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EVALUATION OF PHYSICAL PROPERTIES OF GASES AND MULTICOMPONENT GAS MIXTURES

by

John T. Holmes and
Manfred G. Baerns

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ANL-6951

Mathematics and Computers
(TID-4500, 37th Ed.)

AEC Research and
Development Report

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60440

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Chemical Engineering Division

November 1964

Operated by The University of Chicago
under
Contract W-31-109-eng-38
with the
U. S. Atomic Energy Commission

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NOMENCLATURE

Symbol	Quantity	Unit	Program Name
C_p	Molar heat capacity at constant pressure	cal/mol-°K	CP, CPM
C_v	Molar heat capacity at constant volume	cal/mol-°K	CV
D	Diffusion coefficient	cm ² /sec	DEE, DE
k	Thermal conductivity	cal/cm-°K-sec	KAY, CK
k'	Boltzmann's constant	cal/mol-°K	
M	Molecular weight	g/mol	EM
N	Rate of diffusion	g/mol/sec-cm ²	
P	Total pressure	atm	PK
P_c	Critical pressure	atm	PC
P_r	Reduced pressure	-	PR, PRED
p	Partial pressure	atm	
R	Gas constant	appropriate units	
T_k	Absolute temperature	°K	TK
T_c	Critical temperature	°K	TC
T_r	Reduced temperature	-	TR, TRED
V	Volume	cm ³ /g mol	
V_c	Critical volume	cm ³ /g mol	VC
x	Mole fraction	-	X
y	Distance in direction of diffusion	cm	
Z	Compressibility factor	-	Z
<u>Greek</u>			
ϵ	Force constant	-	
μ	Viscosity	centipoise (g/cm-sec)10 ²	HMU, EMU
ρ	Density	g/cm ³	RHO, ROW
σ	Force constant	-	SIG
Φ	Viscosity and thermal conductivity weighting coefficient	-	PHI
Ω	Collision integral (from table)	-	HMD
Ω_{ij}	Collision integral (interpolated value)	-	HMIP
<u>Constants</u>			
a, b, c, d, e	Constants in the heat capacity equation	appropriate units	A, B, C, D, E
<u>Sub- and Super-scripts</u>			
c	Critical property		--C
i	Component index		(I)
j	Component index		(J)
k	Temperature-Pressure index		(K)
m	Mixture index		
n	Number of components in a mixture		
r	Reduced property		--R

EVALUATION OF PHYSICAL PROPERTIES OF GASES AND MULTICOMPONENT GAS MIXTURES

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ABSTRACT

Relationships which can be used to estimate the density, heat capacity, viscosity, thermal conductivity, and diffusivity of gases and multicomponent gas mixtures are presented and reviewed. These relationships were incorporated into a computer program for calculation and compilation of the properties for the desired components and mixtures at temperatures and pressures specified by the user. The calculations are made either by extrapolation of experimental data given at conditions other than those desired or by using the critical and molecular properties of the gases. The computer program was used to solve a sample problem dealing with the physical properties of CO_2 , O_2 , and N_2 mixtures.

I. INTRODUCTION

In order to describe the transport phenomena in a process involving gaseous reactants and products, one must be able to evaluate the physical properties of the gas or multicomponent gas mixture of interest. A knowledge of the properties is necessary for the prediction of momentum, heat, and mass transfer rates in reacting and nonreacting systems. These rates are necessary for determining reaction mechanisms, kinetics of reactions, process scale-up parameters, and optimum process conditions.

The physical properties commonly of interest are gas density, heat capacity, viscosity, thermal conductivity, and diffusion coefficient. The data in the literature which give these properties for gases are usually for a temperature and pressure such that they must be extrapolated in order to apply them to practical situations.

The physical properties of gas mixtures are seldom available in the literature. It is therefore important to be able to extrapolate or estimate easily the pure-component and multicomponent physical properties of gases using data which are commonly available in the literature.

The evaluation and compilation of the physical properties at various temperatures and pressures for a number of gases, and for a number of multicomponent gas mixtures, is extremely time-consuming if performed with a desk calculator. Therefore, a computer program (CEN-144) was developed with the aid of the Applied Mathematics Division to minimize the time and effort involved. The computer program provides a means of determining the physical properties of gases and mixtures of gases by extrapolation of experimental physical property data for the pure components. If experimental data are not available, the properties are estimated from the critical and molecular data of each of the gases by means of relations suggested by theory but containing constants based on experimental data.

The selection of the relationships used for the computer computations was determined by the accuracy of the estimated values (compared with experimental data) and by the most general applicability to various components. It is realized that the applied relations are not equally accurate for all gases; however, the predictions are generally suitable for engineering purposes. Special methods for the computed values of certain properties or for use with a limited class of gases (i.e., hydrocarbons) can be easily incorporated into the existing computer program if the user desired to do so.

This report contains a summary of the selected methods for calculating the physical properties of gases and gas mixtures, as well as a general description of the computer program and its application to a sample problem.

