



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 reactions. Taking 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	$\Delta H^{\circ}_{\text{for.}, 298,15}$ kJ/mol	$\Delta G^{\circ}_{\text{for.}, 298,15}$ kJ/mol	$S^{\circ}_{298,15}$ J/(mol·K)
NaHCO ₃ (cry.)	-949,08	-851,1	101,3
Na ₂ CO ₃ (cry.)	-1129,43	-1045,7	135,0
Na ₂ CO ₃ 10H ₂ O (cry.)	-4077	-3906	2172
Na ₂ S (cry.)	-374,47	-358,13	79,50
H ₂ S (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 ₂ O)	-470,53	-	-
NaOH (sol.; 50H ₂ O)	-470,17	-	-
NaOH (sol.; 100H ₂ O)	-469,98	-	-
NaOH (sol.; 1000H ₂ O)	-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 m³. It contains 8-8.8% H₂S, 3-3.7% CO₂, 1-1.2% water vapor, up to 0.2% MDEA, and the rest is CH₄ gas.

When the expander gases are passed through NaOH and Ca(OH)₂ solutions, the following reactions take place.

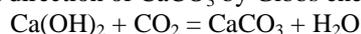
- Ca(OH)₂ + CO₂ = CaCO₃↓ + H₂O
- Ca(OH)₂ + H₂S = CaS↓ + 2H₂O
- 2NaOH + CO₂ = Na₂CO₃ + H₂O
- 2NaOH + H₂S = Na₂S + 2H₂O

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

$$SP_{CaCO_3} = [Ca^{2+}] \cdot [CO_3^{2-}] = 3.8 \cdot 10^{-9} \text{ mol}^2/l^2$$

RESULT

As a result, unreacted hydrogen sulfide forms Na₂S with NaOH. Based on the above data, we determine the reaction direction of CaCO₃ by Gibbs energy.



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

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

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

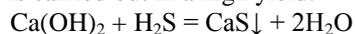
$$\Delta S = (91.7 + 69.91) - (83.4 + 213.67) = -135.46 \text{ J}$$

Enthalpy and entropy were calculated in order to determine the reaction direction of formation of CaCO₃. Gibbs energy is calculated based on the obtained results.

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

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

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



Above, we compare the precipitation formation with CaS.

$$\Delta H = (-476.98 - 2 \cdot 285.83) - (-985.1 - 20.9) =$$

$$(-1048.64) + (1006) = -42.64 \text{ kJ}$$

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

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

Comparing the Gibbs energies of CaCO₃ and CaS, we found that the energy of CaS is higher. This means that the yield of CaCO₃ 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 CaCO₃ in practice.

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