P1.1-3: Conductivity of a polyatomic gas

Equation (1-18) cannot be used to understand the thermal conductivity of a polyatomic ideal gas, such as low pressure oxygen, because the ideal gas thermal conductivity is the sum of two terms corresponding to translational and internal contributions.

$$k = k_{trans} + k_{int} \tag{1}$$

Equation (1-18) only considers the translatonal contribution. Because thermal conductivity and viscosity are analagous transport properties, the translation term for the thermal conductivity of a dilute gas can be estimated as a function of the viscosity (μ) of the gas according to:

$$k_{trans} = \frac{15 R_{univ}\, \mu}{4\, MW} \tag{2}$$

where R_{univ} is the universal gas constant and MW is the molar mass of the of the gas. The internal contribution for a polyatomic molecule results from the transfer of energy associated with rotational and vibrational degrees of freedom. An estimate of the internal contribution is provided by the Eucken[1] correlation

$$k_{int} \approx \frac{\mu}{MW}\left[c_p - \frac{5R_{univ}}{2}\right] \tag{3}$$

where the viscosity is in units of Pa-s and the constant pressure specific heat and gas constant are in units of J/kmol-K. The internal contribution is zero for a monotonic gas.

Choose a gas and use the EES viscosity function to determine its viscosity as a function of pressure and temperature. Then calculate and plot the thermal conductivity as a function of pressure at several temperatures. Compare the values you obtain from the dilute gas theory described above with the values provided at the same conditions obtained from the EES conductivity function. Use your program to answer the following questions.

a.) The thermal conductivity of an ideal gas should only depend on temperature. At what pressure does this requirement fail for the temperature and gas you have selected?

Hydrogen is selected as the gas and the inputs are entered in EES:

```
"Problem 1.1-3"
$UnitSystem SI MASS RAD PA  K J
$TABSTOPS   0.2 0.4 0.6 0.8 3.5 in

T=300 [K]                                   "temperature"
F$='Hydrogen'                               "fluid"
P_MPa=0.1 [MPa]                             "pressure, in MPa"
P=P_MPa*convert(MPa, Pa)                    "pressure"
```

[1] Hirschfelder, J.L., Curtiss, C.F, and Bird, R,B., “Molecular Theory of Gases and Liquids”, John Wiley and Sons, 1967

The viscosity, specific heat capacity at constant pressure, and molecular weight of the gas (μ, c_p, and MW) are obtained using EES' built-in property function:

```
mu=viscosity(F$,T=T,P=P)                    "viscosity"
MW=MolarMass(F$)                            "molecular weight"
cP=cp(F$,T=T,P=P)                           "specific heat capacity"
```

The translation term in the thermal conductivity is estimated using Eq. (2):

```
k_trans=15*R#*mu/(4*MW)                     "translational contribution"
```

The internal term in the thermal conductivity is estimated using Eq. (3):

```
cP_molar=cP*MW                      "specific heat capacity on a molar basis"
k_int=(mu/MW)*(cP_molar-5*R#/2)     "internal contribution"
```

The dilute gas estimate of the thermal conductivity (k_{dilute}) is obtained from Eq. (1) and compared to the value obtained from EES (k):

```
k_dilute=k_trans+k_int          "dilute gas estimate of the thermal conductivity"
k=conductivity(F$,T=T,P=P)      "conductivity from EES' internal function"
```

Figure 1 illustrates the conductivity of hydrogen and the dilute gas estimate as a function of pressure at several values of temperature. It appears that the conductivity is independent of pressure up to about 1 MPa for hydrogen, although this value decreases with reduced temperature.

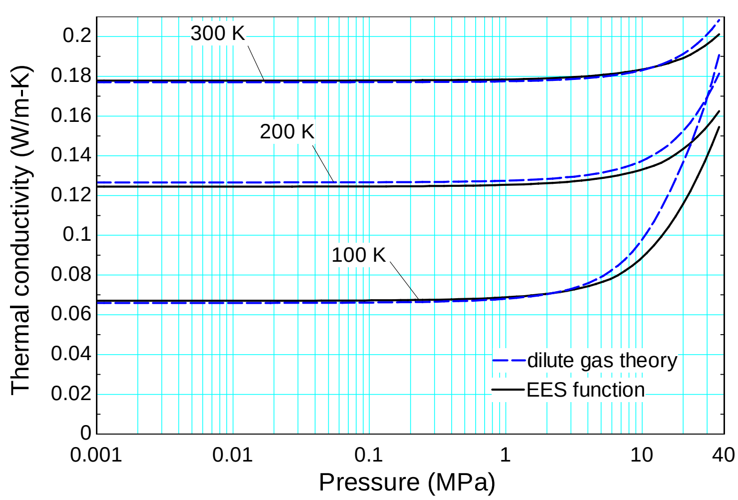

Figure 1: Thermal conductivity as a function of pressure estimated by the dilute gas theory and using EES internal property routines for several temperatures.

b.) How does thermal conductivity vary with temperature? What causes this behavior?

Thermal conductivity increases with temperature. This is due to higher molecular velocities (primarily) but also due to more modes of energy storage being activated with temperature.

c.) How does thermal conductivity vary with the choice of gas. Is there are relationship between the thermal conductivity and the number of atoms per molecule?

Figure 2 illustrates the conductivity of 6 different gases at 300 K and 100 kPa. There does not appear to be a clear correlation between conductivity and the number of atoms per molecule.

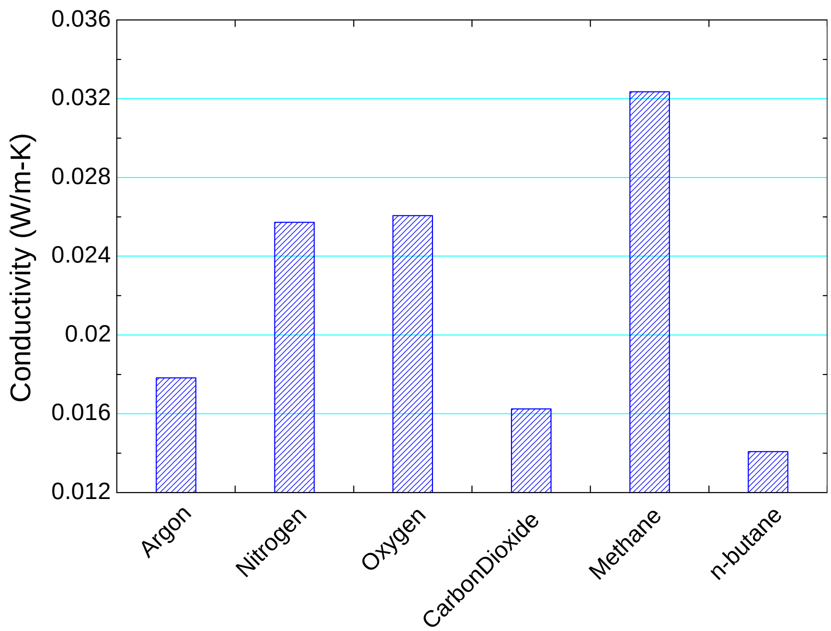

Figure 2: Thermal conductivity for several gases at 300 K and 100 kPa.