II. PROPERTY CALCULATIONS

A. Properties of Pure Gases

1. Density

The density ρ of an ideal gas at conditions P_k and T_k is determined by the following dimensional equation:

$$\rho = P_k M / R T_k, \text{ g/cm}^3. \quad (1)$$

If the gas is not ideal, Equation (1) is modified as follows:

$$\rho = P_k M / Z R T_k, \quad (2)$$

where Z is the compressibility of the gas, which can be obtained from tables and charts. (14,17-19)

2. Heat Capacity

The molal heat capacity at constant pressure of most of the common gases has been measured and correlated as a function of the absolute temperature by the following dimensional equation:(7,12,18)

$$C_p = a + b \times 10^{-3} T_k + c \times 10^{-6} T_k^2 + \frac{d \times 10^5}{T_k^2} + e \times 10^{-9} T_k^3, \text{ cal/mol-}^\circ\text{K. (3)}$$

The maximum deviation using this equation for common gases is about 3%.(12) This type of relationship is empirical and requires the evaluation of a, b, c, d, and e from experimental data. If these constants are not available, they can be estimated by common methods.(18,19)

Equation (3) does not predict the effect of pressure on the heat capacity. At pressures near atmospheric, the effect of pressure is small. Therefore, it is suggested that the graphical method of Watson and Smith(20) based on a reduced temperature and reduced pressure correlation be used, if warranted.

3. Viscosity

The viscosity μ of a gas at low pressure ($P_r \ll 1$) can be predicted by the following dimensional equation, which was originally derived by Hirschfelder et al.(10) and later modified by Bromley and Wilke:(3)

$$\mu = \frac{3.33 \times 10^{-3} (MT_c)^{0.5}}{V_c^{2/3}} [f(1.33 T_r)], \text{ centipoise or (g/cm-sec)}10^2 \quad (4)$$

where $1.33 T_r$ approximately equals $k'T/\epsilon$ and the function, based on the Lennard-Jones potential, is given by

$$f(1.33 T_r) = 1.058 T_r^{0.645} - \frac{0.261}{(1.9 T_r) 0.9 \log (1.9 T_r)} \quad (5)$$

which can be applied for $T_r > 0.3$.(18)

The average error of the predicted viscosities amounts to $\pm 3\%$, whereas the maximum error can be about $\pm 15\%$. If the viscosity μ_2 is known for a certain temperature T_2 , the viscosity μ_1 at a different temperature T_1 can be conveniently extrapolated based on Equation (4):

$$\mu_1 = (\mu_2) \frac{f(1.33 T_{r1})}{f(1.33 T_{r2})} \quad (6)$$

The effect of pressure on gas viscosity can be determined by means of graphical correlations presented by Carr et al.,⁽⁴⁾ Perry et al.,⁽¹⁸⁾ and Reid and Sherwood,⁽¹⁹⁾ which depend on the reduced temperature and pressure.

4. Thermal Conductivity

A number of methods are available for estimating the thermal conductivity of gases, and a critical review is given by Reid and Sherwood.⁽¹⁹⁾ The method chosen for the case when thermal conductivity data are not available is the method of Eucken⁽⁵⁾ combined with a method developed by Bromley and Wilke⁽³⁾ for estimating gas viscosities. The resulting dimensional equation is as follows:

$$k = \frac{333 \times 10^{-7} (T_c/M)^{1/2} f(1.33 T_r)}{V_c^{2/3}} (C_v + 4.47), \text{ cal/cm}^{\circ}\text{K-sec.} \quad (7)$$

The function $f(1.33 T_r)$ is the viscosity temperature function based on the Lennard-Jones potential given by Equation (5). The heat capacity at constant volume C_v is calculated assuming ideal gas behavior by means of the relationship $C_v = (C_p - R)$. The average error of this method for calculating k is reported as 5 to 13% for common gases.⁽¹⁹⁾

If the thermal conductivity k_2 is known at a given temperature T_2 , the following relationship is used to extrapolate the data to another temperature T_1 :

$$k_1 = k_2 \frac{f(1.33 T_{r_1})(C_{v_1} + 4.47)}{f(1.33 T_{r_2})(C_{v_2} + 4.47)} \quad (8)$$

At pressures near and below atmospheric, the effect of pressure on thermal conductivity is small. A graphical method proposed by Lenoir et al.⁽¹³⁾ and based on a reduced temperature and reduced pressure correlation is available, and can be applied to the results at low pressures if the correction is justified.

It should be noted that Bromley⁽²⁾ has proposed a method for estimating the thermal conductivity which gives average errors of 3.5 to 7.5%, but this method was not chosen for this work because of its relative complexity.

5. Diffusion Coefficient

The diffusion coefficient $D_{i,j}$ of a component i into component j (or j into i) is calculated from the dimensional equation which follows:⁽²³⁾

$$D_{i,j} = \frac{T^{3/2} [(M_i + M_j)/M_i M_j]^{1/2}}{P \sigma_{i,j}^2 \Omega_{i,j}} \left[2.14 \times 10^{-3} - 4.92 \times 10^{-4} \left(\frac{M_i + M_j}{M_i M_j} \right)^{1/2} \right], \text{ cm}^2/\text{sec}, \quad (9)$$

where the force constant $\sigma_{i,j} = (1/2)(\sigma_i + \sigma_j)$ and the "collision integral" $\Omega_{i,j}$ is given in a tabulated form⁽¹⁰⁾ as a function of $k'T/\epsilon_{i,j}$ (where $\epsilon_{i,j} = \sqrt{\epsilon_i \epsilon_j}$). The force constants σ_i and ϵ_i for component i can be estimated by empirical relations:

$$\sigma_i = 0.833 V_{c_i}^{1/3} \quad (10)$$

and

$$\epsilon_i = 0.77 k'T_{c_i}. \quad (11)$$

Thus, $k'T/\epsilon_{i,j}$ can be expressed by the following equation:

$$k'T/\epsilon_{i,j} = 1.30 (T_{r_i} T_{r_j})^{0.5}. \quad (12)$$

The average error of the diffusion coefficients obtained by Equation (9) is about 10%.⁽¹⁹⁾

B. Mixture Properties

1. Density

In predicting the density of a multicomponent gas mixture, it is assumed that the total volume of the mixture equals the sum of the volumes of the individual components at constant pressure (Amagat's law), which is usually valid only at low densities. The density of the mixture is then given by

$$\rho_m = \sum_{i=1}^n \rho_i x_i, \text{ g/cm}^3, \quad (13)$$

where ρ_i is the density of component i and x_i is the mole (volume) fraction of component i . The effect of temperature and pressure on the density of each component is taken into account before the density of the mixture is evaluated.

