Numerical Studies of Shock Reflection and Ignition

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Abstract: A new computational-fluid-dynamics code has been developed for the simulation of hydrogen combustion events concerning hydrogen safety analysis. This code describes the feedback of the flow fields with chemical reactions. It considers detailed chemical kinetics for two-dimensional flow fields. Also it is possible to use a two-step kinetic model for global reaction processes. First validation of calculations were performed for ignition induced by shock reflections from an axis of symmetry and from a flat wall with a long narrow gap. The results show a remarkable agreement. With the two-step model, the experimentally observed physical-chemical phenomena can be reproduced. It is also found that the calculated results are strongly dependent on the kinetic scheme applied. Therefore, several schemes from the literature have been studied.

Introduction

For the safety analysis of nuclear power plants, hydrogen risk is a key issue with respect to the containment failure of Light-Water-Reactors (LWRs)[1]. The reason is the large amount of hydrogen that could be released following a severe accident with core meltdown, mainly produced by the zirconium/steam reaction. High loads on the containment structure could be generated by hydrogen combustion. Depending on the time and frequency scales, the resulting combustion loads inside the containment can be divided into two main categories: static and dynamic loading. Slow deflagrations generate global static pressure loads which could be critical for existing safety systems and containment designs. More dangerous is fast combustion, namely high-speed deflagration, deflagration-to-detonation transition (DDT) and detonation, because this leads to locally strong dynamic effects resulting from the pressure/impulse history.

The development of adequate mitigation measures against hydrogen combustion events needs a clear understanding of all hydrogen combustion sequences: hydrogen production, distribution, ignition and flame propagation. For this purpose, a modern field code cluster (MFCC) on the CRAY computer complex has been established at FZ-Jülich for the numerical simulation of various hydrogen combustion processes, including DDT. To enhance these research activities, a new fluid-dynamics-combustion computer code (SHOCKIN) has been recently developed, based on preparations performed at the Shock Wave Laboratory of the RWTH Aachen. Especially, it adopts detailed chemical kinetic schemes for two-dimensional flow fields.

In this paper, we describe the new code and we present some first test results for validation of the calculations. The calculations were carried out for two kinds of experiments: shock-induced ignition at the entrance of a narrow gap in the end wall of a quadratic shock tube[2] and at the axis of a round shock tube[3].

Description of the SHOCKIN code

SHOCKIN is based on a two-dimensional (planar or axis-symmetric), adaptive Euler/Navier-Stokes solver designed by Yu[4], which has been successfully used to simulate complicated flow structures with shock waves. To extend the application into the area of reactive flow, substantial improvements have been made in the new SHOCKIN. The most important one is the introduction of detailed chemical kinetics. The new code can take into account all species and elementary reactions defined by the user and calculates thermodynamic parameters from a thermodynamic database[5]. It can also use a two-step

kinetic model for the global reaction behaviour. Since an adaptive mesh refinement/unrefinement technique is implemented, a high resolution can be obtained, even with many species.

In SHOCKIN, the governing continuum equations of the viscous, reactive gas flow are written in the following conservative form

$$\vec{U}_t + \vec{F}_x + \vec{G}_y + \vec{H} = \vec{R}_x + \vec{S}_y + \vec{Q} \tag{1}$$

where $\vec{U} = \begin{vmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho \vec{Y} \end{vmatrix}$, $\vec{F} = \begin{vmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uE + up \\ \rho u \vec{Y} \end{vmatrix}$, $\vec{G} = \begin{vmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ \rho vE + vp \\ \rho v \vec{Y} \end{vmatrix}$, $\vec{H} = \frac{i}{y} \begin{pmatrix} \rho v \\ \rho vu \\ \rho v^2 \\ \rho vE + vp \\ \rho v \vec{Y} \end{pmatrix}$,

