

QC  
807.5  
.U66  
no.211  
c.2

NOAA TR ERL 211-WPL 15

# NOAA Technical Report ERL 211-WPL 15

U.S. DEPARTMENT OF COMMERCE  
National Oceanic and Atmospheric Administration  
Environmental Research Laboratories

## A Note on Terminologies Used in Gaseous Absorption Processes

R. F. CALFEE

BOULDER, COLO.  
AUGUST 1971



## ENVIRONMENTAL RESEARCH LABORATORIES

The purpose of the Environmental Research Laboratories is to study the oceans, inland and upper atmosphere, the space environment, and the earth, in search of knowledge needed to provide more useful services in improving man's prospects and well-being influenced by the physical environment. Laboratories contributing to these

**Earth Sciences Laboratories (ESL):** Geomagnetism, seismology, geodesy, and related earthquake processes, internal structure and accurate figure of the Earth, and distribution of the Earth's mass.

**Atlantic Oceanographic and Meteorological Laboratories (AOML):** Oceanography, with emphasis on the geology and geophysics of ocean basins, oceanic processes, sea-air interactions, hurricane research, and weather modification (Miami, Florida).

**Pacific Oceanographic Laboratories (POL):** Oceanography; geology and geophysics of the Pacific Basin and margins; oceanic processes and dynamics; tsunami generation, propagation, modification, detection, and monitoring (Seattle, Washington).

**Atmospheric Physics and Chemistry Laboratory (APCL):** Cloud physics and precipitation; chemical composition and nucleating substances in the lower atmosphere; and laboratory and field experiments toward developing feasible methods of weather modification.

**Air Resources Laboratories (ARL):** Diffusion, transport, and dissipation of atmospheric contaminants; development of methods for prediction and control of atmospheric pollution (Silver Spring, Maryland).

**Geophysical Fluid Dynamics Laboratory (GFDL):** Dynamics and physics of geophysical fluid systems; development of a theoretical basis, through mathematical modeling and computer simulation, for the behavior and properties of the atmosphere and the oceans (Princeton, New Jersey).

**Research Flight Facility (RFF):** Outfits and operates aircraft specially instrumented for research; and meets needs of NOAA and other groups for environmental measurements for aircraft (Miami, Florida).

**National Severe Storms Laboratory (NSSL):** Tornadoes, squall lines, thunderstorms, and other severe local convective phenomena toward achieving improved methods of forecasting, detecting, and providing advance warnings (Norman, Oklahoma).

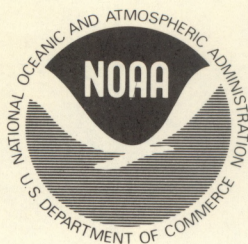
**Space Environment Laboratory (SEL):** Conducts research in solar-terrestrial physics, provides services and technique development in areas of environmental monitoring, forecasting, and data archiving.

**Aeronomy Laboratory (AL):** Theoretical, laboratory, rocket, and satellite studies of the physical and chemical processes controlling the ionosphere and exosphere of the earth and other planets.

**Wave Propagation Laboratory (WPL):** Development of new methods for remote sensing of the geophysical environment; special emphasis on propagation of sound waves, and electromagnetic waves at millimeter, infrared, and optical frequencies.

NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION

BOULDER, COLORADO 80302



U.S. DEPARTMENT OF COMMERCE

Maurice H. Stans, Secretary

NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION

Robert M. White, Administrator

ENVIRONMENTAL RESEARCH LABORATORIES

Wilmot N. Hess, Director

QC  
807.5  
-466  
70.211  
c.2

## NOAA TECHNICAL REPORT ERL 211-WPL 15

# A Note on Terminologies Used in Gaseous Absorption Processes

R. F. CALFEE

ATMOSPHERIC SCIENCES  
LIBRARY

FEB 1 1972

N.O.A.A.  
U. S. Dept. of Commerce

BOULDER, COLO.  
August 1971

For sale by the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402  
Price 25 cents

'72 578

A NOTE ON TERMINOLOGIES USED IN GASEOUS  
ABSORPTION PROCESSES

R. F. Calfee

The relationships among the many systems of units for absorption coefficients, optical paths, and intensities for gaseous processes are discussed. A table showing the inter-connecting factors is presented.

