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Unified Gas-Kinetic Scheme for Gas-Particle Flow in Shock-Induced Fluidization of Particles Bed

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***Abstract*—**In this paper, a unified-gas kinetic scheme (UGKS) for the gas-particle flow is constructed. UGKS is a direct modeling method for both continuum and rarefied flow computations. The dynamics of particle and gas are described as rarefied and continuum flow, respectively. Therefore, we use the Bhatnagar-Gross-Krook (BGK) equation for the particle distribution function. For the gas phase, the gas kinetic scheme for Navier-Stokes equation is solved. The momentum transfer between gas and particle is achieved by the acceleration term added to the BGK equation. The new scheme is tested by a 2cm-in-thickness dense bed comprised of glass particles with 1.5mm in diameter, and reasonable agreement is achieved.

***Keywords*—**Gas-particle flow, unified gas-kinetic scheme, momentum transfer, shock-induced fluidization.

I. Introduction

MANY situations in engineering processes or in nature lead to nonstationary two phase flow: shock-induced powder compaction; behavior of the particles cloud ejected from the free surface of a plate subjected to a strong shock and etc. [1]. The numerical investigation of the gas-particle flow has made great progress since two decades ago.

It is well known that the two main approaches are Baer-Nunziato (B-N) model [2]–[4] and multiphase particle-in-cell (MP-PIC) method [5]–[9]. The meaning of physical quantities is different due to the different modeling scales. Firstly, the B-N model and its derived Saurel-Abgrall (S-A) model [3] are established based on the macroscopic scale, for which the particle is a special type of fluid, and the macroscopic phase interface between gas and particle can be captured. Therefore, the S-A model is also applicable to the calculation of multifluid flow such that the particle volume fraction needs to be updated by a transport equation. While the MP-PIC is based on the mesoscopic scale, and the particles are considered as solid with fixed size. The density of the particles is defined relative to its own volume. For MP-PIC, the motion of particles is described by the distribution function, in which the apparent density of particle is used. So the particle volume fraction can be directly obtained through the ratio of particle density to apparent density instead of the similar transport equation in the B-N model.

In addition, the definition of particle pressure is also different. For B-N model, the particle pressure is determined by the stiffened gas equation of state with the parameters of liquid water [3]. For MP-PIC, the pressure obtained by the integration of the distribution function is only indicative of the thermal motion of the particles, which corresponds to the ideal equation of state. Meanwhile, the part of pressure, which is different from the ideal state equation, is reflected by buoyancy and the solid stress [9]. Another key difference is the characterization of temperature. For the B-N model, the temperature of the particles is the expression of heat, but its specific microscopic meaning is not clear. As far as MP-PIC is concerned, when the size of particle is small enough, it can be assumed that the temperature of the particles is dominated mainly by the thermal motion, which is similar to that for dusty gas [10]. Whereas the particles are relatively large, the temperature of the particles is primarily the characterization of the thermal contribution made by the molecules inside the particles. In this case, it is reasonable to add the temperature as another dimension to the distribution function [6].

Through the above comparison, it can be found that MP-PIC method is superior to B-N model, the reason for which is that the modeling scale of former is mesoscopic and the description of physical quantities is more profound than the latter. However, the computational cost of MP-PIC method is quite expensive due to the lagrangian characteristics of PIC technique and the decoupling of transport and collision term.

Recently, a unified gas-kinetic scheme (UGKS) has been developed for the whole Knudsen number regime based on the gas-kinetic BGK model, with discretized particle velocity space [11]. UGKS is a direct modeling method for both continuum and rarefied flow computations. The method has achieved great success in the non-equilibrium flow [12]–[14]. Compared with the B-N model, UGKS is better to describe the non-equilibrium effect of the particles. Furthermore, there is no need to solve the volume fraction transport equation. Compared with MP-PIC, the coupling of transport and collision terms is the main advantage of UGKS. Therefore, the calculation cost is relatively small.

