Summary of multicomponent diffusion model implementation in MFIX

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Summary

This document summarizes our chronological understanding and implementation of the multicomponent or multispecies diffusion model in MFIX CFD code during FY25. Derivation of this model is provided here for completeness. Several simple case studies were conducted in MFIX and discussed here as part the code verification process. One case was conducted using both MFIX and Fluent CFD codes for added confidence in the code implementation.

Derivation of species *i* diffusion molar flux j_i in a multicomponent system

The diffusion driving force in a multicomponent system is expressed by equation (2.1.15)[1]

$$\vec{d}_i = \vec{\nabla} X_i = -\sum_{j=1}^{n} \frac{X_i X_j}{\mathcal{D}_{ij}} \left(\vec{u}_i - \vec{u}_j\right) \qquad (1)$$

Dropping the vector notation and noting that: $j_i = c_i(u_i - u)$, let's express equation (1) in terms of mole fluxes *j* (capital *J* is the mass flux):

$$d_i = \sum_{j=1}^{n} \frac{X_i X_j}{\mathcal{D}_{ij}} \left(\frac{j_j}{cX_j} - \frac{j_i}{cX_i}\right)$$

$$cd_i = \sum_{j=1}^{n} \left(\frac{X_i j_j - X_j j_i}{\mathcal{D}_{ij}}\right) = \sum_{\substack{j=1 \\ j\neq i}}^{n} \left(\frac{X_i j_j}{\mathcal{D}_{ij}}\right) - \sum_{\substack{j=1 \\ j\neq i}}^{n} \left(\frac{X_j j_i}{\mathcal{D}_{ij}}\right)$$

Since MFIX solves for *n* chemical species, it is tempting to solve the above equation as: $cd_i = A_{ij} X_j$ with $A_{ij} = \sum_{\substack{j=1 \\ j\neq i}}^{n} \frac{X_i}{\mathcal{D}_{ij}}$ and $A_{ii} = -\sum_{\substack{j=1 \\ j\neq i}}^{n} \frac{X_j}{\mathcal{D}_{ij}}$. However, this matrix is singular as we can prove that $\left|A_{ij}\right| = 0$ (this was done for a 3x3 matrix).

All literature examined so far solves for a (n-1) multicomponent system as $j_n = -\sum_{k=1}^{(n-1)} j_k$, thus

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[1] Taylor, R., & Krishna, R. (1993). multicomponent mass transfer. New York: John Wiley & Sons, Inc.

$$cd_i = \sum_{\substack{j=1\\ j\neq i}}^{n-1}\left(\frac{X_i j_j}{\mathcal{D}_{ij}}\right) - \sum_{\substack{j=1\\ j\neq i}}^{n-1}\left(\frac{X_i j_j}{\mathcal{D}_{in}}\right) - \frac{X_i j_i}{\mathcal{D}_{in}} - \sum_{\substack{j=1\\ j\neq i}}^{n}\left(\frac{X_j j_i}{\mathcal{D}_{ij}}\right)$$

$$= -\sum_{\substack{j=1\\ j\neq i}}^{n-1}\left(\frac{X_i}{\mathcal{D}_{in}} - \frac{X_i}{\mathcal{D}_{ij}}\right) j_j - \left(\frac{X_i}{\mathcal{D}_{in}} + \sum_{\substack{j=1\\ j\neq i}}^{n}\left(\frac{X_j}{\mathcal{D}_{ij}}\right)\right) j_i$$

$$cd_i = -A_{ii} j_i - \sum_{\substack{j=1\\ j\neq i}}^{n-1} A_{ij} j_j$$

$A_{ii} = \frac{X_i}{\mathcal{D}_{in}} + \sum_{\substack{j=1\\ j\neq i}}^{n}\left(\frac{X_j}{\mathcal{D}_{ij}}\right)$; $A_{ij} = -X_i\left(\frac{1}{\mathcal{D}_{ij}} - \frac{1}{\mathcal{D}_{in}}\right)$

The above derivation ended up with the exact same equations (2.1.20 – 2.1.22) in the textbook[1] with the matrix notation $A = B$. The above shows the ease of deriving a multicomponent diffusion model with molar concentration fractions X_i. However, we must use mass fractions Y_i per our CFD code (and others) approach.

