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Report title
Continuing Numerical Simulations of the Flow in a Closed Electrothermal-Chemical Bomb

Abstract (not more than 200 words)
In the present report continuing numerical simulations of the flow in a closed electrothermal-chemical bomb has been conducted. The work has been concentrated on numerical stabilization of the computational code, local mesh refinement, and on the implementation of a "booster charge emulator". A first set of routines to handle deposition of electric energy has also been implemented.

Keywords
Interior ballistics, numerical simulation, electrothermal-chemical, ETC

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Rapportens titel (i översättning)
Fortsatta numeriska simuleringar av strömningen i en sluten elektrotermisk-kemisk bomb

Sammanfattning (högst 200 ord)
Fortsatta numeriska simuleringar av strömningen i en sluten elektrotermisk-kemisk bomb har genomförts. Arbetet har koncentrerats på numerisk stabilisering av beräkningskoden, lokal beräkningsnätsförfining, och implementationen av en "boosterladdningsemulator". En första uppsättning av rutiner för att hantera deponering av elektrisk energi har också implementerats.

Nyckelord
Innerballistik, numerisk simulering, elektrotermisk-kemisk, ETC

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Contents

1 Introduction

The topic of this report is the present capability to computationally simulate closed bomb firings including electric discharge phenomena, which is necessary for simulating systems that use an electrothermal-chemical (ETC) concept. The computer code is based on an extension of the model presented in [3] and further development of the code used in a previous study [4]. The four simulations described in this report is also fundamental for further development of the code as well as for studying the effects of the usage of different numerical schemes, different combustion models, and couplings in the combustion–acoustics–turbulence-system.

The conducted work has been concentrated on numerical stabilization of the computational code and on a few topics put forward in the authors' previous study, namely the usage of local mesh refinement and the implementation of a "booster charge emulator" to closer mimic the actual physical course of events during the initial stage of the propellant burning. Further, a first set of routines to handle the deposition of electric energy in the combustion volume has been implemented and tested.

The report is organized as follows. Section 2 describes the flow modeling and the numerical methods used in this study. Section 3 is devoted to the specific simulations of two particular ETC bomb firings. The report is rounded up by conclusions in Section 4.

This report was typeset by $\mathcal{AMS}$-LaTeX, the LaTeX macro system of the American Mathematical Society.

2 The Computational Approach

As the flow modeling has been covered at some length earlier, [3, 4], only the flavor of the modeling is given and the system of governing equations is merely stated.

The model is based on the Eulerian approach for multiphase flow, specialized to one gas phase and one non-moving, incompressible solid phase, with the continuum representation of each phase constructed by a volume averaging, denoted $\langle \cdot \rangle$, of the conservation equations for a single phase. It is also assumed that the phases are in local thermodynamic equilibrium with each other and that Fourier heat conduction applies.

As the phase-averaged equations do not reflect the physical properties, but rather pseudoproperties, they must be recasted. A way to proceed is to define intrinsic averages, denoted $\langle \cdot \rangle_i$, by $\langle \psi_k \rangle = \alpha_k \langle \psi_k \rangle_i$ where α_k is the volume fraction of phase k. To make the equations more manageable one also introduces Favré-averaged quantities $\widetilde{\langle \psi_k \rangle_i} = \langle \rho_k \psi_k \rangle_i / \langle \rho_k \rangle_i$, where ρ_k is the density of phase k. The system of equations governing the flow is then