$$\vec{R} = \begin{vmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ u\tau_{xx} + v\tau_{xy} + \kappa T_x \\ 0 \end{vmatrix}, \vec{S} = \begin{pmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ u\tau_{xy} + v\tau_{yy} + \kappa T_y \\ 0 \end{pmatrix}, \vec{Q} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho \vec{\omega} \end{pmatrix}, \quad \vec{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \cdots \\ Y_N \end{pmatrix}, \vec{\omega} = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \cdots \\ \omega_N \end{pmatrix}, \tag{2}$$

and $\tau_{xx} = (\lambda + 2\mu)u_x + \lambda v_y, \quad \tau_{xy} = \tau_{yx} = \mu(u_y + v_x), \quad \tau_{yy} = (\lambda + 2\mu)v_y + \lambda u_x$, (3)

here p, ρ, T, E, u and v denote pressure, density, temperature, total specific energy and velocity vector components in the Cartesian coordinates, respectively. Y_j and ω_j represent the mass fraction and production rate of jth species. λ and μ indicate coefficients of viscosity, and κ the thermal conductivity. In the above equations $i = 0$ and $i = 1$ correspond to a planar and an axis-symmetric flow.

For the application of a detailed kinetic scheme, the production rate of the jth species is given by

$$\omega_j = \sum_{m=1}^{m=Nr} \left(\nu_{jm}^r - \nu_{jm}^l\right)\left(\omega_{fm} - \omega_{bm}\right), \tag{4}$$

where ν_{jm}^r and ν_{jm}^l are the coefficients of the jth species in the mth reaction on the right- and left-hand side, respectively. The forward and backward reaction rates of the mth reaction, ω_{fm} and ω_{bm}, must be defined by the user. The total specific energy is expressed as

$$E = e + \frac{1}{2}(u^2 + v^2), \tag{5}$$

where e denotes the specific internal energy, which can be calculated according to the thermodynamic database.

In case of utilising the two-step kinetic model, $\vec{Y} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ and $\vec{\omega} = \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix}$. α and β ($0 < \alpha$ and $\beta < 1$) represent the remainder of the progress of the induction reaction and that of the exothermal reaction. The increasing rates of α and β are expressed as

$$\omega_1 = \frac{d\alpha}{dt} = -k_1 \rho \exp(-\frac{E_1}{RT}),$$

$$\omega_2 = \frac{d\beta}{dt} = -k_2 p^2 (\beta^2 \exp(-\frac{E_2}{RT}) - (1-\beta)^2 \exp(-\frac{E_2 + q}{RT})), \quad (6)$$

and the total specific energy is determined by

$$E = \frac{p}{(\gamma - 1)\rho} + q\beta + \frac{1}{2}(u^2 + v^2), \quad (7)$$

where γ indicate the specific heat ratio.

The unstructured triangular meshes used in SHOCKIN are achieved by an implementation of the Voronoi-Delaunay triangulation technique. The classical h-refinement/unrefinement method is utilised adaptively to reconstruct the computation mesh. The governing equation (1) is resolved by a second-order extension of Godunov's approach, including the Piecewise Linear Method. The details of the applied numerical approaches for resolving the gas dynamic problem are described in detail by Yu[4].

For the calculations of chemical kinetic and thermodynamic terms, the subroutines of a chemical kinetic package are applied. A detailed description of the package is given by Kee et. al[5].

Shock reflection from an entrance of a narrow gap

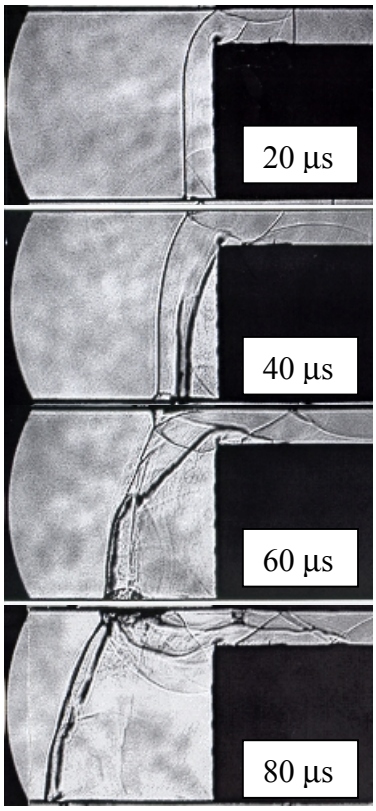

Fig. 1 Experimental schlieren pictures of shock-induced ignition at a gap entrance (mixture: 15%H_2 +85%air; initial pressure: 4 kPa; initial temperature: 293 K; incident shock Mach-no.: 2.87; gap height: 10 mm).

