The Numerical Simulation of the Shock Wave of Coal Gas Explosions in Gas Pipe*

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Abstract: For the problem of large deformation and vortex, the method of Euler and Lagrange has both advantage and disadvantage. In this paper we adopt special fuzzy interface method(volume of fluid). Gas satisfies the conditions of conservation equations of mass, momentum, and energy. Based on explosion and three-dimension fluid dynamics theory, using unsteady, compressible, inviscid hydrodynamic equations and state equations, this paper considers pressure gradient's effects to velocity, mass and energy in Lagrange steps by the finite difference method. To minimize transport errors of material, energy and volume in Finite Difference mesh, it also considers material transport in Euler steps. Programmed with Fortran PowerStation 4.0 and visualized with the software designed independently, we design the numerical simulation of gas explosion with specific pipeline structure, check the key points of the pressure change in the flow field, reproduce the gas explosion in pipeline of shock wave propagation, from the initial development, flame and accelerate the process of shock wave. This offers beneficial reference and experience to coal gas explosion accidents or safety precautions.

1. Introduction

In recent years, people have done many researches on the gas Explosion. Zhiyuan Wu derived the theoretical maximum values in different gas volume fraction, compared with the data of field experiments, and then discussed the relation between the gas concentration and explosion pressure, and reasoned out the conclusion that explosive pressure decreases towards two sides of optimal gas concentration[1-2]. Liang Zhang and others researched gas mixture features of air and carbon monoxide*(CO)* in placing obstacle pipe under different initial temperature. The flame speed and deflagration pressure increased quickly in the site of obstacle. When *CO* equivalence ratio is 1.1, the deflagration pressure reaches the maximum, and with increasing of temperature, pressure buildup slow down about 550m/s[3]. Bangzhi Zhou researched the explosion limit of the gas mixture of air and coal

gas[4]. Juanjuan Luo and others analyzed the gas mixture explosion limit in enclosed space, and analyzed the influence of oxygen content and inert gas to the explosion limit[5]. In 2001, based on the finite difference method, Yuling Shen and others used fluid in cell method to make numerical simulation of gas explosion in 2D visualization software, and analyzed the numerical simulation result, visualize the gas explosion procedure[6]. Because of the practical living space is 3D, the 2D axisymmetric appearance is limit to object and angle of view. We need 3D numerical simulation method to research the gas explosion, to visualize the real gas explosion procedure, to get all of features of the gas explosion, including the shock wave spread characteristic. After that we can defend and control explosion accidents, and minimize the losses.

2. Model and numerical method

A fluid model is adopted, and its basic equations are composed by conservation equations of mass, momentum, energy, and state equations. There are inviscid, no heat conduction, and ignore force of gravity partial difference equations of 3D-unsteady compressible flow[7]:

The conservation equation of mass:

$$\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \tag{1}$$

The conservation equations of momentum:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = \frac{1}{\rho}(-\frac{\partial(P-S_x)}{\partial x} + \frac{\partial S_{xy}}{\partial y} + \frac{\partial S_{xz}}{\partial z}) \tag{2}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = \frac{1}{\rho}(-\frac{\partial(P-S_y)}{\partial y} + \frac{\partial S_{xy}}{\partial x} + \frac{\partial S_{yz}}{\partial z}) \tag{3}$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = \frac{1}{\rho}(-\frac{\partial(P-S_z)}{\partial z} + \frac{\partial S_{xz}}{\partial x} + \frac{\partial S_{yz}}{\partial y}) \tag{4}$$

The conservation equation of energy:

$$\rho[\frac{\partial e}{\partial t} + u\frac{\partial e}{\partial x} + v\frac{\partial e}{\partial y} + w\frac{\partial e}{\partial z} = -[(P-S_x)\frac{\partial u}{\partial x} + (P-S_y)\frac{\partial v}{\partial y} + (P-S_z)\frac{\partial w}{\partial z}] +$$

$$S_{xy}(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}) + S_{xz}(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}) + S_{yz}(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}) \tag{5}$$

Where ρ is the density; u, v and w are the velocity on these directions of x, y and z respectively; P is the pressure; e is the specific internal energy; $S_{xx}, S_{yy}, S_{zz}, S_{xy}, S_{yz}$, and S_{zx} are the partial stress.