Derivation of species *i* diffusion mass flux *J*$_i$ in a multicomponent system

$\vec{d}_i = -\sum_{j=1}^{n} X_i X_j \left(\frac{\vec{u}_i - \vec{u}_j}{\mathcal{D}_{ij}}\right)$ (1) Corresponding to equation (2.1.15) [1]. Dropping the vector notation and noting that $J_i = \rho_i(u_i - v)$ yields:

$$d_i = -\sum_{j=1}^{n} \frac{X_i X_j}{\mathcal{D}_{ij}}\left(\frac{J_i}{\rho_i} - \frac{J_j}{\rho_j}\right)$$

$d_i = \nabla X_i = \sum_{j=1}^{n} \frac{X_i X_j}{\mathcal{D}_{ij}}\left(\frac{J_j}{\rho_j} - \frac{J_i}{\rho_i}\right)$ (2) corresponding to equation (8.9.6) (Fluent 12.0 Manual)

Let's modify equation (2) while noting that $\rho_i = \rho Y_i = \frac{\rho M_i}{M} X_i$

$$-d_i = \sum_{j=1}^{n} \frac{M X_i X_j}{\rho \mathcal{D}_{ij}}\left(\frac{J_i}{M_i X_i} - \frac{J_j}{M_j X_j}\right)$$

$$-\rho d_i = -\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{M}{\mathcal{D}_{ij}} \frac{X_i}{M_j} J_j + \sum_{\substack{j=1\\ j\neq i}}^{n} \frac{M}{\mathcal{D}_{ij}} \frac{X_j}{M_i} J_i$$

Since MFIX solves for *n* chemical species, it is tempting to solve the above equation as: $-\rho d_i = A_{ij}J_j$ with $A_{ij} = \frac{M}{\mathcal{D}_{ij}}\frac{X_i}{M_j}$ and $A_{ii} = -\sum_{\substack{j=1 \\ j\neq i}}^{n}\frac{M}{\mathcal{D}_{ij}}\frac{X_j}{M_i}$. However, this matrix is also singular as we can show that $|A_{ij}| = 0$.

Since we solve for (n-1) species, then:

$$-\rho d_i = -\sum_{\substack{j=1 \\ j\neq i}}^{n-1}\frac{M}{\mathcal{D}_{ij}}\frac{X_i}{M_j}J_j - \frac{M}{\mathcal{D}_{in}}\frac{X_i}{M_n}J_n + \sum_{\substack{j=1 \\ j\neq i}}^{n}\frac{M}{\mathcal{D}_{ij}}\frac{X_j}{M_i}\,J_i$$

Since $J_n = -\sum_{j=1}^{n-1}J_j = -\sum_{\substack{j=1 \\ j\neq i}}^{n-1}J_j - J_i$

$$-\rho d_i = \sum_{\substack{j=1 \\ j\neq i}}^{n-1}\left(\frac{M}{\mathcal{D}_{in}}\frac{X_i}{M_n} - \frac{M}{\mathcal{D}_{ij}}\frac{X_i}{M_j}\right)J_j + \left(\frac{M}{\mathcal{D}_{in}}\frac{X_i}{M_n} + \sum_{\substack{j=1 \\ j\neq i}}^{n}\frac{M}{\mathcal{D}_{ij}}\frac{X_j}{M_i}\right)J_i$$

Simplifying the above equation to read:

$$-\rho d_i = A_{ij}J_j + A_{ii}\,J_i$$

$$A_{ii} = \frac{M}{\mathcal{D}_{in}}\frac{X_i}{M_n} + \sum_{\substack{j=1 \\ j\neq i}}^{n}\frac{M}{\mathcal{D}_{ij}}\frac{X_j}{M_i}$$

$$A_{ij} = \frac{M}{\mathcal{D}_{in}}\frac{X_i}{M_n} - \frac{M}{\mathcal{D}_{ij}}\frac{X_i}{M_j}$$

Note that the same equations are given in the Fluent manual as equations (8.9-9 and 8.9-10):

$$A_{ii} = -\left(\frac{M}{\mathcal{D}_{in}}\frac{X_i}{M_n} + \sum_{\substack{j=1 \\ j\neq i}}^{n}\frac{M}{\mathcal{D}_{ij}}\frac{X_j}{M_i}\right)$$

$$A_{ij} = X_i\left(\frac{1}{\mathcal{D}_{ij}}\frac{M}{M_j} - \frac{1}{\mathcal{D}_{in}}\frac{M}{M_n}\right)$$

The overall negative sign in above equations could be just propagated from another B matrix used in Fluent, which has to do with the transformation of gradient ∇X_i to ∇Y_i to do next.

Let's now shift attention to the LHS of equation (1) and noting that $d_i = \nabla X_i$. The relation between mole fraction X_i and mass fraction Y_i is simply: $X_i = \frac{M}{M_i} Y_i$, with $\frac{1}{M} = \sum_{j=1}^{n} \frac{Y_j}{M_j}$. Thus:

$$\nabla Y_i = \frac{M_i}{M} \nabla X_i + M_i X_i \sum_{j=1}^{n} \frac{\nabla Y_j}{M_j}$$

$$\mathrm{d}_i = \nabla X_i = \frac{M}{M_i} \nabla Y_i - M X_i \sum_{j=1}^{n} \frac{\nabla Y_j}{M_j}$$

$$-\nabla X_i = -\left(\frac{M}{M_i}(1 - X) + \frac{M X_i}{M_n}\right) \nabla Y_i - \sum_{\substack{j=1 \\ j \neq i}}^{n-1} \left(\frac{M X_i}{M_n} - \frac{M X_i}{M_j}\right) \nabla Y_j$$