2. Heat Capacity

The molal heat capacity of a mixture of gases, assuming that Amagat's law of additive volumes holds, is given by the following equation:

$$C_{Pm} = \sum_{i=1}^n C_{Pi} x_i, \text{ cal/mol-}^\circ\text{K}, \quad (14)$$

where x_i is the mole fraction of component i and C_{Pi} is the heat capacity of component i .

Before the heat capacity of the mixture is calculated, the effect of temperature on the heat capacity of the pure component is taken into account. The correction for the effect of pressure should be made as indicated in the discussion of heat capacity for pure gases,⁽²⁰⁾ except that the pseudoreduced temperature and pressure of the mixture should be used to obtain the correction for the heat capacity of the mixture. The pseudo-reduced temperature and pressure are defined as follows:

$$T_{rm} = \sum_{i=1}^n x_i T_{ri}, \quad (15)$$

and

$$P_{rm} = \sum_{i=1}^n x_i P_{ri}. \quad (16)$$

3. Viscosity

The viscosity of a gas mixture is determined with a semi-empirical equation of Wilke:⁽²²⁾

$$\mu_m = \frac{\sum_{i=1}^n \frac{x_i \mu_i}{\sum_{j=1}^n x_j \Phi_{ij}}}, \text{ centipoise or (g/cm-sec)} 10^2 \quad (17)$$

The weighting factor Φ is given by the equation

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2 \quad (18)$$

Equation (17) predicts the viscosities of mixtures of nonpolar gases at low reduced pressures ($P_r \ll 1$) within an accuracy of about 2%;⁽¹⁾ caution is recommended in applying this equation to highly polar gases.

The effect of pressure on the viscosity of a multicomponent gas mixture is determined by, first, calculating the low-pressure viscosity of the mixture and, then, correcting for the different pressures using Carr's charts.^(4,18,19) Instead of the reduced temperatures and pressures of the pure components, the pseudoreduced temperature T_{r_m} and pseudoreduced pressure P_{r_m} of the mixture are applied [see Equations (15) and (16)].

4. Thermal Conductivity

The thermal conductivity of a gas mixture at low pressure is most conveniently calculated by the following equation proposed by Mason and Saxena⁽¹⁵⁾ as modified by Bird et al.:⁽¹⁾

$$k_m = \sum_{i=1}^n \frac{x_i k_i}{\sum_{j=1}^n x_j \Phi_{i,j}}, \text{ cal/cm}^\circ\text{K-sec}, \quad (19)$$

in which $\Phi_{i,j}$ is given by Equation (18). The x_i and x_j are mole fractions, and k_i are the thermal conductivities of the pure components. The average deviation from experimental results of mixtures of nonpolar polyatomic gases was about ± 4 percent.^(1,15)

The effect of temperature on the thermal conductivity is taken into account for the pure components before the mixture k is calculated. The effect of pressure should be made as indicated in the discussion of thermal conductivity of pure gases,⁽¹³⁾ but the pseudoreduced temperature and pressure of the mixture [Equations (15) and (16)] should be used to obtain the correction to the thermal conductivity of the mixture.

5. Diffusion Coefficient

The diffusion coefficient for diffusion of a gas into a multicomponent mixture of stagnant gases is defined by

$$-D_{im} = \frac{N_i P}{RT p_n} \frac{dp_i}{dy}, \quad (20)$$

where p_n refers to the partial pressure of nondiffusing gases and D_{im} is the effective average diffusion coefficient of i with respect to the composition of the gas.

Wilke(21) simplified the Stefan-Maxwell diffusion equation so that D_{im} can be calculated from a knowledge of the diffusion coefficients of the binary pairs:

$$D_{im} = \frac{1 - x_i}{\sum_{\substack{j=1 \\ j \neq i}}^n x_j / D_{ij}}, \text{ cm}^2/\text{sec}, \quad (21)$$

where D_{ij} is the binary diffusion coefficient. The applicability of this equation was demonstrated by Fairbanks and Wilke⁽⁶⁾ for a three-component system.

The effects of temperature and pressure are accounted for in evaluation of the binary diffusion coefficients.

III. DISCUSSION OF THE COMPUTER PROGRAM

The program (CEN-144) for the calculation and compilation of the physical properties of gases and multicomponent gas mixtures was developed in "3600 Fortran" language for the Control Data Corporation 3600 Digital Computer. A listing of the Fortran statements is given in Appendix A. In the following sections, application of the program to a sample problem is described.

A. Input Data

In applying the program to a problem, input data such as those given in Table 1 are entered on cards.

