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Evolution of Species in TNT Explosions*

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Abstract

Evolution of species at thermodynamic-equilibrium were computed for TNT explosions via the thermodynamic code Cheetah. These include species along the CJ isentrope of the detonation products, and species corresponding to stoichiometric combustion of the TNT products with air. These are used to predict the species waveforms in the detonation wave (Fig. 1), in the initial expansion of the blast wave (Fig. 2), and in the turbulent combustion cloud of a 1-kg TNT explosion (Fig. 3). For convenience, results are compiled in Tables 1, 2 and 3 respectively. When combined with the temperature field, these species provide information needed to predict the optical emissions from TNT fireballs at different times. LLNL-ABS-645234

Data Tables

Table 1. Concentrations Ci(r) at t = 0.xlsx

Tables 2. Concentrations Ci(r) at t = 10 mus.xlsx

Table 3. Concentrations Ci(x,0,0) at 1.1 ms.xlsx

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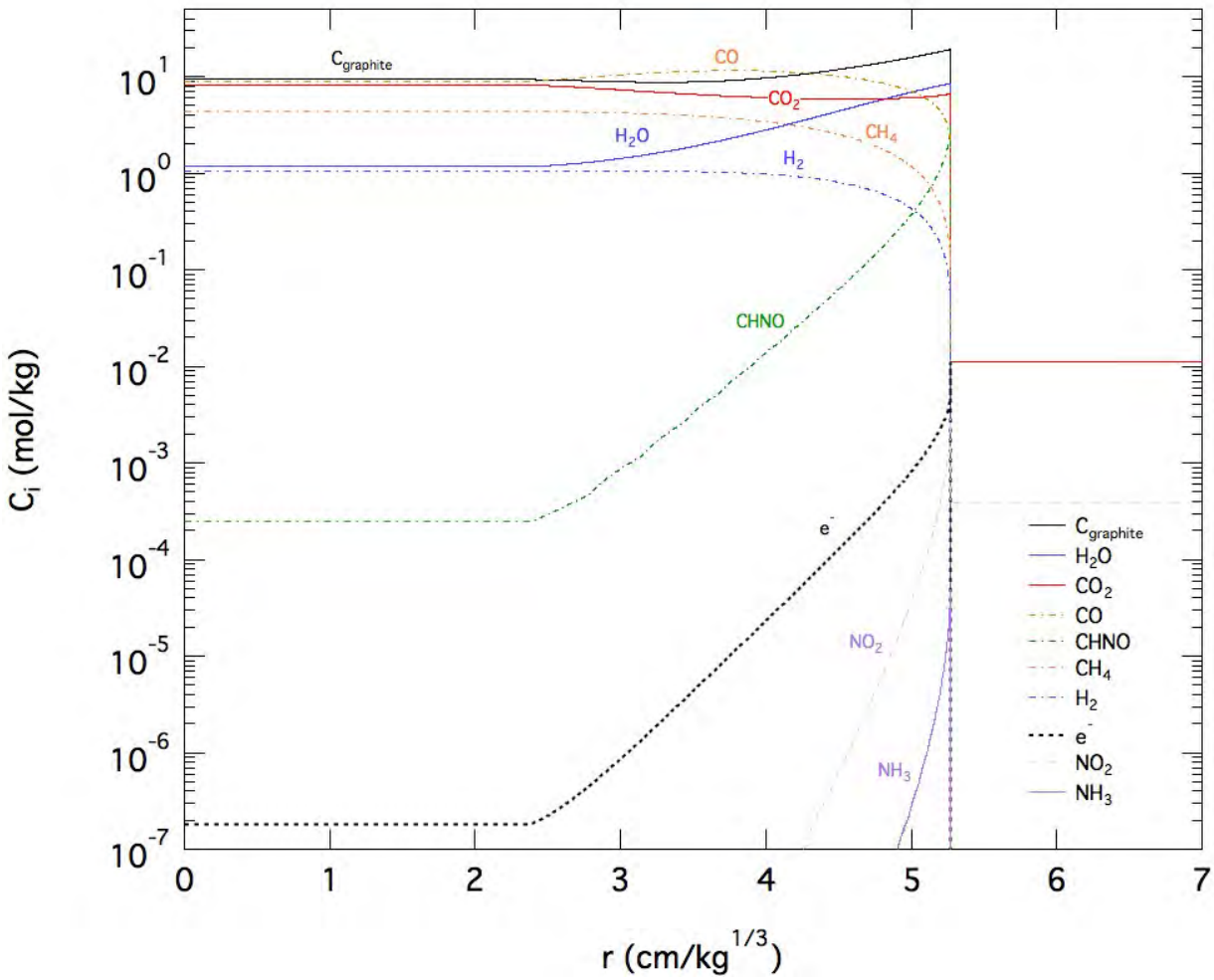

Figure 1. Species profiles in the detonation wave of a spherical TNT charge ($S_{CJ} = 1.58$). See Table 1 for this data.

