

RELATIVE DENSITY OF GAS MIXTURES BY CALCULATION FROM COMPOSITION

UOP Method 948-96

SCOPE

This method is for calculating the relative density of gas mixtures, generated by typical refinery processes run under typical conditions, from their composition as determined by UOP Method 539 or any other suitable method. This method can be used in place of UOP Method 114. The relative density of air is defined as unity (1.00).

OUTLINE OF METHOD

The sample composition is determined by UOP Method 539 or any other suitable method. The relative density of the sample is calculated using a commercially available software program and either mol-% or mass-% data input. A manual calculation that yields an approximate relative density value using the relative densities of the individual components is also included in this method. The software program provides the more accurate value.

APPARATUS

In addition to the apparatus specified in UOP Method 539, the following are required if the user wishes to perform the calculations in house. Alternatively, the user can send the composition data to Matheson Gas Products, who will perform the calculation for a fee.

Computer, personal, capable of supporting K-Flash software application

Software, K-Flash, Kesler Engineering, no substitutions allowed

REAGENTS AND MATERIALS

The materials and reagents specified in UOP Method 539 are required.

IT IS THE USER'S RESPONSIBILITY TO ESTABLISH APPROPRIATE PRECAUTIONARY PRACTICES AND TO DETERMINE THE APPLICABILITY OF REGULATORY LIMITATIONS PRIOR TO USE. EFFECTIVE HEALTH AND SAFETY PRACTICES ARE TO BE FOLLOWED WHEN UTILIZING THIS PROCEDURE. FAILURE TO UTILIZE THIS PROCEDURE IN THE MANNER PRESCRIBED HEREIN CAN BE HAZARDOUS. MATERIAL SAFETY DATA SHEETS (MSDS) OR EXPERIMENTAL MATERIAL SAFETY DATA SHEETS (EMSDS) FOR ALL OF THE MATERIALS USED IN THIS PROCEDURE SHOULD BE REVIEWED FOR SELECTION OF THE APPROPRIATE PERSONAL PROTECTION EQUIPMENT (PPE).

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UOP Methods are available through ASTM International, 100 Barr Harbor Drive, PO Box C700, West Conshohocken PA 19428-2959, United States. The Methods may be obtained through the ASTM website, www.astm.org, or by contacting Customer Service at service@astm.org, 610.832.9555 FAX, or 610.832.9585 PHONE.

PROCEDURE

Obtain a gas analysis of the sample using UOP Method 539 or any other suitable method.

CALCULATIONS

Preferred Method of Calculation

Install the software on the personal computer and enter the composition data into the program. The program will calculate the sample relative density, and it is reported to two decimal places. The program computes the relative density taking into account deviations from the Ideal Gas Law. If the software is not available, Matheson Gas Products will perform the calculations using the Kesler Engineering software for a fee.

Optional Method of Calculation

If a relative density value is needed immediately, and the software is not available, a manual calculation that yields an approximate relative density value for the sample can be performed as follows:

Use all available figures for the gas component values used in the calculations below, and report the final sample relative density to one decimal place.

If the values for the components in the sample are in mol-%, convert them to mass-% as follows:

$$W = \frac{100YZ}{T} \quad (1)$$

where:

- T** = sum of the products **YZ** for all components in the sample
- W** = component concentration, mass-%
- Y** = component concentration, mol-%
- Z** = molecular weight of component (from Table), g/mol
- 100** = factor to convert to mass-%

Using the mass-% values, calculate the sample relative density as follows:

$$D = \frac{X}{100} \quad (2)$$

where:

- D** = calculated sample relative density
- X** = sum of the products **WR** for all components in the sample

where:

W = each component's concentration, mass-% (previously defined, Eq. 1)
R = each component's relative density (from Table)

100 = factor to convert to mass-%

The optional calculation procedure does not take into account deviations from the Ideal Gas Law, and is therefore less accurate than the preferred method.

PRECISION

The precision of this method is limited by the precision of UOP Method 539 or other method used to determine the composition of the sample. If component values can be reported to two decimal places, then the relative density determined using the preferred method of calculation is also good to two decimal places.

ACCURACY

The accuracy of this method is limited by the accuracy of the composition data input to the software program. The software program itself is capable of one percent (relative) accuracy when working with typical refinery gas mixtures at temperatures and pressures commonly in use in typical refinery processes. At temperatures or pressures near critical conditions (at which some or all of the components compress to the liquid state), the accuracy is limited to five percent (relative). Accuracy of data generated on atypical gas mixtures cannot be guaranteed.

TIME FOR ANALYSIS

The elapsed time and labor requirement for the calculations specified in this method are the same, 0.1 hour for the preferred method of calculating, and 0.25 hour for the optional method. See UOP Method 539 for its time requirements.

REFERENCES

UOP Method 114, "Relative Density of Gas by Schilling Effusion Method"
 UOP Method 539, "Gas Analysis by Gas Chromatography"

SUGGESTED SUPPLIERS

In addition to the suppliers listed in UOP Method 539:

Kesler Engineering, 330 Milltown Rd., East Brunswick, NJ 08816 (908-238-6700)
 Matheson Gas Products, Manhattan Rd. & Richards St., P.O. Box 96, Joliet, IL 60434 (815-727-4848)

Table
Molecular Weight and Relative Density
(Air = 1.00) of Refinery Gas Components

Component	Molecular Weight, g/mol	Relative Density
Hydrogen	2.016	0.0696
Argon*	39.95	1.379
Oxygen*	32.00	1.105
Nitrogen	28.01	0.967
Carbon Monoxide	28.01	0.967
Carbon Dioxide	44.00	1.519
Methane	16.04	0.554
Ethane	30.07	1.038
Ethylene	28.05	0.968
Propane	44.11	1.523
Propylene	42.08	1.453
Isobutane	58.12	2.007
<i>n</i> -Butane	58.12	2.007
1-Butene	56.12	1.938
Isobutylene	56.12	1.938
<i>trans</i> -2-Butene	56.12	1.938
<i>cis</i> -2-Butene	56.12	1.938
1,3-Butadiene	54.09	1.867
C ₅ Paraffins	72.15	2.491
C ₅ Olefins	70.14	2.422

* Oxygen and argon are not separated by UOP Method 539. Use values appropriate to the expected sample composition.

The relative density values shown in the Table were taken from the *Handbook of Chemistry and Physics*, **1993**, CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, FL 33431.