Table 1

EXAMPLE OF DATA ENTERED ON INPUT CARDS FOR CEN-144 COMPUTER PROGRAM

CARD TYPE	THE PHYSICAL PROPERTIES OF CO ₂ , O ₂ , AND N ₂ MIXTURES									
(1)	1	CEN 144								
(2)	3	2	1							
(3)	304.2	72.9	94.	44.01	1.	6.339	10.14	-3.415	0.	0. 1.CO ₂
(3)	154.4	49.7	74.	32.	1.	6.117	3.167	-1.005	0.	0. 1.O ₂
(3)	126.2	33.5	90.	28.01	1.	6.457	1.389	-0.069	0.	0. 1.N ₂
(4)		0.133		0.0						
(4)		0.039		0.21						
(4)		0.828		0.79						
(5)		293.		1.0						
(6)	0.0019769	273.0	1.0	0.01462	293.	0.0000383	293.			
(6)	0.00142896	273.0	1.0	0.02031	293.	0.0000612	293.			
(6)	0.00125050	273.0	1.0	0.01754	293.	0.0000627	293.			

- Type 1) A title card with a 1 in column 1, then up to 71 characters, numbers or words, for the run designation. Format 72H.
- Type 2) A card with the number of compounds (≤ 9), number of mixtures (≤ 20), and number of temperature-pressure combinations (≤ 20). Format 3I3.
- Type 3) A set of cards (≤ 9) which include the following information for each compound: T_c , P_c , V_c , M , Z , a , b , c , d , e . The appropriate units are given in the Nomenclature. If ρ , μ , or k or more than one of these are given as input on a later card (6), a 1.0 is placed in positions 71, 72, and 73, and if these are not known experimentally, a 0.0 is substituted for the 1.0. Finally, a 7-character (or less) name of the compound can be supplied at the end of the card. Format 10E 7.0, F3.0, A7.
- Type 4) A set of cards giving (≤ 20) combinations of the mole fraction composition of each mixture. Format 6E12.0.
- Type 5) A set of cards giving (≤ 20) combinations of temperatures ($^{\circ}\text{K}$) and pressures (atm). Format 2E12.0.
- Type 6) A set of cards (≤ 9) giving additional input if ρ , T_ρ , P_ρ , μ , T_μ , k , and T_k are available; T_ρ , P_ρ , T_μ , and T_k are the conditions at which ρ , μ , and k are known. The appropriate units are given in the Nomenclature. A card of this nature must be supplied for each card having a 1.0 designation in positions 71, 72, and 73 of card type (3) above. Format 7E10.0.

The deck of cards which contains the program instructions also includes the tabulated values of $k'T/\epsilon$ and $\Omega^{(10)}$ which are needed for calculating the binary diffusion coefficients [Equation (9)]. An interpolation subroutine⁽¹¹⁾ is used by the computer to evaluate Ω as a function of $k'T/\epsilon$.

The user of the program must realize that the calculated or extrapolated physical properties will be, at the best, as accurate as the input data which are used. It is suggested that, if ρ , k , or μ are known for any of the components of interest, these data be given as input rather than computing these properties from the critical and molecular constants.

The critical constants, compressibility factor, and heat capacity constants which are contained on the input cards can be obtained from several sources.^(7,8,12,14,16-19) The data must be chosen with care, however, since data from different sources are not always in agreement. If

the critical and molecular properties of a component are not available, and are approximated by standard methods,^(12,18,19) the calculated physical properties must then be used with caution.

B. Output Results

The calculated output from the sample problem (see Table 1) is listed in Table 2. A table of dimensional conversion factors for each property

Table 2

THE PHYSICAL PROPERTIES OF CO₂, O₂, AND N₂ MIXTURES*

CEN 144 THE PHYSICAL PROPERTIES OF CO ₂ , O ₂ , AND N ₂ MIXTURES										
COMPOUND	TC	PC	VC	M	Z	A	B	C	D	E
CO ₂	304.20	72.90	94.00	44.01	1.00	6.3390	10.1400	-3.4150	0.0000	0.0000
O ₂	154.40	49.70	74.00	32.00	1.00	6.1170	3.1670	-1.0050	0.0000	0.0000
N ₂	126.20	33.50	90.00	28.01	1.00	6.4570	1.3890	-0.0690	0.0000	0.0000

ADDITIONAL INPUT PROPERTIES							
COMPOUND	DENSITY GRAM/CCM	T(DENSITY) DEG K	P(DENSITY) ATM	VISCOSITY CENTIPOISE	T(VISCOSITY) DEG K	TH.CONDUCTIVITY CAL/CM*DEG K*SEC	T(TH.COND.) DEG K
CO ₂	1.97690-003	273.0	1.000	1.46200-002	293.0	3.83000-005	293.0
O ₂	1.42896-003	273.0	1.000	2.03100-002	293.0	6.12000-005	293.0
N ₂	1.25050-003	273.0	1.000	1.75400-002	293.0	6.27000-005	293.0

TEMPERATURE(DEG K)= 293.0				TEMPERATURE(DEG K)= 293.0			
PRESSURE(ATM)= 1.0000				PRESSURE(ATM)=1.000			

COMPOUND	T REDUCED	P REDUCED	DENSITY GRAM/CCM	HEAT CAPACITY CAL/MOL*DEG K	VISCOSITY CENTIPOISE	TH.CONDUCTIVITY CAL/CM*DEG K*SEC
CO ₂	0.963	0.01372	1.8420-003	9.0168-000	1.4620-002	3.8300-005
O ₂	1.898	0.02012	1.3314-003	6.9587-000	2.0310-002	6.1200-005
N ₂	2.322	0.02985	1.1651-003	6.8581-000	1.7540-002	6.2700-005

