New Models and Numerical Codes for

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# Shock Wave Processes in Condensed Media

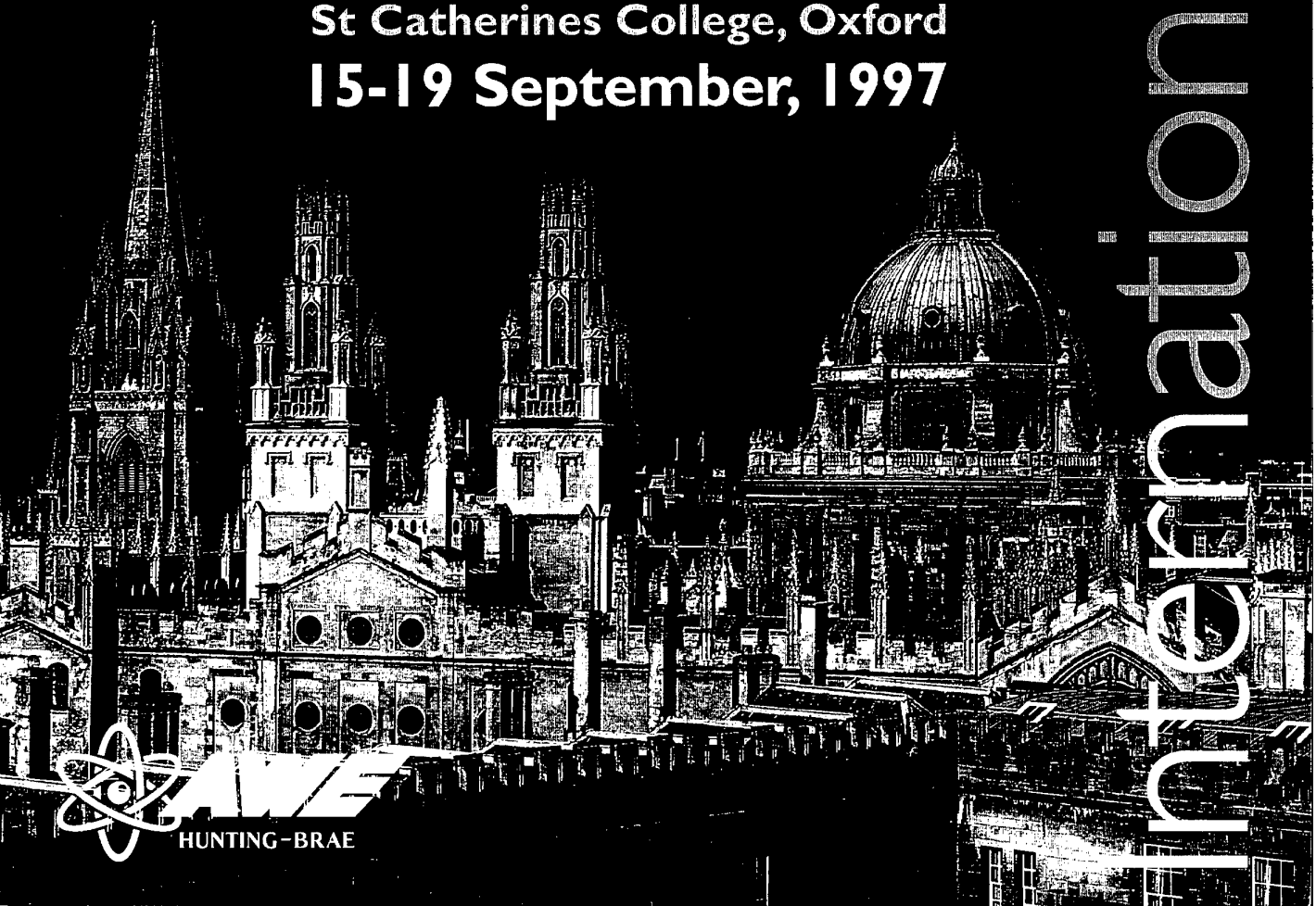
International workshop

## Abstracts

(In presentation order & Poster sessions)