When the finite difference method is adopted to solve discrete equation, the shock wave spreads to produce strong discontinuity. In order to get smooth solutions, artificial viscosity pressure is used. The method is the following:

$$q_x = \rho(\left|\Delta u_x\right| - \Delta u_x) \cdot (a_n(\left|\Delta u_x\right| - \Delta u_x) + b_n \cdot c) \tag{6}$$

$$q_y = \rho(\left|\Delta v_y\right| - \Delta v_y) \cdot (a_n(\left|\Delta v_y\right| - \Delta v_y) + b_n \cdot c) \tag{7}$$

$$q_z = \rho(\left|\Delta w_z\right| - \Delta w_z) \cdot (a_n(\left|\Delta w_z\right| - \Delta w_z) + b_n \cdot c) \tag{8}$$

Where a_n, b_n is the second-order artificial viscosity and first-order viscosity coefficient, c is a constant relative to media.

The state equation of air and gas:

$$p = (k_\alpha - 1)e\rho \tag{9}$$

k_α is the isentropic index of gas, ρ is the instantaneous density, e is the specific internal energy.

The method of numerical calculation and simulation is "sum" splitting finite difference pattern. Time is the forward difference, and space is the centered difference. Firstly, we consider pressure effect in Lagrange's steps, suppose that there are not transports of mass, calculations of material velocity, specific internal energy, momentum, and energy. Secondly, we consider transport of material in Euler's steps, calculate transport value: mass, momentum, and energy. The disposal of material interface is fuzzy interface methods[8-9].

In order to calculate boundary, we add a row of virtual grids. For rigid wall boundary, the shock wave is total reflection; for free continuum boundary, we use extrapolation to calculate physical quantity; for free boundary far away from the explosion center, physical quantity is equal to zero; the empty grids is the same as the free boundary.

The approximation formula of solutions of momentum equation (2), (3) and (4) is as follow:

$$\tilde{u}_{ijk}^{(n+1)} = u_{ijk}^{(n)} - (\Delta t^n / \rho_{ijk})\{[(p+q^{(x)}-S_x)_{i+1/2,j,k}^{(n)} - (p+q^{(x)}-S_x)_{i-1/2,j,k}^{(n)}]/\Delta x_i$$

$$+ [S_{xyi+1/2,j,k} - S_{xyi-1/2,j,k}]\Delta y_j + [S_{xzi,j,k+1/2} - S_{xzi,j,k-1/2}]/\Delta z_k\} \qquad (10)$$

$$\tilde{v}_{ijk}^{(n+1)} = v_{ijk}^{(n)} - (\Delta t^n / \rho_{ijk})\{[(p+q^{(y)}-S_y)_{i,j+1/2,k}^{(n)} - (p+q^{(y)}-S_y)_{i,j-1/2,k}^{(n)}]/\Delta y_j$$

$$+ [S_{xyi+1/2,j,k} - S_{xyi-1/2,j,k}]\Delta x_i + [S_{yzi,j,k+1/2} - S_{yzi,j,k-1/2}]/\Delta z_k\} \qquad (11)$$

$$\tilde{w}_{ijk}^{(n+1)} = w_{ijk}^{(n)} - (\Delta t^n / \rho_{ijk})\{[(p+q^{(z)}-S_z)_{i,j,k+1/2}^{(n)} - (p+q^{(z)}-S_z)_{i,j,k-1/2}^{(n)}]/\Delta z_k$$

$$+ [S_{xzi+1/2,j,k} - S_{xzi-1/2,j,k}]/\Delta x_i + [S_{yzi,j+1/2,k} - S_{yzi,j-1/2,k}]/\Delta y_j\} \qquad (12)$$