DIFFUSIVITY(SQ CM/SEC)			
COMPOUND	CO ₂	O ₂	N ₂
CO ₂	1.1713-001	1.5798-001	1.5968-001
O ₂	1.5798-001	2.0604-001	2.0516-001
N ₂	1.5968-001	2.0516-001	2.0387-001

MIXTURE PROPERTIES			
MIX	CO ₂	O ₂	N ₂
1	0.13300	0.03900	0.82800
2	0.00000	0.21000	0.79000

TEMPERATURE(DEG K)= 293.0				TEMPERATURE(DEG K)= 293.0			
PRESSURE(ATM)= 1.0000				PRESSURE(ATM)=1.000			

MIX	T REDUCED	P REDUCED	DENSITY GRAM/CCM	HEAT CAPACITY CAL/MOL*DEG K	VISCOSITY CENTIPOISE	TH.CONDUCTIVITY CAL/CM*DEG K*SEC
1	2.124	0.02733	1.2616-003	7.1491-000	1.7143-002	5.8427-005
2	2.233	0.02781	1.2001-003	6.8792-000	1.8123-002	6.2401-005

DIFFUSIVITY(SQ CM/SEC)			
MIX	CO ₂	O ₂	N ₂
1	1.5961-001	1.9702-001	1.5814-001
2	1.5932-001	2.0516-001	2.0516-001

*The program labeling is identified in the Nomenclature.

is given in Appendix B. The output format is divided into three parts:

- 1) labeled columns of the input parameters (Compound , T_c , P_c , V_c , M , Z , a , b , c , d , e , ρ , T_ρ , P_ρ , μ , T_μ , k , T_k),
- 2) for each set of T_k and P_k , the calculated values for each pure component (T_r , P_r , ρ , C_p , μ , k), along with a tabulation of all of the binary diffusion coefficients (D_{ij}), and
- 3) for each set of T_k and P_k , a tabulation of the input compositions (x_i), labeled columns of the calculated properties of each mixture (T_{rm} , P_{rm} , ρ_m , C_{pm} , μ_m , k_m) and a tabulation of the diffusion coefficient of each component into each mixture (D_{im}).

The values of C_p , μ , and k for each component and each mixture are always listed at 1.0 atm, since the effect of pressure must be evaluated graphically as discussed previously.

The calculated value of ρ , C_p , μ , and k for each component of the sample problem is within the expected accuracy of the method of calculation when experimental data are compared with the calculated values.

Table 3 gives calculated and experimental binary diffusion coefficients. The agreement in all of these cases is better than $\pm 8\%$ if the calculated data are extrapolated to the temperatures of the experimental data.

Table 3

CALCULATED AND EXPERIMENTAL VALUES OF DIFFUSION
COEFFICIENTS FOR $\text{CO}_2\text{-N}_2$, $\text{N}_2\text{-O}_2$, $\text{CO}_2\text{-O}_2$

Binary Mixture	Diffusion Coefficient (cm^2/sec)	
	Calculated at 293°K	Experimental ⁽¹⁹⁾
$\text{CO}_2\text{-N}_2$	0.160	0.158 at 298°K
$\text{N}_2\text{-O}_2$	0.205	0.181 at 273°K
$\text{CO}_2\text{-O}_2$	0.158	0.139 at 273°K

Table 4 shows calculated and experimental values of C_p , μ , and k of the two gas mixtures (see Table 2 for compositions).

In the case of the diffusion coefficients for a mixture, the value calculated when the mole fraction of a component equals zero should be considered as the coefficient at infinite dilution. A calculated value of

0.159 cm²/sec at 293°C compares quite well with the experimental value of 0.136 cm²/sec at 273°C⁽¹⁹⁾ for the diffusion of CO₂ into air.

Table 4

COMPARISON OF CALCULATED AND EXPERIMENTAL VALUES
FOR HEAT CAPACITY, VISCOSITY, AND THERMAL CONDUCTIVITY
OF CO₂-O₂-N₂ MIXTURES

Mixture	C _p , cal/mol-°K		μ x 10 ² , centipoise		k x 10 ⁵ , cal/cm-°K-sec	
	Calc	Expt	Calc	Expt	Calc	Expt
1	7.15	-	1.71	1.79 ⁽⁹⁾	5.84	-
2 ^a	6.87	7.25	1.81	1.79	6.24	6.20

^aExperimental values for air were used for comparison with the 21% O₂, 79% N₂ mixture.

The sample problem was presented to illustrate the format of the input and output of a typical set of data and are not meant to imply that the properties of other gases and other mixtures will be calculated to as high a degree of accuracy. If the input data are accurate and if there are no chemical or physical interactions which cause nonidealities, the results of the computations should be satisfactory for most engineering purposes.

IV. ACKNOWLEDGMENTS

The authors' sincere thanks are due to John L. Anderson (Applied Mathematics Division) who developed the computer program embodied in this report. They also wish to acknowledge the critical review of the work by Lowell Koppel.*

*Consultant from Purdue University.

