Workshop in honor of M. Ivanov's birthday
June 15-18, 2015, Novosibirsk, Russia

Improvement of Eucken correction for high-temperature gases

V.Istomin,E.Kustova, M.Mekhonoshina

Saint Petersburg State University

Motivation

- Simple engineering formulas are necessary for the calculation of the transport coefficients in high-temperature gases.
- Transport properties of electronically excited gases are actively studied during the last decade due to their importance in re-entry problems.
- For gases with electronic excitation simple relation for thermal conductivity coefficient hasn't been assessed up to now.

- 1913 – E.Eucken on the basement of mean free path concept proposed an approximate analytical expression for the thermal conductivity coefficient.
- 1957 – Using the Chapman-Enskog method Hirschfelder introduced a correction to refine the Eucken formula.
- 1990-2000 – Transport properties of electronically excited gases were investigated by Capitelli, Bruno, Kustova, Istomin and others.
- Applicability of Eucken formula to high temperature conditions, when electronic excitation is important, was not discussed in the literature except some papers.

Objectives

- Using methods of the kinetic theory
  - to develop an accurate model for calculating the thermal conductivity coefficient of gases with excited rotational, vibrational and electronic degrees of freedom,
  - to modify Eucken formula for gases with electronic excitation.
- Using the accurate model to estimate the limits of applicability of simplified Eucken and Hirschfelder relations in the temperature range $200 - 25000$ K.

If the molecules do not have the internal energy, the following approximate relation can be used: $\lambda = \frac{5}{2}\eta c_v$.
For particles with internal energy, on the basis of the mean free path consideration, Eucken suggests to separate λ into two parts:

$$\lambda = \lambda_{tr} + \lambda_{int} = (c_{v,tr} f_{tr} + c_{v,int} f_{int})\, \eta,$$

factors:

$$f_{tr} = \frac{5}{2}, \qquad f_{int} = 1.$$

Components of the specific heat due to the translational motion and internal energy of the molecules: factors:

$$c_{v,tr} = \frac{3k}{2m}, \qquad c_{v,int} = c_v - c_{v,tr}.$$

Using the Chapman-Enskog theory the Eucken formula can be improved. Hirschfelder has shown that the thermal conductivity can be expressed as follows:

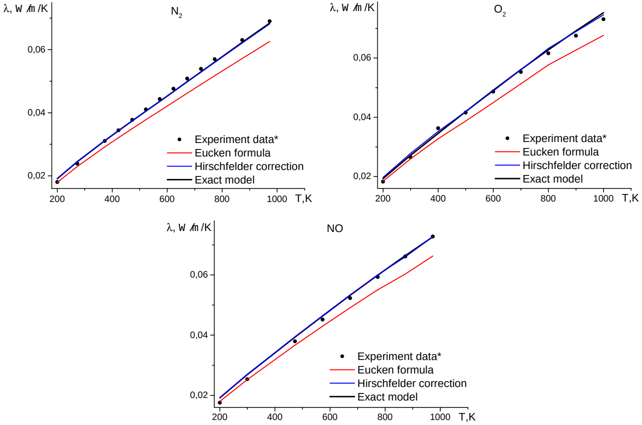
$$\lambda = \left(\frac{5}{2} c_{v,tr} + \frac{\rho D}{\eta} c_{v,int} \right) \eta.$$

The mean value $f_{int} = \frac{\rho D}{\eta} = 1.328$ provides a good approximation for the Lennard-Jones model.
This expression is more accurate than the Eucken formula, but for some cases it gives inaccuracy exceeding the experimental uncertainty.

- We consider a non-equilibrium gas mixture flow under condition of fast relaxation of internal energy and slow chemical reactions (one-temperature approximation)
- Algorithm for calculating the transport coefficients is based on zero- and first-order approaches of the modified Chapman-Enskog method.
- Thermal conductivity coefficient expressed as $\lambda' = \frac{k}{3}[\mathbf{A}, \mathbf{A}] = \lambda_{tr} + \lambda_{int}$ and describes in one-temperature approximation transfer of translational λ_{tr} and all λ_{int} internal energy types.
- In this work we consider gases O, N, O_2, N_2, NO
- We take into account 170 and 204 excited electronic states of the nitrogen and oxygen atoms
- 5, 7 and 4 electronic terms of the nitrogen,oxygen and nitric oxide molecules
- Temperature range $200 - 20000$ K

Results
Comparison with experiment at low temperatures

Figure : Thermal conductivity coefficient as a function of T



*Uribe F.J., Kestin J. and Mason E.A. Thermal conductivity of nine polyatomic gases at low density // J. Phys. Chem. Ref. Data, V. 19. 5. P. 1123-1136, 1990.