Based on the above considerations, the construction of UGKS for the gas-particle flow is necessary. For UGKS, the dynamics of particle and gas are described as rarefied and continuum flow, respectively. The new scheme is tested by the shock-induced fluidization of a particles bed. The experimental results are used for the validation of the UGKS, and reasonable agreements have been achieved.This paper is organized as follows. The UGKS is presented in Section II. Section III is the numerical test case to validate the proposed method. The last section is the concluding remarks.

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II. Methodology

In this section, we describe the details of the governing equations of particle and gas, respectively, and based on which the UGKS for gas-particle flow is constructed. In reality, the gas flow is treated as continuum. Therefore, in order to reduce the computational cost, the gas-kinetic scheme (GKS) [15] is used to describe the gas flow.

A. Unified Gas-Kinetic Scheme for Particle Phase

1) Model: For the particle phase equation, we use the Bhatnagar-Gross-Krook (BGK) ([16]) for the particle distribution function$f_p\left(x_p,u_p,t\right)$,

$$\frac{\partial f_p}{\partial t}+\frac{\partial u_p f_p}{\partial x}+\frac{\partial \omega_p f_p}{\partial x}=\frac{M_p-f_p}{\tau_p}, \tag{1}$$

where x_p is the particle position, u_p is the particle velocity, τ_p is the relaxation time of particles, M_p is the equilibrium distribution function, and ω_p is the particle acceleration which is given by

$$\omega_p=D_p\left(U_g-u_p\right)-\frac{1}{\rho_p}\frac{\partial P_g}{\partial x}+\frac{1}{\theta\rho_p}\frac{\partial \eta_P}{\partial x}. \tag{2}$$

In the above equation, D_p is the drag experienced by particles, U_g is the macroscopic velocity of gas, ρ_p is the density of particle material, θ is the particle volume fraction, and P_g is the gas pressure. Numerically, the interface between a single particle and gas cant be resolved, while the grid size is smaller than the particle size, the simulated virtual particles cant retain their shape as the real particles. Thus, η_P is the equivalent attraction which prevents the virtual particles from being scattered. Taking into account the more virtual particles, the greater the equivalent attraction, the specific form of η_P is modeled as

$$\eta_P=C_{af}\theta\rho_P, \tag{3}$$

where C_{af} is the coefficient of attractive force which can be determined by the experiment [1].

In addition, the drag experienced by particles, D_p is given by

$$D_p=C_d\frac{3}{8}\frac{\rho_g}{\rho_p}\frac{\left|U_g-u_p\right|}{r_p}, \tag{4}$$

where ρ_g is the density of gas, r_p is the radius of the particles and C_d is the drag coefficient. The value of C_d is also obtained by experiment [1].

It should be emphasized that considering that the thermal motion of the particles plays a minor role [1], the collision term at the right end of (1) is negligible. That is to say, for the sake of simplicity, the following equation can be used to describe the dynamic of the particle phase,

$$\frac{\partial f_p}{\partial t}+\frac{\partial u_p f_p}{\partial x}+\frac{\partial \omega_p f_p}{\partial u_p}=0. \tag{5}$$

2) Reduced Model: The UGKS is a scheme for capturing the time evaluation of particle distribution function $f_p\left(x_p,u_p,t\right)$, in which the particle velocity space u_p is discretized. In order to reduce the computational cost, reduced distribution functions [17] are used in the computation, and defined as,

$$H_p=\int f_p dvdw, B_p=\int\left(v^2+w^2\right)f_p dvdw. \tag{6}$$

As a result, the relationship between the macroscopic flow variables and distribution functions can be written in terms of the moments of H_p and B_p,

$$W_p=\begin{pmatrix}\widetilde{\rho_p}\\ \widetilde{\rho_p}U^{(1)}\\ \widetilde{\rho_p}E^{(1)}\end{pmatrix}=\int\begin{pmatrix}H_p\\ u_pH_p\\ \frac{u_p^2}{2}H_p+\frac{1}{2}B_p\end{pmatrix}du_p, \tag{7}$$

where $\widetilde{\rho_p}$ is the density of particle relative to the mesh size. Then, the particle volume fraction θ can be obtained by,

$$\theta=\frac{\widetilde{\rho_p}}{\rho_p} \tag{8}$$

Multiplying (5) by vector and integrating the vector equation, the following system is obtained,

$$\frac{\partial \phi_p}{\partial t}+\frac{\partial u_p\phi_p}{\partial x}+\frac{\partial \omega_p\phi_p}{\partial u_p}=0, \tag{9}$$

where $\phi_p=\left(H_p,B_p\right)^T$. The construction of UGKS for particle phase is based on (9).

