KINTECH LABORATORY

# Calculation of transport properties of Air in wide range of Temperatures

## Background

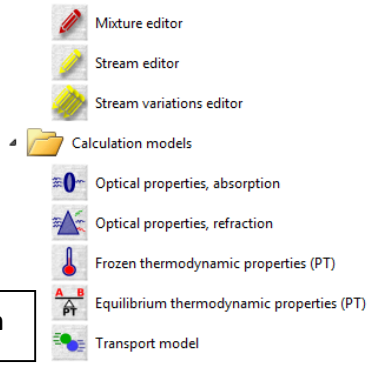
Transport and thermophysical properties (heat capacity, enthalpy, viscosity, heat conduction, electrical conductivity, diffusion coefficients) are important characteristics used for modeling and conceptual design of the set-up and apparatus for combustion, discharges, chemical technologies. Accessibility of these properties are key moment for applicability of state-of-art CFD codes.

## Problem statement

It is required to calculate thermophysical and transport properties of Air for a wide range of the temperatures 300 – 30000 K in Local Thermodynamic Equilibrium (LTE) approache with high accuracy 1-3 %.

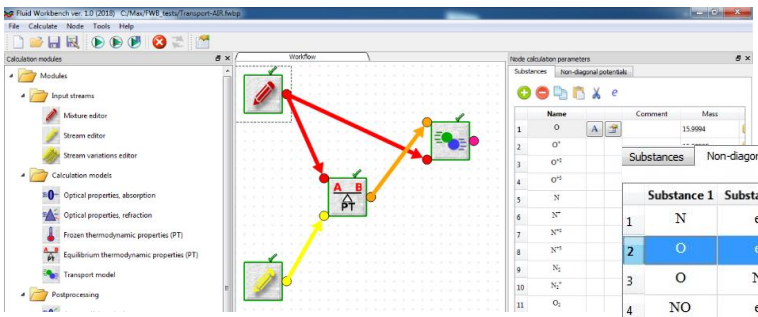
## Problem setup in Fluid Workbench

To calculate transport and thermodynamic properties in LTE approach for Air, we use four 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 and **Transport model** to calculate transport properties.




**List of available 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 collision properties data for more than 4100 substances. 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 along with their thermodynamic and collision characteristic from database.



**Work Flow diagram**

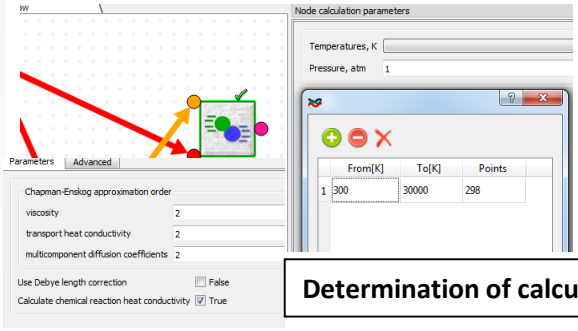
**Data of species collisions for calculation transport properties.**

Substances | Non-diagonal potentials

| | Substance 1 | Substance 1 |
|---|---|---|
| 1 | N | e |
| 2 | O | e |
| 3 | O | N |
| 4 | NO | e |
| 5 | NO | N |
| 6 | NO | O |
| 7 | $N_2$ | e |

