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Non-Condensable Gases in RELAP-7

Joshua E Hansel, Matthias S Kunick, Ray A Berry, David Andrs

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1 Introduction

This report considers how the model PDEs in RELAP-7 can be amended to account for the presence of non-condensable gases (NCGs) in the flow system. Let the number of NCGs be denoted by N_{NCG}. The primary (and condensable) vapor, e.g., steam, will be referred to as the "primary vapor" and will have the subscript "$v, 0$", and the other constituents are assumed to be non-condensable and will be referred to as "NCGs" and will use the subscript "v, i", with $i = 1, \ldots, N_{\text{NCG}}$. Mixture quantities will use the subscript "v" (without any numeric index).

Before distinguishing between condensable and non-condensable gases, the mixture equations are derived generally; there the mixture components are just referred to as "species" and will just have a subscript "i" instead of the corresponding vapor subscript "v, i". The total number of species is denoted by N_{species}.

This report is organized as follows: Section 2 discusses mixture models, Section 3 discusses the governing equations for transport of the mixture species, and Section 4 gives the system of equations to be used for the inclusion of NCGs.

2 Mixture Models

State-of-the-art mixture models are formulated as functions of the dimensionless Helmholtz free energy

$$\phi(\delta, \tau, \psi) = \phi^{\mathrm{o}}(\delta, \tau, \psi) + \phi^{\mathrm{r}}(\delta, \tau, \psi)\,, \tag{1}$$

where the reducing parameters of the reduced density $\delta = \rho/\rho_c(\psi)$ and the inverse reduced temperature $\tau = T_c(\psi)/T$ are composition-dependent functions, ϕ^{o} is the ideal-gas part of the mixture, and ϕ^{r} is the residual part of the non-ideal mixture. The ideal and residual parts are commonly written as

$$\phi^{\mathrm{o}}(\rho, T, \psi) = \sum_{i=1}^{N_{\text{species}}} \psi_i[\phi^{\mathrm{o}}_{\mathrm{o}i}(\rho, T) + \ln \psi_i]\,, \tag{2}$$

$$\phi^{\mathrm{r}}(\delta, \tau, \psi) = \sum_{i=1}^{N_{\text{species}}} \psi_i \phi^{\mathrm{r}}_{\mathrm{o}i}(\delta, \tau) + \Delta\phi^{\mathrm{r}}(\delta, \tau, \psi)\,. \tag{3}$$

In Eqs. (2) and (3), the subscript o indicates the pure component equation of state, and $\Delta\phi^{\mathrm{r}}$ is the empirical departure function that describes the difference in the residual Helmholtz free energy of the mixture with regard to that obtained from the linear combination of the residual Helmholtz free energies of the pure components. The state-of-the-art mixture model requires the reduced Helmholtz free energies of the pure components along with continuous first, second, and third derivatives. The calculation of phase equilibria and inverse functions is especially computationally expensive, and convergence cannot be guaranteed. For these reasons, simplified mixture models are often used in extensive process simulations. The resulting inaccuracies in the calculated fluid properties must be accepted.

In this section, two different models, A and B, for the ideal mixing of non-ideal gases are discussed. These models will turn out to be equivalent for ideal-gas mixtures but lead to different results when applied to non-ideal gases. These differences, along with potential pitfalls and possible enhancements, are discussed.

2.1 Mixture Model A - Components Under Partial Pressures

For this model it is assumed that all of the N_{species} components are under their partial pressures p_i and possess the entire volume V of the mixture as illustrated in Figure 1.

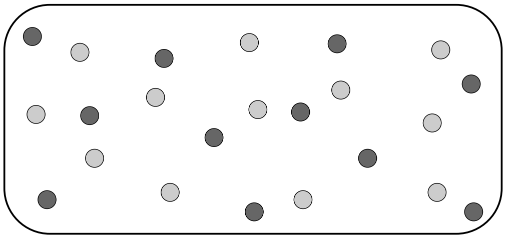

Figure 1. Illustration of model A – Components under partial pressures possess mixture volume

