KINTECH LABORATORY

Air optical properties calculation

Background

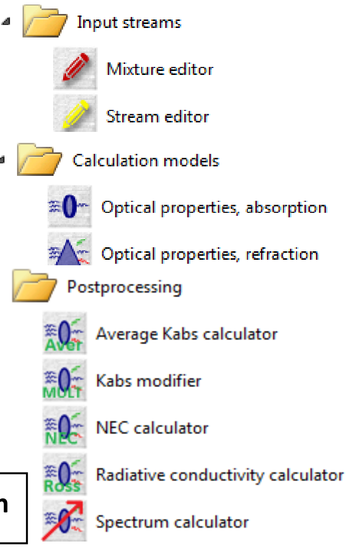
Optical properties of gases, fluids and plasma are important characteristic of the media at high temperature, because of essential or dominant input of radiation in the energy balance. These characteristics are significant also for cold media when absorption of radiation is point of interest. Absorption coefficient, refraction index, net emission coefficient, radiative heat conductivity and radiation spectrum – all these characteristics are used often for modeling of gases at high temperature, combustion and plasma.

Problem statement

It is required to calculate optical properties of Air for a wide range of the temperatures 300 – 30000 K and pressures 0.1-100 atm in Local Thermodynamic Equilibrium (LTE) approach.

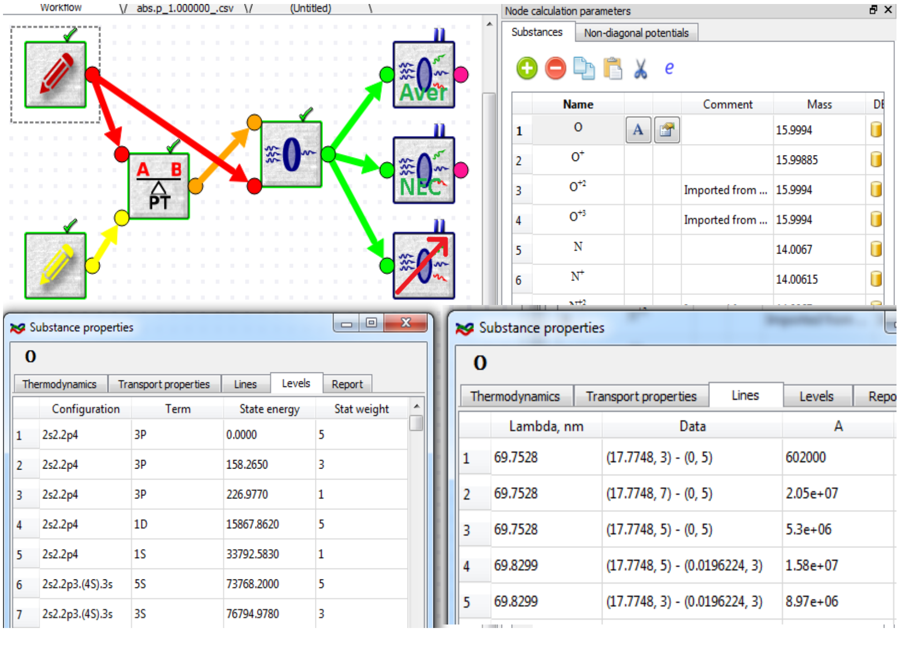
Problem setup in Fluid Workbench

To calculate optical properties in LTE approach for Air, we use set of modules from FWB library: **Mixture editor** to set initial composition, **Stream editor** to take all necessary information about species properties from Kintech DB, **Equilibrium thermodynamic properties** to calculate chemical equilibrium composition at given Pressure and Temperature, **Optical properties, absorption** model to calculate absorption coefficient, Average Kabs calculator for average absorption coefficient, **NEC calculator** for Net Emission coefficient and **Spectrum calculator** for calculation of emission spectrum at given profile of gas temperature..



List of available optical models in Fluid Workbench

The **list of possible species (mechanism)** is generated automatically by query to KintechDB database, which is tightly integrated with Fluid Workbench and provide reference thermodynamic and atoms, molecules electronic structure and radiation probabilities data for principal elements and molecules. For Air the query to database generates the list of 15 species formed from elements O, N and e including atoms, molecules and ions. Species are loaded automatically along with their thermodynamic properties and information about electronic, rotational, vibrational energy structure and possible transition with radiation probabilities.



Work Flow diagram and generated list of species

Data of species for electronic, vibrational, rotational energy structure, transition probabilities and broadening parameters.

Parameters of **Equilibrium Model** determine the range of the pressure (P=0.1-100 atm) and temperature (from 300 to 30000 K) of calculations. Parameters of **Optical properties, absorption** model set of range of investigated wavelengths and accuracy of calculation.

