Detonation Modelling for the Mining and Quarrying Industries:

Use of the NAG Fortran Library

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In many open cast mining operations, tonnes of explosives are used in individual blasts and there is a strong commercial incentive to optimize blast design. Factors in mining operations include limiting downstream processing costs associated with fines and large boulders, limiting ground vibration and associated damage, avoiding gaseous fume from detonation products and controlling explosive and ancillary accessories (delays, detonators etc.) costs. Blast optimization can be achieved by appropriate choice of blast design (layout, explosive type and quantity, time delays on charges etc). It should be emphasized that cost of a recovery operation from a failed blast can be substantial.

In support of this mining activity, computer models have been developed that combine the steady state detonation aspects of the explosive and the geo-mechanical response of the confining rock media [1]. The work described here is solely concerned with modelling how the explosive and detonation products behave and, in this activity, there has been a need for robust numerical algorithm software and routines from the Nag Fortran library (C05, D02N, E04 chapters). End users will be inclined to run the simulation solver on modest performance computers and failures in the software are not acceptable: they may well be remote from any source of assistance with software failures.

Commercial blasting explosives are heterogeneous and typically comprise of separate oxidizer and fuel with a mechanical sensitizer e.g. a gassed water-in-oil ammonium nitrate based emulsion with gas voids or micro-balloons, ANFO and water-gels. In contrast to high explosives used in defence related applications, the energetic media in this work does not detonate ideally, that is to say its performance cannot be predicted by thermo-hydrodynamic theory [2] alone i.e.

chemical equilibrium is not attained in the detonation process
the detonation state is dependent on charge diameter and confiner: it does not behave linearly with explosive density

the shock front is curved and the detonation reaction zone is comparatively long
there is a critical failure diameter, confiner dependent, below which a detonation cannot be sustained

In terms of numerical simulation the above physics can be divided into two mathematical problems:

(i) the determination of chemical equilibria in multi-phase supercritical media at high temperature and density [3]
(ii) the solution of reactive Euler equations (cylindrical geometry) in 1 and 2-D [4]

The output of these simulations form a source term is the modelling of the whole rock fragmentation and heave process: basically, the geotechnical model requires a pressure history term that describes the pressure the rock experiences at the detonation product/ rock interface during the detonation and subsequent rarefaction.

The first problem that has to be solved is the ideal detonation state and associated isentrope [3]. A fluid equation of state has been developed with a sound statistical mechanical basis and is provided in a Chebyshev polynomial form covering the density-temperature domain of interest. Since solid products are a minor component in these applications a simple Murnaghan Eos form is used [5]. The code using Nag Fortran library routines (E04UCF, CO5NDF) solves a constrained optimization problem for different states of interest and this is of the form:

$\min A(n_{g_i}, n_{s_i} : V, T)$ subject to $0 \le n_{g_i}, n_s \le N_{\max}$

where A is the reduced Helmholz Free Energy: n_{g_i} & n_{s_i} are moles of gas and solid phase species $i : V, T$ represent the total volume and temperature in the system.

The shortcoming of the first calculation is that it does not allow for finite reaction and radial flow against a confining medium: it represents the fastest detonation velocity attainable in rigid confinement/ infinite diameter media. A further simulation is carried out to determine non-ideal detonation behaviour [4]. This requires the solution of steady reactive Euler equations which comprise:

- mass, momentum and energy conservation
- unreacted and product thermodynamic equations of state for a fluid (simplified representations based on ideal detonation isentrope for the products and shock compression data for the unreacted media)
- stress-strain relationship for confiner
- lumped rate expression

Strictly speaking, this second analysis requires the solution of a boundary value problem but an alternative approach based an iterative solution using an initial value problem (using D02NBF) has been developed for this application because of the need for rapid computation. The code runs in two modes. The first fits the rate parameters in the rate expression to measured experimental data, normally based on a set of detonation velocity vs inverse diameter test data in a well defined confinement. The second determines the behaviours of the same explosive, based on the established rate law coefficients but in different confinement (see below).

Figure 1 illustrates typical results with the detonation velocity decreasing with inverse diameter and increasing according to the strength of the confining medium. The asymptotic behaviour in some rocks is due to the influence of the sound wave in the confiner when this exceeds the detonation velocity wave in the explosive: theory is weak in this area !

All the numerical solvers used in this work, with the exception of ODRPACK (NIST, Boulder, USA) [6] has employed Nag routines from the chapters indicated. The computer codes developed, latterly linked to GUIs running under different versions of Windows, are used widely in the mining and explosives industries worldwide with the companies (AEL, DYNO, DeBeers, Sandvik Tamrock, Rio Tinto, LKAB, Anglo American & Codelco) both sponsoring the work and applying the codes to real problems in blast optimization.

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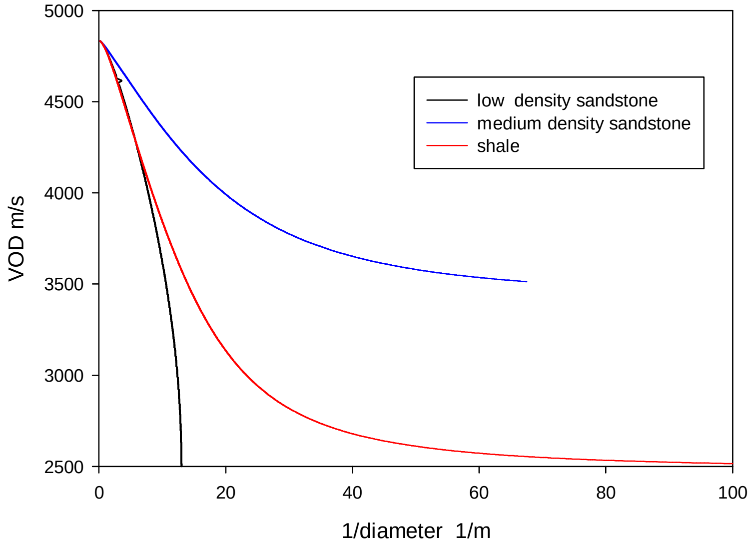

Figure 1 Detonation velocity of a typical ANFO explosive as a function charge diameter in different confinement

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