The partial pressures p_i are defined in terms of the molar fractions ψ_i as

$$p_i = \psi_i \, p \, , \tag{4}$$

where the molar fraction ψ_i is calculated from

$$\psi_i = \frac{n_i}{n} \, , \tag{5}$$

with

$$n = \sum_{i=1}^{N_{\text{species}}} n_i \, . \tag{6}$$

The symbol n refers to the amount of substance (number of moles). The mass fraction ξ_i of each component is defined as

$$\xi_i = \frac{m_i}{m} \, , \tag{7}$$

where the mass of the mixture m is

$$m = \sum_{i=1}^{N_{\text{species}}} m_i \, . \tag{8}$$

The molar mass M of the mixture is computed from

$$M = \sum_{i=1}^{N_{\text{species}}} \left(\psi_i M_i \right) \, , \tag{9}$$

or from

$$M = \frac{1}{\displaystyle\sum_{i=1}^{N_{\text{species}}} \frac{\xi_i}{M_i}} \, . \tag{10}$$

The mass fraction ξ_i can be obtained from the molar fraction using

$$\xi_i = \frac{M_i}{M}\,\psi_i\,. \tag{11}$$

2.1.1 Calculation of density

If the molar fraction equals the volume fraction, the density $\rho = m/V$ can be written as

$$\rho = \sum_{i=1}^{N_\text{species}} \frac{m_i}{V} = \sum_{i=1}^{N_\text{species}} \rho_i(p_i, T)\,. \tag{12}$$

Eq. (12) with the partial densities computed form partial pressures only holds for ideal gas mixtures, where

$$\rho = \sum_{i=1}^{N_\text{species}} \rho_i(p_i, T) = \sum_{i=1}^{N_\text{species}} \frac{p_i M_i}{\bar{R}T} = \frac{p}{\bar{R}T} \sum_{i=1}^{N_\text{species}} \psi_i M_i = \frac{pM}{\bar{R}T}\,. \tag{13}$$

Eqs. (4) and (13) are known as Dalton's law, which only applies to ideal-gas mixtures as shown in Section 2.4. For non-ideal components, Eq. (12) should not be used. The use of Eq. (15) is recommended instead.

2.1.2 Calculation of mass-specific properties

All mass-specific properties z, including specific volume, should be calculated from

$$z = \sum_{i=1}^{N_\text{species}} \frac{Z_i}{m} = \sum_{i=1}^{N_\text{species}} \frac{m_i z_i(p_i, T)}{m} = \sum_{i=1}^{N_\text{species}} \xi_i z_i(p_i, T)\,. \tag{14}$$

For specific volume, Eq. (14) yields

$$v = \sum_{i=1}^{N_\text{species}} \frac{V_i}{m} = \sum_{i=1}^{N_\text{species}} \frac{m_i v_i(p_i, T)}{m} = \sum_{i=1}^{N_\text{species}} \xi_i v_i(p_i, T)\,. \tag{15}$$

For the ideal-gas mixture, this is consistent with Eqs. (12) and (13) since

$$v = \sum_{i=1}^{N_\text{species}} \xi_i v_i(p_i, T) = \sum_{i=1}^{N_\text{species}} \xi_i \frac{\bar{R}, T}{p_i M_i} = \frac{\bar{R}, T}{pM}\,. \tag{16}$$

This equation is more suitable for ideal mixtures of real gases since thermodynamic consistency of the mass-specific properties can be assured. For the specific entropy it must be noted that the entropy of mixing is already included when using Eq. (14).

2.1.3 Calculation of transport properties

All transport properties z, such as dynamic viscosity and thermal conductivity, should be calculated from

$$z = \sum_{i=1}^{N_{\text{species}}} \psi_i z_i(p_i, T)\,. \tag{17}$$

The volume fraction is approximated with the molar fraction, and it is assumed that the transport properties of the mixture depend on that volume fraction and the pure component transport properties only.

2.2 Mixture Model B - Components Possess Partial Volumes

For this model it is assumed that all of the N_{species} components are under the pressure of the mixture p and reside in a fraction of the total volume as illustrated in Figure 2.