$$
\begin{cases}
\partial_t \langle \rho \rangle_i + \nabla \cdot \left(\langle \rho \rangle_i \widetilde{\langle \mathbf{u} \rangle_i} \right) = 0 \\
\partial_t \left(\langle \rho \rangle_i \widetilde{\langle \mathbf{u} \rangle_i} \right) + \nabla \cdot \left(\langle \rho \rangle_i \widetilde{\langle \mathbf{u} \rangle_i} \widetilde{\langle \mathbf{u} \rangle_i} \right) = -\nabla \langle p \rangle_i + \nabla \cdot \langle \mathbf{S} \rangle_i \\
\qquad\qquad + \dfrac{1}{V} \displaystyle\int_{A_1} \mathbf{S}_1 \cdot \mathbf{n}_1 dA \\
\partial_t \left(\langle \rho \rangle_i \widetilde{\langle h \rangle_i} \right) + \nabla \cdot \left(\langle \rho \rangle_i \widetilde{\langle \mathbf{u} \rangle_i} \widetilde{\langle h \rangle_i} \right) = \langle \dot{p} \rangle_i \\
\qquad\qquad - \nabla \cdot \left(\alpha_1 \langle \mathbf{j}_{q,1} \rangle_i + \alpha_2 \langle \mathbf{j}_{q,2} \rangle_i \right) \\
\qquad\qquad + \alpha_1 \langle \phi_1 \rangle_i + \alpha_2 \langle \phi_2 \rangle_i \\
\qquad\qquad - \dfrac{1}{V} (\kappa_1 - \kappa_2) \displaystyle\int_{A_1} \nabla T \cdot \mathbf{n}_1 dA \\
\qquad\qquad - \dfrac{1}{V} \displaystyle\int_{A_1} (\rho_2 h_2 - \rho_1 h_1) \langle p \rangle_i^n dA \\
\partial_t \alpha_2 = -\dfrac{a}{V} \displaystyle\int_{A_1} \langle p \rangle_i^n dA
\end{cases}
\tag{2.1}
$$

given the same notation as in [4].

The equation of state that is used to close the set of equations is a fourth-order accurate Boltzmann virial expansion, see e.g. [2], for a hard sphere-model of the gas molecules.

As described in a previous report [4], the deposition of electric energy in the combustion volume is given by the Joule heating term P_J, which can be

expressed as

$$P_J = \mathbf{j} \cdot \mathbf{E} = \sigma(\nabla\varphi \cdot \nabla\varphi)$$

where $\mathbf{j}$ is the electric current density, $\mathbf{E}$ the electric field strength, σ the electric conductivity, and φ the electric potential. The electric conductivity, which is temperature dependent, is a material property that is estimated by thermochemical equilibrium calculations using the CEC93 code [5]. The electric potential is calculated using Laplace's equation

$$\nabla^2\varphi = 0 \tag{2.2}$$

in the combustion chamber, with the following boundary conditions: $\varphi = \varphi_0$ on the high-voltage electrode, $\varphi = 0$ on the earthed electrode, and $\frac{\partial\varphi}{\partial\mathbf{n}} = 0$ everywhere else.

To facilitate the calculations, only the part of the electrodes that was in contact with the propellant was included in the simulations. This simplification is not believed to be detrimental to the results, since the major part of the current will be conducted through the region of the flame front. In this model, it is assumed that no arc is formed in the combustion volume. This assumption is consistent with the first few milliseconds after the application of the electric pulsed power.

One important quantity is the total current that is conducted through the combustion chamber. This current, I, can be calculated by

$$I = \int_S \sigma\nabla\varphi \cdot d\mathbf{S} \ ,$$

where S is the area of one of the electrodes.

Just as in [4], the Monotone Integrated LES (MILES) concept has been used in this study in favor of conventional LES modeling. As the details of the MILES approach applied to the equations governing this flow has already been described the reader is referred to the authors' previous study.

3 Closed Bomb Firing Simulations

Continuing numerical simulations of the flow in an ETC bomb similar to the experimental one at FOI, see e.g. [1], have been performed. The differences between the experimental and computational configurations is that the high voltage insulation of Bakelite and part of the electrodes are omitted in this study. The simulations without and with electric discharge phenomena tries to mimic Experiment 41 and Experiment 71 in the ETC experiment test series, respectively, where the propellant is pasted inside the rectangular cavity.

The first simulation was performed on the same mesh as in the previous study, consisting of about $2.2 \cdot 10^5$ cells, with the burning exponent and coefficient for the Saint Robert–Vieille burn law, given by $r = ap^n$ with r being the linear burnt distance of the propellant and p being the pressure, set to $a = 1.533 \cdot 10^{-3}$ m/s and $n = 0.92$, based on data from Experiment 40. This simulation was, just as in the previous study, initialized with zero velocity throughout the computational domain and a uniform pressure of 102.87 MPa and a uniform temperature of 3 148 K in the gas phase. These pressure and temperature figures were computed with the thermo-chemistry computer code CEC93, see e.g. [5], for the specific kind and amount of booster propellant used in Experiment 41. The pressure and the temperature in the solid is initiated with a linear ramping function so that the end of the propellant that is farthest away from the gas–solid interface is at $p = 101.3$ kPa and $T = 300$ K. The computer code was partially rewritten prior to this simulation in order to obtain more numerically stable computations. This goal was achieved and it was then possible to use a twice as large simulation time-step, resulting in substantially shorter computing times; approximately 55 % of the computing time of the previous implementation.

