Estimating The Tertiary Gaseous Diffusion Concentration Of Volatile Organic Compounds Using Stephen Maxwell's Mathematical Model

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ABSTRACT

Emissions of volatile organic compounds (VOCs) from certain solid or liquid materials have recently become a concern for states and environmental protection organizations. They are commonly found in a wide range of household products such as detergents, disinfectants, and even paints, all of which contain organic solvents, and gases emitted into the atmosphere. It can lead to harmful health effects, some of which may pose a risk to human health in the short and long term. In addition, polluted air spreads over long distances in a way that cannot be practically avoided or controlled, causing damage to the surrounding environment and living organisms. Air pollution has led to global warming, resulting in higher temperatures and climate change. This article used Stephen Maxwell's equation model with Polymath software to determine the molar flows of a mixture of gases polluting the surrounding environment and divided into two compounds A and B from point 1 to point 2. This process is summarized first by analyzing the binary diffusion of acetone (A) only through Air (C) and then separately studying the diffusion of methanol (B) only through air (C) to find a first approximation of the solution. This concept has also been used to calculate the molar flow and concentration of substances A, B, and C at different distances. Calculations were performed by knowing the diffusion coefficient of the previously mentioned compounds, which depends mainly on the temperature surrounding this gaseous mixture.

Keywords: Volatile organic compound (VOC), Polymath software, Concentration Profile

الملخص

أصبحت انبعاثات المركبات العضوية المتطايرة (VOCs) من بعض المواد الصلبة أو السائلة في الآونة الأخيرة مصدر قلق للدول ومنظمات حماية البيئة. وهي توجد عادة في مجموعة واسعة من المنتجات المنزلية مثل المنظفات والمطهرات وحتى الدهانات، والتي تحتوي جميعها على مذيبات عضوية وغازات منبعثة في الغلاف الجوي. يمكن أن يؤدي إلى آثار صحية ضارة، قد يشكل بعضها خطراً على صحة الإنسان على المدى القصير والطويل. بالإضافة إلى ذلك، ينتشر الهواء الملوث لمسافات طويلة بشكل لا يمكن تجنبه أو السيطرة عليه عمليا، مما يسبب ضررا للبيئة المحيطة والكائنات الحية. أدى تلوث الهواء إلى ظاهرة الاحتباس الحراري، مما أدى إلى ارتفاع درجات الحرارة وتغير المناخ. استخدمت هذه المقالة نموذج معادلة ستيفن ماكسويل مع برنامج Polymath لتحديد التدفقات المولية لخليط من الغازات الملوثة للبيئة المحيطة والمقسمة إلى مركبين A وB من النقطة 1 إلى النقطة 2. يتم تلخيص هذه العملية أولاً من خلال تحليل الإنتشار الثنائي لـ الأسيتون (A) فقط من خلال الهواء (C) ثم دراسة إنتشار الميثانول (B) فقط من خلال الهواء (C) بشكل منفصل للعثور على أول حل تقريبي. تم إستخدام هذا المفهوم أيضًا لحساب التدفق المولي وتركيز المواد A وB وC على مسافات مختلفة. تم إجراء الحسابات من خلال معرفة معامل الإنتشار للمركبات المذكورة سابقاً والذي يعتمد بشكل رئيسي على درجة الحرارة المحيطة بهذا الخليط الغازي.

الكلمات المفتاحية: المركبات العضوية المتطايرة (VOC)، برنامج Polymath، سلوك التركيز