**St Catherines College, Oxford**

**15-19 September, 1997**



AWE

HUNTING-BRAE

*International Workshop*
*on*
*New Models and Numerical Codes*
*for Shock Wave Processes in*
*Condensed Media*

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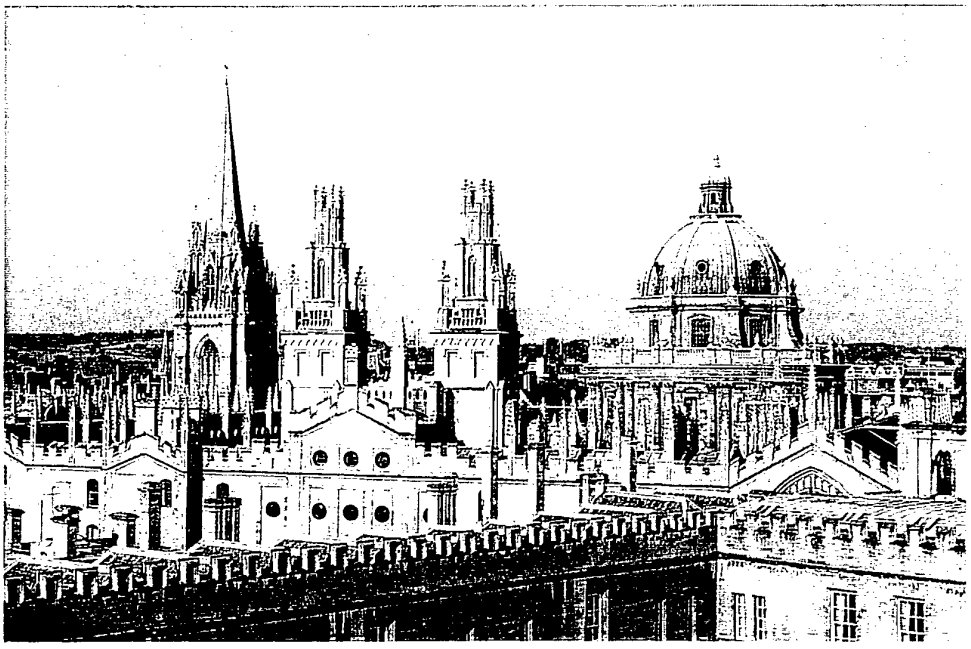



# *ABSTRACTS*

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impractical only few years ago. The large deformations and slow in such problems often require sophisticated numerical rezoning and/or advection procedures that cause diffusion of material EOS (#) parameters and material interfaces. Furthermore, the EOS parameters of interest include not only the classical pressure, volume, and temperature, but also the internal state strength variables that govern the evolution of plastic flow and material failure. Installation of EOS models in hydrocodes is of course very code-specific, and is typically very challenging for complex EOS models. In this paper we confine ourselves to discussing general guidelines for construction EOS models that are as "hydrocode-friendly' as possible.

We focus in this paper on three main guidelines, (1) thermodynamic respectability (obeys the second law), (2) uniqueness (well-posed and independent of cell size and other numeric features), and (3) simplicity (minimisation of model parameters that must be carried in the calculation).

We illustrate the guidelines with examples from mesomechanics.

(*) We use the term "hydrocode" to cover a large range of explicit continuum codes, including free Lagrange, Eulerian, mixed Eulerian-Lagrange, and "smooth particle hydrodynamics" (SPH).

(#) We use the term "EOS" to denote the subroutine that calculated the increment in the complete stress tensor from the increment in the complete strain tensor, i.e. the constitutive relations.