Using Fluent notation, we can write above equation as: $-\nabla X = -B\ \nabla Y$

$$i \neq j \quad B_{ij} = X_i \left(\frac{M}{M_n} - \frac{M}{M_j}\right)$$

$$i = j \quad B_{ij} = \frac{M}{M_i}(1 - X) + \frac{M X_i}{M_n}$$

Here again, there is a sign difference between the B matrices derived here and in Fluent. Thus, this sign will cancel in the following expression written in matrix notation:

$-\rho \nabla X = -\rho B \nabla Y = AJ$. And the diffusive mass flux J is obtained simply as: $J = -\rho A^{-1} B \nabla Y = -\rho D \nabla Y$, or by using index notation: $J_i = -\sum_{j=1}^{n-1} \rho D_{ij}\ \nabla Y_j$, where D_{ij} are the Fickian diffusion coefficients. The mass diffusion flux contributes to the species mass fraction conservation equation as: $\frac{\partial \rho Y_i}{\partial t} + \nabla . \rho \vec{v} Y_i = -\nabla . \vec{J}_i + R_i$.

Comparison of computed Fickian diffusion coefficients with published data

Let's compare our computed Fickian diffusion coefficient D_{ij} (not to be confused with molecular or Maxwell-Stefan coefficients $\mathcal{D}_{ij}$) obtained for a multicomponent diffusion case in Example 4.2.5 on Page 86 of Taylor and Krishna textbook. It involves diffusion of CO (1), H2 (2), CH4 (3), and H2O (4) at the molar concentrations of $x_1 = 0.05$, $x_2 = 0.75328$, $x_3 = 0.09809$, $x_4 = 0.09809$. The Maxwell-Stefan coefficients were taken from the textbook and not computed from kinetic theory of low-density gases. This was done for accurate comparison between the two methods.

Taylor and Krishna obtained the following results:

$$D_{ij} = \begin{bmatrix} 8.3828 & -1.4960 & 0.0469 \\ 0.4612 & 13.5835 & -0.1589 \\ -0.1531 & -1.6809 & 8.5718 \end{bmatrix} \times 10^{-6}\, m^2/s$$

We computed the following in MFIX: $D_{ij} = \begin{bmatrix} 8.3829 & -1.4960 & 0.04695 \\ 0.4612 & 13.5835 & -0.1589 \\ -0.1531 & -1.6809 & 8.5718 \end{bmatrix} \times 10^{-6}\, m^2/s$

The dominance of the diagonal terms is evident but is not always the case as seen in other examples in the textbook. The agreement is almost exact which was expected. The molecular mass of the diffusing elements and the transformation from mole fraction to mass fraction was verified to be almost identical.

Model implementation in MFIX, a ternary diffusion test case in a Loschmidt tube

The ternary: CH4 (1) – Ar (2)– H2 (3) diffusion system is shown in the figure below and consists of a closed tube divided into two regions, top and bottom, where the initial concentrations are set differently as shown in the figure. Initially, the separation between these two regions is removed and species diffuse freely at isothermal condition. The purpose of this exercise is to compute the transient space-averaged concentration of species in the upper and lower parts of the Loschmidt tube. Note that the domain is wall-bounded and essentially 1D.

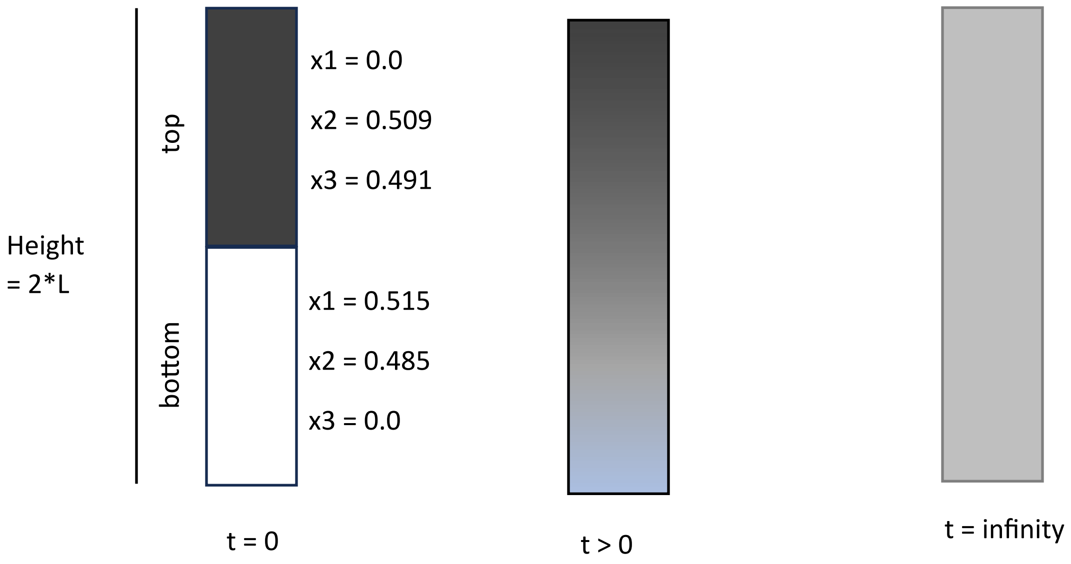

Figure: Ternary diffusion example taken from Taylor and Krishna (example 5.5.1 page 112-114).

