How is the Mass Diffusivity evaluated based on Kinetic Theory within Ansys Fluent?

/ Solution

When the Species Transport Model is invoked, one of the additional fluid property inputs required is Mass Diffusivity (m²/s). Of the various options to input this value, one of them is using kinetic theory to evaluate the mass diffusivity.

When using kinetic theory, the solver does not prompt any other user inputs. The mass diffusivity gets evaluated internally using the Chapman-Enskog formula:

$$D_{ij} = 0.00186 \frac{\sqrt{T^3\left(\frac{1}{M_{w,i}} + \frac{1}{M_{w,j}}\right)}}{P_{abs}\sigma_{ij}^2\Omega_D} \times 10^{-4} \quad \text{(m}^2\text{/s)}$$

where

M_w = Molecular Weight (g/mol)

T = Temperature (K)

P_{abs} = Pressure (atm)

σ_{ij} = L-J Characteristic Length of Binary Mixture (Angstrom) = $\frac{1}{2}(\sigma_i + \sigma_j)$

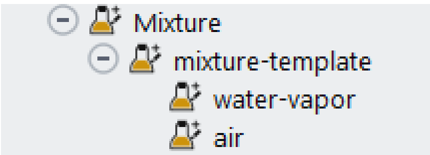
Ω_D = Non-dimensional Diffusion Collision Integral = $\frac{1}{T_D^{*0.145}} + \frac{1}{(T_D^* + 0.5)^2}$

T_D^* = Reduced Temperature = $T/(\varepsilon/k_B)_{ij}$

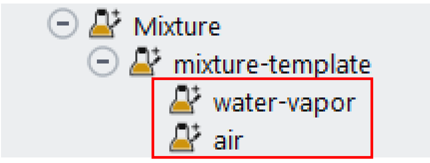
$(\varepsilon/k_B)_{ij}$ = L-J Energy Parameter of Binary Mixture (K) = $\sqrt{(\varepsilon/k_B)_i(\varepsilon/k_B)_j}$

L-J parameters used by the solver for each species in the above calculations will get populated under species materials considered within the mixture material.

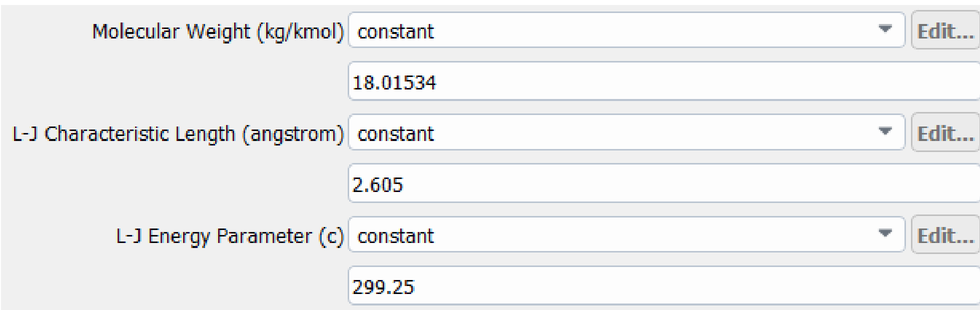
Example: Consider a mixture of air and water-vapor at a pressure of 1 (atm) and a temperature of 300 (K)



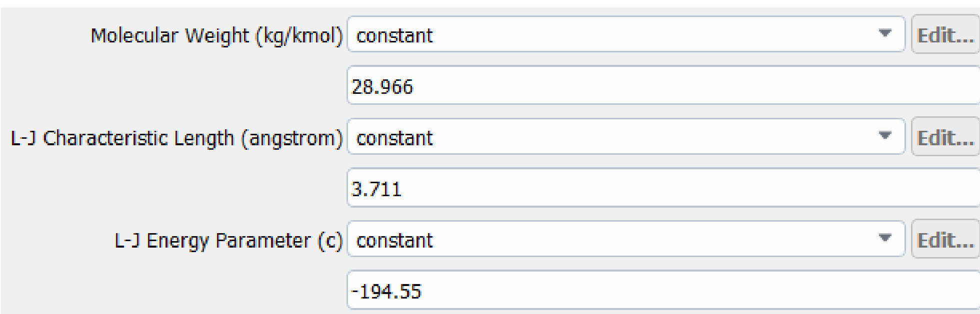
Mixture of water-vapor and air, using Mass Diffusivity based on kinetic-theory



L-J parameters considered by the solver can be looked at by visiting each species



water-vapor



air

Note: $(\varepsilon/k_B)_i$ must be converted to Kelvin (K) before using it to evaluate $(\varepsilon/k_B)_{ij}$

Sample calculations for operating conditions of T = 300 (K) and P_{abs} = 1 (atm) for air and water-vapor mixture:

$$\sigma_{ij} = 0.5(\sigma_i + \sigma_j) = 3.158 \text{ (Angstrom)}$$

$$(\varepsilon/k_B)_{ij} = \sqrt{(\varepsilon/k_B)_i(\varepsilon/k_B)_j} = 212.11 \text{ (K)}$$

$$T_D^* = T/(\varepsilon/k_B)_{ij} = 1.41436$$

$$\Omega_D = \frac{1}{T_D^{*0.145}} + \frac{1}{(T_D^* + 0.5)^2} = 1.22384$$

$$D_{ij} = 2.376 \times 10^{-5} \text{ (m}^2\text{/s)}$$

Comparing the evaluated values with those reported from Fluent solver:

```
                    Max
  Lam Diff Coef of h2o                  (m2/s)
------------------------ --------------------
                   fluid        2.3701217e-05
        ---------------- --------------------
                     Net        2.3701217e-05

                    Min
  Lam Diff Coef of h2o                  (m2/s)
------------------------ --------------------
                   fluid        2.3701217e-05
        ---------------- --------------------
                     Net        2.3701217e-05
```

Evaluated D_{ij} = 2.376e-5 (m^2/s)

Keywords: kinetic-theory; mass diffusivity; L-J parameters

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