1. Introduction

One of the most common terms in the solvents industry is “Volatile Organic Compound”, abbreviated to “Volatile Organic Compounds”. Volatile organic compounds are a large group of organic chemicals that readily evaporate at room temperature. The original definition of volatile organic compounds referred to each compound's vapor pressure above 133.3 Pa at room temperature as the determinant of volatility [1]. Although in effect since December 29, 2004, the definition is based solely on all carbon compounds other than carbon monoxide, carbon dioxide, carbonic acid, metal carbides or carbonates, and ammonium carbonates involved in photochemical reactions in the atmosphere (U.S. Environmental Protection). United States) Agency, U.S. Environmental Protection Agency, Definition of Volatile Organic Compounds: Code of Federal Regulations: Title 40, Part 51, Section 51.100). Volatile organic chemicals (VOCs) are emitted as gases from some solids or liquids that contain organic compounds. Volatile organic compounds are a common ingredient in many household products. Paints, varnish, and waxes contain organic solvents, as do many clear-out, disinfection, beauty, and degreasing products. The fuel is made from organic chemicals. All of these products can release organic compounds during use and sometimes also during storage. When these organic compounds are released into the atmosphere, they contribute significantly to the formation of smog [2]. VOC emissions are not necessarily a health or environmental concern. Ground-level ozone, the main component of smog, is formed when nitrogen oxides (NOx) and volatile organic compounds react in the presence of sunlight. Ozone is not normally emitted directly into the air but is created at ground level by a chemical reaction between nitrogen oxides and volatile organic compounds in the presence of sunlight. Vehicle exhaust, industrial exhaust, gasoline fumes, chemical solvents, and natural sources emit nitrogen oxides, and volatile organic compounds that contribute to the formation of ozone. Sunlight and warm weather cause ground-level ozone to create harmful levels in the air [3].

Diffusion is a time-dependent process arising from the movement of certain entities spread out in space. The most classical description of the phenomenon of diffusion comes from Fick [6, 7]. He assumes that the flow moves from regions of high concentration to regions of low concentration, with a magnitude proportional to the concentration gradient. We refer to [4] for a physical and mathematical description of Fickian diffusion.

The direct relationship between the flow gradient and the focus provides a reasonable approximation of the diffusion process in many common situations. However, as empirically observed, this assumption can sometimes be oversimplified. In fact, there are situations where the magnitude of the flow does not quite match the concentration gradient, or where the flow moves from areas of low concentration to areas of high concentration. For example, the first behavior has been observed in porous media [5]. The second type of behavior was observed, among other things, in multi-component gas mixtures. The phenomenon of diffusion in a multi-component gas mixture was first described in detail by Maxwell [8] and Stefan [9]. They proposed an explanation of the process based on the dual interaction of the gas molecules. The result of his analysis is a system of paired nonlinear partial differential equations in which diffusion occurs in a much more complex way than Fick's law predicts. In the early 1980s, interactive numerical software packages with graphical capabilities began to emerge as the primary computing tool for solving engineering problems. For example, Shacham and Cutlip developed such a package for the PLATO educational computer system. It was soon ported to the personal computer and has been used under the name "POLYMATH" ever since. When using an interactive software package, the student is asked to enter the mathematical model and numerical information, but the programs extract all the scientific steps from the solution. These advantages of mathematical packages have led to the replacement of calculators and spreadsheets as the main means of calculation in many subjects [10].

2. Theory and Calculations

The multi-component molecular diffusion of gases can be described using the Stefan-Maxwell equations. Numerical integration of a system of simultaneous ordinary differential equations with two-parameter optimization to fit the split boundary conditions [11].

$$\frac{dC_i}{dz} = \sum_{i=1}^{n} \frac{(x_i N_j \;\; x_i N_j)}{D_{ij}} \tag{1}$$

$$\frac{dC_A}{dz} = \frac{(x_A N_B \;\; x_B N_A)}{D_{AB}} + \frac{(x_A N_C \;\; x_C N_A)}{D_{AC}} \tag{2}$$

$$\frac{dC_B}{dz} = \frac{(x_B N_A \;\; x_A N_B)}{D_{AB}} + \frac{(x_B N_C \;\; x_C N_B)}{D_{BC}} \tag{3}$$

$$\frac{dC_C}{dz} = \frac{(x_C N_A \;\; x_A N_C)}{D_{AC}} + \frac{(x_C N_B \;\; x_B N_C)}{D_{BC}} \tag{4}$$

where the appropriate equalities for the binary molecular diffusivities have been substituted for $D_{BA} = D_{AB},\ D_{CA} = D_{AC}, and\ D_{CB} = D_{BC}.$

The physical or chemical process dictates the typical boundary conditions of the above equations.

2.1 Problem Statement and Objectives

This research generally aims to study the behavior of the spread of volatile organic substances in the surrounding environment and estimate their concentration through transport paths. Gases A and B diffuse through stagnant gas C at a temperature of 55 °C and a pressure of 0.2 atmospheres. This process involves molecular diffusion between two points where the compositions are known, as summarized in the table (1) The space between the points is 10^{-3} m.

