Estimations of thermal hazards based on calorimetric experiments can be resource consuming. Therefore, reactive hazards predictions using computational techniques are an attractive option. Typically, prior to detailed experimentation, a screening test is performed on the set of potential reactive chemicals using a differential scanning calorimeter (DSC). The screening tests help to focus the resources on the more reactive systems. The onset temperature ($T_o$) and the energy of reaction (- $DH_{rxn}$) are two important parameters obtained from a DSC run.

Prediction of thermal stability requires the knowledge of both the thermodynamics and kinetics for the given system. In this paper, the energy of reaction (- $DH_{rxn}$) is approximated by the maximum enthalpy of decomposition (as calculated by the CHETAH program) and transition state theory (TST) is employed to estimate the decomposition kinetics of aromatic nitro compounds. The activation energy is approximated as a fraction of the bond dissociation energy (BDE), calculated for the C-NO$_2$ bond, at the B3P86 level of theory with the cc-pVDZ basis set. BDE values are also reported from the semi-empirical AM1 theory. These quantum mechanical calculations are combined with an unsteady state model for a batch reactor to predict onset temperatures for nineteen nitro compounds, which are compared with experimental values.