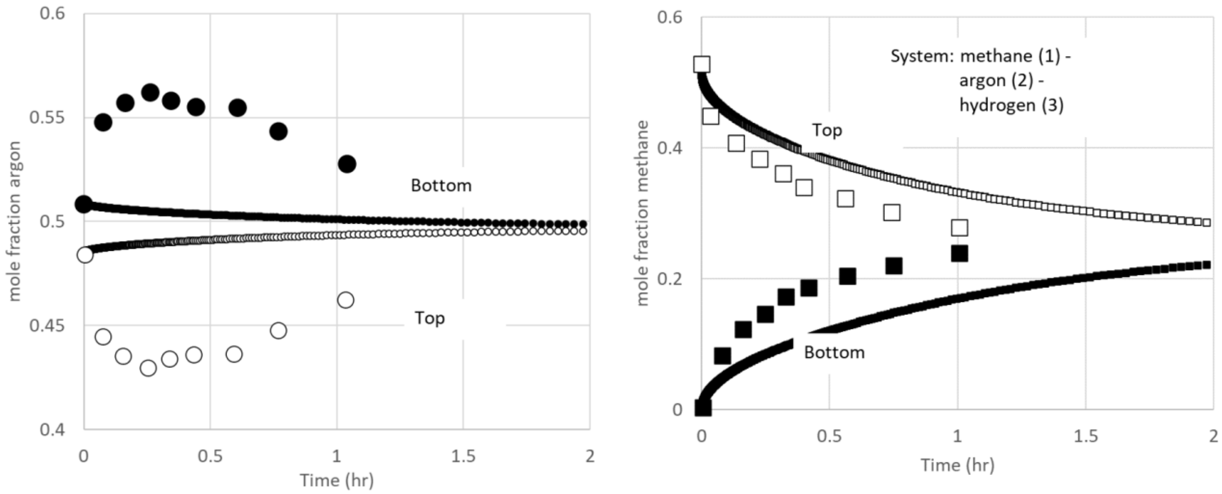

Figure: Results obtained with the dilute mixture approximation in MFIX.

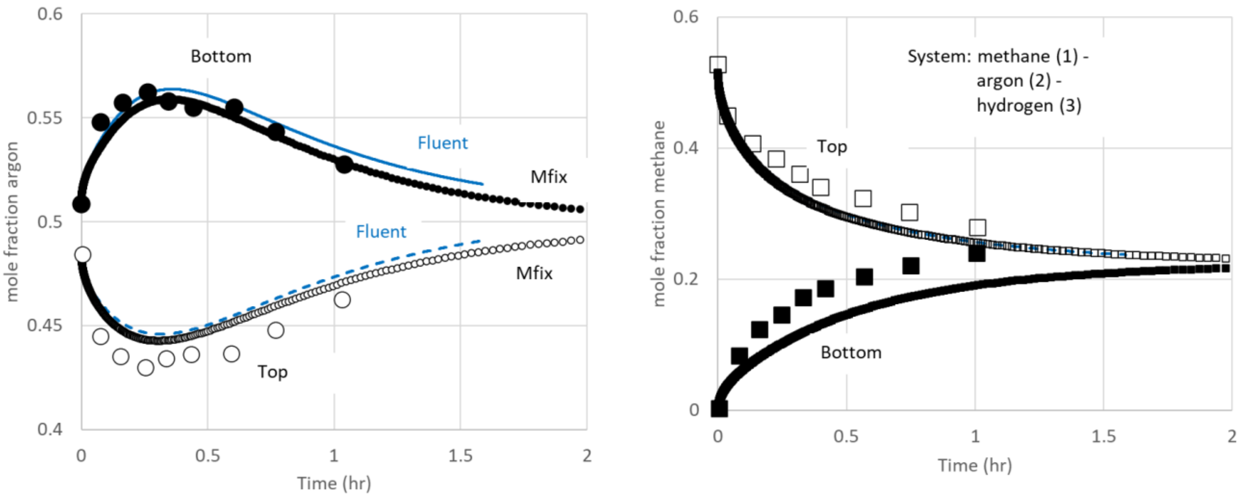

Figure: Results obtained with the new multicomponent diffusion model.