A simple device is sometimes used to measure the diffusion coefficients of binary vapor mixtures. At the bottom of the tube is a pool of quiescent liquid. The vapor that evaporates from this puddle propagates through the pipe. Gas flow through the top of the tube keeps the mole fraction of vapor diffused there reduced to zero. The mole fraction of vapor at the vapor-liquid interface is its equilibrium value [12].

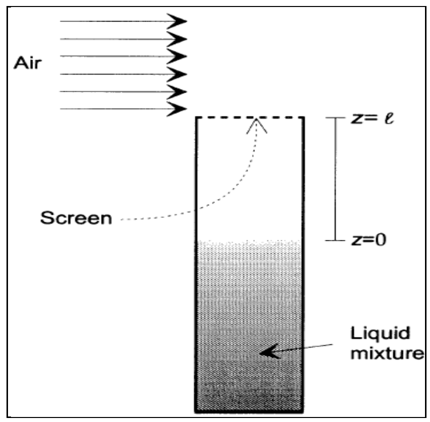

Fig.1 Schematic diagram of a Stefan diffusion tube [12].

a) Use Stefan Maxwell's equations to calculate the molar fluxes of both gases A and B from point 1 to point 2. Hint: A first approximate solution can be obtained by first considering the binary diffusion of A alone through the C component and then separately
binary diffusion of B only through the C component.

(b) Plot the gas mole fractions as a function of the distance from point 1 to point 2.

Table 1. Data for Multicomponent Diffusion [6]

Component	Point 1 Concentration kg-mol/m^3	Point 2 Concentration kg-mol/m^3	Diffusivities at 0.2 atm m^2/s
A	2.229×10^{-4}	0	$D_{AC} = 1.075\times10^{-4}$
B	0	2.701×10^{-3}	$D_{BC} = 1.245\times10^{-4}$

C	7.208×10^{-3}	4.730×10^{-3}	$D_{AB} = 1.470\times10^{-4}$

3. Results and Discussion

This research presents some of the results obtained by applying the POLYMATH program to the aforementioned case, and by looking at the following Figures.

Let it be known to us that compound A represents acetone, compound B represents compound methanol, and air represents compound C based on previous studies and after relying on the data available in Table 1 and including them in the calculations available in the POLYMATH program to calculate the gradient of the molar fraction through the length of the tube shown in Figure 1 As well as the change in the concentration of acetone and methanol with the length of the tube and the rate of molar flow of these substances into the air, we reached some results shown in the following figures:

Since Figure 2 represents the change in the molar fraction of acetone and methanol, as well as air, with the length of the transition path through the tube, we note that this change is small for acetone compared to methanol, and this is due to the fact that the diffusivity of compound B is higher than that of compound A in air, as shown previously.