Unfortunately there does not seem to be any agreement on the system of units to be used for the measurement of absorption processes of gases. It is the purpose of this note to interrelate some of the more commonly used terminologies. It is assumed that the transmission,  $T$ , through a layer of gas is the ratio of the emerging intensity,  $I$ , to the incident intensity,  $I_0$ , and that the transmission is a function of the frequency and depends upon the amount of the absorbing medium,  $U$ . If the Beers-Lambert Law is assumed to hold, then an absorption coefficient,  $K(\nu)$ , is defined by

$$T(\nu) = \frac{I(\nu)}{I_0(\nu)} = e^{-K(\nu)U} \quad (1a)$$

or

$$K(\nu) = \frac{-\ln T(\nu)}{U} \quad (1b)$$

where  $U$  is referred to as the optical path (not to be confused with optical depth which is  $-\ln T$  or  $UK$ ).

Part of the problem comes from the fact that  $U$  is defined in several ways. Physicists frequently use

$$U(\text{atm cm}) = p(\text{atm}) \times L(\text{path in cm}) . \quad (2a)$$

In other cases the density of the absorber,  $\rho$ , is used in defining the optical path resulting in a different set of units.

$$U(\text{gm cm}^{-2}) = \rho(\text{gm cm}^{-3}) \times L(\text{path in cm}). \quad (2b)$$

Since densities are also expressed in  $\text{gm m}^{-3}$  and  $\text{Kg m}^{-3}$ , and path lengths in meters and kilometers, the optical path may come out in units of

$\left(\frac{\text{gm}}{\text{m}^2}\right)$ ,  $\left(\frac{\text{Kg}}{\text{m}^2}\right)$ ,  $\left(\frac{\text{gm}}{\text{m}^3} \text{ km}\right)$  or possible combinations of mass and distance units.

The concentration of the absorbing gas is sometimes expressed in parts per million (ppm) by volume. Then the optical path is

$$U(\text{atm cm}) = \text{ppm} \times P(\text{total pressure in atm}) \\ \times L(\text{path in cm}) \times 10^{-6} \quad (3)$$

From (1) we see that  $K(\nu)$  has units which are the reciprocal of the units used for optical path description.

$$K(\nu) = - \frac{\ln T(\nu)}{pL} (\text{atm cm})^{-1} \quad (4a)$$

$$K(\nu) = - \frac{\ln T(\nu)}{\rho L} (\text{gm cm}^{-2})^{-1} \quad (4b)$$

The two sets of units for optical path measurements are related through the ideal gas law  $p = \rho R \theta / M$  where  $p$ ,  $\rho$  and  $\theta$  are the partial pressure, the density and the temperature of the absorbing gas;  $M$  is the molecular weight of the absorber and  $R$  is the universal gas constant. The coefficients used in the following expression arise from the combinations of constants appearing in the gas law.

If the partial pressure,  $p$  (atm) at  $\theta$  ( $^{\circ}\text{K}$ ) and the length of absorbing

path, L (cm), are known then at STP,

$$U(\text{atm cm STP}) = p(\theta) L \frac{273}{\theta} \quad (5)$$

When the partial pressure, p, at  $\theta$  ( $^{\circ}\text{K}$ ) is known, but the optical path designation is preferred in terms of density,  $\rho$ , then from the gas law

$$\rho(\theta)(\text{gm cm}^{-3}) = 1.219 \times 10^{-2} \frac{p(\text{atm})M}{\theta} \quad (6)$$

Then the optical path term in either set of units can be found from (2).

The absorption coefficient may be found expressed in terms of decibels. To see how this nomenclature is related to the other units of absorption coefficient, note that

$$\ln T(\nu) = \frac{\log_{10} T(\nu)}{.4343} \equiv \frac{10 \log_{10} \left( \frac{I(\nu)}{I_0(\nu)} \right)}{4.343} \quad (7)$$

and

$$\frac{10 \log_{10} \left( \frac{I(\nu)}{I_0(\nu)} \right)}{U} \equiv \frac{k(\nu) \text{ (decibels)}}{\text{(optical path units)}} \cdot$$

