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Experimental Measurements of Molecular Force Parameter for Ar-CO_2 Gas Mixture

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ABSTRACT

A binary mixture of Ar-CO2 with equal percentage was used in the thermal diffusion column. A set of different temperature and pressures were applied. Through the operation of separation, the separation factor and the thermal diffusion factor were calculated. The molecular force parameter was calculated through a special computer program using the well known Lennard-Jones (12-6) molecular model. The results are in agreement with those extracted from viscosity measurement.

قياسات تجريبية لمعلم القوة الجزيئي لخليط من غاز Ar-CO_2

الملخص

تم في هذا البحث استخدام مزيج ثنائي من غازي Ar-CO_2 وبنسبة متعادلة في عمود الانتشار الحراري وبدرجات حرارية وضغوط مختلفة. من خلال عملية الفصل تم حساب عامل الفصل وعامل الانتشار الحراري كما تم حساب معلم القوة الجزيئية من خلال برنامج حاسوب استخدم فيه نموذج ليونارد-جونز(6-12). النتائج كانت متطابقة مع تلك المستخدمة بقياسات اللزوجة.

INTRODUCTION

Thermal diffusion phenomena can be used to separate gases and nuclear isotopes of materials in the gaseous state when the gas mixture is acted upon by a temperature gradient.

In such a case, the lighter component tends to move towards the hot side while the heavier component moves towards the cold side (Rijab, 2000). Ordinary gas diffusion processes work against this effect and when an equivalent state is reached, a net separation effect is established. This separation effect is usually described in terms of a parameter called the thermal diffusion factor α_T which is given by:-

$$\alpha_T = \frac{\ln(q)}{\ln(T_1 / T_2)} \qquad \text{.....(1)}$$

Where
q is the separation factor

$$q = \frac{(C_1 / C_2)Top}{(C_1 / C_2)Bottom}$$

And C_1 and C_2 are the concentrations of the components of the gas mixture, and T_1, T_2 being the hot and the cold ends of the temperature gradient respectively.

The parameter α_T is theoretically related to the force constant of the particular potential force function being used to describe the interactive force that is acting between the molecules and thus considered as an important transport parameter thus α_T measurements can give understanding of molecular force (Azooz, 1994).

Thermal diffusion Column is one of the main types of thermal diffusion equipment used to study the molecular interaction.

Theoretical Part:-

The large temperature gradient acts to create convection currents with the overall equilibrium effect on gas components being separated, with the lighter one concentrating at the top, while the heavy component concentrating sat the bottom. This type of equipment has the advantage of producing large separation effects which are fairly easy to detect. Nevertheless it suffers from the disadvantage that the thermal diffusion factor α_T can only be obtained from the relation (AL-Faydhi, 1998):-

$$Ln(q) = \alpha_T F_s (r_c, r_h, L, T)$$

Where F_s is the calibration factor function, which depends on the geometrical dimensions off the column including the hot tube radius r_h, the cold tube radius r_c, and the Length of the column L in addition to its dependence on the mean temperature T through the annular spacing (Fig. 1)

$$T = \frac{T_C + T_h}{2}$$

T_c and T_h represent the cold and hot temperature respectively. Although, F_S has been calculated mathematically for some T.D.Cs (Thermal diffusion columns) (Youssef,1989), these calculation are model dependent. It was demonstrated that experimental calibration using gases with known α_T can give better results (Acharyya, 1987).

Fig. 1: Thermal diffusion column used in this work.

EXPERIMENTAL SETUP

Thermal diffusion column is basically consists of two coaxial cylindrical tubes with a small annular spacing between them. The inner tube is usually heated from the inside by an electric wire heater and thus forms the hot surface, while the outer tube is surrounded by a cooling jacket thus, forming the cold surface. The gas mixture kept within the annular space between the two tubes.

The effective length of the thermal diffusion column was (3) cm. the outer diameter of the hot tube was (2.14) cm, while the inner diameter of the cold tube was (3.2) cm. The water jacket tube used in this work was of inner diameter of (8.0) cm. More details may obtained in reference (AL-Faydhi,1998).

A binary mixture consists of Ar-CO_2 with equal percentages was let to occupy the annular spacing of the T.D.C. used. A set of different temperatures and pressures were taken. The samples of mixture taken from special parts were analyzed using a gas analyzer (VGA-100) model no(978-1000) [NEVA].Figure (2) illustrate the results of the operation Ar- CO_2 separation at pressure 1.5 bar and temperature 350 k.

Fig. 2: Mass Analysis Spectrum of Ar-CO_2 Separation Process.

THE RESULTS

The results, obtained are illustrated in tables (1 and 2). These results were used to calculate the molecular force parameter through the

Table 1: The Separation Factor.

T / q / p	310	326	338	350
1.5	2.0	2.8	3.5	4.3
2.0	1.9	2.6	3.2	3.5
2.5	1.6	2.2	2.7	3.1
3.0	1.5	1.9	2.3	2.9

Table 2: Thermal Diffusion Factor.

T / α_T / p	310	326	338	350
1.5	0.0125	0.0170	0.0194	0.0222
2.0	0.0129	0.01622	0.0185	0.0197
2.5	0.0169	0.0135	0.01557	0.0177
3.0	0.00948	0.0108	0.0133	0.0158

Lennard-Jones(12-6) model with the molecular potential function given by:-

$$\phi(r) = 4\in[(\frac{\delta}{r})^{12} - (\frac{\delta}{r})^{6}]$$

Where δ is the distance parameter (Bates, 1966).

Through a special computer program written for this purpose the molecular force parameter were calculated using the experimental results gained are shown in table (3).

Table 3: the Molecular Force Parameter.

T / ∈/k / p	310	326	338	350
1.5	163.15	120.74	105.625	99.54
2.0	155	125.38	120.71	106.06
2.5	167.56	155.23	140.83	120.68
3.0	182.35	176.21	160.952	140.00

DISCUSSION

In table 3 which represent the values of force parameter ($\in$) according to the temperature (T) and pressures (P).

Obviously, the values of ($\in$) is varying through changing D and B (99.54-182.35) k, which means that temperature and pressure have a little effect on the force parameter but still the values of ($\in$) lies in the same range and as average ($\in$) = 139.9 k.

CONCLUSIONS

Molecular force parameter can be determined experimentally with a good agreement with that estimated value taken from viscosity measurements which is equal to 153 k° for Ar-CO_2 mixture. While the force parameter which determined experimentally through several sets of run was 139,9 k° as an average. Thus the T.D.C measurements confirm the fact of being more specific way for determining the molecular force parameter than of that calculated from any other transport properties.

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