Humidity Thermodynamic Library for OpenFOAM®

Implementation of a new thermodynamic library to account for humidity effects in buoyant driven flows

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The following document summarizes the basic equations for the humidity library developed by Tobias Holzmann.

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1 Introduction

In Heat-Ventilation-Air-Condition (HVAC) simulations it is sometimes important to take humidity effects into account. E.g., investigating into swimming pools inside buildings or mixing air streams with different humidity. Furthermore, it sometimes happens that the humidity influences the flow pattern as wet air is lighter compared to dry air. To account for such phenomenon, the humidity thermodynamic library was introduced. However, it is also possible to use already existing solvers while taking into account a multi-species approach such as reactingFoam without reactions. The approach used in the humidity thermodynamic library is mainly created for HVAC analysis and within temperature ranges from 0 degC to 100 degC.
The following document shows the main ideas and formulas that are implemented in the code.

2 Theory and Equations

The theory is simple. The thermodynamic library has to take into account the density change based on the humidity. For that purpose we need to track the specific humidity ξ (kg water / kg wet air) in our fluid domain. This is done by solving the transport equation for this quantity:

$$\frac{\partial \rho \xi}{\partial t} + \nabla \bullet (\rho \mathbf{U} \xi) = \nabla \bullet (\mu_{\text{eff}} \nabla \xi) + S_\xi \tag{1}$$

For a numerical simulation, one has to set the correct specific humidity. For the boundaries, special types are implemented to use more practical values such as the relative humidity.
To calculate the density of the wet air ρ_{wa}, one needs to calculate the following:

a. The saturation pressure of water vapor $p_{\text{sat,H}_2\text{O}}$

b. The partial pressure of the water vapor $p_{\text{p,H}_2\text{O}}$

Knowing the both above mentioned quantities, the specific humidity ξ, the actual pressure p and the temperature T, one can calculate the density of wet air and other quantities such as the relative humidity ϕ or the mass of water $m_{\text{H}_2\text{O}}$ which is inside the wet air.

2.1 Saturation Pressure of Water Vapor

The library includes two calculation options for estimating the saturation pressure of water vapor. Either the Magnus or the Buck formula is used to estimate the quantity. The Magnus formula, valid between -50 degC to 100 degC and 101325 Pa, is given as:

$$p_{\mathrm{s,H_2O}} = 611.2 \exp\left(\frac{17.62\theta}{243.12+\theta}\right) \tag{2}$$

θ is the temperature given in degree Celsius.
The Buck formula, valid between 0 degC and 100 degC and 101325 Pa – very accurate between 0 deg and 50 degC – is given as:

$$p_{\mathrm{s,H_2O}} = 611.21 \exp\left[\left(18.678 - \frac{\theta}{234.5}\right)\frac{\theta}{257.14+\theta}\right] \tag{3}$$

2.2 Partial Pressure of Water Vapor

Commonly, the partial pressure is simply calculated by knowing the relative humidity as:

$$\phi = \frac{p_{\mathrm{p,H_2O}}}{p_{\mathrm{s,H_2O}}} \tag{4}$$

However, we only know the specific humidity ξ and the saturation pressure $p_{\mathrm{s,H_2O}}$. Hence, we need to combine the following equations.
Specific humidity:

$$\xi = \frac{\rho_{\mathrm{H_2O}}}{\rho_{\mathrm{w.A.}}} = \frac{\rho_{\mathrm{H_2O}}}{\rho_{\mathrm{d.A.}} + \rho_{\mathrm{H_2O}}} \tag{5}$$

$\rho_{\mathrm{H_2O}}$ density of water vapor, $\rho_{\mathrm{w.A.}}$ density of wet air, $\rho_{\mathrm{d.A}}$ density of dry air.
Density water vapor:

$$\rho_{\mathrm{H_2O}} = \frac{p_{\mathrm{p,H_2O}}}{R_{\mathrm{H_2O}}T} \tag{6}$$

$R_{\mathrm{H_2O}} = 461.51$, specific gas constant of water (J/kg/K).
Density dry air:

$$\rho_{\mathrm{H_2O}} = \frac{p - p_{\mathrm{p,H_2O}}}{R_{\mathrm{d.A.}}T} \tag{7}$$

$R_{\mathrm{d.A.}} = 287.058$, specific gas constant of dry air (J/kg/K).

For simplification we define:

$$p_{\mathrm{p,H_2O}} = p_p$$

$$p_{\mathrm{s,H_2O}} = p_s$$

$$\rho_{\mathrm{H_2O}} = p_w$$

$$\rho_{\mathrm{d.A.}} = p_{dA}$$

$$\rho_{\mathrm{w.A.}} = p_{wA}$$

$$R_{\mathrm{H_2O}} = R_w$$

$$R_{\mathrm{d.A.}} = R_{dA}$$

It follows:

$$\xi = \frac{\rho_w}{\rho_{dA} + \rho_w} = \frac{\frac{p_p}{R_w T}}{\frac{p-p_p}{R_{dA}T} + \frac{p_p}{R_w T}} \tag{8}$$

$$\xi \frac{p - p_p}{R_{dA}T} + \xi \frac{p_p}{R_w T} = \frac{p_p}{R_w T} \tag{9}$$

$$\xi \frac{(p - p_p)(R_w T)}{R_{dA}T} + \xi p_p = p_p \tag{10}$$

$$\xi \frac{p R_w T}{R_{dA}T} - \xi \frac{p_p R_w T}{R_{dA}T} + \xi p_p = p_p \tag{11}$$

$$\xi \frac{p R_w T}{R_{dA}T} = \xi \frac{p_p R_w T}{R_{dA}T} - \xi p_p + p_p \tag{12}$$

$$\xi p R_w T = \xi p_p R_w T - \xi p_p R_{dA} T + p_p R_{dA} T \tag{13}$$

$$\xi p R_w T = p_p \left(\xi R_w T - \xi R_{dA} T + R_{dA} T\right) \tag{14}$$

$$p_p = \frac{\xi p R_w T}{\xi R_w T - \xi R_{dA} T + R_{dA} T} \tag{15}$$

$$p_p = \frac{\xi p R_w T}{\xi (R_w T - R_{dA} T) + R_{dA} T} \tag{16}$$

$$p_p = \frac{pR_wT}{R_wT - R_{dA}T + \frac{1}{\xi}R_{dA}T} \tag{17}$$

$$p_p = \frac{pR_wT}{R_wT - R_{dA}T(1 - \frac{1}{\xi})} \tag{18}$$

$$p_p = \frac{pR_wT}{R_wT\left[1 - \frac{R_{dA}T}{R_wT}(1 - \frac{1}{\xi})\right]} \tag{19}$$

$$p_p = \frac{p}{\left[1 - \frac{R_{dA}T}{R_wT}(1 - \frac{1}{\xi})\right]} \tag{20}$$

By using equation (20), we can calculate the partial pressure.