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Modeling thermal ignition and the initial conditions for internal burning in PBX 9501

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Work has been ongoing in our group for several years to produce a thermal ignition model for HMX based plastic bonded explosives valid over the entire temperature range of energetic response. We have made considerable progress recently, resulting in both the first broadly accurate model of this type and the possible identification of a crucial component of the chemical mechanism responsible for thermal ignition and decomposition. I will present a new model of thermal ignition for HMX formulations that is based on this recent progress. The model is similar in kind, but very different in detail from previous models produced by us and others. As has been the case for our previous models it is based entirely on known processes in the decomposition of HMX and is highly constrained by independent measurements. We have applied the model in simple calculations of ignition time over the full temperature range of energetic response for HMX, including directly observed ignition induced by fast shear and compression. I will also present new calculations relevant to the initial conditions for internal burning subsequent to ignition in low boundary temperature thermal explosion experiments. Simplified gas phase chemistry relevant to both dark and bright zone burning in HMX has been included and leads to a second, high temperature and pressure ignition zone in this environment. I will discuss experimental support for these calculations and the ramifications for internal pressures at ignition responsible for driving initial subsonic burning subsequent to ignition.