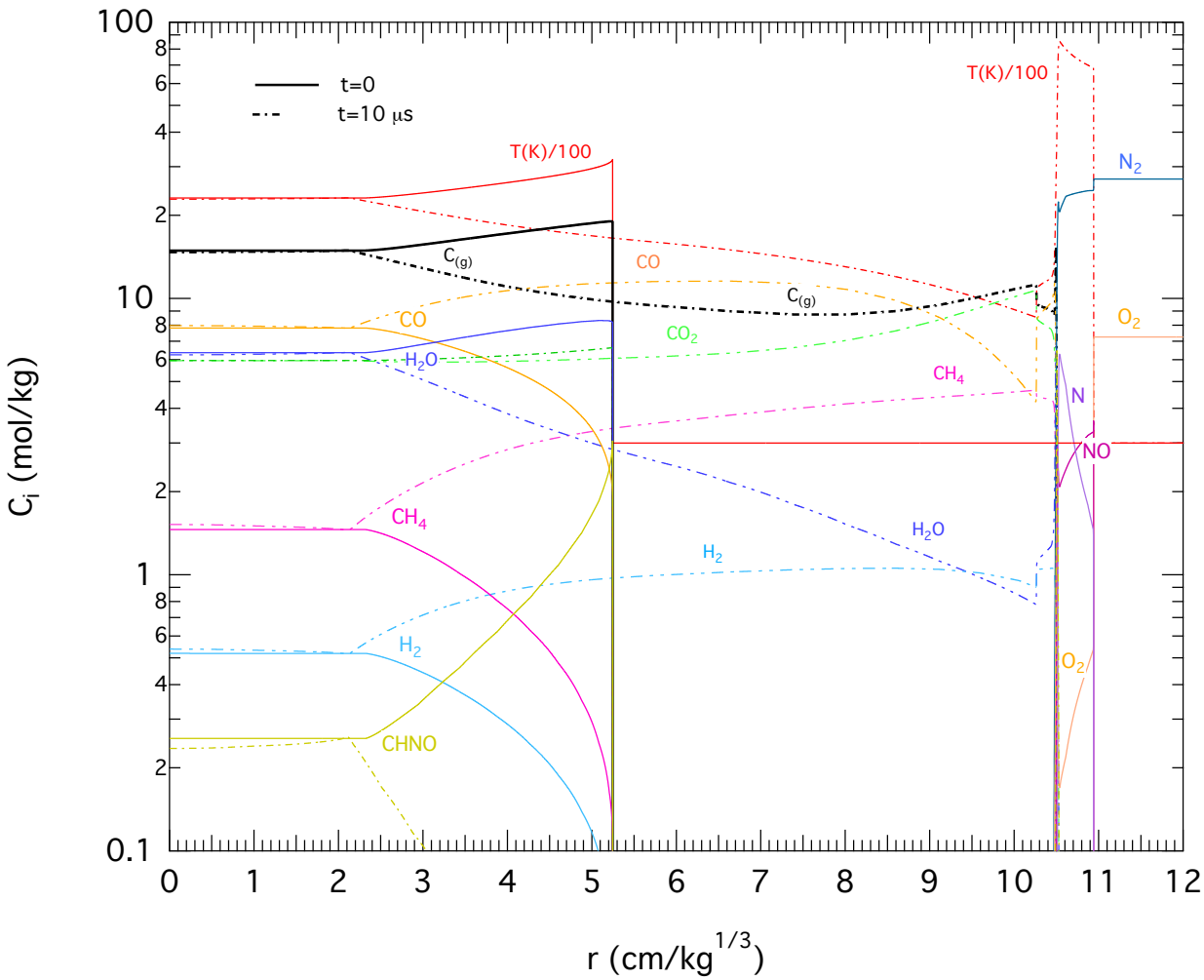

Figure 2a. Species profiles along the CJ isentrope ($S_{CJ} = 1.58$) in the TNT detonation products gases at $t = 0$ and $10\ \mu s / kg^{1/3}$ in a spherical explosion. See Table 2 for this data.