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APPENDIX A

Computer Program CEN-144 for the Calculation and Compilation
of the Physical Properties of Gases and Multicomponent Gas Mixtures

```

PROGRAM CEN144
C   J. ANDERSON   2170/CEN144   JUNE 1964
      DIMENSION TC(9),PC(9),VC(9),EM(9),Z(9),A(9),B(9),C(9),D(9),E(9),
      1X(9,20),TK(20),PK(20),TR(9,20),PR(9,20),SIG(9),ENPUI(9),CP(9,20),
      2RHO(9,20),HMU(9,20),CAY(9,20),TE(2),FI(2),C11(9),C12(9),C13(9),
      3C14(9),C15(9),CAYT(79),HMD(79),AL(156,4),TSR(20),DEE(9,9,20),
      4ROW(20,20),CPM(20,20),EMU(20,20),PHI(9,9,20),CK(20,20),
      5OE(9,20,20),COMP(9),TRED(20,20),PRED(20,20)
      C1=1.0E-03
      C2=1.0E-06
      C3=1.0E+05
      C4=1.0E-09
      C10=3.33E-03
400  FORMAT(72H
      1
401  FORMAT(3I3)
402  FORMAT(10E7.0,F3.0,A7)
403  FORMAT(6E12.0)
404  FORMAT(2E12.0)
405  FORMAT(12E6.0)
406  FORMAT(/////20H TEMPERATURE(DEG K)=F7.1,35X,19HTEMPERATURE(DEG K)=
      1F7.1/15H PRESSURE(ATM)=F9.4,38X19HPRESSURE(ATM)=1.000//)
407  FORMAT(1X,A7,3X,F8.3,4XF9.5,4XE11.4,15XE11.4,5XE11.4,4XE11.4)
408  FORMAT(/////23H DIFFUSIVITY(SQ CM/SEC)/9H COMPOUND,7X,A7,8(5XA7))
409  FORMAT(1X,A7,4X,9(E12.4))
410  FORMAT( * MIX*5X*T REDUCED*5X*P REDUCED*6X*DENSTY*17X,
      1*HEAT CAPACITY*4X*VISCOSITY*4X*TH.CONDUCTIVITY*/38X*GRAM/CCM*16X,
      213HCAL/MOL*DEG K,4X*CENTIPOISE*3X16HCAL/CM*DEG K*SEC)
411  FORMAT(1X,I2,5XF8.3,6XF9.5,5XE11.4,15XE11.4,5XE11.4,4XE11.4)
412  FORMAT(/////23H DIFFUSIVITY(SQ CM/SEC) /4H MIX,9X,A7,8(5XA7))
413  FORMAT(1X,I2,4X,9(F12.5))
414  FORMAT(7E10.0)
415  FORMAT(///// * MIXTURE PROPERTIES*// * MOLE FRACTION*// * MIX*,9X,
      1A7,8(5XA7))
416  FORMAT(//9H COMPOUND,7X2HTC,9X2HPC,9X2HVC,9X1HM,10X1HZ,9X1HA,
      110X1HB,10X1HC,10X1HD,10X1HE)
417  FORMAT(1X,A7,5(F11.2),5(F11.4))
418  FORMAT(1X,I2,4X,9(E12.4))
419  FORMAT(/////28H ADDITIONAL INPUT PROPERTIES/9H COMPOUND,7X,
      17HDENSITY,6X10HT(DENSITY),4X10HP(DENSITY),5X9HVIScosity,3X,
      212HT(VISCOSITY),3X15HTH.CONDUCTIVITY,3X11HT(TH.COND.)/15X,
      39H GRAM/CCM,7X5HDEG K,9X3HATM,10X10HCENTIPOISE,5X,5HDEG K,7X,
      416HCAL/CM*DEG K*SEC,5X5HDEG K)
420  FORMAT(1X,A7,4X,E14.5,4XF8.1,6XF8.3,2XE14.5,4XF8.1,2XE16.5,6XF8.1)
421  FORMAT( * COMPOUND*3X*T REDUCED*3X*P REDUCED*5X*DENSTY*17X,
      1*HEAT CAPACITY*4X*VISCOSITY*4X*TH.CONDUCTIVITY*/38X*GRAM/CCM*16X,
      213HCAL/MOL*DEG K,4X*CENTIPOISE*3X16HCAL/CM*DEG K*SEC)
      READ 405,(CAYT(I),I=1,79)
      READ 405,(HMD(I),I=1,79)
      CALL CCDIS(CAYT,HMD,AL,79,FN)
      5 READ 400
      IF (EQF,60)6,7
      6 CALL EXIT
      7 READ 401,NC,NM,NT
      IX=0
      PRINT 400
      PRINT 416
      READ 402,(TC(I),PC(I),VC(I),EM(I),Z(I),A(I),B(I),C(I),D(I),E(I),
      1ENPUI(I),COMP(I),I=1,NC)
      DO 10 I=1,NC
      PRINT 417,COMP(I),TC(I),PC(I),VC(I),EM(I),Z(I),A(I),B(I),C(I),
      1D(I),E(I)