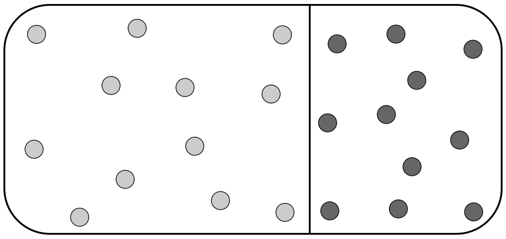

Figure 2. Illustration of model B – Components under pressure of the mixture possess partial volumes

The partial volumes V_i are defined using the molar fractions ψ_i as

$$V_i = \psi_i\, V\,, \tag{18}$$

where the molar fraction ψ_i is calculated from Eq. (5) or, for given mass fractions, from

$$\psi_i = \frac{M}{M_i}\xi_i \,, \tag{19}$$

with the molar mass M of the mixture computed from Eq. (10).

2.2.1 Calculation of density

The specific volume of the mixture is defined as

$$v(p,T) = \frac{V}{m} = \frac{\sum\limits_{i=1}^{N_\text{species}} m_i v_i(p,T)}{m} = \sum_{i=1}^{N_\text{species}} \xi_i v_i(p,T) \,. \tag{20}$$

The density is $\rho = 1/v$. It must be noted that the specific volume v of component i must not be confused with the partial specific volume, i.e., the inverse of the partial density in model A (see Eq. (12)). For model B, the partial volume of component i must be calculated from

$$v_i = \frac{v}{\xi_i} \,, \tag{21}$$

which is in agreement with the definition of the mass-fraction in Eq. (7).

2.2.2 Calculation of mass-specific properties

All mass-specific properties z, including specific volume, are calculated from

$$z(p,T) = \sum_{i=1}^{N_\text{species}} \frac{Z_i}{m} = \sum_{i=1}^{N_\text{species}} \frac{m_i z_i(p,T)}{m} = \sum_{i=1}^{N_\text{species}} \xi_i z_i(p,T) \,. \tag{22}$$

For the ideal-gas mixture, Eq. (20) is equal to Eq. (16) since

$$v(p,T) = \sum_{i=1}^{N_\text{species}} \xi_i v_i\,(p,T) = \sum_{i=1}^{N_\text{species}} \xi_i \frac{\bar{R}T}{pM_i} = \sum_{i=1}^{N_\text{species}} \psi_i \frac{\bar{R}T}{pM} = \frac{\bar{R}T}{pM} \,. \tag{23}$$

Eq. (22) assures thermodynamic consistency of the mass-specific properties for the ideal mixing of real gases. For the specific entropy s, the entropy of mixing must be added when using Eq. (22), so that

$$s(p,T) = \sum_{i=1}^{N_{\text{species}}} \xi_i s(p,T) - \sum_{i=1}^{N_{\text{species}}} \psi_i \, \ln \psi_i \,, \tag{24}$$

where R is the specific gas constant of the mixture $R = \bar{R}/M$, where $\bar{R}$ is the universal gas constant, which has a value of 8.3144598 J/(mol-K).

2.2.3 Calculation of transport properties

All transport properties z, such as dynamic viscosity and thermal conductivity, should be calculated from

$$z\,(p,T) = \sum_{i=1}^{N_{\text{species}}} \psi_i z_i(p,T)\,. \tag{25}$$

The volume fraction is approximated with the molar fraction and it is assumed that the transport properties of the mixture depend on that volume fraction and the pure component transport properties only.

2.2.4 Calculations from given specific volume and internal energy

The independent variables of the mixture model, pressure p and temperature T, are calculated by iteration from

$$\begin{bmatrix} p(v,e,\xi) \\ T(v,e,\xi) \end{bmatrix} = \begin{bmatrix} p \\ T \end{bmatrix} : \begin{cases} v = \sum_{i=1}^{N_{\text{species}}} \xi_i v_i(p,T) \\ e = \sum_{i=1}^{N_{\text{species}}} \xi_i e_i(p,T) \end{cases} . \tag{26}$$