The second simulation was performed on a mesh consisting of about $1.45 \cdot 10^5$ cells where a local mesh refinement had been used in the rectangular cavity and its immediate vicinity. In these parts the mesh is identical to the one used previously, but in the bulk of the combustion chamber the mesh is coarser. All other parameters were the same as in the first simulation. The idea of using local mesh refinement stems from the results of the previous report where it was noted that the flow in the bulk volume seemed to be adequately resolved while the rectangular cavity and its vicinity was under-resolved. As there are no pronounced differences between the results from the first and the second simulation, it seems clear that local mesh refinement can be used to reduce the number of cells in the computation without deteriorating the results. The major advantage is that the computing time of this second simulation is about 70 % of the computing time of the first simulation

in this study.

The third simulation was also carried out on the locally refined mesh, but instead of using the harsh and oversimplified initial conditions used previously a "booster charge emulator" was implemented to closer mimic the actual physical course of events. The booster charge is emulated by "feeding" a cell somewhere in the gas volume with mass for some initial time. The "mass feeding" as a function of time was deduced from data from Experiment 41. The simulation results showed the correct exponential pressure growth although the pressure was somewhat underestimated. This is not too severe as the simulation has only been run on a relatively coarse mesh and this discrepancy may very well disappear on a finer mesh. The most interesting result of this simulation is that the computational time-step had to be reduced to obtain a numerically stable solution. This is, however, not too surprising as the steep pressure rise must be captured, thus implying the need for a good time resolution. As this behavior is rather local in time, it should be possible to use this smaller time-step only during the steep pressure rise period and to use the larger time-step at all other times.

The fourth simulation, which tries to mimic Experiment 71, was run on the same mesh as the first simulation, but with routines for handling the deposition of electric energy in the combustion chamber included in the computer code. This implementation is quite immature at present, but a few things can be deduced from this first simulation including electric energy: As the conductivity is strongly dependent on the temperature, this quantity must be computed with a good accuracy. Coupled to this is also the demand to have a good estimate of the conductivity as a function of temperature. Furthermore, it is not obvious how to implement the surface integral used to calculate the current on an unstructured mesh with both gas and solid phases present. Solving the Laplace equation with the stated boundary conditions, however, is pretty straightforward and poses no actual problems.

4 Concluding Remarks

In this study continuing numerical simulations of the flow in a closed electro-thermal-chemical bomb has been conducted. A partial rewriting of the original code made it more numerically stable, resulting in substantially shorter (almost a factor one half!) computing times, as the computational time-step used could be twice as large. This also alleviates the spectral broadening phenomena in spectral density plots, which was dealt with in the previous study. The other tests and implementation development issues are based on a subset of the "road map" that was built in the previous study of the subject. Most notably is

- The inclusion of a "booster charge emulator" to closer mimic the actual physical course of events, thus remedying the errors originating from the harsh and oversimplified initial conditions of the simulations. The simulation results showed the correct exponential pressure growth although the pressure is a bit underestimated.

- The usage of local mesh refinement in the rectangular cavity and in its immediate vicinity in order to get a sufficient resolution in the combustion zone. It seems clear that local mesh refinement can be used to reduce the number of cells in the computation without deteriorating the results. The major advantage of using this technique is to reduce the computational time.

- A first set of routines to handle the deposition of electric energy in the combustion chamber has been implemented. Laplace's equation is solved and the electric conductivity is estimated by thermochemical equilibrium calculations. Since the conductivity is strongly dependent on the temperature, this property is critical for accurate simulation results. The implementation has to be studied in more detail. For instance, the electric conductivity may be used as a parameter to investigate its influence.

A number of issues put forward in the first study has not been addressed yet and in future studies one should consider the following:

- Several meshes should be used to ensure mesh independency.

- Evaluate the use of higher-order temporal schemes to find out if any pronounced differences arise or if a first order discretization is sufficient.

- Examine if the combustion modeling is sufficient, i.e. if the nonlinearities from the flow and the acoustics dominate over the nonlinearities

inherent in the combustion itself, or if one should resort to more intricate models.

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