Multispecies mass transport library

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The present library is based on *"Novaresio V., García-Camprubí M., Izquierdo S., Asinari P., Fueyo N., An Open-Source Library for the Numerical Modeling of Mass-Transfer in Solid-Oxide Fuel Cells, Computer Physics Communications, Elsevier B.V., pp. 22, 2011, Vol. 183, pag. 125-146, ISSN: 0010-4655, DOI: 10.1016/j.cpc.2011.08.003"*

The contribution of all authors was fundamental in order to develop the theoretical background of the library. In this release I have only rearranged the implementation with small modifications without adding relevant aspects. The paper above is published with a preliminary release of the library. The first version was already compatible with OpenFOAM standard releases. This new version improves the compatibility with OpenFOAM-1.6-ext and contains some bug fix. Dusty gas model (described on the paper) and complete Maxwell-Stefan model (that also considers pressure gradient) are not implemented yet. Moreover Maxwell-Stefan model implementation no longer follow the algorithm described in the paper but it is now coded using formulation 2.0.5.

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1 Chemical-species equation

The equation for the conservation of the chemical species α is:

$$\frac{\partial\left(\rho y_\alpha\right)}{\partial t}+\nabla\cdot\left(\rho y_\alpha\vec{v}\right)+\nabla\cdot\vec{j}_\alpha=S_{y_\alpha} \tag{1}$$

where ρ is the fluid density, $\vec{v}$ is the fluid mass average velocity, y_α is the mass fraction of species α, $\vec{j}_\alpha$ is the mass diffusion-flux of species α relative to the mass-average velocity $\vec{v}$, and S_{y_α} stands for the volumetric sources or sinks of the species α.

2 Diffusion-flux modeling

The binary diffusion coefficients for a couple of species is $\mathcal{D}_{\alpha\beta}$ [3]. For porous media we also define the Knudsen diffusion coefficient $\mathcal{D}_{K\alpha}$ [3.0.11] and the effective diffusion coefficients $\mathcal{D}_{\alpha m}^{eff}=\frac{\varepsilon}{\tau}\mathcal{D}_{\alpha m}$ and $\mathcal{D}_{K\alpha}^{eff}=\frac{\varepsilon}{\tau}\mathcal{D}_{K\alpha}$, where ε and τ are the porosity and the tortuosity factor of the porous medium.

2.0.1 Fick's model

The mass-diffusion flux in a multicomponent mixture is defined as:

$$\vec{j}_\alpha=-\rho\mathcal{D}_{\alpha m}\nabla y_\alpha \tag{2}$$

where $\mathcal{D}_{\alpha m}$ is given by:

$$\mathcal{D}_{\alpha m}=\frac{1-x_\alpha}{\sum_{\beta\neq\alpha}\left(\frac{x_\beta}{\mathcal{D}_{\alpha\beta}}\right)} \tag{3}$$

2.0.2 Fick's model (very diluted mixture)

The mass-diffusion flux in a multicomponent mixture is defined as:

$$\vec{j}_\alpha=-\rho\mathcal{D}_{\alpha m}\nabla y_\alpha \tag{4}$$

where $\mathcal{D}_{\alpha m}$ is the binary diffusion coefficient between species α and the carrier species (indicated by N index):

$$\mathcal{D}_{\alpha m}=\mathcal{D}_{\alpha N} \tag{5}$$

2.0.3 Model based on Schmidt number

The mass-diffusion flux in a multicomponent mixture is defined as:

$$\vec{j}_\alpha=-\rho\mathcal{D}_{\alpha m}\nabla y_\alpha \tag{6}$$

where $\rho\mathcal{D}_{\alpha m}$ is given by:

$$\rho\mathcal{D}_{\alpha m}=\frac{\mu}{Sc_\alpha} \tag{7}$$

and Sc_α is the Schmidt number for species α (constant for all species in this version of the code).

2.0.4 Model based on Lewis number

The mass-diffusion flux in a multicomponent mixture is defined as:

$$\vec{j_\alpha} = -\rho \mathcal{D}_{\alpha m} \nabla y_\alpha \tag{8}$$

where $\rho \mathcal{D}_{\alpha m}$ is given by:

$$\rho \mathcal{D}_{\alpha m} = \frac{\alpha}{Le_\alpha} \tag{9}$$

and Le_α is the Lewis number for species α (constant for all species in this version of the code).

2.0.5 Maxwell-Stefan's model

The Maxwell-Stefan relation between diffusive mass fluxes and molar fractions (neglecting the $\frac{\nabla T}{T}$ term) is defined as:

$$\nabla x_\alpha - (y_\alpha - x_\alpha)\frac{\nabla p}{p} = \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{N} \frac{x_\alpha x_\beta}{\mathcal{D}_{\alpha\beta}} \left(\frac{\vec{j_\beta}}{\rho} - \frac{\vec{j_\alpha}}{\rho} \right) \tag{10}$$

In this version of the code the term $(y_\alpha - x_\alpha)\frac{\nabla p}{p}$ is also neglected. After some mathematical manipulations it is possible to obtain an expression for the diffusive mass flux, $\vec{j_\alpha}$

$$\vec{j_\alpha} = -\sum_{\beta=1}^{N-1} \rho D_{\alpha\beta} \nabla y_\beta \tag{11}$$

where:

$$D_{\alpha\beta} = [D] = [A]^{-1}[B] \tag{12}$$

$$A_{\alpha\alpha} = -\left(\frac{x_\alpha}{\mathcal{D}_{\alpha N}} \frac{1}{W_N} + \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{N} \frac{x_\beta}{\mathcal{D}_{\alpha\beta}} \frac{1}{W_\alpha} \right) \tag{13}$$

$$A_{\alpha\beta} = x_\alpha \left(\frac{1}{\mathcal{D}_{\alpha\beta}} \frac{1}{W_\beta} - \frac{1}{\mathcal{D}_{\alpha N}} \frac{1}{W_N} \right) \tag{14}$$

$$B_{\alpha\alpha} = -\left(x_\alpha \frac{1}{W_N} + (1 - x_\alpha) \frac{1}{W_\alpha} \right) \tag{15}$$

$$B_{\alpha\beta} = x_\alpha \left(\frac{1}{W_\beta} - \frac{1}{W_N} \right) \tag{16}$$

and W_α is the molar weight of species α.