The central difference method:

$$P_{i-1/2,j,k} = (P_{i-1,j,k}\Delta x_i + P_{i,j,k}\Delta x_{i-1})/(\Delta x_i + \Delta x_{i-1})$$

If the consistency or mass of some media is smaller than specified value, then physical quantity F_θ is equal to zeros, that is, empty grid. If the boundary is rigid wall or axis of symmetry, physical quantity F_θ gets the value of central grids. Time steps calculate as follow (satisfying CFL condition*):

$$\Delta t = \Gamma \min[\frac{\Delta x}{|u_x|+1.4}, \frac{\Delta y}{|v_y|+1.4}, \frac{\Delta z}{|w_z|+1.4}] \qquad (0 < \Gamma < 1.0) \qquad (13)$$

The algorithm of internal energy increments:

$$\Delta e_{ijk} = \Delta t^n /(\rho_{ijk}\Delta x_i)[\bar{U}_{ijk}(q_{i+1/2,j,k}^{(x)} - q_{i-1/2,j,k}^{(x)}) - \bar{U}_{i+1/2,j,k}(p_{ijk}+q_{i+1/2,j,k}^{(x)}) + \bar{U}_{i-1/2,j,k}(p_{ijk}+q_{i-1/2,j,k}^{(n)})]$$

$$+ \Delta t^n /(\rho_{ijk}\Delta y_j)[\bar{V}_{ijk}(q_{i,j+1/2,k}^{(y)} - q_{i,j-1/2,k}^{(y)}) - \bar{V}_{i,j+1/2,k}(p_{i,j,k}+q_{i,j+1/2,k}^{(y)}) + \bar{V}_{i,j-1/2,k}(p_{i,j,k}+q_{i,j-1/2,k}^{(y)})]$$

$$+ \Delta t^n /(\rho_{ijk}\Delta z_k)[\bar{W}_{ijk}(q_{i,j,k+1/2}^{(z)} - q_{i,j,k-1/2}^{(z)}) - \bar{W}_{i,j+1/2,k}(p_{ijk}+q_{i,j,k+1/2}^{(z)}) + \bar{W}_{i,j,k-1/2}(p_{ijk}+q_{i,j,k-1/2}^{(z)})]$$

$$+ \Delta t^n /(\rho_{ijk}\Delta x_i)[S_{xijk}(\bar{U}_{i+1/2,j,k} - \bar{U}_{i-1/2,j,k}) + S_{xyijk}(\bar{V}_{i+1/2,j,k} - \bar{V}_{i-1/2,j,k}) + S_{xzijk}(\bar{W}_{i+1/2,j,k} - \bar{W}_{i-1/2,j,k})]$$

$$+ (\Delta t^n \rho_{ijk}\Delta y_j)[S_{yijk}(\bar{V}_{i,j+1/2,k} - \bar{V}_{i,j-1/2,k}) + S_{xyijk}(\bar{U}_{i,j+1/2,k} - \bar{U}_{i,j-1/2,k}) + S_{yzijk}(\bar{W}_{i+1/2,j,k} - \bar{W}_{i-1/2,j,k})]$$

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* Courant, Friedrichs and Lewy in 1928 firstly presented convergence of difference method, and got convergence condition of explicit difference method.

$$+\Delta t^n /(\rho_{ijk}\Delta z_k)[S_{zijk}\left(\overline{W}_{i,j,k+1/2}-\overline{W}_{i,j,k-1/2}\right)+S_{xzijk}\left(\overline{U}_{i,j,k+1/2}-\overline{U}_{i,j,k-1/2}\right)+S_{yzijk}\left(\overline{V}_{i,j,k+1/2}-\overline{V}_{i,j,k-1/2}\right)]$$

(14)