The above figure shows a comparison of MFIX computation results with those obtained using Fluent[2] and experimental data. For the mole fraction of methane profiles, the results obtained with MFIX and Fluent are almost identical and can't be noticed from the graph. Slightly more noticeable difference between the two software can be seen for the mole fraction profiles of Argon. It is interesting that an analytical solution obtained by Taylor and Krishna shows better agreement with measurements.

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[2] Thanks to Hossain Aziz for running the Fluent simulation at NETL.

Implementation of Maxwell-Stefan diffusion coefficients from kinetic theory

A kinetic theory model for low density gases is available in the literature[3] and was implemented in MFIX. It only requires the assumption of the validity of the well-known Lennard-Jones potential between two species *i, j*: $\varphi(r) = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$. An approximation for ideal gas provides the following formula for calculating the diffusivity:

$$\mathcal{D}_{ij} = 0.0018583\sqrt{T^3\left(\frac{1}{M_i} + \frac{1}{M_j}\right)}\frac{1}{P\sigma_{ij}\Omega_{D,ij}}$$

With $\mathcal{D}_{ij}$ expressed in (cm^2/s), and T (K), P (atm), σ_{ij} (Å). The potential pair parameters ϵ_{ij} and σ_{ij} could be obtained from individual parameters following: $\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)$, $\epsilon_{ij} = \sqrt{\epsilon_i \times \epsilon_j}$. The individual potential parameters are available for many molecules in the literature[2].

Finally, the collision integral can be expressed following a curve fitting of data in equation E.2-2 of BSL textbook: $\Omega_{D,ij} = \frac{1.06036}{T^{*0.15610}} + \frac{0.19300}{exp(0.47635T^*)} + \frac{1.03587}{exp(1.52996T^*)} + \frac{1.76474}{exp(3.89411T^*)}$

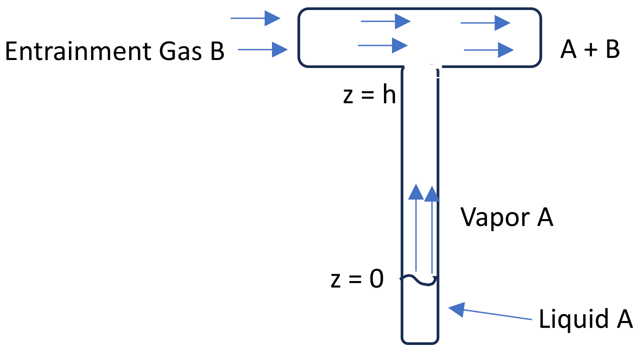
The results obtained with this formula for $\mathcal{D}_{ij}$ were compared with a similar formula obtained online[4] with very good agreement. For example, at normal conditions of 1 atm and 273 K:

$\mathcal{D}_{O_2-H_2}$= 69.1e-6 and 68.9e-6 m^2/s; $\mathcal{D}_{O_2-CO}$= 17.52e-6 and 17.47e-6 m^2/s were obtained with MFIX and online[5], respectively.

Another example at higher pressure and temperature conditions of 2 atm and 310 K:

$\mathcal{D}_{O_2-H_2}$= 42.98e-6 and 42.88e-6 m^2/s; $\mathcal{D}_{O_2-CO}$= 10.97e-6 and 11.00e-6 m^2/s were also obtained with MFIX and the reference [3], respectively.

Binary and ternary gas diffusion in a Stefan tube



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[3] R. Byron Bird, Warren E. Stewart, Edwin N. Lightfoot (aka **BSL**). Transport Phenomena-2nd ed., Wiley, NY (2002).
[4] https://demonstrations.wolfram.com/BinaryDiffusionCoefficientsForGases
[5] See online reference above.

We first derive an analytical solution for the case of binary diffusion in a Stefan tube shown below, then we compare the results obtained with this method and MFIX numerical simulation.

Assumptions for analytical solution: Steady-Flow; 1D in the z-direction; at z = 0, $y_A = y_A^0$ equilibrium at liquid-vapor interface; at z = h, $y_A = y_A^h = 0$.

For a binary system, Fick's law for diffusion can be written as: $J_A = -\rho \mathcal{D}_{AB} \frac{\partial Y_A}{\partial z}$, which can also be obtained from the multicomponent diffusion model developed previously and starting with: $-\rho \frac{\partial X_A}{\partial z} = -\frac{M}{\mathcal{D}_{AB}} \frac{X_A}{M_B} J_B + \frac{M}{\mathcal{D}_{AB}} \frac{X_B}{M_A} J_A$, and while recognizing that $J_B = -J_A$, we obtain after little manipulation: $-\rho \mathcal{D}_{AB} \frac{\partial X_A}{\partial z} = M \left(\frac{X_A}{M_B} + \frac{1 - X_A}{M_A} \right) J_A$.