2.0.6 Bosanquet's model

The mass-diffusion flux in a multicomponent mixture is defined as:

$$\vec{j_\alpha} = -\rho \mathcal{D}_\alpha^{eff} \nabla y_\alpha \tag{17}$$

where $\mathcal{D}_\alpha^{eff}$ is given by:

$$\frac{1}{\mathcal{D}_\alpha^{eff}} = \frac{1 - \Upsilon x_\alpha}{\mathcal{D}_{\alpha m}^{eff}} + \frac{1}{\mathcal{D}_{K\alpha}^{eff}} \tag{18}$$

and where $\mathcal{D}_{\alpha m}$ is the same defined for Fick's model [2.0.1] (Υ is assumed to be zero in this version of the code):

3 Diffusion-coefficient modeling

3.0.7 Constant model

Binary diffusion coefficients don't depend by pressure and temperature

$$\mathcal{D}_{\alpha\beta} = const \tag{19}$$

3.0.8 Champan-Enskog model

Champan-Enskog correlation for binary diffusion coefficients (SI units except for collision diameters σ_α in angstroms) is given by:

$$\mathcal{D}_{\alpha\beta} = 10.1325 \frac{0.001858 T^{1.5} \left(W_{\alpha\beta}\right)^{-0.5}}{p \sigma_{\alpha\beta}^2 \Omega_D} \tag{20}$$

where:

$$\sigma_{\alpha\beta} = \frac{\sigma_\alpha + \sigma_\beta}{2}$$

$$W_{\alpha\beta} = \left(\frac{1}{W_\alpha} + \frac{1}{W_\beta}\right)^{-1}$$

$$\Omega_D = \frac{1.06036}{{T_N}^{0.15610}} + \frac{0.19300}{exp(0.47635 T_N)} + \frac{1.03587}{exp(1.52996 T_N)} + \frac{1.76474}{exp(3.89411 T_N)}$$

$$T_N = \frac{T}{E_{\alpha\beta}}$$

$$E_{\alpha\beta} = \varepsilon_{\alpha\beta}/k_B$$

$$\varepsilon_{\alpha\beta} = \left(\sqrt{\varepsilon_\alpha \varepsilon_\beta}\right)$$

Here k_B is the Boltzmannn constant and ε_α is the characteristic Lennard-Jones energy.

3.0.9 Wilke-Lee model

Wilke-Lee correlation for binary diffusion coefficients (SI units except for collision diameters σ_α in angstroms) is given by:

$$\mathcal{D}_{\alpha\beta} = 10.1325 \frac{\left(0.0027 - 0.0005 W_{\alpha\beta}^{-0.5}\right) T^{1.5} W_{\alpha\beta}^{-0.5}}{p \sigma_{\alpha\beta}^2 \Omega_D} \tag{21}$$

3.0.10 Fuller-Schettler-Giddings model

Fuller-Schettler-Giddings correlation for binary diffusion coefficients (SI units except for diffusion volumes $\sum v_\alpha$) is given by:

$$\mathcal{D}_{\alpha\beta} = 10.1325 \frac{0.001 T^{1.75} W_{\alpha\beta}^{-0.5}}{p \left[\left(\sum v\right)_\alpha^{1/3} + \left(\sum v\right)_\beta^{1/3} \right]^2} \tag{22}$$

3.0.11 Knudsen model

Knudsen diffusion coefficient (SI units) is defined from kinetic theory of gases as:

$$\mathcal{D}_{K_\alpha} = \frac{d_p}{3} \sqrt{\frac{8RT}{\pi\, W_\alpha}} \tag{23}$$

where d_p is the pore diameter expressed in m.

4 Sensible enthalpy equation

The sensible enthalpy equation for multispecies flow is defined as:

$$\frac{\partial (\rho h_s)}{\partial t} + \nabla \cdot (\rho h_s \vec{v}) - \nabla \cdot (\alpha \nabla h_s) + \nabla \cdot \left[\alpha \sum_{\alpha=1}^{N} (h_{s\alpha} \nabla y_\alpha) \right] + \nabla \cdot \left[\sum_{\alpha=1}^{N} \left(\vec{j}_\alpha h_{s\alpha} \right) \right] = S \tag{24}$$

In standard reactingFoam the term

$$\nabla \cdot \left[\alpha \sum_{\alpha=1}^{N} (h_{s\alpha} \nabla y_\alpha) \right] + \nabla \cdot \left[\sum_{\alpha=1}^{N} \left(\vec{j}_\alpha h_{s\alpha} \right) \right]$$

is neglected, or better, it vanishes supposing $Le = 1$ for all species. Using the multispecies transport library we can calculate this term coherently with the adopted diffusion-flux model.

5 modifiedReactingFoam solver

The standard reactingFoam needs only few changes in order to use the library:

- the definition of a multiSpeciesTransportModel object at the end of createFields.H;
- YEqn.H only contains the convectionScheme definition and the multiSpeciesTransportModel.correct(...) instruction to solve the species equations with the desired model;
- in hsEqn.H the missed terms are added into sensible enthalpy equation.