Production of an opacity table for air

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Opacities are one of the most crucial ingredients in radiation-hydrodynamic simulations used to model a variety of astrophysical phenomena, laser-produced plasmas, and in shock-induced heating studies. For hot plasmas, it is usually only necessary to consider the opacities of atoms and their ions – a task that can still be very challenging for systems where a number of ion stages are populated and for complex ions where many atomic levels may retain population. For cooler plasmas (roughly temperatures in the range of 1 eV), it may be necessary to consider mixtures of atomic and molecular species. This can also be quite challenging, especially for scenarios where ionization and dissociation of molecules can lead to cases where contributions from atoms, molecules, and their ions are all important. Here we describe our recent work in calculating the opacity of air for a range of temperatures and densities. For room temperature cases, the opacity of air is dominated by the diatomic molecule contributions from N2 and O2. At temperatures of a few thousand Kelvin other molecular species, such as NO and NO2, make important contributions. At higher temperatures (approaching tens of thousands of Kelvin), molecular and atomic contributions are both significant. At even higher temperatures, atomic contributions finally start to dominate.

Our approach starts from the LANL Magpie code [1], which computes the equation-of-state of the air components for a given temperature and pressure in local thermodynamic equilibrium. The LANL MOLOP suite [2] is then used to compute the molecular absorption. We use a combination of detailed quantum chemistry (using the MOLPRO code [3]) and RKR methods to compute the potential energy curves and dipole matrix elements for the diatomic molecules of interest. NO2 contributions are provided from work done at Sandia National Laboratories [4]. The atomic contributions are computed using the LANL suite of atomic physics codes [5]. The LANL MOLOP code then assembles the monochromatic opacity of the air mixture and has recently been used to construct tables of air opacities. Examples of such opacities will be shown at the conference.
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References

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