Humidity Thermodynamic Library for OpenFOAM®

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

Holzmann CFD

Dr. mont. Tobias Holzmann

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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 $p_{\text{sat},\text{H}_2\text{O}}$

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

c. The specific gas constant of wet air R_{wA}

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:

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

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:

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

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. By knowing that we can use the partial pressures to calculate species specific data, it follows for the 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 vapor (J/kg/K).
As the partial pressure of dry air is simple the total pressure minus the partial pressure of the water vapor, we can achieve the same equation for the density of dry air:

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

$R_{\mathrm{d.A.}} = 287.058$, 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

By using equation (20), we can calculate the partial pressure and after that the relative humidity inside the domain. The thermodynamic library will give a warning, if the relative humidity exceeds the value of 100 %.

2.3 Water Vapor Content of the Air

After we know the partical and saturation pressure in each cell, we further can calculate the actual water vapor content inside each cell and in addition the maximum water vapor content before condensation will occur. The latter one is used for stabilization.
Actual water vapor content (kg/m^3):

$$\rho_{\text{vap}} = \frac{p_p}{R_wT} \tag{21}$$

Maximum water vapor content (kg/m^3):

$$\rho_{\text{vap,max}} = \frac{p_s}{R_wT} \tag{22}$$

2.4 Stabilization

For stabilization purposes the maximum water vapor content is taken into account to calculate the maximum specific humidity value ξ_{max} while using equation (8) and replacing ρ_{w} by $\rho_{\text{vap,max}}$. It follows:

$$\xi_{\text{max}} = \frac{\rho_{\text{vap,max}}}{\rho_{dA} + \rho_{\text{vap,max}}} = \frac{1}{\frac{\rho_{\text{dA}}}{\rho_{\text{vap,max}}} + 1} = \left[\frac{\rho_{\text{dA}}}{\rho_{\text{vap,max}}} + 1\right]^{-1} \tag{23}$$

$$\xi_{\text{max}} = \left[\frac{p - p_p}{R_{dA}T}\frac{1}{\rho_{\text{vap,max}}} + 1\right]^{-1} \tag{24}$$

2.5 Density of wet air

At last, the density of wet air ρ_{wA} has to be calculated. Equation (5) or (8) is used here.

$$\rho_{dA} + \rho_w = \rho_{wA} \tag{25}$$

$$\xi = \frac{\rho_w}{\rho_{dA} + \rho_w} = \frac{\frac{p_p}{R_w T}}{\rho_{wA}} \tag{26}$$

$$\rho_{wA} = \frac{p_p}{R_w T \xi} \tag{27}$$

However, this formulation is not working for numerical simulations as we can have a specific humidity of zero. Hence, a division by zero. One could implement a condition by which the density of wet air is equal to the dry air if the specific humidity is zero (or almost close to it). However, as already mentioned this is not a good implementation. The best way is to calculate each term individually of equation (25). It follows:

$$\rho_{wA} = \frac{p - p_p}{R_{dA} T} + \frac{p_{\mathrm{p}}}{R_{\mathrm{H_2O}} T} = \frac{1}{T} \left(\frac{p - p_p}{R_{dA}} + \frac{p_{\mathrm{p}}}{R_{\mathrm{H_2O}}} \right) \tag{28}$$

2.6 Initialize the specific humidity field

The natural initialization for the numerical simulation is to provide the specific humidity in the whole numerical domain. However, it is common practice to use the relative humidity for initialization. Hence, the library first checks if the specific humidity field is given (`thermo:specificHumidity`). If this is not the case, the library checks if the user provides the relative humidity field (`thermo:relHum`).
If the relative humidity field is provided, we need to re-calculate the specific humidity based on the relative humidity data. Therefore, we first calculate the saturation pressure of water vapor as given in section 2.1 by using equation (2) or (3). It is now possible to evaluate the partial pressure of water vapor by using equation (4). Finally, we can use equation (20) to initialize the specific humidity field. The equation implemented in the library is given by:

$$\zeta = \left(1 - \left[1 - \frac{p}{p_p} \right] \frac{R_w}{R_d A} \right)^{-1} \tag{29}$$

and can be derived by reformulating equation (20).