3) Unified Gas-Kinetic Scheme: The unified gas-kinetic scheme is a finite volume method. The physical space in 1D is divided into control volumes Ω_i . The temporal discretization is denoted by t_n the n-th time step. The particle velocity space is discretized in order to capture the non-equilibrium distribution. The discrete distribution functions in physical and velocity spaces are denoted by

$$H_{p,i}^n=H_{p,i,\alpha}^n=H_p\left(t_n,x_i,u_{p,\alpha}\right),B_{p,i}^n=B_{p,i,\alpha}^n=B_p\left(t_n,x_i,u_{p,\alpha}\right). \tag{10}$$

With the discrete particle velocity points, the moments of the particle distribution functions can be obtained by numerical quadrature over velocity space,

$$W_{p,i}^n=\sum\begin{pmatrix}\kappa_\alpha H_{p,i}^n\\ \kappa_\alpha H_{p,i}^n u_{p,\alpha}\\ \kappa_\alpha\left(\frac{u_{p,\alpha}^2}{2}H_{p,i}^n+\frac{1}{2}B_{p,i}^n\right)\end{pmatrix}, \tag{11}$$

where κ_α is the weight of numerical quadrature. The UGKS method for particle phase is constructed in the following.

Firstly, for convenience, the model equation (9) is split into following two equations,

$$\frac{\partial \phi_p}{\partial t}+\frac{\partial u_p\phi_p}{\partial x}=0, \tag{12}$$

$$\frac{\partial \phi_p}{\partial t}+\frac{\partial \omega_p\phi_p}{\partial u_p}=0. \tag{13}$$

If (12) and (13) are denoted by Υ_0 and Υ_1 respectively, then we can obtain [18],

$$H_p\left(x,t+\Delta t\right)\approx\Upsilon_1\left(\Delta t\right)\Upsilon_0\left(\Delta t\right)H_p\left(x,t\right). \tag{14}$$

Secondly, (12) is solved by the following steps. Through integrating (12) over the control volume Ω_i in a physical space and in a time interval (t_n,t_{n+1}) , we can obtain,

$$\phi_{p,i,\alpha}^{n+1}=\phi_{p,i,\alpha}^{n}+\frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}u_{p,\alpha}\left(\phi_{p,i-1/2,\alpha}-\phi_{p,i+1/2,\alpha}\right)dt. \tag{15}$$

In the above system, the construction of the time-dependent particle distribution function $\phi_{p,i-1/2,\alpha}$ at the cell interface is the central ingredient for the development of UGKS. The detailed method to determine $\phi_{p,i-1/2,\alpha}$ is seen in [11].

Thirdly, the MUSCLE scheme is used to solve (13). The evolution of particle distribution function over time is corresponding to (13),

$$\phi_{p,i,\alpha}^{n+1}=\phi_{p,i,\alpha}^{n}+\frac{1}{\Delta u_p}\int_{t^n}^{t^{n+1}}\begin{pmatrix}\omega_{p,i,\alpha-1/2}\phi_{p,i,\alpha-1/2}\\-\omega_{p,i,\alpha+1/2}\phi_{p,i,\alpha+1/2}\end{pmatrix}dt. \tag{16}$$

For simplicity, the forward temporal integral is used, i.e.

$$\phi_{p,i,\alpha}^{n+1}=\phi_{p,i,\alpha}^{n}+\frac{\Delta t}{\Delta u_p}\begin{pmatrix}\omega_{p,i,\alpha-1/2}^{n}\phi_{p,i,\alpha-1/2}^{n}\\-\omega_{p,i,\alpha+1/2}^{n}\phi_{p,i,\alpha+1/2}^{n}\end{pmatrix}. \tag{17}$$

