THERMOS Toolkit: Software and databases package for properties calculations of LTE and Non-LTE plasmas

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THERMOS Toolkit [1] has been developed at the Keldysh Institute of Applied Mathematics, it consists of set of atomic databases and software package, which is designed for calculation of thermodynamic and radiative properties of plasma at various conditions over wide range of temperatures and densities.

The software package includes codes for numerical simulation of transparent and optically thick plasmas. The local thermodynamic equilibrium (LTE) plasma properties are calculated by using the self-consistent Hartree-Fock-Slater model or Saha-Boltzmann statistics with atomic database. For Non-LTE cases the system of level kinetics equations is solved in the quasi-stationary approach with a fixed radiation field by using the collisional-radiative equilibrium (CRE) model with atomic databases.

The atomic databases calculation process is based on the non-relativistic model, supplemented by a procedure of building the RDCA (**R**educed **D**etailed **C**onfiguration **A**ccounting) database [2]. The latter improves positions and strengths of spectral lines by using data from detailed atomic codes, such as RCG [3], FAC [4] or available experimental data. In addition to that, a special technique has been developed and implemented for averaging the atomic data on a given photon energy grid – **R**adiative **U**nresolved **S**pectra **A**tomic **M**odel or RUSAM [5], [6], which is aimed at reducing calculation time with little to none detriment to accuracy.

Opacity and thermodynamic properties tables are being calculated over wide range of electron temperatures and densities for two limiting cases (transparent and optically thick plasma layer). These tables can be used in RHD calculations with escape-factor interpolation [7]. The interpolation method is efficient and gives reasonable results in a wide range of electron densities.

The THERMOS Toolkit takes part in the NLTE Code Comparison Workshops [8], and its calculation results are comparable to those of some reputed codes from over the world.

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