

INTRODUCTION

Thermodynamics (or the general theory of heat) studies macroscopic processes in bodies and substances[1-5]. At the same time, he also studies the phenomena associated with a large number of atoms and molecules in substances. Thermodynamics studies only the thermodynamic equilibrium states of bodies and slow processes, which can be considered as practically equilibrium states that continuously follow each other[6-11]. Some of their thermodynamic parameters (enthalpy, entropy and Gibbs energy) are needed to determine the direction of chemical reactions [12-16].

MATERIALS AND METHODS

Table 1 presents some thermodynamic parameters of the substances involved in the reactions in the process of cleaning the expander gases from acidic contains.

Table-1.
Standard thermodynamic parameters of substances involved in the purification of expander gases from acid components

Substance and its state	$\Delta H^o_{for., 298,15}$ kJ/mol	$\Delta G^o_{for., 298,15}$ kJ/mol	$S^o_{, 298,15}$ J/(mol•K)
$NaHCO_3$ (cry.)	-949,08	-851,1	101,3
Na_2CO_3 (cry.)	-1129,43	-1045,7	135,0
Na_2CO_3 $10H_2O$ (cry.)	-4077	-3906	2172
Na_2S (cry.)	-374,47	-358,13	79,50
H_2S (g)	-20,9	-33,8	205,69
$CaCO_3$ (cry.)	-1206,8	-1128,4	91,7
$Ca(OH)_2$ (cry.)	-985,1	-897,1	83,4

CaS (cry.)	-476,98	-471,93	56,61
NaOH (cry.)	-495,93	-379,8	64,43
NaOH (sol.; $20H_2O$)	-470,53	-	-
NaOH (sol.; $50H_2O$)	-470,17	-	-
NaOH (sol.; $100H_2O$)	-469,98	-	-
NaOH (sol.; $1000H_2O$)	-470,10	-	-
NaOH (sol;)	-470,45	-419,44	48,0
CO_2 (g)	-393,51	-394,38	213,67

The daily output of expander gases released at the volatile gas processing plant is 200 m^3. It contains 8-8.8% H_2S, 3-3.7% CO_2, 1-1.2% water vapor, up to 0.2% MDEA, and the rest is CH_4 gas.

When the expander gases are passed through NaOH and $Ca(OH)_2$ solutions, the following reactions take place.

a) $Ca(OH)_2 + CO_2 = CaCO_3\downarrow + H_2O$
b) $Ca(OH)_2 + H_2S = CaS\downarrow + 2H_2O$
c) $2NaOH + CO_2 = Na_2CO_3 + H_2O$
d) $2NaOH + H_2S = Na_2S + 2H_2O$

However, the solubility coefficients of precipitates formed by calcium ion differ from each other. $SP_{CaCO3} = 3.8{\bullet}10^{-9}$, $SP_{CaS} = 1.3{\bullet}10^{-8}$. This shows that when the expander is passed through the absorbent solution, only $CaCO_3$ precipitates.

$SP_{CaCO3} = [Ca^{2+}] \bullet [CO_3^{2-}] = 3.8{\bullet}10^{-9}\ mol^2/l^2$

RESULT

As a result, unreacted hydrogen sulfide forms Na_2S with NaOH. Based on the above data, we determine the reaction direction of $CaCO_3$ by Gibbs energy.

$Ca(OH)_2 + CO_2 = CaCO_3 + H_2O$

$\Delta H = H_{prod.} - H_{ini.}$

$\Delta H = (-1206.8 - 285.83) - (-985.1 - 393.51) =$
$(-1492.63) + (1378.61) = -114.02$ kJ

$\Delta S = S_{prod.} - S_{ini.}$

$\Delta S = (91.7 + 69.91) - (83.4+213.67) = -135.46$ J

Enthalpy and entropy were calculated in order to determine the reaction direction of formation of $CaCO_3$. Gibbs energy is calculated based on the obtained results.

$\Delta G = \Delta H - T\Delta S$

$\Delta G = -114.02 - 298{\bullet}(-135.46{\bullet}10^{-3}) = -73.65$ kJ

Gibbs energy was -73.65 kJ. This shows that the reaction is carried out in a high yield.

$Ca(OH)_2 + H_2S = CaS\downarrow + 2H_2O$

Above, we compare the precipitation formation with CaS.