2.3 Calculation of Heat Capacities and Speed of Sound from Thermodynamic Derivatives

For both models A and B, the heat capacities and speed of sound must be calculated according to their definitions from thermodynamic derivatives:

$$c_p = \left(\frac{\partial h}{\partial T}\right)_p , \tag{27}$$

$$c_v = \left(\frac{\partial e}{\partial T}\right)_v , \tag{28}$$

$$c = v\sqrt{-\left(\frac{\partial p}{\partial v}\right)_s} . \tag{29}$$

Since the independent parameters of the mixture model are p and T, the derivatives must be calculated from the following equations:

$$\left(\frac{\partial e}{\partial T}\right)_v = \left(\frac{\partial e}{\partial T}\right)_p - \left(\frac{\partial e}{\partial p}\right)_T \frac{\left(\frac{\partial v}{\partial T}\right)_p}{\left(\frac{\partial v}{\partial p}\right)_T} , \tag{30}$$

$$\left(\frac{\partial p}{\partial v}\right)_s = \left[\left(\frac{\partial v}{\partial p}\right)_T - \left(\frac{\partial v}{\partial T}\right)_p \frac{\left(\frac{\partial s}{\partial p}\right)_T}{\left(\frac{\partial s}{\partial T}\right)_p}\right]^{-1} . \tag{31}$$

2.4 Discussion

2.4.1 Equivalence of model A and B for ideal gases

For ideal gases, the mixture models A and B are equivalent. This can easily be derived from the ideal-gas equation

$$p = \rho\frac{\bar{R}T}{M} , \tag{32}$$

where $\bar{R}$ is the universal gas constant. According to Eq. (32), the partial density of component i as an ideal gas reads

$$\rho_i^A = \frac{m_i}{V} = p_i \frac{M_i}{\bar{R}T}\,, \tag{33}$$

for model A. Eq. (12), in conjunction with Eqs. (4) and (9), gives the density of the mixture:

$$\rho^A = \sum_{i=1}^{N_{\text{species}}} \left(p_i \frac{M_i}{\bar{R}T} \right) = \frac{\sum_{i=1}^{N_{\text{species}}} (p_i M_i)}{\bar{R}T} = \frac{p \sum_{i=1}^{N_{\text{species}}} (\psi_i M_i)}{\bar{R}T} = \frac{pM}{\bar{R}T}\,. \tag{34}$$

For model B, the (molecular) density of the ideal gas for component i is

$$\rho_i^B = \frac{m_i}{V_i} = \frac{m_i}{\psi_i V} = \frac{\rho_i^A}{\psi_i} = p \frac{M_i}{\bar{R}T}\,, \tag{35}$$

and, according to Eq. (20), the density of the mixture is

$$\rho^B = \frac{1}{\sum_{i=1}^{N_{\text{species}}} \left(\frac{\xi_i}{\rho_i\,(p,T)} \right)} = \frac{1}{\sum_{i=1}^{N_{\text{species}}} \xi_i \left(\frac{\bar{R}T}{pM_i} \right)} = \frac{1}{\frac{\bar{R}T}{p} \sum_{i=1}^{N_{\text{species}}} \left(\frac{\xi_i}{M_i} \right)}\,, \tag{36}$$

which finally gives

$$\rho^B = \frac{1}{\frac{\bar{R}T}{p} \sum_{i=1}^{N_{\text{species}}} \left(\frac{\psi_i}{M} \right)} = \frac{pM}{\bar{R}T}\,. \tag{37}$$

The equivalence of the models in terms of the resulting mixture density can be seen in Eqs. (34) and (37).

2.4.2 Inconsistency in model A for non-ideal gases

For real gases, the models A and B are not equivalent. It can be shown that model A implies an inconsistency when it is applied to real fluids. The pressure p as a function of density ρ and temperature T is calculated from a Helmholtz free energy explicit equation of state from

$$p = \rho \frac{\bar{R}}{M} T \left(1 + \delta\, \phi_\delta^{\mathrm{r}} \right)\,, \tag{38}$$

where $\delta = \rho/\rho_c$ is the reduced density, $\tau = T_c/T$ is the inverse reduced temperature, and $\phi = f/\left(\bar{R}T\right)$ is the dimensionless Helmholtz free energy. The superscript r denotes the residual part, the subscript δ denotes the first derivative with respect to the reduced density, and the subscript c denotes the critical point. For consistency, the definition of the mass fraction given in Eq. (7) must lead to Eq. (10). For a binary mixture with the components I and II, Eq. (7) can be rewritten as

$$\xi_{\mathrm{I}} = \frac{\rho_{\mathrm{I}}}{\rho} = \frac{\rho_{\mathrm{I}}}{\rho_{\mathrm{I}} + \rho_{\mathrm{II}}} \,. \tag{39}$$