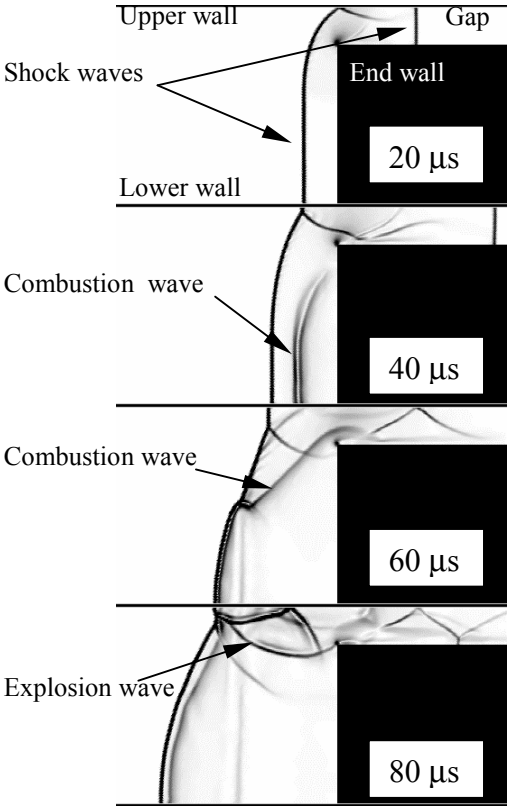

Fig. 2 Numerically simulated schlieren pictures produced with the fluid-dynamics-combustion code SHOCKIN. (Conditions and time step correspond to Fig. 1).

The first calculations for the validations of the SHOCKIN code were performed for experimental results with a series of schlieren pictures (see Fig. 1) which were obtained in a lean H_2-air mixture in a square shock tube with a long gap in the flat end wall. The times at which the photographs were taken after a shock wave originally propagating from left to right had reached the entrance of the gap are marked on the pictures in Fig. 1. This experiment is chosen because of the unsteady high temperature and density gradients which are induced by shock reflections and the interaction between a shock wave and a rarefaction fan. The ignition in such flow fields with changing thermodynamic conditions is an ideal example for validating the reaction model for a wide range.

By adjusting the parameters in the two-step model excellent results are achieved. The simulated schlieren pictures are shown in Fig. 2. In the first frame at t = 20 μs, the main part of the incident shock wave is reflected from the end wall and the rest propagates into the narrow gap. In the second frame at t = 40 μs, a combustion wave can be seen, which is initiated at the end wall due to the compression effect of the reflected shock. In front of the flame front there is a series of pressure waves or a weak shock wave. The combustion wave overtakes the reflected shock in the third frame at t = 60 μs. The overtaking process remains a vertical contact surface which can be also seen at t = 80 μs. The reflection of the weak shock, generated by the flame, at the upper wall of the tube leads to a second ignition zone and a subsequent explosion wave, as can be seen in the last frame. In the gap there are some stationary and nonstationary oblique shock waves. All these phenomena are in good agreement with the experimental observation.

With detailed chemical kinetics the code performs quite well, but the result is strongly dependent on the kinetic scheme applied. Several schemes from the literature have been tested for hydrogen combustion and similar results, as in Fig. 2, are obtained, but a more complete simulation needs an improved kinetic scheme of hydrogen combustion, which is under investigation.