Here

$$\overline{U}_{ijk}=(U_{ijk}+\tilde{U}_{ijk})/2 \quad,\quad \overline{V}_{ijk}=(V_{ijk}+\tilde{V}_{ijk})/2 \quad,\quad \overline{W}_{ijk}=(W_{ijk}+\tilde{W}_{ijk})/2,$$

$$\overline{U}_{i\pm\frac{1}{2},j,k}=(\overline{U}_{ijk}\Delta x_{i\pm1}+\overline{U}_{i\pm1jk}\Delta x_i)/(\Delta x_i+\Delta x_{i\pm1}),\quad \overline{V}_{i,j\pm\frac{1}{2},k}=(\overline{V}_{ijk}\Delta y_{j\pm1}+\overline{V}_{ij\pm1k}\Delta y_j)/(\Delta y_j+\Delta y_{j\pm1}),$$

$$\overline{W}_{i,j,k\pm\frac{1}{2}}=(\overline{W}_{ijk}\Delta z_{k\pm1}+\overline{W}_{ijk\pm1}\Delta z_k)/(\Delta z_k+\Delta z_{k\pm1})$$

Internal energy increments are allocated by the volume fraction:

$$\tilde{e}_{ijk}^{(\theta)}=e_{ijk}^{(\theta)}+\sigma_{ijk}^{(\theta)}\frac{M_{ijk}}{M_{ijk}^{(\theta)}}\Delta e_{ijk} \quad,\quad \theta=1,2,3$$

(15)

Where M_θ is mass of the media θ, $\sigma_{ijk}^{(\theta)}=V_{ijk}^{(\theta)}/\sum_{\theta=1}^{N}V_{ijk}^{(\theta)}$.

3. Numerical simulation

Physical model is shown as figure 1. In order to view shock wave spreading procedure, we design double H type pipes varied from the real environments. The calculation field physical size is like as actual physical size, only to reduce calculation size and the number of calculation meshes. The number of calculation meshes is 60×80×80, which is similar to physical size 37×37×20, and the number of calculation steps is 2000. It was fired from the upper left corner and divided into three phases: kindling stage, compression combustion stage and single shock wave spreading stage.
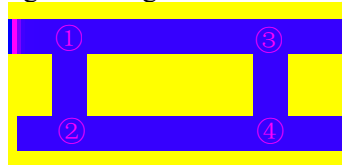

Fig 1: pipe model

The three prerequisites of gas explosion: gas concentration, space limitation and flame or ignition point. Space limitation refers to some concentrations gas without ventilation or in closed space. These several conditions result in gas explosion accident. Industry gas includes blast furnace gas, coke oven gas, converter gas and etc. Domestic gas mainly includes coke oven gas and natural gas. The explosive limits ratio of coke oven gas is 5.0-28.4%, the explosive limits ratio of natural gas is 4.8-13.4%, and blast furnace gas's is 35.8-71.9%. The explosive temperature of coke oven gas is about 600°C, and natural gas's is 650°C.

Gas explosion is instantaneous combustion, and it leads to down pressure and consistency. It produces rarefaction wave in explosion product, and then the expanding gases in high temperature and pressure create a devastating and lethal shock wave.

These sub-graphs one to ten of the figure 2(time is 6.38×10-2,1.76,4.96, 8.28,11.63,15.06,18.53,22.02, 25.52, 31.65 microsecond respectively) and the sub-graphs one to four of figure 3(corresponding four key points of fig 1. The cross axle is time; vertical axis is pressure) are shown as that explosion product expanding to gas initial pressure. Because of inertia, gas produces excessive expansion, until to inertia effect dispels the explosion product volume reaches a maximum. Its average pressure is low the initial pressure and mixed gas in return compress explosion product.