Now

$$K(\nu)(\text{atm cm})^{-1} = \frac{-10 \log_{10} \left( \frac{I(\nu)}{I_0(\nu)} \right)}{4.343 U} = .2303k(\nu) \left( \frac{\text{db}}{\text{atm cm}} \right) \quad (8)$$

or

$$k(\nu) \left( \frac{\text{db}}{\text{atm cm}} \right) = 4.343 K(\nu) (\text{atm cm})^{-1} \quad (9a)$$

or

$$k(\nu) \left( \frac{\text{db}}{\text{gm cm}^{-2}} \right) = 4.343 K(\nu) (\text{gm cm}^{-2})^{-1} \quad (9b)$$

$$1 \text{ db (gm cm}^{-2}) = 10 \text{ db (gm km m}^{-3}) \quad (10)$$

Sometimes  $K$  in decibels per unit length is specified, but this is not enough unless the temperature and pressure or density are also given.

If  $K(\nu)$  is given in  $(\text{atm cm})^{-1}$  and we wish to know its equivalent in  $\text{db}/(\text{gm cm}^{-2})$  using (6) we see that

$$k(\nu) \left( \frac{\text{db}}{\text{gm cm}^{-2}} \right) = 356.3 K(\nu) (\text{atm cm})^{-1} \text{STP} \times \frac{\theta}{M} \quad (11)$$

If the concentration is given in  $\mu\text{g m}^{-3}$  and we wish to express it in ppm we proceed as follows: if  $n_p \ll n_a$

$$\text{ppm} = \frac{V_p}{V_{ol}_a + V_{ol}_p} = \frac{n_p}{n_a + n_p} \cong \frac{n_p}{n_a} \quad (12)$$

$$n_p = \frac{m_p}{M_p} \text{ and } n_a = \frac{m_a}{M_a} \text{ where the subscript } p \text{ denotes}$$

the pollutant molecules, and  $a$ , the air molecules. Since the mass of each is proportional to its density, we may write

$$\text{ppm} = \frac{n_p}{n_a} = \frac{m_p / M_p}{m_a / M_{air}} = \frac{\rho_p}{\rho_a} \times \frac{M_a}{M_p} \quad (13)$$

If  $n_p \approx n_a$ , the approximation in (12) does not hold so

$$\text{ppm} = \frac{n_p}{n_p + N_a} = \frac{\frac{m_p}{M_p} / \frac{m_a}{M_a}}{\frac{m_p}{M_p} + \frac{m_a}{M_a}} = \frac{\frac{\rho_p}{M_p} / \frac{\rho_a}{M_a}}{\frac{\rho_p}{M_p} + \frac{\rho_a}{M_a}} = \frac{1}{1 + \frac{\rho_a}{M_a} \times \frac{M_p}{\rho_p}} \quad (14)$$

For water vapor,  $1 \text{ gm cm}^{-2}$  is numerically equivalent to the frequently used precipitable centimeter and is customary to use (2b) to determine U. Here  $\rho$  is the actual density of water vapor present at temperature  $\theta$ . More often the relative humidity, rh, is given. In this case we must look up  $\rho_s(\theta)$ , the saturation density at temperature  $\theta$  ( $^{\circ}\text{K}$ ). Then for water vapor

$$U \frac{\text{gm}}{\text{cm}^2} \text{ H}_2\text{O} = U(\text{pr cm H}_2\text{O}) = \text{rh} \times \rho_s(\theta) \times L(\text{cm}). \quad (15)$$

Closely related to this subject is the notation used for the strength or intensities of absorption lines and bands. For water vapor, the convention is to use

$$S\left(\frac{\text{cm}^{-1}}{\text{gm cm}^{-2}}\right).$$

For carbon dioxide and most other gases, the usage is

$$S\left(\frac{\text{cm}^{-1}}{\text{atm cm}}\right).$$

From (6) we can convert from  $(\text{gm cm}^{-2})$  to  $(\text{atm cm})$  by

$$\rho P = 1.217 \times 10^{-2} p (\text{atm}) L \frac{M}{\theta};$$



so

$$\left( S \frac{\text{cm}^{-1}}{\text{gm cm}^{-2}} \right) = S \left( \frac{\text{cm}^{-1}}{\text{atm cm}} \right) \times \frac{\theta}{M} \times 82.06 \quad (16a)$$

or

$$\left( S \frac{\text{cm}^{-1}}{\text{atm cm}} \right) = \left( \frac{\text{cm}^{-1}}{\text{gm cm}^{-2}} \right) \times 1.219 \times 10^{-2} \frac{M}{\theta} \quad (16b)$$