From previous analysis, we showed that: $\frac{\partial Y_A}{\partial z} = \frac{M_A}{M} \frac{\partial X_A}{\partial z} + M_A X_A \left(\frac{\partial Y_A}{M_A \partial z} + \frac{\partial Y_B}{M_B \partial z} \right)$, and after some algebraic manipulation we obtain: $\frac{\partial X_A}{\partial z} = \frac{M}{M_A M_B} (M_B(1 - X_A) + M_A X_A) \frac{\partial Y_A}{\partial z}$

Therefore, we obtain the well-known Fick's law: $-\rho \mathcal{D}_{AB} \frac{\partial Y_A}{\partial z} = J_A$. So we just demonstrated that the multicomponent diffusion model reduces to Fick's law for a binary system. Furthermore, the code implementation of the same multicomponent model works for binary mixture by reducing to Fick's law with zero off-diagonal fluxes, and so no special treatment is done for the binary mixture case. An analytical solution for the diffusion in Stefan tube can be obtained by combining the previously derived Fick's law while also considering the species mass fraction conservation equation: $\frac{\partial \rho v Y_A}{\partial z} = -\frac{\partial J_A}{\partial z}$. The gas velocity is deduced from the steady gas continuity equation: $\frac{\partial \rho v}{\partial z} = \rho \frac{\partial v}{\partial z} = 0$ for constant gas density. Thus, the gas velocity is a constant: $v = v_0$. We can eliminate the flux to obtain: $\frac{\partial^2 Y_A}{\partial z^2} = \frac{v_0}{\mathcal{D}_{AB}} \frac{\partial Y_A}{\partial z}$. By a change of variable assuming $\xi = \frac{\partial Y_A}{\partial z^*}$, $z = hz^*$, and $\alpha = \frac{v_0 h}{\mathcal{D}_{AB}}$ and then we obtain a solution for: $\xi = k e^{\alpha z^*}$ and a final solution for mass fraction as: $Y_A = \frac{{Y_A}^0}{1 - e^{\alpha}} \left(e^{\alpha z^*} - e^{\alpha} \right)$, which was subjected to boundary conditions already mentioned. A similar analytical solution was derived for molar fractions and fluxes and is available online[6]. Note that this solution is for $\alpha \neq 0$. For $\alpha = 0$ (no convection), the solution for Y_A is a linear function of z derived from $\frac{\partial^2 Y_A}{\partial z^2} = 0$.

To set-up this case in MFIX, an inlet condition with concentration ${Y_A}^0$ and velocity v_0 subjected to the dimensionless number $\alpha = 5$ was used ($\mathcal{D}_{AB}$=1e-5 m^2/s, h= 0.24 m, v_0 = 2.08e-4 m/s). An extra pressure drop (Darcy's law) was added at the top of the Stefan tube to avoid gas B entering the tube (semipermeable surfaces block species diffusion and were avoided). The MFIX simulation results are shown below and compare reasonably well with the analytical solution. The reason for using a large value for α (convection dominant) is

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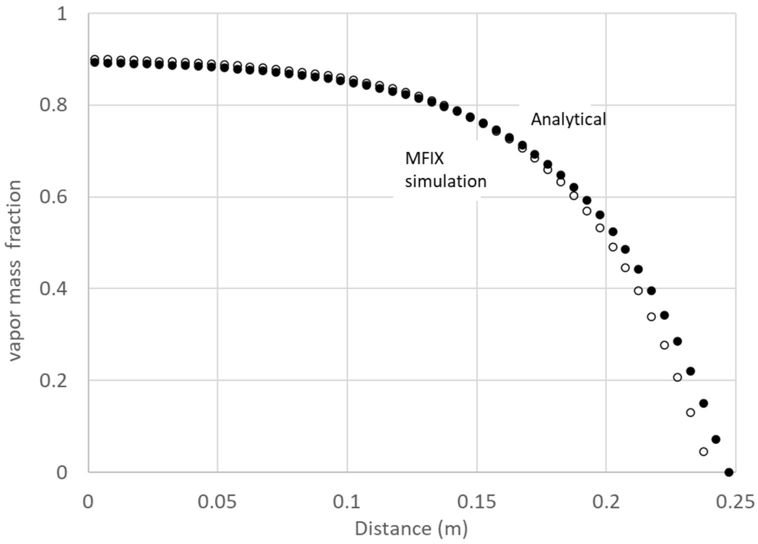
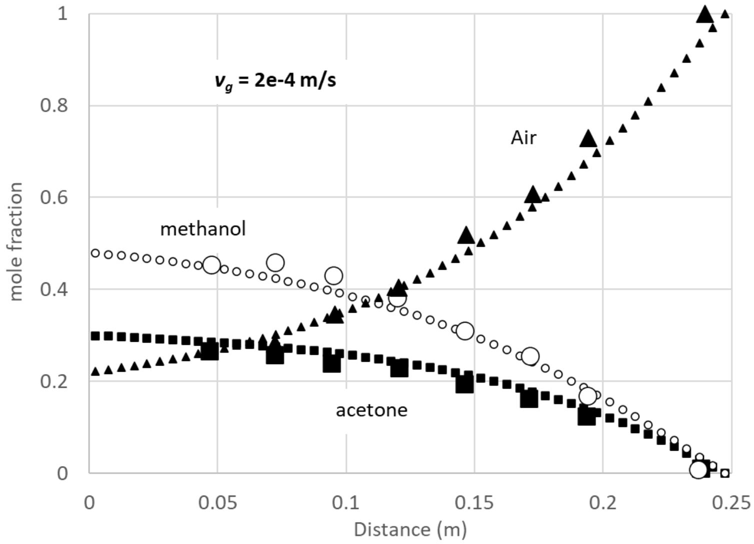
[6] https://www3.nd.edu/~dtl/cbe30356/notes/l17/lecture17.pdf

