KAPPA: Kinetic Approach to Physical Processes in Atmospheres library in C++

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Abstract

KAPPA is an open-source object-oriented C++ library for calculation of physico-chemical relaxation rates and transport properties in various approximations of kinetic theory, including multi-temperature and state-to-state (STS) suited for strongly non-equilibrium reacting flows. An overview of the KAPPA implementation along with the computation of transport properties is presented for the STS model.

Mathematical model

Experimental results show that relaxation times of different processes in reacting mixtures [1] often verify the following relation:

$$\tau_{el} < \tau_{rot} \ll \tau_{vibr} < \tau_{react} \sim \theta \tag{1}$$

A closed set of macroscopic equations for the macroscopic parameter $n_{ci}(\mathbf{r},t)$, $\mathbf{v}(\mathbf{r},t)$ and $T(\mathbf{r},t)$ consists of the conservation equations for the momentum and total energy coupled with the detailed vibration-chemical kinetics for vibrational levels [2]:

$$\frac{d\rho}{dt} + \nabla\cdot(\rho\mathbf{v}) = 0 \tag{2}$$

$$\rho\frac{d\mathbf{v}}{dt} + \nabla\cdot\mathbf{P} = 0 \tag{3}$$

$$\rho\frac{dU}{dt} + \nabla\cdot\mathbf{q} + P:\nabla\mathbf{v} = 0 \tag{4}$$

$$\frac{dn_{ci}}{dt} + n_{ci}\nabla\cdot\mathbf{v} + \nabla\cdot(n_{ci}\mathbf{V}_{ci}) = R_{ci} \tag{5}$$

$$c = 1,...,L, \quad i = 0....,L_c \tag{6}$$

where the number density of molecules of species c at the vibrational level i is: The specific total energy U is given by:

$$\rho U(\mathbf{r},t) = \frac{3}{2}nkT + \sum_{ci}\langle\varepsilon^{ci}\rangle n_{ci} + \sum_{ci}\varepsilon_i^c n_{ci} + \sum_c \varepsilon_c n_c \tag{7}$$

$\langle\varepsilon^{ci}\rangle$, ε_i^c and ε_c are the average rotational, vibrational and formation energy, respectively. The pressure tensor $\mathbf{P}$ is obtained as:

$$\mathbf{P} = (p - p_{rel})\,\mathbf{I} - 2\eta\mathbf{S} - \zeta\nabla\cdot\mathbf{v}\mathbf{I} \tag{8}$$

$$\eta = \frac{kT}{10}[\mathbf{B},\mathbf{B}], \quad \zeta = kT[F,F], \quad p_{rel} = kT[F,G] \tag{9}$$

p_{rel} is the relaxation pressure, η and ζ are the coefficients of shear and bulk viscosity, respectively. Bracket integrals $[A,B]$ are introduced in [2]. The diffusion velocity is specified by:

$$\mathbf{V}_{ci} = -\sum_{dk} D_{cidk}\mathbf{d}_{dk} - D_{Tci}\nabla\ln T \tag{10}$$

$$D_{cidk} = \frac{1}{3n}[\mathbf{D}^{ci},\mathbf{D}^{dk}], \quad D_{Tci} = \frac{1}{3n}[\mathbf{D}^{ci},\mathbf{A}] \tag{11}$$

$$\mathbf{d}_{ci} = \nabla\left(\frac{n_{ci}}{n}\right) + \left(\frac{n_{ci}}{n} - \frac{\rho_{ci}}{\rho}\right)\nabla\ln p \tag{12}$$

where D_{cidk} and D_{Tci} are the multicomponent and thermal diffusion coefficients and $\mathbf{d}_{ci}$ the species specific driving forces. The total heat flux is:

$$q = -\lambda'\nabla T - p\sum_{ci} D_{Tci}\mathbf{d}_{ci} + \sum_{ci}\left(\frac{5}{2}kT + \langle\varepsilon_j^{ci}\rangle_{rot} + \varepsilon_i^c + \varepsilon_c\right)n_{ci}\mathbf{V}_{ci} \tag{13}$$

Thermal conductivity coefficient coefficients are:

$$\lambda' = \lambda_{tr} + \lambda_{rot} = \frac{k}{3}[\mathbf{A},\mathbf{A}] \tag{14}$$

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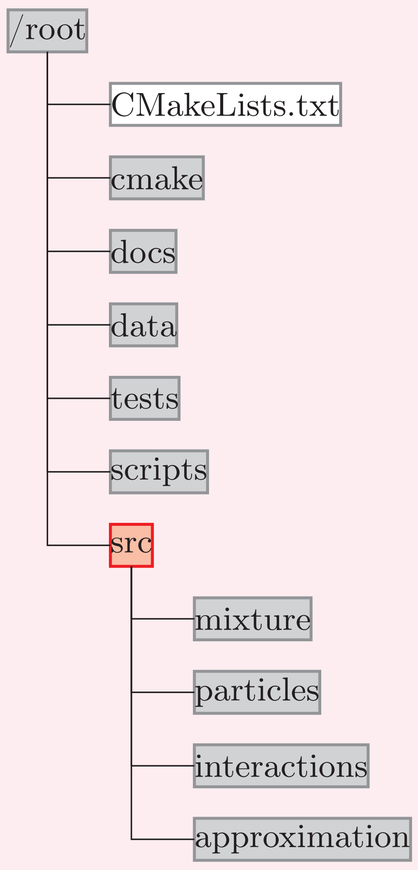
KAPPA API



Interaction models currently available in KAPPA:

- Collision integrals: Rigid Sphere, Variable Soft Sphere, Lennard–Jones, Born–Mayer, ESA phenomenological potentials;
- VT, VV-exchanges: SSH, FHO QCT-based models;
- Exchange reaction: the Arrhenius law, Rusanov-Fridman, Polak, Warnatz, Aliat, QCT-based models;
- Dissociation: Arrhenius law, Treanor-Marrone, (along with its modification), QCT-based models;
- Ionization: Arrhenius law;
- Relaxation times: Parker, Millikan-White, Park models.