For simplicity, Eq. (38) is rewritten for the partial density as a function of partial pressure and temperature

$$\rho_i = \frac{p_i M_i}{\bar{R}T} \frac{1}{\left(1 + \delta\, \phi^{\mathrm{r}}_{\delta}\right)} = \frac{p_i M_i}{\bar{R}T} X_i \,. \tag{40}$$

Inserting Eq. (40) in Eq. (39) gives

$$\xi_{\mathrm{I}} = \frac{p_{\mathrm{I}} M_{\mathrm{I}} X_{\mathrm{I}}}{p_{\mathrm{I}} M_{\mathrm{I}} X_{\mathrm{I}} + p_{\mathrm{II}} M_{\mathrm{II}} X_{\mathrm{II}}} \,. \tag{41}$$

Using Eq. (4) with Eq. (41) yields to

$$\xi_{\mathrm{I}} = \frac{\psi_{\mathrm{I}} M_{\mathrm{I}}}{\psi_{\mathrm{I}} M_{\mathrm{I}} + \psi_{\mathrm{II}} M_{\mathrm{II}} + \psi_{\mathrm{II}} M_{\mathrm{II}} \left(\dfrac{X_{\mathrm{II}}}{X_{\mathrm{I}}} - 1\right)} = \frac{\psi_{\mathrm{I}} M_{\mathrm{I}}}{M + \psi_{\mathrm{II}} M_{\mathrm{II}} \left(\dfrac{X_{\mathrm{II}}}{X_{\mathrm{I}}} - 1\right)} \,. \tag{42}$$

Eq. (42) only agrees with Eq. (7) if $X_{\mathrm{I}}/X_{\mathrm{II}} = 1$. This condition is only fulfilled for ideal gases. Similarly, only the density of ideal-gas mixtures can be calculated with Eq. (12). For non-ideal gases the definition of the partial pressures does not lead to volume fractions that are equal to the molar fractions.

For model A, the following relation is assumed:

$$V = m v\left(p, T, \boldsymbol{\psi}\right) = m_i v_i\left(p_i, T\right) \,. \tag{43}$$

It can be shown that Eq. (43) is always fulfilled for ideal-gas mixtures since

$$V = m \frac{\bar{R}T}{pM} = m_i \frac{\bar{R}T}{p_i M_i} \,. \tag{44}$$

is fulfilled with Eqs. (4), (7), and (11). For non-ideal gases this will not be the case.

Mixture model A is used by TRACE, where the components are considered to be ideal gases. For mixing non-ideal gases, model A is not fully consistent. Therefore, the application of this model is not planned for RELAP-7.

2.4.3 Potential pitfall of model B

The fluid properties of the individual components of model B are evaluated at the pressure of the mixture. For mixtures with condensable components, this restricts the applicability of model B to temperatures above the highest saturation temperature in the considered pressure domain. For example, humid air is a mixture of water vapor and non-condensable gases. At ambient conditions, the water vapor properties of the unsaturated humid air need to be calculated at conditions, where pure water would be liquid. In this case, the lowest temperature where model B is applicable would be $T_\mathrm{s}\left(p = 0.1\,\mathrm{MPa}\right) \approx 373$ K. An extrapolation into the metastable vapor phase would allow for a minimum temperature $T_\mathrm{min}\left(p = 0.1\,\mathrm{MPa}\right) \approx 326$ K at the vapor spinodal.

3 Species Equations

Assuming that each species can have its own velocity, the 1-D mass conservation equation for species i is as follows:

$$\frac{\partial \xi_i \rho}{\partial t} + \frac{\partial \xi_i \rho u_i}{\partial x} = S_i \, , \tag{45}$$

where S_i is the volumetric mass source of the species, if any.

