

# Ideal Gas Law and its Treatment in LBM

LatticeX

## 1 Introduction

People are often confused by the units of the ideal gas constant. This confusion is compounded by the fact that there are two forms of the gas constant: the universal gas constant and the specific gas constant. To avoid confusion and error, these are defined below, along with their relationships with mol and molecular weight. For completeness, numerical values are given in S.I. units.

### 1.1 Mol and Molecular Weight

- (1) A mol (sometimes gmol, g-mol, or mole, not to be confused with the rodent) denotes an amount of matter. Specifically one mol is  $6.0251 \times 10^{23}$  molecules of a substance, a standard number of molecules known as Avogadro's number. Strictly speaking, mol does not have dimensions of mass; rather, mol is a primary dimension in and of itself, i.e., the amount of matter. Note that some authors, however, treat mol as a unit of mass. The number of mols of a substance is denoted by the letter  $n$ .
- (2) Molecular weight ( $M$ ) is defined as the number of grams (g) per mol of a substance.  $M$  is obtained from standard periodic charts or periodic tables of the elements. For example, molar weight of water is 18 g/mol. One mole of  $H_2O$  is made up of 2 moles of Hydrogen atoms and 1 mole of Oxygen atom. Molecular weight of 1 mole of Hydrogen atoms is 1 g/mol; Molecular weight of 1 mole of Oxygen atoms is 16 g/mol. Thus, molecular weight of 1 mole of water = 2 g/mol + 16 g/mol = 18 g/mol. Another example, the molecular weight of nitrogen is  $M_{nitrogen} = 14.0067$  g/mol. Nitrogen in its gaseous or vapor state occurs as a diatomic molecule,  $N_2$ ; thus,  $M_{gaseous\_nitrogen} = 28.0134$  g/mol. Since air is made up predominantly of nitrogen gas, the molecular weight of air is very close to that of nitrogen,

$$M_{air} = 28.97 \text{ g/mol}$$

### 1.2 Ideal gas law<sup>[1]</sup>

The ideal gas law, also called the general gas equation, is the equation of state of a hypothetical ideal gas. It is a good approximation of the behavior of many gases under many conditions, although it has several limitations. The ideal gas law is often written as

$$PV = nRT$$

Where  $P$ ,  $V$  and  $T$  are the pressure, volume and absolute temperature;  $n$  is the number of moles of gas; and  $R$  is the ideal gas constant. It is the same for all gases. It can also be derived from the microscopic kinetic theory.

The state of an amount of gas is determined by its pressure, volume, and temperature. The modern form of the equation relates these simply in two main forms. The temperature used in the equation of state is an absolute temperature: the appropriate SI unit is the kelvin.

#### 1.2.1 Common forms

The most frequently introduced form is

$$PV = nRT = Nk_B T$$

where:

$P$  is the pressure of the gas,

$V$  is the volume of the gas,

$n$  is the amount of substance of gas (also known as number of moles),

$N$  is the number of gas molecules of gas (or the Avogadro constant times the amount of substance  $N_A n$ ), For  $n = 1$  mol,  $N$  is equal to the number of particles in one mole (Avogadro's number).

$R$  is the ideal, or universal, gas constant, equal to the product of the Boltzmann constant and the Avogadro constant,

$k_B$  is the Boltzmann constant, As part of the 2019 redefinition of SI base units, The Boltzmann constant is defined to be exactly  $1.380649 \times 10^{-23}$  J/K,

$T$  is the absolute temperature of the gas.

In SI units,  $P$  is measured in pascals,  $V$  is measured in cubic metres,  $n$  is measured in moles, and  $T$  in kelvins (the Kelvin scale is a shifted Celsius scale, where  $0.00 \text{ K} = -273.15 \text{ }^\circ\text{C}$ , the lowest possible temperature).  $R$  has the value  $8.3144621 \text{ J/(K}\cdot\text{mol)}$ .

### 1.2.2 Molar form

How much gas is present could be specified by giving the mass instead of the chemical amount of gas. Therefore, an alternative form of the ideal gas law may be useful. The chemical amount ( $n$ ) (in moles) is equal to total mass of the gas ( $m$ ) (in grams) divided by the molar mass ( $M$ ) (in grams per mole):

$$n = \frac{m}{M}$$

By replacing  $n$  with  $m/M$  and subsequently introducing density  $\rho = m/V$ , we get:

$$PV = \frac{m}{M} RT$$

$$P = \frac{m}{V} \frac{RT}{M}$$

$$P = \rho \frac{R}{M} T$$

Defining the specific gas constant  $R_{\text{specific}}$  as the ratio  $R/M$ ,

$$P = \rho R_{\text{specific}} T$$

This form of the ideal gas law is very useful because it links pressure, density, and temperature in a unique formula independent of the quantity of the considered gas.