Then, the distribution function of the interface in velocity space can be reconstructed from the initial distribution. That is,

$$\omega_{p,i,\alpha-1/2}^{n}\phi_{p,i,\alpha-1/2}^{n}=\begin{cases}\omega_{p,i,\alpha-1}^{n}\phi_{p,i,\alpha-1}^{n}+\sigma_{\alpha-1}^{\omega\phi}\dfrac{1}{2}\Delta u_p,\\ \omega_{p,i,\alpha-1/2}^{n}>0\\ \quad\omega_{p,i,\alpha}^{n}\phi_{p,i,\alpha}^{n}-\sigma_{\alpha}^{\omega\phi}\dfrac{1}{2}\Delta u_p,\\ \quad\omega_{p,i,\alpha-1/2}^{n}<0\end{cases} \tag{18}$$

where $\sigma_\alpha^{\omega\phi}$ is the slope of $\omega_{p,i,\alpha}^{n}\phi_{p,i,\alpha}^{n}$ at the velocity point $u_{p,\alpha}$. The value of $\sigma_\alpha^{\omega\phi}$ can be obtained by van Leer limiter, i.e.

$$\sigma_\alpha^{\omega\phi}=\left(sign\left(s_1\right)+sign\left(s_2\right)\right)\frac{\left|s_1\right|\left|s_2\right|}{\left|s_1\right|+\left|s_2\right|}, \tag{19}$$

in which, $sign\left(s_1\right)$ is the signal function, and $s_1=\left(\omega_{p,i,\alpha}^{n}\phi_{p,i,\alpha}^{n}-\omega_{p,i,\alpha-1}^{n}\phi_{p,i,\alpha-1}^{n}\right)/\left(u_{p,\alpha}-u_{p,\alpha-1}\right),s_2=\left(\omega_{p,i,\alpha+1}^{n}\phi_{p,i,\alpha+1}^{n}-\omega_{p,i,\alpha}^{n}\phi_{p,i,\alpha}^{n}\right)/\left(u_{p,\alpha+1}-u_{p,\alpha}\right)$.

As described above, inserting (15) and (17) into (14), one obtains the reduced distribution functions $\phi_{p,i,\alpha}^{n+1}$. Then the macroscopic variables can be updated by (11). In the next step, we will show you how to construct the gas-kinetic scheme for gas phase.

B. Gas-Kinetic Scheme for Gas Phase

For the gas phase, according to the conservation principle, the evolution equation of the macroscopic variables can be written as,

$$\varepsilon_i^{n+1}W_{g,i}^{n+1}=\varepsilon_i^{n}W_{g,i}^{n}+\frac{1}{\Delta x}\left(\vec{F}_{g,i-1/2}-\vec{F}_{g,i-1/2}\right)+S_i^n, \tag{20}$$

in which, $W_{g,i}^{n}$ is the macroscopic variables of gas, i.e. $W_{g,i}^{n}=\left(\rho_{g,i}^{n},\rho_{g,i}^{n}U_{g,i}^{n},\rho_{g,i}^{n}E_{g,i}^{n}\right)^T$. ε_i^n is the gas volume fraction, therefore, $\varepsilon_i^n=1-\theta_i^n$. $\vec{F}_{g,i-1/2}$ is the interfacial flux of macroscopic variables, thus

$$\vec{F}_{g,i-1/2}=\int_{t_n}^{t_{n+1}}\int u_g\left(\psi_1H_{g,i-1/2}+\psi_2B_{g,i-1/2}\right)dudt, \tag{21}$$

where $\psi_1=\left(1,u,\frac{u^2}{2}\right)^T,\psi_2=\left(0,0,\frac{1}{2}\right)^T$.