Let the mixture velocity be defined as follows:

$$u \equiv \sum_{i=1}^{N_\text{species}} \xi_i u_i \, . \tag{46}$$

Summing Equation (45) over all species gives

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = \sum_{i=1}^{N_\text{species}} S_i \, , \tag{47}$$

which looks identical to the single-vapor mass conservation equation. However, it is undesirable to track velocities for each species, so now we attempt to eliminate u_i. First we define the diffusion velocity for each species:

$$\hat{u}_i \equiv u_i - u \, . \tag{48}$$

Inserting this definition into Equation (45) gives

$$\frac{\partial \xi_i \rho}{\partial t} + \frac{\partial \xi_i \rho (\hat{u}_i + u)}{\partial x} = S_i \, . \tag{49}$$

Defining a diffusive flux,

$$J_i \equiv \xi_i \rho \hat{u}_i \, , \tag{50}$$

this equation becomes

$$\frac{\partial \xi_i \rho}{\partial t} + \frac{\partial \xi_i \rho u}{\partial x} = S_i - \frac{\partial J_i}{\partial x} \, . \tag{51}$$

Note that at this point, no approximations have been made yet. Now we make the approximation; the diffusive flux is approximated using Fick's first law:

$$J_i \approx -\rho D_i \frac{\partial \xi_i}{\partial x} \, . \tag{52}$$

However, it is important to note that now, summing Equation (51) gives

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = \sum_{i=1}^{N_{\text{species}}} S_i - \sum_{i=1}^{N_{\text{species}}} \frac{\partial J_i}{\partial x}\,, \tag{53}$$

which is only equivalent to the single-vapor equations if the sum of the diffusive fluxes is zero:

$$\sum_{i=1}^{N_{\text{species}}} \frac{\partial J_i}{\partial x} = 0\,. \tag{54}$$

Taking the gradient of Equation (52) and using the partition-of-unity property of the mass fractions, one can see that one trivial solution for this condition is that all species have the same diffusion coefficient. Otherwise, if one assumes this condition is met and thus uses Equation (47), along with Equation (51) for all species excluding species i, then the following is required to ensure consistency:

$$\frac{\partial J_i}{\partial x} = -\sum_{j \neq i}^{N_{\text{species}}} \frac{\partial J_j}{\partial x}\,. \tag{55}$$

Bringing the sum inside the derivative on the right side and then integrating (which does make the condition more strict but is still useful for this analysis) gives the following definition for the diffusion coefficient for species i:

$$D_i = \frac{-\sum\limits_{j \neq i}^{N_{\text{species}}} D_j \frac{\partial \xi_j}{\partial x}}{\frac{\partial \xi_i}{\partial x}}\,. \tag{56}$$

Note that if the vapor mixture equation is used along with $N_{\text{species}} - 1$ species equations, with Equation (54) assumed to be satisfied, then one does not actually need to use Equation (56); it is used implicitly. For a binary mixture ($N_{\text{species}} = 2$), this simply reduces to $D_1 = D_2$.

4 Vapor Mixture Equations

Recall the vapor equations for the seven-equation model, *without any NCGs*:

$$\frac{\partial \alpha_v \rho_v A}{\partial t} + \frac{\partial \alpha_v \rho_v u_v A}{\partial x} = S_v A \,, \tag{57}$$

$$\frac{\partial \alpha_v \rho_v u_v A}{\partial t} + \frac{\partial \alpha_v (\rho_v u_v^2 + p_v) A}{\partial x} = p_{\text{int}} A \frac{\partial \alpha_v}{\partial x} + p_v \alpha_v \frac{\partial A}{\partial x} + F_v A \,, \tag{58}$$

$$\frac{\partial \alpha_v \rho_v E_v A}{\partial t} + \frac{\partial \alpha_v u_v (\rho_v E_v + p_v) A}{\partial x} = p_{\text{int}} u_{\text{int}} A \frac{\partial \alpha_v}{\partial x} + Q_v A \,, \tag{59}$$

where the source terms are the following:

$$S_v A \equiv S_v^{\text{int}} A + S_v^{\text{wall}} A \,, \tag{60}$$

$$S_v^{\text{int}} A \equiv \Gamma_{\ell \to v}^{\text{int}} a_{\text{int}} A \,, \tag{61}$$

$$S_v^{\text{wall}} A \equiv \Gamma_{\ell \to v}^{\text{wall}} P_{\text{hf}} \,, \tag{62}$$