It is common, especially in engineering and meteorological applications, to represent the specific gas constant by the symbol  $R$ . In such cases, the universal gas constant is usually given a different symbol such  $R^*$  to distinguish it. In any case, the context and/or units of the gas constant should make it clear as to whether the universal or specific gas constant is being referred to.

### 1.3 Calculations

The universal gas constant ( $R_u$ ) is, as its name implies, universal, i.e., the same regardless of the gas being considered. In SI units,

$$R_u = 8.3143 \frac{\text{J}}{\text{mol} \cdot \text{K}}$$

The specific gas constant ( $R$ , sometimes  $R_{\text{gas}}$ ) is not universal, and its value depends on the specific gas being considered.  $R$  is defined as the universal gas constant divided by the molecular weight of the substance,  $R = R_u/M$ . The dimensions of  $R$  are not the same as those of  $R_u$ , since molecular weight is not a dimensionless quantity, although some authors treat it as such. For air in S.I. units,

$$R_{air} = \frac{R_u}{M} = \frac{8.3143 \frac{J}{mol \cdot K}}{28.97 \frac{g}{mol}} = 287.0 \frac{J}{kg \cdot K} = 287.0 \frac{N \cdot m}{kg \cdot K} = 287.0 \frac{Pa \cdot m^3}{kg \cdot K}$$

The density of dry air can be calculated using the ideal gas law, expressed as a function of temperature and pressure<sup>[2]</sup>:

$$\rho = \frac{p}{R_{specific} T}$$

where:

$\rho$  = air density (kg/m<sup>3</sup>);

$p$  = absolute pressure (Pa);

$T$  = absolute temperature (K);

$R_{specific}$  = specific gas constant for dry air (J/(kg·K));

The specific gas constant for dry air is 287.058 J/(kg·K) in SI units. This quantity may vary slightly depending on the molecular composition of air at a particular location.

### 1.4 Sound speed in gases

The ideal gas law is based on a simple picture of a gas as a large number of molecules which move independently of one another, except for occasional collisions with each other or with the walls of their container. When they do collide, the collision occurs with no net loss of energy -- that is, it is an elastic collision. Thus, the ideal gas model predicts that the speed of sound in a pure gas will be [3][4]

$$v_{sound} = \sqrt{\frac{\gamma R T}{M}} = \sqrt{\frac{\gamma p}{\rho}}$$

Where,

$R$  = the universal gas constant = 8.314 J/mol K,

$T$  = the absolute temperature

$M$  = the molecular weight of the gas in kg/mol

$\gamma$  = the adiabatic constant, characteristic of the specific gas

For air, which is a mixture of molecules, you will need to use average values for the adiabatic constant and molecular mass. Air is mostly  $N_2$  and  $O_2$ , which are both simple diatomic molecules with almost the same masses. The adiabatic constant will be very close to 1.4 for both molecules for a wide range of temperatures near room temperature. Hence the adiabatic constant will also be close to 1.4 for air.

If we select  $\gamma = 1$  in lattice unit (here reference is needed):

$$v_{sound} = \sqrt{\gamma p / \rho}$$

We can obtain  $p = \frac{v_{sound}^2 \rho}{\gamma} = \frac{1}{3} \rho$ . Also in LBM, refer to [5], that  $p = c_s^2 \rho$ , and  $c_s = c/\sqrt{3}$  with  $c$  the lattice speed, thus  $c_s^2 = 1/3$ .

### Reference

- [1] [https://en.wikipedia.org/wiki/Ideal\\_gas\\_law](https://en.wikipedia.org/wiki/Ideal_gas_law)
- [2] [https://en.wikipedia.org/wiki/Density\\_of\\_air](https://en.wikipedia.org/wiki/Density_of_air)
- [3] <https://pages.mtu.edu/~suits/SpeedofSound.html>

[4] <http://hyperphysics.phy-astr.gsu.edu/hbase/Sound/souspe3.html>

[5] Anthony Ladd, R. Verberg, Lattice-Boltzmann simulations of particle-fluid suspensions. Journal of statistical physics, 2001, pp.1191-1251.