Features

- accurate and efficient computation of transport and chemical kinetic properties for multicomponent, non-equilibrium flows;
- easily extendable and maintainable;
- couple with existing CFD tool;
- self-documenting database format;
- open-source, to promote code and data sharing.

Application: transport coefficients

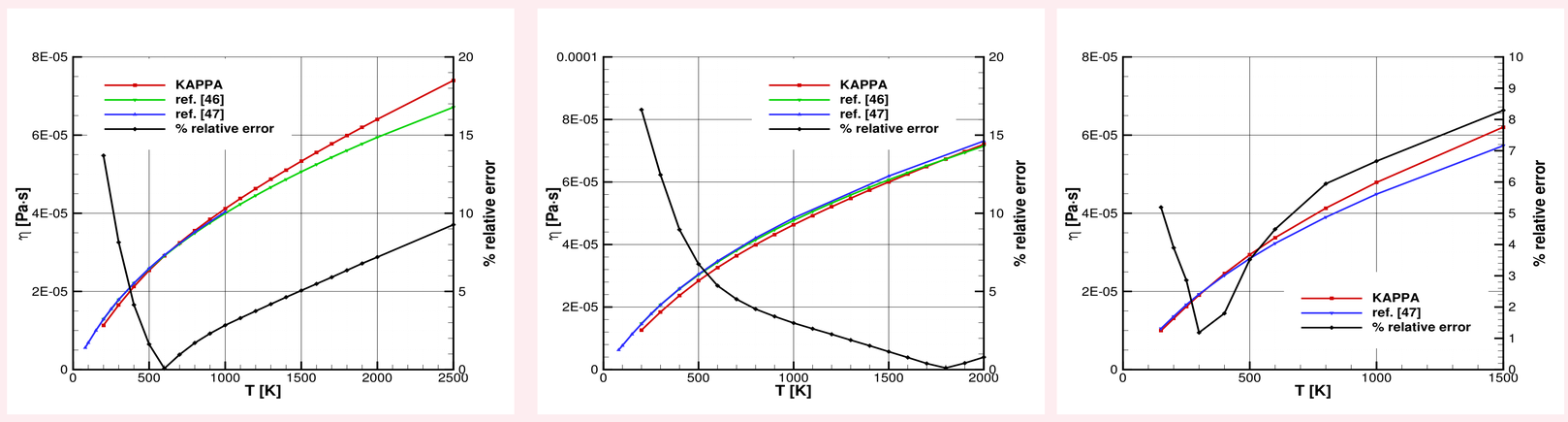


Figure 1. Shear viscosity η for N_2 (left), O_2 (center), NO (right) at ambient pressure. Comparison of numerical [2] and experimental [3, 4] results.

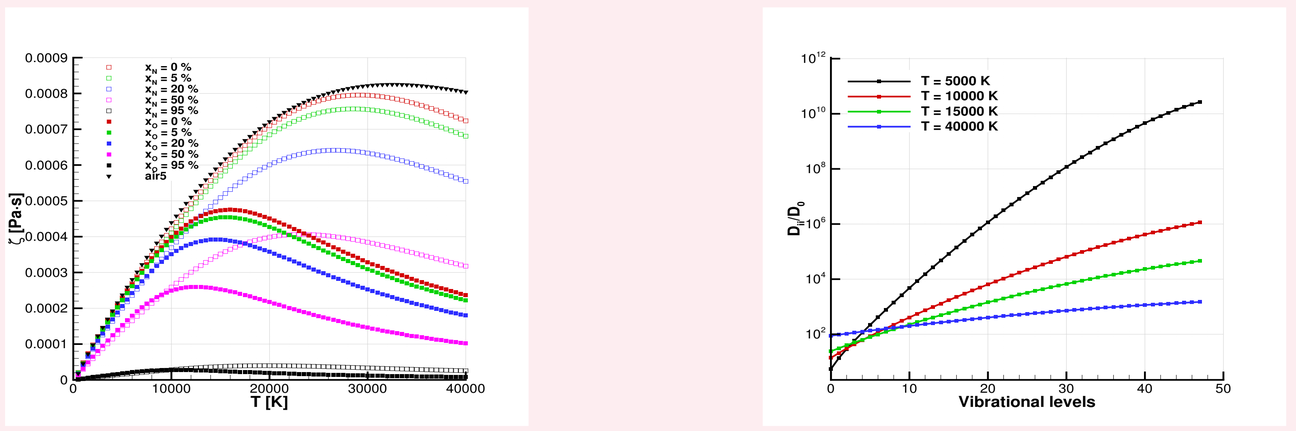


Figure 2. Bulk viscosity coefficients ζ (left) computed for $N_2 - N$, $O_2 - O$ and air5 at fixed atomic molar fractions at ambient pressure. Dimensionless **self-diffusion** coefficients (right) for $N_2 - N$ with $x_N = 50$.

Conclusion and Perpectives

- The KAPPA library for kinetic theory computation in strongly non-equilibrium reacting flow is presented, its capabilities, structure and implementation are discussed;
- Results of the computation of transport properties according to the STS approach are given;
- Parallelization, ionization flow extension, 1T and 2T validation, CFD solver interface.

References

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[4] Y. Touloukian, S. Saxena, P. Hestermans, Viscosity, 1974.