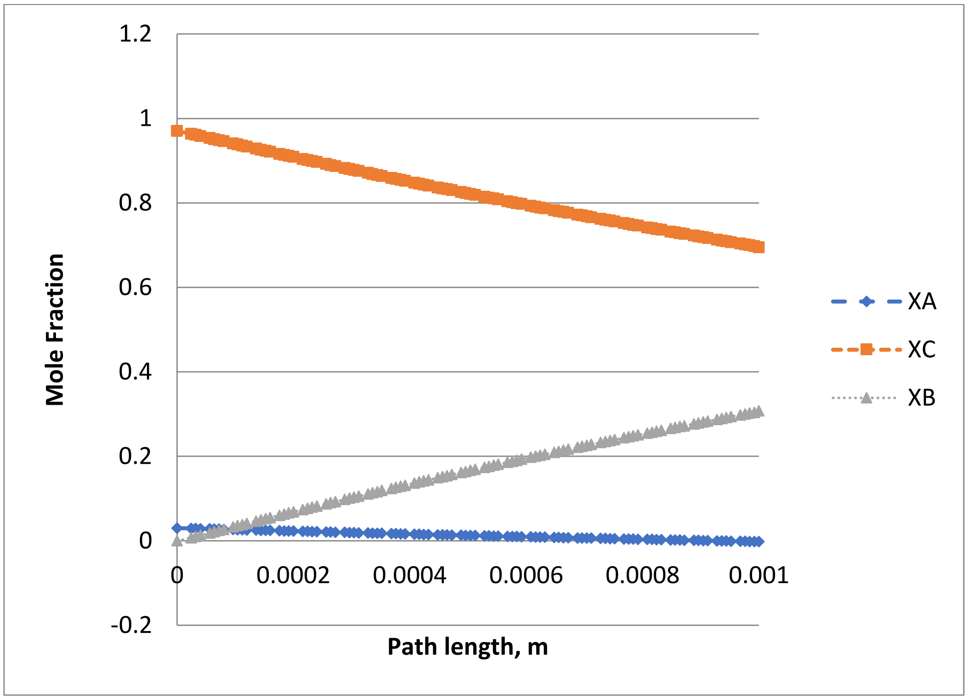

Fig.2 The relationship between Mole Fraction of VOCs and diffusion path length

We notice in Figure 3 that the aforementioned volatile substances behave the same as in Figure 2 in case the concentration of these changes with the length of the transition path in the tube.

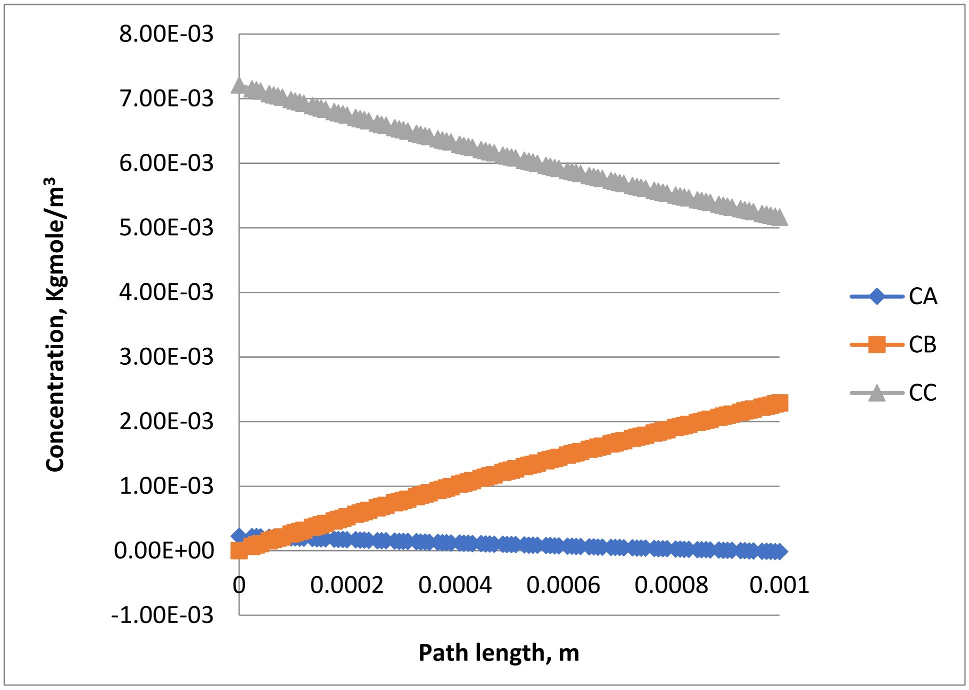

Fig.3 The relationship between Concentration of VOCs and diffusion path length

As for Figure 4, it shows the state of the molar flow of acetone and methanol compound in the air. It is noted from the figure that the molar flow rate remains constant with the length of the path as a result of the stability of the factors affecting the flow rate of pressure and temperature.

Based on the above explanation of these results, these results are presented and summarized in Appendix at the end of this paper.