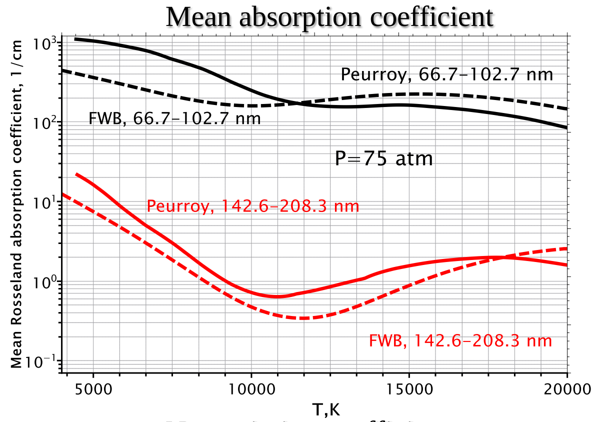
CS-FWB-2

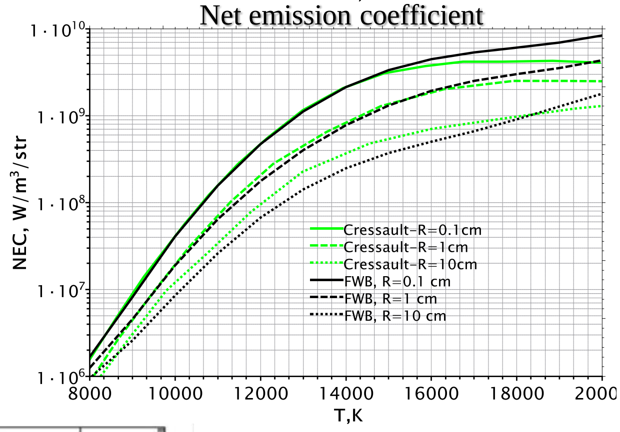
Results

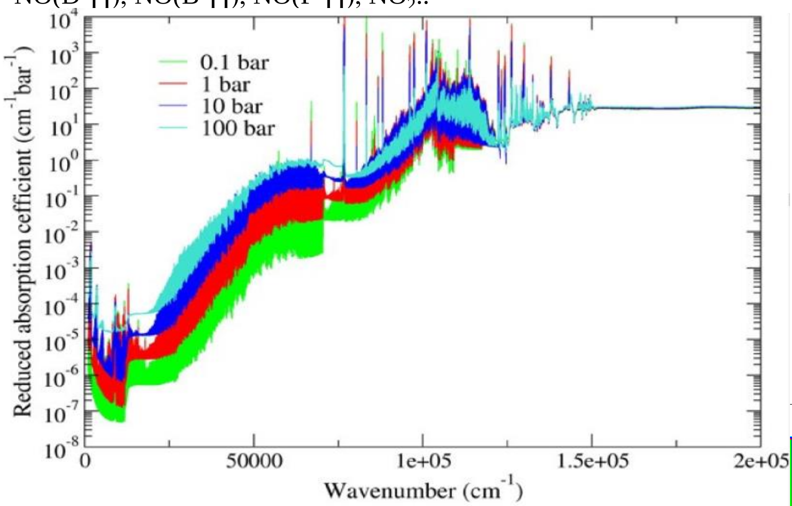
Air optical properties are calculated for the range of pressure and temperature: P=0.1-100 atm, T=300 - 30000 K.

The results of FWB calculation for air reduced absorption coefficient (k_{abs}/P), mean Rosseland absorption coefficient and Net Emission Coefficient (NEC) are presented in plots and compared with published results.

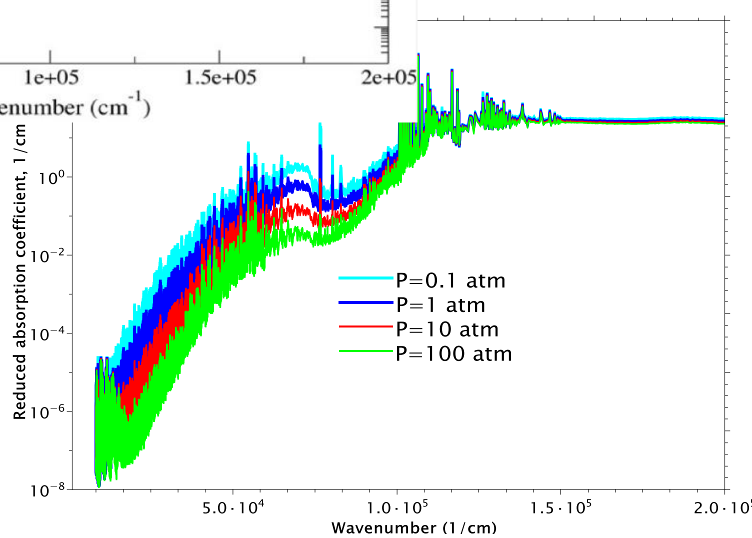
For comparison, appropriate calculation results from literature are presented in plots: Bogatyreva et al. [1] for absorption coefficient, Perroy et al. [2] for mean Rosseland absorption coefficient and Cressault et al. [2] for Net Emission Coefficient. The agreement of FWB results with literature data is good for [1], [3] and satisfactory for [2]. The reason of difference with work [2] is high sensitivity of the results to the data base of the radiation lines and probabilities of the transitions. Following electronic states were regarded in the calculations for low temperatures: $N_2(X^1\Sigma)$, $N_2(A^3\Sigma)$, $N_2(B^3\Pi)$, $N_2(B^3\Sigma)$, $N_2(a^1\Sigma)$, $N_2(a^1\Sigma)$, $N_2(C^3\Sigma)$, $N_2(B^3\Pi)$, $O_2(X^3\Sigma)$, $O_2(B^3\Sigma)$, $O_2(A^3\Sigma)$, $O_2(C^1\Sigma)$, $O_2(b^1\Sigma)$, $O_2(a^1\Sigma)$, $NO(X^2\Pi)$, $NO(A^2\Pi)$, $NO(B^2\Pi)$, $NO(C^2\Pi)$, $NO(D^2\Pi)$, $NO(B^2\Pi)$, $NO(F^2\Pi)$, NO_2..







Absorption coefficient in accordance to work [1]



Absorption coefficient by FWB

References

1. N Bogatyreva et al 2011 J. Phys.: Conf. Ser. 275 012009
2. B.Peyrou e.a, 2012 J. Phys. D: Appl. Phys. 45 455203
3. Y Naghizadeh-Kashani, Y Cressault and A Gleizes, 2002 J. Phys. D: Appl. Phys. 35 2925
4. Y Naghizadeh-Kashani, Y Cressault and A Gleizes 2002 J. Phys. D: Appl. Phys. 35 2925