```



```

      IF(IX)10,8,10
8  IF(ENPUT(I))9,10,9
9  IX=1
10 READ 403,(X(I,J),J=1,NM)
    READ 404,(TK(K),PK(K),K=1,NT)
    IF(IX)13,15,13
13 PRINT 419
15 DO 24 I=1,NC
    C13(I)=0.0
    C14(I)=0.0
    C15(I)=0.0
    CUBER=CUBERTF(VC(I))
    SIG(I)=0.833*CUBER
    C11(I)=C10*SQRTF(EM(I)*TC(I))/(CUBER*CUBER)
    C12(I)=EM(I)/Z(I)
    IF(ENPUT(I))24,24,16
16 READ 414,RHOI,TEE,PEA,HMUI,TE(1),CAYI,TE(2)
    PRINT 420,COMP(1),RHOI,TEE,PEA,HMUI,TE(1),CAYI,TE(2)
    DO 18 I1=1,2
    IF(TE(I1))17,18,17
17 TRI=TE(I1)/TC(I)
    EX=0.39086503362*LOGF(1.9*TRI)
    FI(I1)=1.058*(TRI**.645)-.261/((1.9*TRI)**EX)
18 CONTINUE
    IF(RHOI)19,20,19
19 C13(I)=TEE*RHOI/PEA
20 IF(HMUI)21,22,21
21 C14(I)=HMUI/FI(1)
22 IF(CAYI)23,24,23
23 TES=TE(2)*TE(2)
    CPI=A(I)+B(I)*C1*TE(2)+C(I)*C2*TES+D(I)*C3/TES+E(I)*C4*TE(2)*TES
    CVI=CPI-1.987
    C15(I)=CAYI/(FI(2)*(CVI+4.47))
24 CONTINUE
    DO 30 K=1,NT
    TSR(K)=TK(K)**1.5/PK(K)
    TKS=TK(K)*TK(K)
    C5=C1*TK(K)
    C6=C2*TKS
    C7=C3/TKS
    C8=C4*TK(K)*TKS
    C9=PK(K)/TK(K)
    DO 30 I=1,NC
    TR(I,K)=TK(K)/TC(I)
    PR(I,K)=PK(K)/PC(I)
    EX=0.39086503362*LOGF(1.9*TR(I,K))
    FIK=1.058*(TR(I,K)**.645)-.261/((1.9*TR(I,K))**EX)
    CP(I,K)=A(I)+B(I)*C5+C(I)*C6+D(I)*C7+E(I)*C8
    CVIK=CP(I,K)-1.987
    IF(C13(I))725,25,725
25 RHO(I,K)=C12(I)*C9/82.057
    GO TO 726
725 RHO(I,K)=C9*C13(I)
726 IF(C14(I))727,27,727
727 HMU(I,K)=C11(I)*FIK
    GO TO 728
728 IF(C15(I))729,28,729
28 CAY(I,K)=HMU(I,K)*(CVIK+4.47)/(EM(I)*100.0)
    GO TO 30
729 CAY(I,K)=FIK*(CVIK+4.47)*C15(I)
30 CONTINUE

```

```

DO 40 I=1,NC
DO 40 IQ=1,NC
ILL=1
EMR=SQRTF((EM(I)+EM(IQ))/(EM(I)*EM(IQ)))
EMC=EMR*(.00214-.000492*EMR)
PA=EM(I)/EM(IQ)
PB=SQRTF(8.0*(1+PA))
PQ=(EM(IQ)/EM(I))**.250
IF(SIG(I))31,32,31
31 IF(SIG(IQ))33,32,33
32 ILL=0
GO TO 733
33 SIGPS=(SIG(I)*SIG(I)+2.0*SIG(I)*SIG(IQ)+SIG(IQ)*SIG(IQ))/4.0
DC=EMC/SIGPS
733 DO 40 K=1,NT
IF(ILL)735,734,735
734 DEE(I,IQ,K)=0.0
GO TO 39
735 GAMP=1.30*SQRTF(TR(I,K)*TR(IQ,K))
J=2
34 IF(GAMP-CAYT(J))38,38,36
36 J=J+1
GO TO 34
38 N1=2*J-3
N2=2*J-2
CD=GAMP-CAYT(J-1)
CY=HMD(J-1)+((HMD(J)-HMD(J-1))/(CAYT(J)-CAYT(J-1)))*CD
CN=(CAYT(J)-GAMP)*(AL(N1,1)+AL(N2,1)*CD)*CD
HMIP=CY+CN
DEE(I,IQ,K)=TSR(K)*DC/HMIP
39 PHI(I,IQ,K)=((1.0+SQRTF(HMU(I,K)/HMU(IQ,K))*PQ)**2)/PB
40 CONTINUE
DO 50 K=1,NT
DO 50 J=1,NM
CK(J,K)=0.0
EMU(J,K)=0.0
CPM(J,K)=0.0
ROW(J,K)=0.0
TRED(J,K)=0.0
PRED(J,K)=0.0
DO 45 I=1,NC
ROW(J,K)=ROW(J,K)+RHO(I,K)*X(I,J)
CPM(J,K)=CPM(J,K)+CP(I,K)*X(I,J)
TRED(J,K)=TRED(J,K)+TR(I,K)*X(I,J)
PRED(J,K)=PRED(J,K)+PR(I,K)*X(I,J)
SUM1=0.0
SUM2=0.0
DO 42 IQ=1,NC
SUM1=SUM1+X(IQ,J)*PHI(I,IQ,K)
IF(I-IQ)41,42,41
41 SUM2=SUM2+X(IQ,J)/DEE(I,IQ,K)
42 CONTINUE
DE(I,J,K)=(1.0-X(I,J))/SUM2
EMU(J,K)=EMU(J,K)+(X(I,J)*HMU(I,K))/SUM1
CK(J,K)=CK(J,K)+(X(I,J)*CAY(I,K))/SUM1
45 CONTINUE
50 CONTINUE
DO 100 K=1,NT
IF(K-1)56,58,56
56 PRINT 400
58 PRINT 406,TK(K),TK(K),PK(K)
PRINT 421