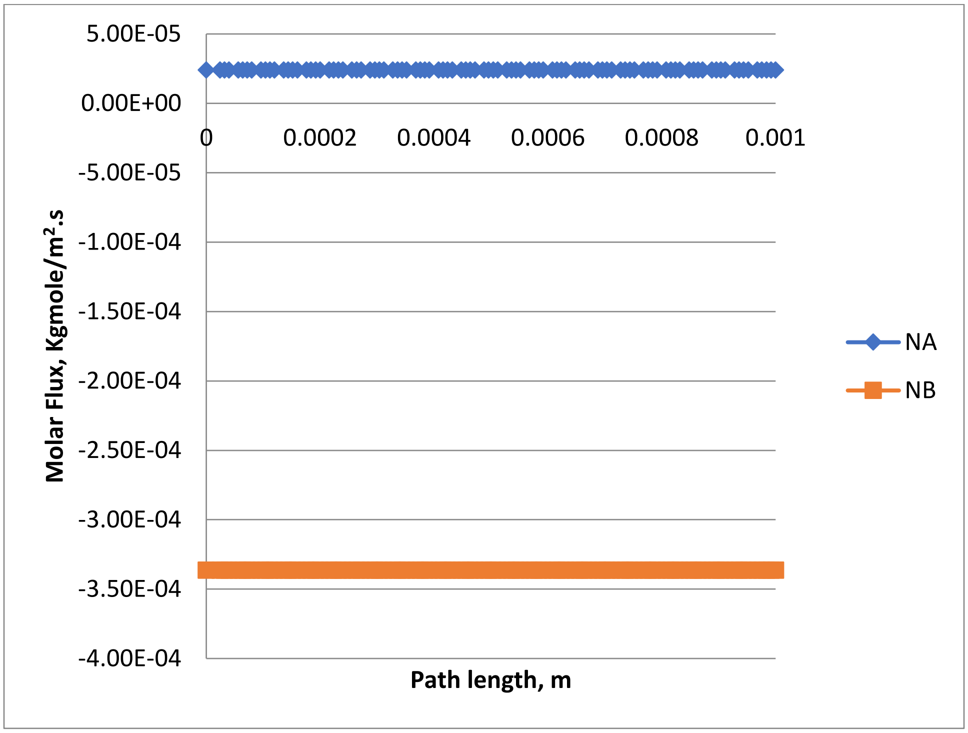

Fig.4 The relationship between molar flux and diffusion path length

4. Conclusion

The Stephen Maxwell equations were applied to describe the Multicomponent molecular diffusion of gases, to find the flow performance of volatiles in air. An analytical view of the result is obtained through simple algebraic models. These results indicate when the Maxwell and Stefan diffusivity, which is more complex to implement in many notations computationally, should be used in the rate calculations of the diffusivity and flow of volatiles. A Stefan tube among a falling gas-liquid boundary can be used to evaluate the liquid-liquid diffusion coefficient, provided that the gas-phase binary diffusion coefficients of the vaporized type are recognized.

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Appendix

POLYMATH Results

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Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
Z	0	0	0.001	0.001
CA	2.229E-04	-1.692E-05	2.229E-04	-1.692E-05
CB	0	0	0.002284	0.002284
CC	0.007208	0.0051638	0.007208	0.0051638
NA	2.396E-05	2.396E-05	2.396E-05	2.396E-05
NB	-3.363E-04	-3.363E-04	-3.363E-04	-3.363E-04
DAB	1.47E-04	1.47E-04	1.47E-04	1.47E-04
NC	0	0	0	0
DBC	1.245E-04	1.245E-04	1.245E-04	1.245E-04
DAC	1.075E-04	1.075E-04	1.075E-04	1.075E-04
CT	0.0074309	0.0074309	0.0074309	0.0074309
ERRA	2.229E-04	-1.692E-05	2.229E-04	-1.692E-05
ERRB	-0.002701	-0.002701	-4.17E-04	-4.17E-04

XB	0	0	0.3073667	0.3073667
XA	0.0299964	-0.0022769	0.0299964	-0.0022769
XC	0.9700056	0.6949123	0.9700056	0.6949123

ODE Report (RKF45)

Differential equations as entered by the user
[1] d(CA)/d(Z) = (XA*NB-XB*NA)/DAB+(XA*NC-XC*NA)/DAC
[2] d(CB)/d(Z) = (XB*NA-XA*NB)/DAB+(XB*NC-XC*NB)/DBC
[3] d(CC)/d(Z) = (XC*NA-XA*NC)/DAC+(XC*NB-XB*NC)/DBC

Explicit equations as entered by the user
[1] NA = 2.396E-5
[2] NB = -3.363E-4
[3] DAB = 1.47E-4
[4] NC = 0
[5] DBC = 1.245E-4
[6] DAC = 1.075E-4
[7] CT = 0.2/(82.057E-3*328(
[8] ERRA = CA-0
[9] ERRB = CB-2.701E-3
[10] XB = CB/CT
[11] XA = CA/CT
[12] XC = CC/CT

Independent variable
variable name : Z
initial value : 0
final value : 0.001

Precision
Step size guess. h = 0.1
Truncation error tolerance. eps = 0.000001

General
number of differential equations: 3
number of explicit equations: 12
Data file: D\:POLLUTION PAPERS AND POLYMATH\CASE 1.pol