In addition, $H_{g,i-1/2}$ and $B_{g,i-1/2}$ are the reduced distribution function of gas, therefore similar to (6),$H_{g,i-1/2}=\int f_{g,i-1/2}dvdwd\xi,B_{g,i-1/2}=\int\left(v^2+w^2\right)f_{g,i-1/2}dvdwd\xi$, and ξ is microscopic velocity corresponding to the internal degrees of freedom. Furthermore, $f_{g,i-1/2}$ is the gas distribution function at the cell interface. Since gas is treated as continuum, the GKS scheme is used to obtain $f_{g,i-1/2}$, and its expression is as [15],

$$\begin{aligned}f_{g,i-1/2}\left(u,t,\xi\right)&=\left(1-e^{-t/\tau_g}\right)M_{g0}\\&+\left(\tau_g\left(-1+e^{-t/\tau_g}\right)+te^{-t/\tau_g}\right)\begin{pmatrix}\bar{a}^LH[u]\\+\bar{a}^R\left(1-H[u]\right)\end{pmatrix}uM_{g0}\\&+\tau_g\left(t/\tau_g-1+e^{-t/\tau_g}\right)\bar{A}M_{g0}\\&+e^{-t/\tau_g}\begin{pmatrix}\left(1-\left(t+\tau_g\right)ua^L\right)H[u]M_g^L\\+\left(1-\left(t+\tau_g\right)ua^R\right)\left(1-H[u]\right)M_g^R\end{pmatrix}\\&+e^{-t/\tau_g}\left(-\tau_gA^LH[u]M_g^L+-\tau_gA^R\left(1-H[u]\right)M_g^R\right)\end{aligned}, \tag{22}$$

where H[u] is the Heaviside function, τ_g is the relaxation time of gas. M_{g0} is the equilibrium gas distribution function at the cell interface at the initial moment of each iteration. M_g^L and M_g^R are the equilibrium gas distribution functions at the left and right of cell interface respectively. In addition, $\bar{a}^L,\bar{a}^R,\bar{A},a^L,a^R,A^L,A^R$ are local constants. How to determine the above spatial and temporal gradients for the equilibrium distribution function was explained in [15].

Once the distribution function at the cell interface $f_{g,i-1/2}\left(u,t,\xi\right)$ is determined, the flux in (20) can be obtained through (21). Then, the next step to consider is the source term S_i^n in (20). Based on the conservation of momentum and energy exchange between gas and particle, it is available that,

$$S_i^n=-\Delta W_{p,i}^n, \tag{23}$$

in which,

$$\Delta W_{p,i}^n=\sum\begin{pmatrix}\kappa_\alpha\Delta H_{p,i}^n\\\kappa_\alpha\Delta H_{p,i}^nu_{p,\alpha}\\\kappa_\alpha\left(\frac{u_{p,\alpha}^2}{2}\Delta H_{p,i}^n+\frac{1}{2}\Delta B_{p,i}^n\right)\end{pmatrix}, \tag{24}$$

where $\Delta\phi^n_{p,i} = \left(\Delta H^n_{p,i}, \Delta B^n_{p,i}\right)^T$ is the changes of particle distribution functions contributed by the interaction between gas and particle, i.e.

$$\Delta\phi^n_{p,i} = \frac{\Delta t}{\Delta u_p}\left(\Omega^n_{p,i,\alpha-1/2}\phi^n_{p,i,\alpha-1/2} - \Omega^n_{p,i,\alpha+1/2}\phi^n_{p,i,\alpha+1/2}\right). \tag{25}$$

In (25), $\Omega^n_{p,i,\alpha-1/2} = D^n_{p,i}\left(U^n_{p,i} - u_{p,\alpha-1/2}\right) - \frac{1}{\rho_p}\frac{\partial P^n_{p,i}}{\partial x}$.

It can be seen that inserting (21) and (23) into (20), one can update the macroscopic variables of gas.

C. Numerical Procedure

In summary, the procedure of UGKS for the gas-particle two phase flow is as follows:

a. Equations (15) and (21) are used to obtain flux of particle and gas respectively at the cell interface in physical space.
b. Equation (16) is used to obtain the flux of particle at the cell interface in velocity space, and then update the macroscopic variables of particle by (11).
c. Obtain the source term in (20) by (23). Therefore, the macroscopic variables of gas are updated.
d. The time evolution solution of the flow field can be obtained by iterating through the above three steps.

III. Numerical Test

In order to validate the proposed method above, the shock-induced fluidization of a particles bed [1] is tested.

A. A Single Layer of Particles

As described above at Section II-A1, the drag coefficient C_d in (4) and attractive coefficient C_{af} in (3) are both determined by experiment result. So a single layer of 2mm diameter particles is used to obtain the exact values of these two coefficients. The parameters of the problem are given in Table 1.