Potentials — Table of collision integrals

| T | $\Omega_{11}$ | $\Omega_{12}$ | $\Omega_{13}$ | $\Omega_{14}$ | $\Omega_{15}$ | $\Omega_{16}$ | $\Omega_{17}$ | $\Omega_{22}$ | $\Omega_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| 200 | 1.45692 | 1.61367 | 1.67824 | 1.71307 | 1.75075 | 1.77926 | 1.79963 | 1.5152 | 1.64323 |
| 300 | 1.67283 | 1.82433 | 1.884 | 1.91392 | 1.94628 | 1.97077 | 1.98827 | 1.73975 | 1.88498 |
| 400 | 1.89943 | 2.0485 | 2.1046 | 2.13045 | 2.15842 | 2.17958 | 2.1947 | 1.9754 | 2.1383 |
| 500 | 2.07323 | 2.21651 | 2.26789 | 2.28923 | 2.31233 | 2.3298 | 2.34228 | 2.15616 | 2.33177 |
| 600 | 2.23431 | 2.37162 | 2.4183 | 2.43525 | 2.45359 | 2.46747 | 2.47738 | 2.32368 | 2.51057 |
| 700 | 2.3606 | 2.49039 | 2.53195 | 2.54445 | 2.55798 | 2.56822 | 2.57554 | 2.45503 | 2.64999 |
| 800 | 2.48132 | 2.60382 | 2.64044 | 2.64867 | 2.65756 | 2.6643 | 2.6691 | 2.58057 | 2.78288 |
| 900 | 2.57549 | 2.68991 | 2.72145 | 2.72548 | 2.72984 | 2.73314 | 2.7355 | 2.67851 | 2.88579 |
| 1000 | 2.6673 | 2.77399 | 2.80067 | 2.80067 | 2.80067 | 2.80067 | 2.80067 | 2.77399 | 2.98585 |
| 1100 | 2.75672 | 2.85595 | 2.87792 | 2.87402 | 2.86979 | 2.8666 | 2.86432 | 2.86699 | 3.08305 |
| 1200 | 2.84382 | 2.93579 | 2.95318 | 2.94547 | 2.93714 | 2.93084 | 2.92633 | 2.95757 | 3.17747 |
| 1300 | 2.91083 | 2.99519 | 3.00801 | 2.99667 | 2.9844 | 2.97511 | 2.96848 | 3.02726 | 3.24929 |




**Determination of calculation parameters**

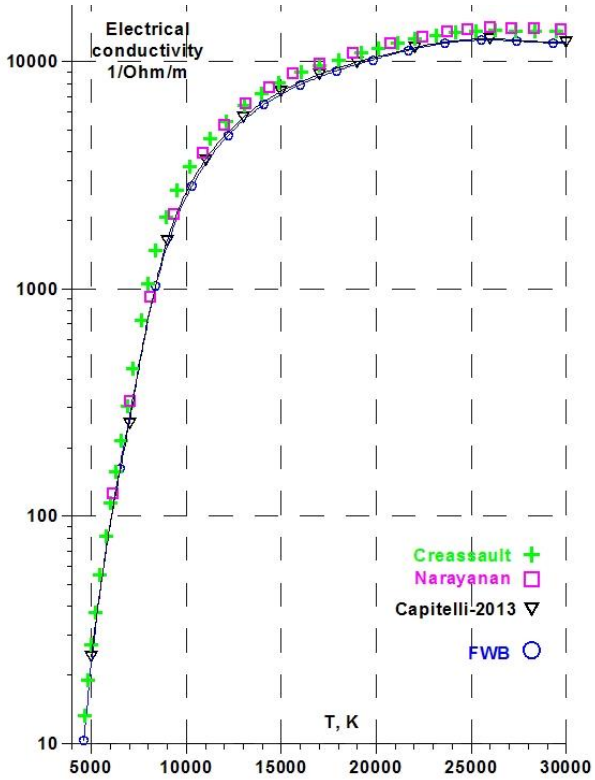
Parameters of Equilibrium Model determine the range of the pressure (P=1 atm) and temperature (from 300 to 30000 K) of calculations. Parameters of Transport Model set order of approximation in framework of Chapman-Enskog theory and approaches to take into account input of reactions and internal degree of freedom in heat conduction and heat capacity.