```

```

DO 60 I=1,NC
60 PRINT 407,COMP(I),TR(I,K),PR(I,K),RHO(I,K),CP(I,K),HMU(I,K),
1CAY(I,K)
PRINT 408,(COMP(I),I=1,NC)
DO 70 I=1,NC
70 PRINT 409,COMP(I), (DEE(I,IA,K),IA=1,NC)
PRINT 415,(COMP(I),I=1,NC)
DO 75 J=1,NM
75 PRINT 413,J,(X(I,J),I=1,NC)
PRINT 406,TK(K),TK(K),PK(K)
PRINT 410
DO 80 J=1,NM
80 PRINT 411,J,TRED(J,K),PRED(J,K),ROW(J,K),CPM(J,K),EMU(J,K),CK(J,K)
PRINT 412,(COMP(I),I=1,NC)
DO 90 J=1,NM
90 PRINT 418,J,(DE(I,J,K),I=1,NC)
100 CONTINUE
GO TO 5
END

SUBROUTINE CCDIS ( X,Y,A,N,FN)
DIMENSION X(79),Y(79),A(156,4)
A(1,1)=0.0
A(1,2)=-2.0
A(1,3)=2.0*(X(2)-X(1))
A(1,4)=0.0
N3 = N-1
N1 = N3-1
J = 1
DO 10 I = 1,N1
J = J+1
A(J,1)=(X(I+1)-X(I))/(X(I+2)-X(I+1))
A(J,2)=A(J,1)*(X(I+1)-X(I))
A(J,3)=1.0
A(J,4)= (Y(I+1)-Y(I))/((X(I+1)-X(I))*(X(I+2)-X(I+1)))
A(J,4)=A(J,4)-(Y(I+2)-Y(I+1))/((X(I+2)-X(I+1))*(X(I+2)-X(I+1)))
K=I
J = J+1
A(J,1) = (X(K+1)-X(K))/(X(K+2)-X(K+1))
A(J,2)=-((X(K+2)-X(K))/((X(K+2)-X(K+1))*(X(K+1)-X(K))))
A(J,3)=1.0
A(J,4)=(Y(K+2)-Y(K+1))/((X(K+1)-X(K))*(X(K+2)-X(K+1)))
A(J,4)=A(J,4)/(X(K+2)-X(K+1))
R=(Y(K+1)-Y(K))/((X(K+1)-X(K))*(X(K+1)-X(K)))
R=R/(X(K+2)-X(K+1))
10 A(J,4)=A(J,4)-R
N2 = 2*N3
A(N2,1)=-2.0
A(N2,2) = -4.0*(X(N3+1)-X(N3))
A(N2,3)=0.0
A(N2,4)=0.0
CALL TDSEQ (A,N2,FN)
RETURN
END
SUBROUTINE TDSEQ (A,N,FN)
DIMENSION A(156,4)
IF(A(1,2)) 12,11,12
11 FN = 1.0
GO TO 50
12 A(1,3)=A(1,3)/A(1,2)
A(1,1)=A(1,4)/A(1,2)
N=N
DO 10 I=2,N

```

```
A(I,2)=A(I,2)-A(I,1)*A(I-1,3)
IF(A(I,2)) 13,11,13
13 A(I,3)=A(I,3)/A(I,2)
10 A(I,1) = (A(I,4) - A(I,1)*A(I-1,1))/A(I,2)
I=N
20 I=I-1
IF(I)40,40,30
30 A(I,1) = A(I,1) - A(I,3)*A(I+1,1)
GO TO 20
40 FN=0.0
50 RETURN
END
```

APPENDIX B

Conversion Factors

1. Density

Multiply $\frac{\text{g/cc}}{\text{by:}}$	to get
1000	$\frac{\text{kg}}{\text{m}^3}$
1.000027	kg/liter
62.428	lb_m/ft^3
0.036127	$\text{lb}_m/\text{in.}^3$

2. Heat Capacity

Multiply $\frac{\text{cal/mol-}^\circ\text{K}}{\text{by:}}$	to get
1/molecular weight	$\text{cal/g-}^\circ\text{K}$
1/molecular weight	Btu/lb- $^\circ\text{F}$
4.186/molecular weight	Joule/g- $^\circ\text{K}$
1.0	Btu/lb-mol- $^\circ\text{F}$

3. Viscosity

Multiply $\frac{\text{centipoise}}{\text{by:}}$	to get
1/density of gas	centistokes
0.01	poise
0.001	kg/m-sec
6.7197×10^{-4}	$\text{lb}_m/\text{ft-sec}$
2.0886×10^{-5}	$\text{lb}_f\text{-sec}/\text{ft}^2$
2.4191	$\text{lb}_m/\text{ft-hr}$

4. Thermal Conductivity

Multiply $\frac{\text{cal/cm-}^\circ\text{K-sec}}{\text{by:}}$	to get
4.1840×10^7	$\text{g-cm}/\text{sec}^3\text{-}^\circ\text{K}$
4.1840×10^7	ergs/sec-cm- $^\circ\text{K}$
4.1840×10^5	W/m- $^\circ\text{K}$
1.6813×10^3	$\text{lb}_m\text{-ft}/\text{sec}^3\text{-}^\circ\text{F}$
52.256	$\text{lb}_f/\text{sec-}^\circ\text{F}$
241.75	Btu/hr-ft- $^\circ\text{F}$

5. Diffusivity

Multiply $\frac{\text{cm}^2/\text{sec}}{\text{by:}}$	to get
10^{-4}	m^2/sec
3.8750	ft^2/hr