Recently a move has been made to express strengths in terms of  $\text{cm}^{-1}/(\text{molecules cm}^{-2})$ . To convert from  $\text{cm}^{-1}/(\text{gm cm}^{-2})$  we multiply by the molecular weight,  $M$ , of the gas and divide by Avagadrós number,  $A$ ,

$$S \left( \frac{\text{cm}^{-1}}{(\text{molecule cm}^{-2})} \right) = S \left( \frac{\text{cm}^{-1}}{\text{gm cm}^{-2}} \right) \times \frac{M}{A} \quad (17a)$$

$$S \left( \frac{\text{cm}^{-1}}{(\text{molecule cm}^{-2})} \right) = S \left( \frac{\text{cm}^{-1}}{\text{atm cm}} \right) \times \frac{\theta}{A} \times 82.06 \quad (17b)$$

The conversions of optical paths to  $\text{molecules/cm}^2$  are as follows:

$$1 (\text{atm cm}) \text{ STP} = 2.69 \times 10^{19} \text{ molecules cm}^{-2}$$

$$1 (\text{gm cm}^{-2}) \text{ of H}_2\text{O} = 3.34 \times 10^{22} \text{ molecules cm}^{-2} \quad .$$

It is hoped that these relations will be useful. They are summarized in Table 1 for convenience.

TABLE 1  
SUMMARY OF UNIT RELATIONSHIPS

U (atm cm) STP	x	$1.219 \times 10^{-2} \times \frac{M}{\theta}$	gm cm <sup>-2</sup>
U (gm/cm <sup>2</sup> )	x	$82.06 \times \frac{273}{M}$	(atm cm) STP
U (atm cm) STP	x	$2.689 \times 10^{19}$	molecules cm <sup>-2</sup>
U (gm/cm <sup>2</sup> ) H <sub>2</sub> O	x	$3.34 \times 10^{22}$	molecules cm <sup>-2</sup>
K(v)(atm cm) <sup>-1</sup> STP	x	$82.06 \frac{\theta}{M}$	(gm cm <sup>-2</sup> ) <sup>-1</sup>
K(v)(gm cm <sup>-2</sup> ) <sup>-1</sup>	x	$1.219 \times 10^{-2} \frac{M}{273}$	(atm cm) <sup>-1</sup> STP
K(v)(atm cm) <sup>-1</sup> STP	x	$3.72 \times 10^{-20}$	(molecules cm <sup>-2</sup> ) <sup>-1</sup>
K(v)(gm cm <sup>-2</sup> ) <sup>-1</sup>	x	$\frac{A}{M}$	(molecules cm <sup>-2</sup> ) <sup>-1</sup>
K(v)(atm cm) <sup>-1</sup> STP	x	$356.3 \frac{\theta}{M}$	db/(gm cm <sup>-2</sup> )
K(v)(atm cm) <sup>-1</sup> STP	x	4.343	db/(atm cm) STP
K(v)(gm cm <sup>-2</sup> ) <sup>-1</sup>	x	4.343	db/(gm cm <sup>-2</sup> )
$S\left(\frac{\text{cm}^{-1}}{\text{atm cm}}\right)$ STP	x	$82.06 \frac{\theta}{M}$	$\left(\frac{\text{cm}^{-1}}{\text{gm cm}^{-2}}\right)$
$s\left(\frac{\text{cm}^{-1}}{\text{gm cm}^{-2}}\right)$	x	$1.219 \times 10^{-2} \frac{M}{273}$	$\left(\frac{\text{cm}^{-1}}{\text{atm cm}}\right)$ STP
$S\left(\frac{\text{cm}^{-1}}{\text{atm cm}}\right)$ STP	x	$3.72 \times 10^{-20}$	$\left(\frac{\text{cm}^{-1}}{(\text{molecules cm}^{-2})}\right)$
$S\left(\frac{\text{cm}^{-1}}{\text{gm cm}^{-2}}\right)$	x	$\frac{M}{A}$	$\left(\frac{\text{cm}^{-1}}{(\text{molecules cm}^{-2})}\right)$

θ = temperature deg K,

M = molecular weight,

A = Avadadros number.