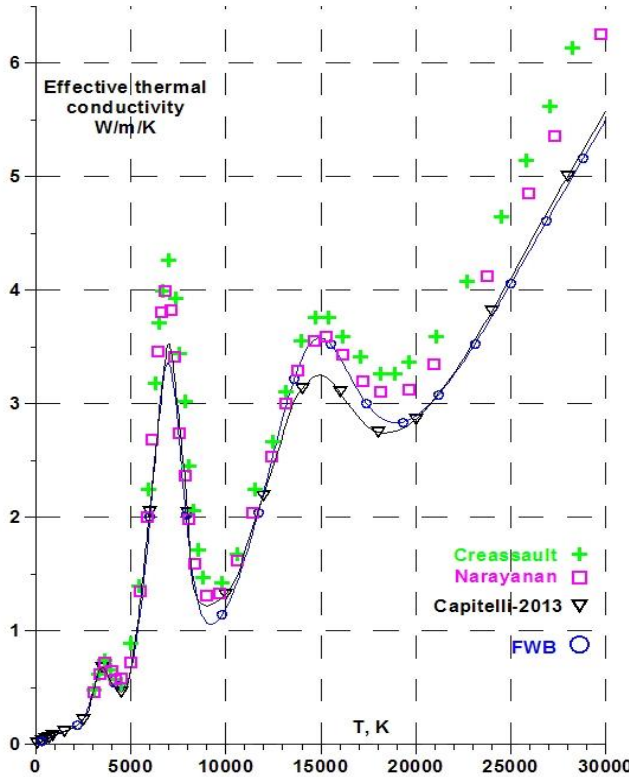
## Results

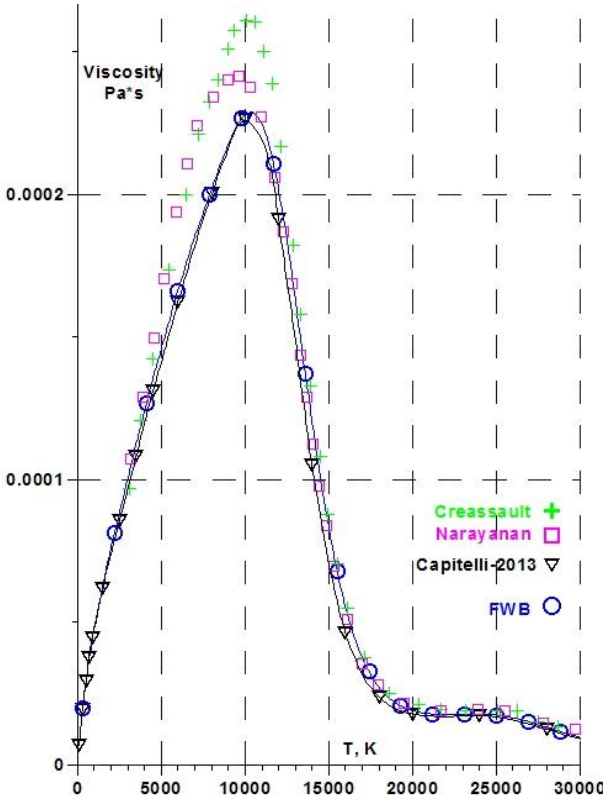
Air transport coefficients are calculated in the second approximation of Chapman-Enskog theory with taking into account input of chemical reactions in heat capacity and thermal conductiviry. Calculations are made for P=1 atm, T=300 - 30000 K.

The results of FWB calculation for air effective thermal conductivity $\lambda_{eff}$, viscosity $\mu$ and electrical conductivity are presented in plots by the blue lines with circles.

For comparison, appropriate calculation results from literature are presented in plots: Capitelli et al. [1] (black line with triangles), Cressault et al. [2] (green pluses), and Narayanan [3] (magenta squares). The agreement of FWB results with literature data is good for [1] and satisfactory for [2, 3]. The deviation of FWB results from [2, 3] at high temperatures T> 15000K is due to the correction by Debye length $r_D$ for screened Coulomb potential: in the works [2, 3] this correction is not taken into account for ions; in FWB and in [1] - with account for ions.




## References

1.Capitelli M., Bruno D., Laricchiuta A. Fundamental Aspects of Plasma Chemical Physics. Transport. Springer, N.Y. 2013

2.Cressault Y. et al. Influence of metallic vapours on the properties of air thermal plasmas. Plasma Sources Science and Technology. 2008, Vol.17. No.3, p.035016

3.Narayanan V.R.T. Numerical modeling of post current-zero dielectric breakdown in a low voltage circuit breaker. A dissertation submitted to the faculty of the graduate school of the University of Minnesota. USA. 2014