

Example:

Assuming that the following variables are known from a simulation run in ANSYS-CFX : $r_1, r_2, \rho_1, \rho_2, MW_1, MW_2, V_{\text{mix}} = 1\text{m}^3$ find the concentration at a measured point from a volume fraction contour plot.

The solution is as follows: The summation of the total volume fractions of the two species should sum up to 1.

$$r_1 + r_2 = 1$$

The mixture density can be calculated from the following:

$$\rho_{\text{mix}} = \rho_1 r_1 + \rho_2 r_2$$

Knowing that the volume fraction for species 1 is in reference to 1 m^3 volume.

$$r_1 = \frac{V_1}{V_{\text{mix}}} = V_1$$

The same applies for the volume fraction for species 2 is in reference to 1 m^3 volume.

$$r_2 = \frac{V_2}{V_{\text{mix}}} = V_2$$

We calculate the mass of species 1 is as follows:

$$m_1 = \rho_1 \cdot r_1$$

Mass of Species 2 is calculated using this:

$$m_2 = \rho_2 \cdot r_2$$

Leading to calculate the number of moles for species 1:

$$n_1 = \frac{m_1}{MW_1}$$

Leading to calculate the number of moles for species 2:

$$n_2 = \frac{m_2}{MW_2}$$

Calculating concentration for species 1

$$C_1 = \frac{n_1}{V_{\text{mix}}} = \frac{\rho_1 \cdot r_1}{MW_1}$$

Calculating concentration for species 2

$$C_2 = \frac{n_2}{V_{\text{mix}}} = \frac{\rho_2 \cdot r_2}{MW_2}$$

This tutorial was written by Ahmed Al Makky to answer the regular question of how to find the concentration of a gas species using known volume fractions.