Shock reflection from an axis of symmetry

Another validation test case of calculation was performed for an experiment in an axis-symmetric system. As shown in Fig. 3, a shock wave moves from left to right in a round shock tube. When the shock wave enters the ring obstacle, a bow-shaped reflected shock wave is generated on the surface of the conic inlet. The reflected shock wave will be further converged and reflected at the axis of the tube. This can lead to ignition at the axis.

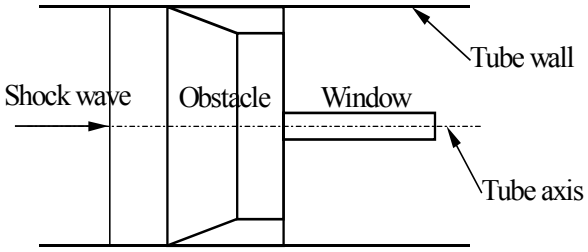

Fig. 3 Sketch of the experiment geometry.

Depending on the initial conditions, different shapes of the ignition zone were observed[3]. A typical case is shown in Fig. 4. The obstacle is located at the left-hand side of the pictures. The thickest vertical line on the pictures is the front of the incident shock. Between the leading shock and the obstacle there are some other vertical lines which are induced by vortex behind the obstacle and shock reflections at the tube wall. The ignition takes place along the axis, and appears coarsely as a long horizontal zone. The most difficult aspect to explain concerning the shape of the ignition zone is the head, which looks like a hat. This question is clarified by the numerical simulation with SHOCKIN. The shape is induced by a jet along the axis, as can be seen in Fig. 5. This jet results from the meeting of two shock reflection regions, which occurs before the picture shown in Fig. 5.

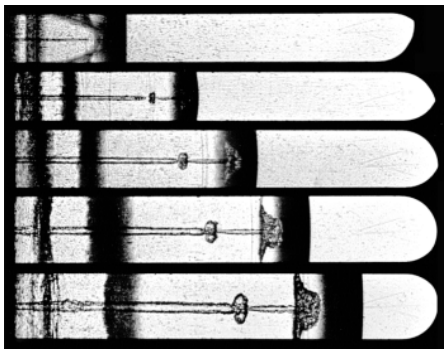

Fig. 4 Experimental schlieren pictures of shock-induced ignition at a tube axis (mixture: 20.1%H_2 +79.9%air; initial pressure: 0.1 MPa; initial temperature: 293 K; incident shock Mach-no.: 1.84; width of the optical window: 20 mm).

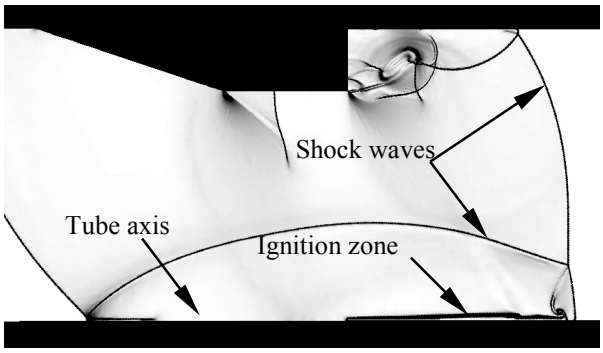

Fig. 5 Numerical simulation (density gradient in axis-radius plane) of the hat-shaped head of the ignition zone in Fig. 4 with SHOCKIN. (Conditions correspond to Fig. 4, t = 30 µs).

Conclusions

A new two-dimensional CFD code (SHOCKIN), which describes the feedback of the flow fields with chemical reactions, has been successfully developed. This code takes into account all species and elementary reactions defined by the user, or uses a two-step kinetic model for the global reaction processes. First test cases for validation of the calculations were carried out for experimental results with schlieren pictures obtained in a square and a round shock tube. The results show that the code works quite well. With the two-step model, the experimentally observed physical-chemical phenomena can be reproduced. It is also found that the calculated results are strongly dependent on the kinetic scheme applied. Several schemes from the literature for hydrogen combustion have been tested. A more complete simulation needs an improved kinetic scheme of hydrogen combustion, which is under investigation. By means of the SHOCKIN code experimental results with complicated phenomena can be explained in more detail.

References

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