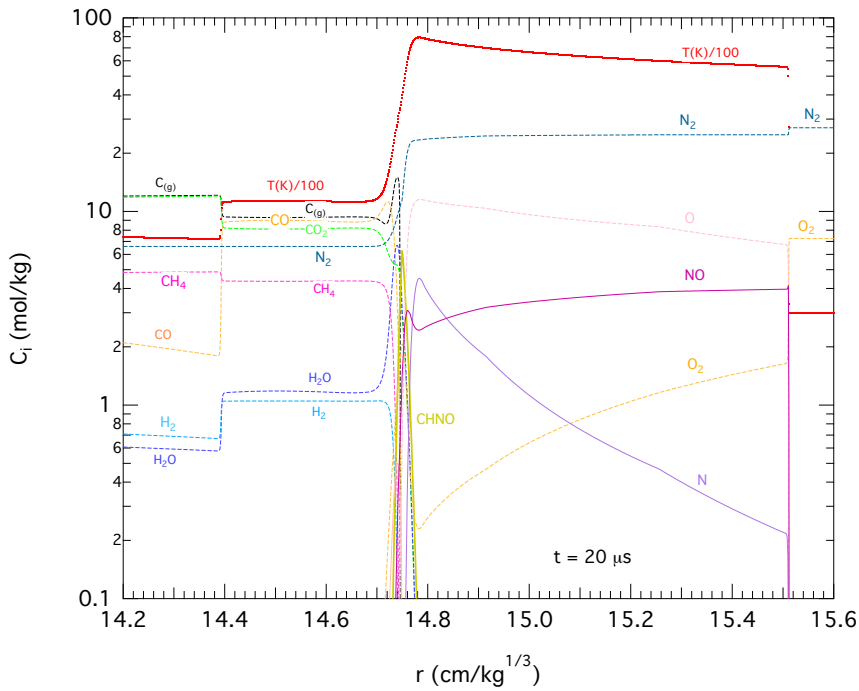

Figure 2b. Species profiles in the shock-heated air layer of the blast wave at $t = 20\ \mu s / kg^{1/3}$. In the shock-heated air layer one finds: N_2, O, NO, O_2 and N at temperatures ranging from 6,000 K to 8,000 K. In the outer layer of the DP one finds: $C_{(g)}$, CO, CO_2, N_2, CH_4, H_2O and H_2 at temperatures ranging from 800 K to 1,200 K. Air molecules will be the dominant radiators.

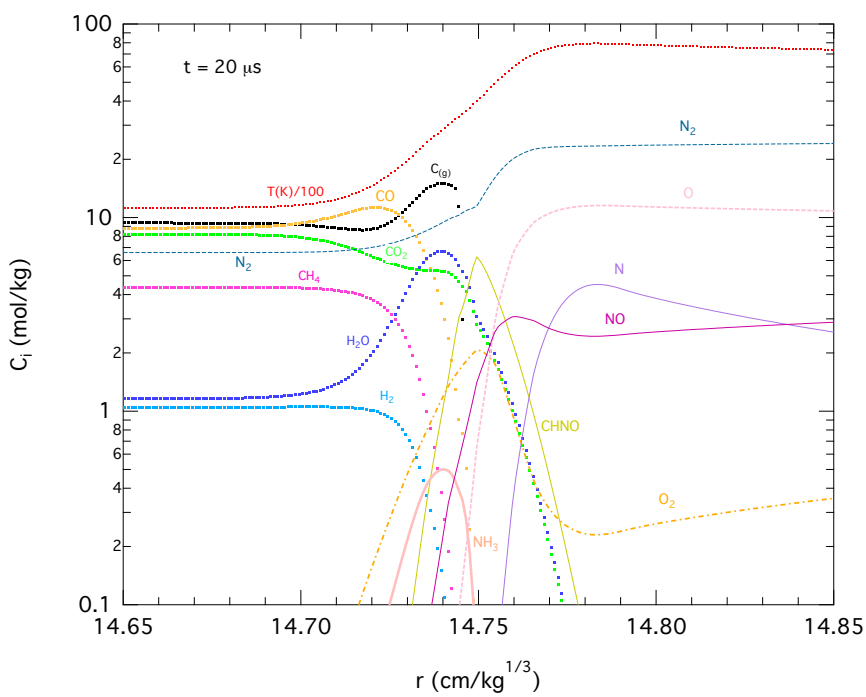

Figure 2c. Blow-up of the DP-air interface region at $t = 20\ \mu s / kg^{1/3}$.

