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Numerical Simulation of
Shock Wave Structure in Gas Explosion

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Abstract

In order to study the characteristics of gas explosion in coal mine, on the basis of theoretical analysis and experimental research, the ignition and propagation characteristics of gas explosion is simulated by the introduction of elementary chemical reaction. This essay is also on the research of the transmission and simulation characteristics of exploration flame in an barrier tube. Especially the 17-component, 58-step chemical reaction modeling is introduced. The results of simulation match with theoretical analysis and experimental research. In order to provide effective argument for the investigation of gas explosion, field exploration and the reconstruction of the accident.

1. Introduction

1.1. Significance of the numerical simulation of gas explosion

At present, the theory system of gas explosion is not perfect; especially the mechanism of shock wave generated by the explosion is still not well-argued. Moreover, in consideration of the actual conditions,
there are still limitations pertaining to the scale and the comprehensiveness of the test [1]. Numerical simulation is the extension of theoretical and experimental researches, which can make up for these deficiencies as well as provide a complementary form [2]. Compared to the theoretical and experimental research, numerical simulation has the advantages of being effective and economical [3,4]. With the ever-growth of computer technology and computation fluid mechanics and computation fuel study, more precision and economics have been introduced. Numerical simulation has hence become an important method of the reproduction and the research for explosion. Meanwhile, the information provided by numerical simulation is not available from the experimental tests [5,6,7,8,9,10].

1.2. Numerical calculation of the structure of the gas exploration wave

Currently, there are several main difficulties in the calculation of gas explosion.

The complexity of the interior tube structure (including barrier), the computational grid which approach to the barrier and focus on the ignition point would be numerous. Therefore, the calculation of integrated flow field is huge.

The mechanism of methane combustion is complicated. Also the ignition of methane usually involves hundreds of elementary chemical reactions.

The ignition of hydrocarbon fuels is difficult, and the ignition delay (chemical delay) of hydrocarbon fuels is long. The physical and chemical processes of ignition are also quite complicated. Strictly speaking, the ignition is an unsteady process and usually placed in the sealed end. Also, there are usually vortexes in the tubes, namely the oscillation flow. The diversity of ignition might give rise to the difficulty of the description, which inevitably affects the calculation of the fuel chamber.

To solve all of the above, a computer package which can deal with a large variety of elementary chemical reaction in gas explosion is needed. That is, however, what this essay is focused on.

2. Simulation examples

2.1. Physical modeling

The experimental testing system of gas explosion is shown as Figure 1, which includes ignition controller, tube of methane explosion experiment, pressure relief tank, measurement system of explosion pressures and flame data system, gas distribution system, laser trigger delay systems, laser schlieren system, etc.

Figure 1: The structure of experimental testing system
Tube segment is made up of ignition section (ignition flange and ignition), transition section, experimental section and vacuum chamber (vacuum before the experiment) which could be connected by membrane to keep the experiment safe. Gas, data acquisition and power cables are isolated from each other by a trench and placed on control panel with gas supply system. Test section and transition section are both equipped with optical window for flow visualization and spectral measurements (components, temperature). Continuous and pulsed laser light sources are designed for flow visualization in order to obtain a single and continuous (high-speed photography) imaging of the combustion flow field. Measurement and data acquisition system of multi-channel pressure (piezoelectric and piezoresistive sensors) and flame speed are designed. The designed diaphragm can be used to measure strong deflagration and detonation. In the height-adjustable stand, pipe supports are located in a fixed track to ensure flexible movement both back and forth. For the safety of experiments, CCD monitoring system, alarm lights, alarm reminder system are also designed.

2.2. Mathematical modeling

The three-dimensional unsteady, viscous, compressible gas mixture explosion can be established as the following mathematical modeling [1].

\[
\frac{\partial Q_k}{\partial t} + \frac{\partial E_k}{\partial x} + \frac{\partial F_k}{\partial y} + \frac{\partial G_k}{\partial z} = \frac{\partial E_{g,v}}{\partial x} + \frac{\partial F_{g,v}}{\partial y} + \frac{\partial G_{g,v}}{\partial z} + S \tag{1}
\]

2.2.1. Ignition modeling

Internal combustion engine ignition modeling (similar to the way the spark discharge), i.e. to incorporate a certain internal energy in designated area at certain times:

\[
E^{n+1} = E^n + (\rho \cdot C_p \cdot \Delta T)^n \tag{2}
\]

In which, \( \Delta T \) is decided by the numerical experiments.

2.2.2. Chemical reaction modeling

In this essay, 17-component, 58-step reaction modeling is used to describe CH4/O2 fuel chemical reactions, which accurately simulated ignition of combustion and flow component of heat release base. Specifically listed in Table 1:

Table 1: Chemical component of CH4/O2/N2 reaction system
2.3. Numerical scheme

2.3.1. Discretion of equation

Gas equation applies implicit LU for decomposition, in which uses 2-step upwind TVD scheme for explicit convection-order and centered difference for diffusion. Chemical source term is processed by implicit.

