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Calibration of reaction rates for the CREST reactive-burn model

CAROLINE HANDLEY, AWE — In recent years, the hydrocode-based CREST reactive-burn model has had success in modelling a range of shock initiation and detonation propagation phenomena in polymer bonded explosives. CREST uses empirical reaction rates that depend on a function of the entropy of the non-reacted explosive, allowing the effects of initial temperature, porosity and double-shock desensitisation to be simulated without any modifications to the model. Until now, the sixteen reaction-rate coefficients have been manually calibrated by trial and error, using hydrocode simulations of a subset of sustained-shock initiation gas-gun experiments and the detonation size-effect curve for the explosive. This paper will describe the initial development of an automatic method for calibrating CREST reaction-rate coefficients, using the well-established Particle Swarm Optimisation (PSO) technique. The automatic method submits multiple hydrocode simulations for each "particle" and analyses the results to determine the "misfit" to gas-gun and size-effect data. Over ∼40 "generations," the PSO code finds a best set of reaction-rate coefficients that minimises the misfit. The method will be demonstrated by developing a new CREST model for EDC32, a conventional high explosive.

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