The pressure increases constantly and explosion product was compressed in the opposite direction until opposite inertia dispels. In this time explosion product expands again and create pulsation procedure.
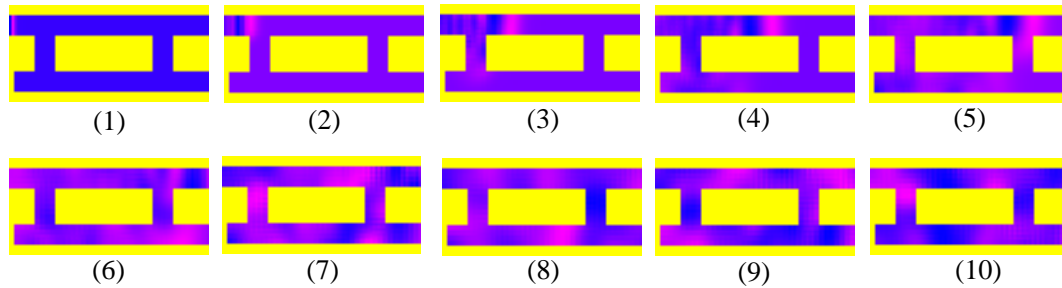

(1)   (2)   (3)   (4)   (5)

(6)   (7)   (8)   (9)   (10)

Fig 2: two-dimension
simulation

(1)   (2)

(3)   (4)

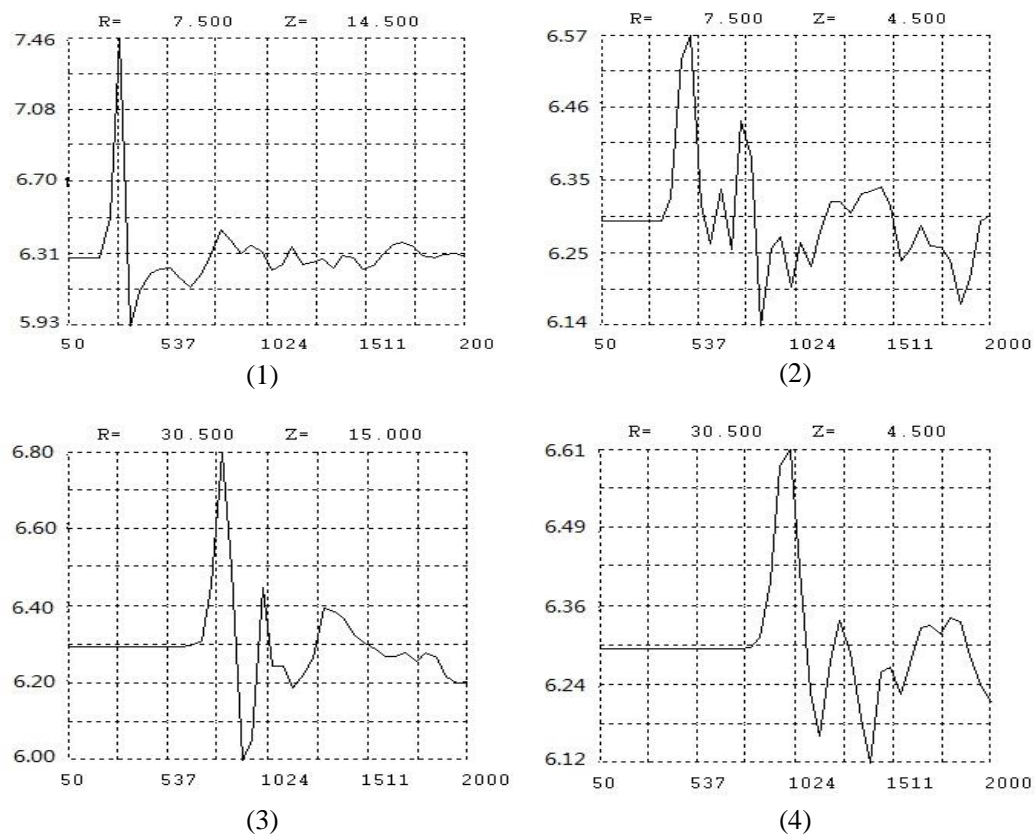Fig 3: time-press curve on key
points

4. Experiment contrasting

City gas consists mainly of hydrogen(H_2), methane(CH_4) and carbon monoxide(CO). Each ingredient's experiment overpressure is shown in the Table 1[10]:

table 1: overpressure value contrast: experiment and numerical simulation

ingredient	H_2	CH_4	CO	numerical simulation
V1（10^5Pa）	8.6	9.0	7.0	8.0~9.0

V2（10^5Pa）	6.6	7.7	6.5	7.46

V1: constant overpressure in gas explosion.   V2: observed peak overpressure.