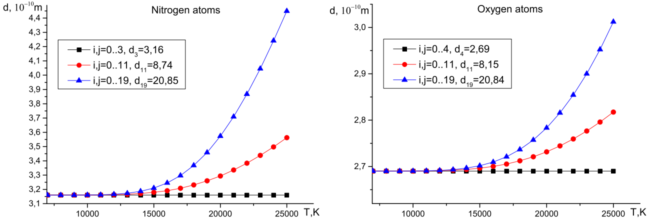
We introduce the effective diameter:

$$d_{eff}^2 = \frac{1}{Z_{int}^2} \sum_{nm} s_n s_m exp\left(\frac{-\varepsilon_n - \varepsilon_m}{kT}\right)\left(\frac{d_n + d_m}{2}\right)^2,$$

and obtain a simplified averaging operator:

$$< F >= \left(\frac{kT}{\pi m}\right)^{1/2} \pi d_{eff}^2 \int F(\gamma)\gamma^3 \exp\left(-\gamma^2\right) d\gamma,$$

Figure : Effective diameters as functions of T



The average value for the factor f_{tr} equal $\frac{5}{2}$ in the whole temperature range.

Figure : Eucken factor f_{int} for air species as a function of T

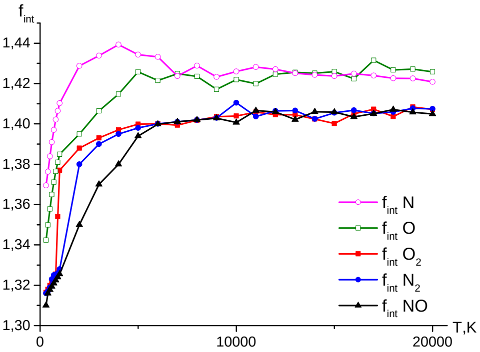
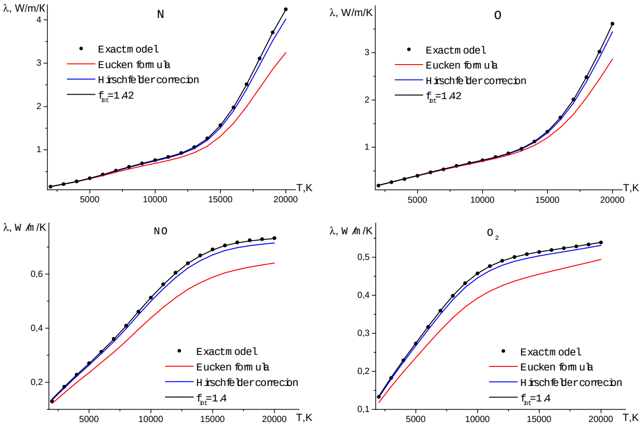


Figure : Thermal conductivity coefficients of air species as functions of T



Conclusions

Table : The values of the Eucken factor f_{int} which provide the best accuracy.

c	$T < 20000$ K		
N	1.42		
O	1.42		
c	$T < 1000$ K	$1000 < T < 5000$ K	$5000 < T < 20000$ K
NO	1.328	$-2 \cdot 10^{-9} T^2 + 3 \cdot 10^{-5} T + 1.2988$	1.40
O_2	1.328	$-3 \cdot 10^{-9} T^2 + 3 \cdot 10^{-5} T + 1.3436$	1.40
N_2	1.328	$-8 \cdot 10^{-9} T^2 + 6 \cdot 10^{-5} T + 1.2783$	1.40

Our model provides satisfactory accuracy for temperatures lower than 20000 K.

The research leading to these results has received funding from the Saint Petersburg State University (project 6.37.163.2014).

Thank you for your attention!