the absence of diffusion at inlets in MFIX. A constant gas density (the value is not important as it cancels out) was set in MFIX to mimic the analytical derivation.

Stefan tube for a ternary system of acetone (1), methanol (2), and air (3) was conducted experimentally and described in example 2.1.1 on page 21 of Taylor and Krishna textbook. We use the same approach as in the binary system described above. The vapor mixture of acetone and methanol was fed at the bottom inlet at a guessed gas velocity of 2e-4 m/s (the rate of evaporation and v_0 are not known) that provided good agreement with experimental data found in the graph below.



Analytical solution compared with simulation results for binary species diffusion in Stefan tube.



MFIX simulation results compared with experimental data for ternary diffusion in a Stefan tube.

Implementation of thermal diffusion flux in MFIX

The numerical implementation of the thermal diffusion flux is straightforward due to the already implemented multicomponent diffusion flux. The generalized flux that includes thermal diffusion can be obtained by slightly modifying the multicomponent flux as:

$$J_i = -\sum_{j=1}^{n-1} \rho D_{ij} \nabla Y_j - D_{T,i} \frac{\nabla \mathrm{T}}{T}$$

An expression for the thermal diffusion provided in the Fluent 13 manual and mentioned in the literature[7] as an approximation of this coefficient:

$$D_{T,i} = -2.59 \times 10^{-7} T^{0.659} \left(\frac{M_i^{0.511} X_i}{\sum_{j=1}^{n} M_j^{0.511} X_j} - Y_i \right) \left(\frac{\sum_{j=1}^{n} M_j^{0.511} X_j}{\sum_{j=1}^{n} M_j^{0.489} X_j} \right)$$

This form of the thermal diffusion was tested for a diffusion tube with a binary mixture of Air-Acetone, initially fully mixed with a mass fraction $Y_{Acetone} = Y_{Air} = 0.5$ subject to a constant temperature difference of 1000 K between a cold and hot wall. The initial uniform concentration of species does not change if we ignore the contribution of thermal diffusion. However, accounting for the thermal diffusion creates a species mass fraction gradient with larger concentration of the heavy species (Acetone) at the cold wall. For this case, the Acetone-Air diffusion coefficient was calculated from kinetic theory model described earlier with Lennard-Jones parameters determined from viscosity data[8].

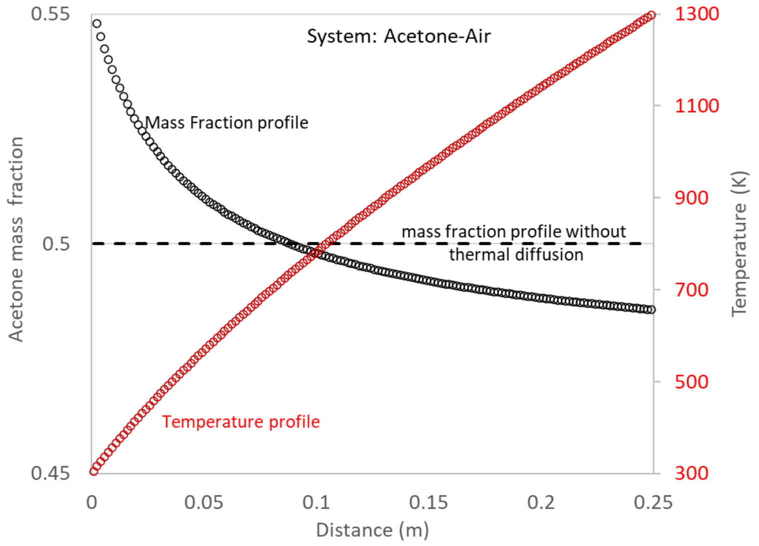


Figure: Effect of thermal diffusion in a binary Acetone-Air system

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[7] Kennett K Kuo and Ragini Acharya. Applications of Turbulent and Multiphase Combustion, 2012, John Wiley & Sons, Inc. See page 267, equation 4.159.

[8] Robert C Reid, John M Prausnitz and Thomas K Sherwood. The properties of gases and liquids, 1977, McGraw-Hill, Inc. See Page 678, Appendix C.