## EQUATION OF STATE IN MATHEMATICAL MODELS OF CONTINUOUS MECHANICS

V F Kuropatenko

Russian Federal Nuclear Center - VNIIEF, Chelyabinsk-70, Russia

The system of conservation laws for mass, momentum and energy is closed by evolutionary equations for processes taking place in a substance and equations of state (EOS) describing the materials properties in stable state. A wide range of physical states and, hence, a wide range of variation of pressure P, temperature T and other thermodynamical parameters are typical for many applied problems (managed thermonuclear fusion, development of antimeteoroid protection for space crafts, accidents in nuclear reactions, etc). EOS should describe material properties with sufficient accuracy in wide range of P, T.

A semiempirical approach for EOS construction is considered in the present work. The form of one of thermodynamical potentials is stated using a theoretical conception. The experimental data are used to determine the numerical values of coefficients in these dependencies. Such approach allows to use the experimental and calculational information and gives an opportunity to construct EOS in the compact form convenient information and gives an opportunity to construct EOS in the compact form convenient for numerical calculations. Mathematical models for the nonstationary dynamical processes impose on EOS the requirements of their effective including into computational procedure. The caloric EOS with regard to pressure P, density p, internal energy E and the thermal EOS with regard to variables P, p, T are considered. The conceptual issues of EOS constructing, the general issues concerning the totality of EOS, the particular EOS for metals, rocks, plastic materials and explosives are presented in the work. A comparison of the developed EOS with the theoretical models and the experimental data are given.

A special consideration is given for the phase transition description. On the phase boundaries many thermodynamical parameters (sonic velocity, compressibility, heat capacity, etc) are discontinue. These discontinuities are the sources of finite errors. To eliminate them one should modify the

difference conservation laws. The ways allowing to restrict the error while simulating flows with phase transition are considered.

## CALCULATION OF SHOCK COMPRESSION DATA AND PHASE DIAGRAM FOR CHLORINE SUBSTITUTED METHANE COMPOUNDS

V V Dremov, D G Modestov

Russian Federal Nuclear Center - VNIIEF, Chelyabinsk-70, Russia

The chlorine substituted methane compounds are of interest because of their application in the so called indicator method that allows to study high-rate processes in shock waves. In the basis of this method there are measurements of shock wave luminosity when the shock wave travelling through a studied sample enters into an indicator. As usually, a chlorine substituted methane compound is used as the indicator. A reliable interpretation of experimental data requires a full description of physical processes in the indicator and a possibility for numerical simulation of hydrodynamic flow in the experimental set up during experiment.

Here we present the physical model which describes the processes in these materials under shock loading and takes into account the experimental conditions.

The variational perturbation theory and an analogue of the Lindemann melting law namely a constancy of packing fraction along a melting curve have been applied for calculation of melting curves for some substituted methane compounds (di-chloromethane, chloroform and tetrachloromethane). The obtained results have been compared with the experimental ones. On the basis of these calculations we have made a conclusion about the nature of the methane compounds transformation under shock compression.

The equation of state for the chlorine substituted methane compounds taking dissociation into account has been constructed on the basis of the variational perturbation theory and the van der Waalse one fluid model. When comparing the calculated Hugoniots with the experimental ones it has been shown that relaxation processes may strongly affect a shape of the experimental Hugoniots. Having provided for the rate of a dissociation reaction it became possible to obtain results that rather well agree with experimental ones.

## WIDE-RANGE HUGONIOTS OF POROUS SUBSTANCES

N N Kalitkin, I V Kuzmina

Institute for Mathematical Modelling, Moscow, Russia

Modern static compressions reach pressures up to 1-2 Mbar. Shock wave experiments give much higher pressures: up to 5-10 Mbar in light gas guns with plane geometry and 25 Mbar in semi-spherical explosion devices (up to 500 Mbar in underground nuclear explosions, but treatment of these measurements is complicated and less reliable).

Dynamic experiments give only Hugoniot but not the whole equation of state (EOS) of substance. At $P < 2$ Mbar it is possible to reconstruct EOS from Hugoniot with descent accuracy using models connecting cold compression curve with heat terms. At larger pressures these models have insufficient accuracy. But one *ab initio* method is known which constructs EOS from a series of Hugoniots for different initial densities.