TABLE I
Parameters of a Single Layer of Particles

Quantity	Value
Air preshock density	1.2kg/m^3
Incident shock Mach number	1.3
Particle density	2500kg/m^3

Through numerical calculations, as Fig. 1 shown, the cloud front trajectories between UGKS and experiment matches good when $C_d = 12, C_{af} = 20$.

B. Dense Bed

In order to validate the proposed scheme, as Fig. 2 shown, a dense bed which consists of 2cm of 1.5mm diameter glass particles is tested. The parameters of the problem are identical with that in Table I. In addition, the initial particle volume fraction in the bed is 0.65. The initial pressure is uniform and set to 10^5Pa.

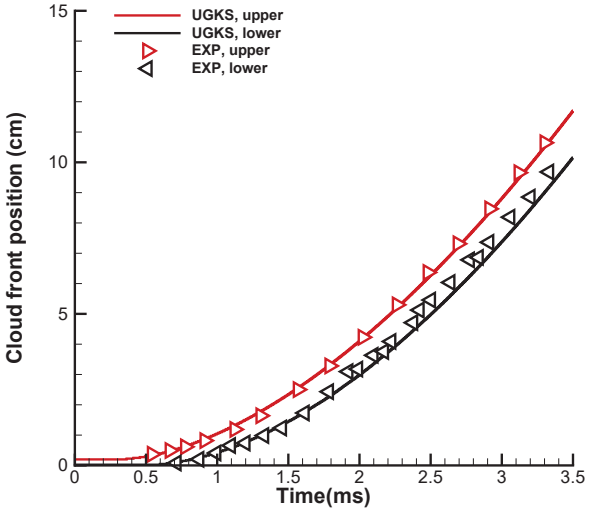

Fig. 1 Cloud front trajectories from single layer bed of 2mm diameter glass spheres subject to Mach 1.3 shock in air

As far as UGKS for gas-particle flow is concerned, the computational domain is divided into 1400 cells and CFL=0.9. For particle phase, the velocity space [-284m/s, 284 m/s] is discretized with 140 mesh points. Fig. 3 shows the comparison of pressure signals upstream and downstream of the cloud with time between UGKS and experiment as well as the code by Rouge in [1]. It is seen that the result computed by UGKS is better than that by Rouge, and matches better with experiment. Fig. 4 shows the upper and lower front trajectories. Similarly, the trajectories calculated by UGKS and measured by experiment are in good agreement. It should be stated that for UGKS, as Fig. 5 shown, the particle cloud is divided into two parts, the dense and dilute ones. Therefore, we choose the boundary of the dense and dilute regions as the lower and upper front of one-dimensional cloud.

From the above analysis, the conclusion can be drawn that UGKS for gas-particle is successfully constructed. However, it is unsatisfactory that pressure value downstream of the cloud rising too fast after 4ms, resulting in a poor match with the experiment. This is an issue that needs to be taken care of in further research.

IV. Conclusion

In this paper, a unified gas-kinetic scheme for gas-particle flow is developed. UGKS is a direct modeling method for both continuum and rarefied flow computations due to the couplng of transport and collision terms, which is suitable for describing the non-equilibrium effect of the particles based on the mesoscopic scale. The new scheme has been tested in shock-induced fluidization of a particles bed. The experimental results are used for the validation of the UGKS, and reasonable agreement is achieved. In order to further develop the current scheme for engineering applications, the collisions between the particles and the heat conduction between the particles and gas will be implemented into UGKS in the near future.