Solving for (n-1) species equations in MFIX: Reacting flows

Solving for (n-1) gas species mass fraction conservation equations is required due to the derivation of the multicomponent diffusion model. Here we verify that such modification to the algorithm in MFIX will not generate errors in reacting flows with/without mass transfer between phases. The multicomponent fluxes are implemented in MFIX as source terms in solve_species_eq.f subroutine where the loop of n species was modified to a loop over (n-1) species with the last species mass fraction calculated as: $Y_n = 1 - \sum_{i=1}^{n-1} Y_i$.

It is simple to note that when the stiff chemistry algorithm is invoked, the reaction rates and mass transfer between phases is not used in solve_species_eq.f subroutine but rather in the stiff chemistry subroutines. Thus, the results obtained with the stiff chemistry solver are identical for both approaches, i.e solving for either (n) or (n-1) species. We have checked that this is the case with the Silane decomposition tutorial case, and the results are not shown here.

The Silane decomposition case mentioned above will not work without the stiff chemistry solver due to very large pre-exponent reaction rates. A reduction of 6 orders of magnitude in all gas-phase homogeneous reactions was required to make this case run without stiff chemistry solver. As shown in the SiH4 reacting gas-phase species mass fraction and Si solids-phase species mass fraction variation with time, the results solving for (n) or (n-1) species equations are identical. Furthermore, considering either an inert species (N2 and Al2O3) or a reacting species (SiH4 and Si) as the nth species (i.e. not solving for this nth species), show almost identical results as seen in the figures below. These results are understandable because MFIX algorithm was already designed to work for (n) species, even inert species. Let's explain further: In this Silan decomposition case, the solids-phase consisted initially of 100% inert species Al2O3. A mass transfer between gas-solids phases deposits Si on the Al2O3 particle effectively reducing the mass fraction of Al2O3. MFIX solves for the inert Al2O3 mass fraction and must, thus, compute a reduction in its mass fraction. This is done in MFIX by having a mass transfer term in all species equations (even inert ones), and that's the reason why the new algorithm works as well as the previous algorithm solving for (n) species mass fractions.

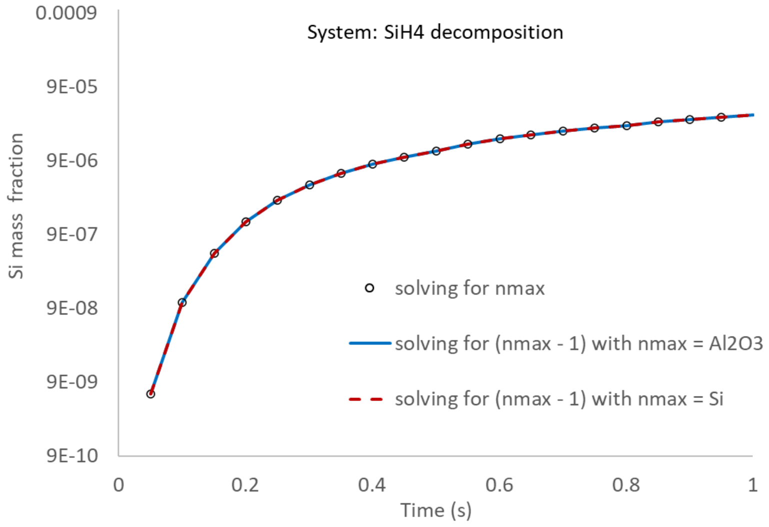

Figure: Transient profile of mass fraction of deposited Si

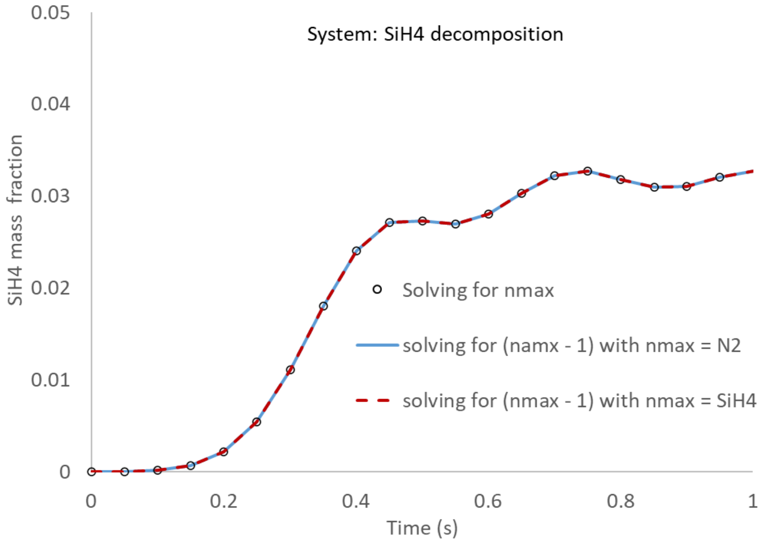

Figure: Transient profile of mass fraction of reactant SiH4