From these waveforms of pressure wave, explosion procedure can divide into three phase:(1) The phase of ascendancy of explosion pressure. In this phase the energy given out from explosion reaction is more than the energy lost by thermal conduction around. The constantly accumulation of energy result in pressure steadily ascending. The velocity of pressure accumulation is related to chemical reaction kinetics and the rate of combustion.(2) The peak value zone of explosion pressure. When the energy given out from explosion reaction is equal to the energy of thermal conduction, explosion pressure curve appears the highest value.(3) The degradation zone of explosion pressure. When the energy given out from explosion reaction is less than the energy of thermal conduction, pressure begins to slide. The degradation velocity is related to thermal conduction and compressible gas flow. Because of complex construction in pipe, explosion shock wave appears reflection phenomenon, and it makes a series smaller peak.

5. Conclusions

Base on explosion and fluid dynamics theory, using unsteady, compressible, nonviscous hydrodynamic equations and state equations, this paper is to apply the finite difference method to specific-structure coal gas explosions in gas pipe, program by Fortran PowerStation 4.0 and visualize the results by the special software designed independently. The law was analyzed in all the explosions procedure: the flame stage, initial development of explosive field, accelerative stage, shock wave spread and the end. By the overpressure value contrast of experiment and numerical simulation, it proves that the numerical model and simulation result is effective and appropriate. This offers beneficial reference and experience to coal gas explosion accidents or safety precautions.

Reference:
[1] Zhiyuan Wu, Shuangqi Hu, Yunxin Tan. Simplified calculation on max explosion press of multi-element mixed inflammable gas[J]. *Journal of combustion science and technology*, (16):118-122(2010) (in Chinese)
[2] Zhiyuan Wu, Yunxin Tan, Jinglin Zhang. Influence of gas concentration on its detonation press. *Journal north of China institute e of technology*. 25(2): 117-120(2004) (in Chinese)
[3] Liang Zhang, Xiaoling Wei , Lixin Xul. Deflagration characteristics of a preheated CO-air mixture in a pip[J]e. *Explosion and Shockwaves*. (30): 191-195(2010) (in Chinese)
[4] Bangzhi Zhou, Zhen Guo, Yongsheng Wei. Study of limiting range of explosive reaction for polybasic explosive mixed gas in coalgas-air[J]. *Journal of Qinghai Normal University (Natural Science)*, (4):46-48(2003)
[5] Juanjuan Luo, Wenjun Li, Liang Jie. Research on explosion Limit of coal Gas in underground coal gasification[J]. *Coal Mining Technology,* （15）：29-31(2010) (in Chinese)
[6] Yuling Shen, Jianguo Ning. Numerical simulation of gaseous explosions some typical conduits[J]. *Journal of safety and environment,* 1(3):11-16 (2001) (in Chinese)
[7] Deyuan Li, Guorong Xu, Hongshou Shuil. 2D unsteady fluid dynamics numerical simulation[M]. *Beijing: Science Press,*(1998,9) (in Chinese)
[8] Jianguo Ning,Longwei Chen. Fuzzy Interface dispose in Euler method[J]. Science in China Ser. *E Engineering and Materials Science*, 47(5):550-568(2004)
[9] Jianguo Ning,Tianbao Ma. Computational Explosion Mechanics[M]. National Defense Industry Press.101-108(2015) (in Chinese)
[10] Hengyang Zhao. The Theory of Explosion of Gas and Dust[M]. *Beijing institute of technology* Press, 34-37(1996) (in Chinese)