Phase interaction terms are not considered in equation for the gas phase, only the N-S discretion of equation is considered for description of chemical reaction flow.

\[
\frac{\partial Q_i}{\partial \tau} + \frac{\partial E_i}{\partial \xi} + \frac{\partial F_i}{\partial \eta} + \frac{\partial G_i}{\partial \zeta} = \left( \frac{\partial E_{i,\nu}}{\partial \xi} + \frac{\partial F_{i,\nu}}{\partial \eta} + \frac{\partial G_{i,\nu}}{\partial \zeta} \right) + \hat{S}
\]

For the chemical reaction flow, the characteristic time of chemical reaction is much shorter than characteristic time of flow. Sometimes the difference could be several orders of magnitude. Therefore, in solving equation (3), rigid questions of the chemical reaction source terms might be encountered. For equation (3), the size of rigidity can be defined by Damkohler numbers.

\[
D_a = \frac{\tau_{flow}}{\tau_{chem}}
\]
In which $\tau_{flow}$, $\tau_{chem}$ are the characteristic time of flow and chemical reaction, each elementary reaction has its own Damkohler number, $D_a$ of the entire system is depend on the elementary reaction which consume the shortest characteristic time. And for rigidity problem, $D_a >> 1$.

There are two approaches for the rigidity problem. One is called the decoupling method, i.e. to decouple the oncoming chemical reactions (mainly in the components of the source terms of the equation) and the flow equations. In each time step, the first step is to freeze chemical reaction to compute the flow field, then to solve chemical reaction without consideration of the impact of the flow field. Of which, the advantage are not only easy to implement and take respectively numerical method for flow field and chemical reactions, but also to solve multi-step chemical reaction even in a flow field time step. But when the chemical non-equilibrium is violent, the flow-field coupling and the decoupling methods might show poor stability, convergence problems and other shortcomings. Fully coupled approach i.e. to solve the equations of chemical reactions and flow control simultaneously is more stable than the decoupling method, which is just used in this essay. As the chemical reaction characteristic time is much shorter than the characteristic flow time, so if you want to solve the flow field and chemical reactions simultaneously, chemical reactions must be implicit processing. Coupling methods mainly include the whole point of implicit and fully implicit, which are all involved in the calculation of this essay.

Another feature of Supersonic combustion flow field is that shock is included in the flow field. High-precision shock capturing format convection is required to capture the shock wave, and 2-order central difference is used for viscous term.

### 2.3.2. Mesh generation

Orthogonality of the grid, the grid and the continuity of the derivative of the grid will result in numerical oscillations, convergence consequences, even failure of calculation, so the generation of a good mesh is vital to the success of the calculation. There are mainly three categories of generation methods for structured grid: algebraic methods, analytical methods and differential equation methods. The algebraic method is easy to calculate and facilitate the grid distribution control, but difficult to ensure the continuity of the derivative for complex boundary. Orthogonality is difficult to ensure the continuity of the derivative, too.

For complex areas, the approach is: algebraic methods is used for the initial mesh, attracting to the walls, barrier as well, while for complex computational domain, in order to ensure orthogonality of the grid, the solution of Laplace equation is demanded for the correction of initial grid.

### 2.4. Results analysis

As illustrated in Table 2:

<table>
<thead>
<tr>
<th>conditions</th>
<th>Static pressure (KPa)</th>
<th>static temperature (K)</th>
<th>with / without barrier</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>112.81</td>
<td>300</td>
<td>no</td>
</tr>
<tr>
<td>Case 2</td>
<td>112.81</td>
<td>300</td>
<td>yes</td>
</tr>
</tbody>
</table>

As illustrated in Figure 2 (a), (b) and (c) are the flame Schlieren and simulation results of methane explosion under the condition of no barrier.
From the schlieren and simulation results of explosion flame taken at different times, the whole explosion of methane flame is not continuous, partial or pull-off along (intermittent) phenomenon exists also, and non-reaction air exists between the flame cross-section air mass; It is these non-equilibrium process that the explosion of methane is the combined reaction of hot and chain reaction and the state of chemical reaction vary with the strength of shock wave, leads to the change of the gas amount after wave of change, which is exactly accordance with experimental observations and furthermore illustrates the chemical reaction as well as positive incentive effects of blast.

As illustrated in Figure 3 (a) and (b) are the flame Schlieren and simulation results of methane explosion under the condition of barrier
Figure 3 experimental simulation control chart of flame and barrier effect
Barrier has relatively greater impact on shock wave structure and propagation of explosive flame when methane is under the propagation of weak explosion. Explosion flame front curled around barrier, and inside the flame wave has produced a significant disturbance, forming vortex in flow field of explosion and increasing flow turbulence of explosion, which indicate the barrier in the flow field of methane explosion exacerbated the transformation of large turbulent flow and small vortex, hence making the large-scale fluctuations of vorticity and turbulent energy transfer to the pulse of a small vortex. This results in a substantial acceleration of explosion flames spread forward.

3. Conclusion

Through optical diagnostics of explosion flow and electrical measurements of explosion parameter, the non-continuity of the flame, partially pull off (intermittent) phenomenon and no reaction between the flame cross-section air mass are all confirmed.

The flame of methane explosion accelerate small under the conditions of no barrier, whose acceleration mechanism is due to chemical reaction of methane from the explosion incentive and the energy released by the wave-driven is an acceleration of flame propagation. While under barrier conditions, the transmission speed of fire blast increases through the barrier. The very reason why barrier have a significant impact on the acceleration of on flame propagation is mainly because that the presences of barrier increased turbulent flow, making the explosion reaction rate to accelerate.

The comparison of experimental result and numerical simulation structure are basically consistent, which verify the reliability simulating gas explosion program with the chemical reaction.

References