$$\begin{aligned} F_v A \equiv \lambda (u_\ell - u_v) A - F_{\text{wall},v}^{\text{friction}} A - F_{\text{int},\ell \to v}^{\text{friction}} A \\ + \alpha_v \rho_v A g_x + \left(S_v^{\text{int}} + S_v^{\text{wall}} \right) u_{\text{int}} A \,, \end{aligned} \tag{63}$$

$$\begin{aligned} Q_v A \equiv \bar{p}_{\text{int}} \mu (p_\ell - p_v) A + \bar{u}_{\text{int}} \lambda (u_\ell - u_v) A \\ - F_{\text{wall},v}^{\text{friction}} u_v A - F_{\text{int},\ell \to v}^{\text{friction}} u_{\text{int}} A \\ + \alpha_v \rho_v u_v A g_x + Q_v^{\text{int}} a_{\text{int}} A + (q_v^{\text{wall}} + q_\ell^{\text{wall,boil}}) P_{\text{hf}} \\ + S_v^{\text{int}} \left(H_v^{\text{int}} - \frac{p_{\text{int}}}{\rho_{\text{int}}} \right) A + S_v^{\text{wall}} H_\ell A \,. \end{aligned} \tag{64}$$

Now the presence of NCGs is considered. Assuming that there is no volumetric source of non-condensable gases, i.e., $S_i = 0$ for $i = 1, \ldots, N_{\text{NCG}}$, the vapor mixture equation is simply the following:

$$\frac{\partial \alpha_v \rho_v A}{\partial t} + \frac{\partial \alpha_v \rho_v u_v A}{\partial x} = S_{v,0} A \,. \tag{65}$$

This equation replaces the single vapor equation, given by Equation (57). With the addition of the NCGs, there are N_{NCG} new unknowns in the system: $\xi_{v,i}$ for $i = 1, \ldots, N_{\text{NCG}}$

and thus N_{NCG} new equations are required. The associated equations will be the species equations for each NCG:

$$\frac{\partial \alpha_v \xi_{v,i} \rho_v A}{\partial t} + \frac{\partial \alpha_v \xi_{v,i} \rho_v u_v A}{\partial x} = -\frac{\partial J_{v,i}}{\partial x} \,, \tag{66}$$

where the diffusive flux is

$$J_{v,i} = -\alpha_v \rho_v D_{v,i} \frac{\partial \xi_{v,i}}{\partial x} A \,. \tag{67}$$

4.1 Spatial Discretization and Boundary Conditions

This section describes how Equation (66) is spatially discretized. Note that Equation (65) appears in the PDE system as well, but it looks the same as its no-NCG version, so it does not need discussion.

The time derivative, advection, and volumetric source terms of Equation (66) are discretized just as the corresponding terms in the vapor mixture mass equation, so the only term that needs to be discussed is the the new term, containing the diffusion flux. For the continuous Galerkin finite element, the term is integrated by parts:

$$\left(\frac{\partial J_{v,m}}{\partial x} \,, \varphi_i \right)_\Omega = -\left(J_{v,m} \,, \frac{\partial \varphi_i}{\partial x} \right)_\Omega + \langle J_{v,m} \,, \varphi_i n_x \rangle_\Gamma \,. \tag{68}$$

The boundary term is usually evaluated according to boundary conditions, but here an approximation is made to avoid these complications: the diffusive flux at the boundary is assumed to be zero. Thus,

$$\left(\frac{\partial J_{v,m}}{\partial x} \,, \varphi_i \right)_\Omega = -\left(J_{v,m} \,, \frac{\partial \varphi_i}{\partial x} \right)_\Omega \,. \tag{69}$$

Note that this is not an approximation for wall boundary conditions, only for inlets and outlets.

For finite volume discretization, the diffusion term is integrated over the volume, leading to the following:

$$\int\limits_{V_i} \frac{\partial J_{v,m}}{\partial x} \, \mathrm{d}V = J_{v,m,i+1/2} - J_{v,m,i-1/2} \,, \tag{70}$$

where again, the diffusive flux is assumed to be zero if it corresponds to a boundary edge.

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