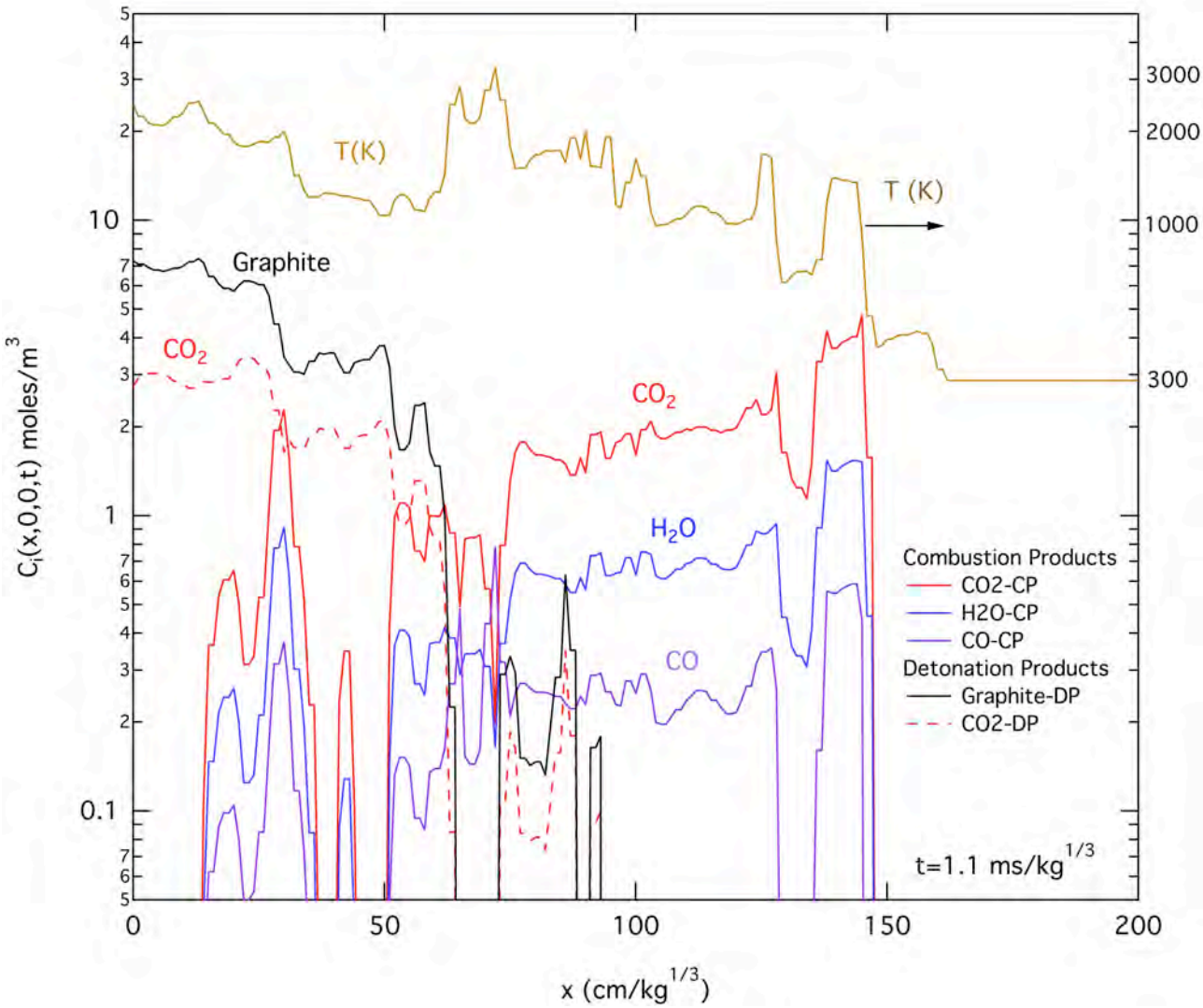

Figure 3. Major species profiles along the *x-axis*, in the turbulent combustion fireball of a TNT explosion at $t = 1.1\, ms / kg^{1/3}$. See Table 3 for this data.