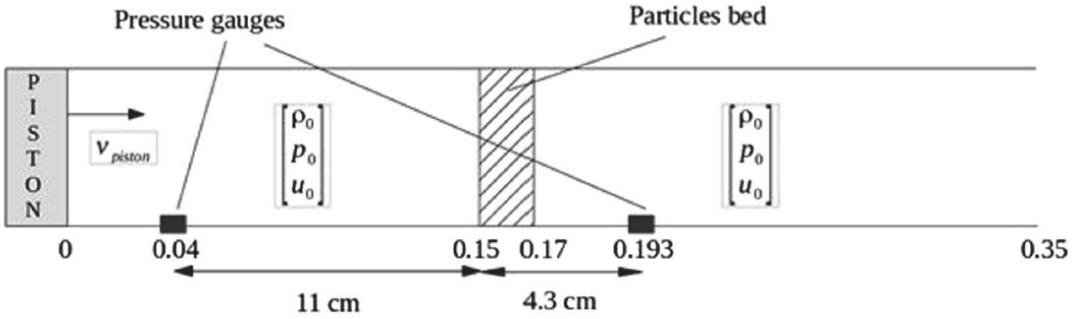

Fig. 2 Rogue et al. (1998) fluidization shock tube test. A shock at Mach number 1.3 is created by the expansion of the high pressure gas, equivalent to a shock created by a piston moving at 151 m/s [1]

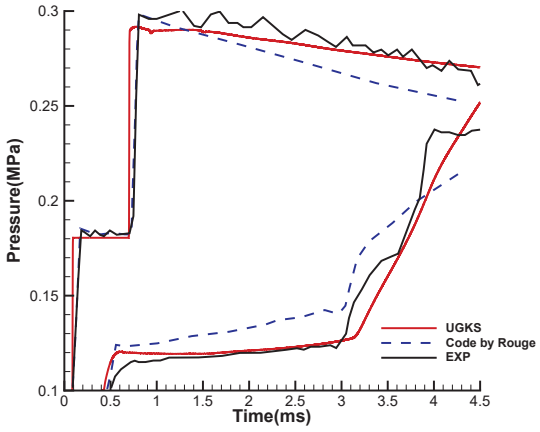

Fig. 3 Pressure signals upstream and downstream of the cloud; transducer location 11cm below and 4.3 mm above the support, 2 cm bed of 1.5mm diameter glass spheres subject to Mach 1.3 shock in air ($C_d = 12, C_{af} = 20$)

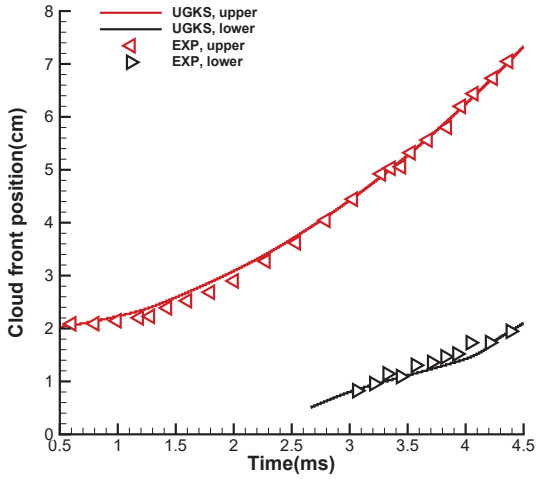

Fig. 4 Cloud upper and lower front trajectories from 2 cm bed of 1.5mm diameter glass spheres subject to Mach 1.3 shock in air ($C_d = 12, C_{af} = 20$)

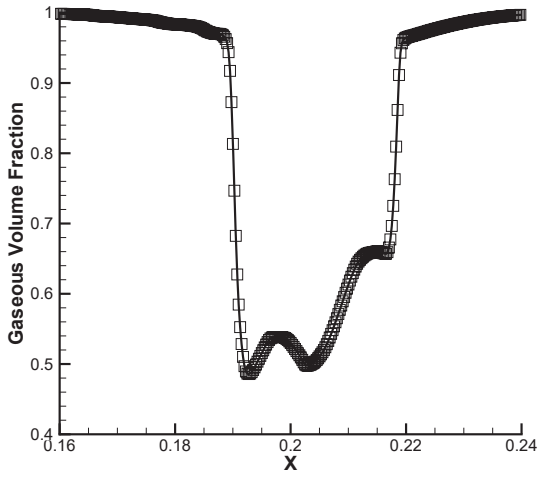

Fig. 5 Gaseous volume fraction distribution from 2 cm bed of 1.5mm diameter glass spheres subject to Mach 1.3 shock in air ($C_d = 12, C_{af} = 20$,4.5ms)

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