$\Delta H = (-476.98 - 2{\bullet}285.83) - (-985.1 - 20.9) =$
$(-1048.64) + (1006) = -42.64$ kJ

$\Delta S = (56.61 + 2{\bullet}69.91) - (83.4+205.69) = -92.66$ J

$\Delta G = -42.64 - 298{\bullet}(-92.66{\bullet}10^{-3}) = -15.03$ kJ

Comparing the Gibbs energies of $CaCO_3$ and CaS, we found that the energy of CaS is higher. This means that the yield of $CaCO_3$ precipitation is high.

CONCLUSION

In short, it is very convenient to calculate the thermodynamic parameters of processes when determining the direction of any chemical reaction and whether it will occur or not. In this article, thermodynamic processes were used to determine the deposits formed during cleaning of expander gases from acidic additives. As a result, we theoretically proved the formation of $CaCO_3$ in practice.

REFERENCES

1. *Olimov B., Akhmedov V. The effect of reaction duration and catalyst on the synthesis of arylvinyl esters //Збірник наукових праць ΛΌГOΣ. – 2020. – С. 33-37.*
2. *Ахмедов В. Н., Олимов Б. Б. Способ получения виниловых эфиров на основе винилацетилена //Gaydar Aliyevning. – 2020. – Т. 97.*
3. *Olimov B., Akhmedov V., Gafurova G. Production and use of corrosion inhibitors on the basis of two-atomic phenols and local raw materials //Главный редактор. – 2021. – Т. 7. – С. 85.*
4. *Bobir O., Vokhid A., Gulnoz G. Production and use of corrosion inhibitors on the basis of two-atomic phenols and local raw materials //Universum: химия и биология. – 2021. – №. 11-2 (89). – С. 85-88.*
5. *Olimov B. B., Yoldosheva N. J. Gravimetric study of the mechanism of action of corrosion inhibitors used in the oil and gas industry //Международный научно-образовательный электронный журнал «Образование и наука в xxi веке». Выпуск. – №. 19.*
6. *Назаров Ш. и др. Синтез мономеров при участии винилацетилена из одноатомных фенолов содержащих ариловую группу //Universum: химия и биология. – 2020. – №. 11-2 (77).*
7. *Олимов Б. Б., Ахмедов В. Н. Винилацетилен асосида фенолларнинг винил эфирлари синтези.“Замонавий ишлаб чикаришнинг мухандислик ва технологик*

муаммоларини инновацион ечимлари" Халкаро илмий анжуман материаллари //Замонавий ишлаб чикаришнинг мухандислик ва технологик муаммоларини инновацион ечимлари" Халкаро илмий анжуман материаллари Бухоро. – 2019. – С. 37-39.

8. *Shomurod N., Vokhid A., Bobir O. Preliminary quantum chemical analysis of synthesized monomers with the participation of vinylacetylene //International journal of progressive sciences and technologies. – 2020. – Т. 22. – №. 2. – С. 50-56.*
9. *Ахмедов В. Н., Олимов Б. Б. У., Назаров Ш. К. Электронная структура и квантово-химические расчёты виниловых эфиров фенолов //Universum: химия и биология. – 2020. – №. 4 (70).*
10. *Olimov B. B., Ahmedov V. N., Hayitov S. Ikki atomli fenollar asosida vinilli efirlarni olish usullari //Fan va texnologiyalar taraqqiyoti ilmiy–texnikaviy jurnal. – 2020. – №. 1.*
11. *Olimov B. B., Akhmedov V. N., Gafurova G. A. Application of derivatives of diatomic phenols as corrosion inhibitors //Euro Asian Conference on Analytical Research (Germany. – 2021. – Т. 15. – С. 136-138.*
12. *Ахмедов В., Олимов Б., Гафурова Г. Винилачетилен иштирокида винил эфирлар олиш. НамДУ илмий ахборотномаси-Научный вестник НамГУ. – 2021.*
13. *Bahodirovich, Olimov B., et al. "Synthesis of Resorcinol Vinyl Ether in the Mono-position, Influence of the Catalyst, Temperature and Solvent on the Reaction Yield."* JournalNX*, 2020, pp. 44-51.*
14. *Olimov B.B., Sadiqova M.I., Beshimov I.A. Technology of obtaining effective corrosion inhibitors in the oil and gas industry // Universum: технические науки : электрон. научн. журн. 2022. 1(94). URL: https://7universum.com/ru/tech/archive/item/12950*
15. *Олимов Б.Б., Гафурова Г.А., Кудратов О.Х. Production and properties of corrosion inhibitors in the oil and gas industry // Universum: химия и биология : электрон. научн. журн. 2022. 2(92). URL: https://7universum.com/ru/nature/archive/item/13009*