A Computational Model for Gas-Particle Flows with Distributed Phase Interfaces

by

Chak M. Tsui

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Graduate Department of Aerospace Science and Engineering
University of Toronto

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Abstract

A new method of computing unsteady gas-particle flows with smoothly distributed phase interfaces is introduced to facilitate computations in which the gas flow a continuum about particles that have independent paths (non-continuum). However, a viscous-flow resistance is imposed such that flow restricted more strongly further inside the particle interface where the particle become solid. The resulting force on the moving particle from the viscous-flow resistance and gas pressure around the particle is used to determine its acceleration and trajectory. Two unsteady one-dimensional problems are solved to assess the advantages and limitations of the new model. The first involves the reflection of a shock wave from a closed duct end for which the wall has a stationary distributed interface, and the second involves the acceleration of a projectile in a duct by a high-pressure gas, for which the projectile has smoothly distributed interfaces with the gas.
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Nomenclature

Alphanumeric Letters

- \( a \) speed of sound of the gas flow \([m/s]\), acceleration \([m/s^2]\)
- \( \vec{a} \) vector acceleration \([m/s^2]\)
- \( A \) cross-sectional area \([m^2]\)
- \( B(x) \) dimensionless modification term in viscous-flow resistance
- \( c_{visc} \) second dimensionless coefficient of viscous-flow resistance
- \( C_{visc} \) first coefficient of viscous-flow resistance \([m^{-1}]\)
- \( C_p \) specific heat of the material at constant pressure \([J/kg\cdot K]\)
- \( C_d \) dimensionless drag coefficient
- \( d \) equivalent diameter of the particle \([m]\)
- \( e \) energy per unit volume \([J/m^3]\)
- \( f_{visc} \) viscous-flow resistance per unit volume \([N/m^3]\)
- \( F_{back} \) gas pressure force on the rear surface of a projectile \([N]\)
- \( F_{front} \) gas pressure force on the frontal surface of a projectile \([N]\)
- \( F_{drag} \) aerodynamic drag force \([N]\)
- \( F_{grav} \) gravitational force \([N]\)
- \( F(U) \) flux term in \( x \) direction
- \( G(U) \) flux term in \( y \) direction
- \( \tilde{G} \) modified spatial derivatives of flux term in chapter 3
- \( H(U) \) term of spatial derivatives
- \( k \) thermal conductivity of the gas phase \([J/m\cdot s\cdot K]\)
- \( m \) mass \([kg]\)
- \( M_i \) incident shock Mach number
- \( M_r \) reflected shock Mach number
- \( n \) exponent in viscous-flow resistance
- \( N \) total number of cells
- \( Nu \) Nusselt number
- \( p \) static pressure of the gas flow \([N/m^2]\)
- \( Pr \) Prandtl number
- \( \dot{q} \) heat transfer \([J/m^3\cdot s]\)
- \( R \) gas constant \([J/kg\cdot K]\)
- \( Re \) Reynolds number
\( R \)  
Riemann solver operator

\( S(U_y, U_r) \)  
source term in the Euler's equations

\( \dot{S} \)  
modified source term in chapter 3

\( t \)  
time

\( T \)  
temperature [K]

\( T(V) \)  
source term in the VODE subroutine

\( u \)  
velocity in \( x \) direction [m/s]

\( \bar{u} \)  
vector velocity [m/s]

\( U \)  
conservative variables

\( \bar{U} \)  
modified conservative variables in chapter 3

\( v \)  
velocity in \( y \) direction [m/s]

\( V \)  
volume [m³]

\( \tilde{V} \)  
independent variable array used in the VODE subroutine

\( x \)  
displacement [m]

\( \bar{x} \)  
vector displacement [m]

**Greek Letters**

\( \gamma \)  
ratio of specific heats

\( \delta t \)  
time between successive plotted spatial distributions of variables [s]

\( \Delta t \)  
time step [s]

\( \Delta x \)  
width of a cell [m]

\( \eta \)  
normalized free parameter in the Bézier's polynomial \((0 \leq \eta \leq 1)\)

\( \zeta \)  
normalized free parameter in the Bézier's polynomial \((0 \leq \zeta \leq 1)\)

\( \varepsilon \)  
volume fraction

\( \varepsilon_{g_{\min}} \)  
minimum allowed gas-volume fraction

\( \mu \)  
viscosity [N·s/m²]

\( \rho \)  
density [kg/m³]

\( \sigma \)  
partial phase density [kg/m³]

**Superscripts**

\(+\)  
left side of this location

\(-\)  
right side of this location

\textit{init}  
initial condition

\textit{old}  
state at the last time level

\textit{new}  
state at the next time level

\( T \)  
matrix transpose

**Subscripts**

1  
first point for Bézier's polynomials, also used in cell indexing, and the gas state in front of the incoming shock

2  
second point for Bézier's polynomials, also used in cell indexing, and the gas state behind the incoming shock
third point for Bézier's polynomials, also used in cell indexing, and the gas state behind the reflected shock

fourth point for Bézier's polynomials, also used in cell indexing

index for the \( i \)th cell

index for the left boundary of the \( i \)th cell

index for the right boundary of the \( i \)th cell

gas phase

at the left side of the projectile

at a reference condition

particle phase, projectile

at the right side of the projectile

property of a sphere

\( x \) direction

\( y \) direction

**VODE Parameters**

- **NEQ** number of variables
- **T** current time
- **TOUT** time for the output
- **ITOL** an indicator for the type of error control
- **RTOL** relative error tolerance parameter
- **ATOL** absolute error tolerance parameter
- **ITASK** an index specifying the task to be performed
- **ISTATE** an index to specify the state of the calculation
- **IOPT** an indicator for optional input
- **LRW** size of the double precision work array
- **LIW** size of the integer work array
- **ML** number of sub-diagonals under the main diagonal
- **MU** number of sub-diagonals above the main diagonal
- **MF** method flag
- **RPAR** user specified double-precision scalar or array variable
- **IPAR** user specified integer scalar or array variable
- **H0** the step size to be used on the first step
- **HMAX** maximum step size allowed
- **HMIN** minimum step size allowed
- **MAXORD** maximum order allowed
- **MXSTEP** maximum number of steps allowed
- **MXHNL** maximum number of message printed
Chapter 1

Introduction

Flows of a dusty-gas or gas-particle mixture constitute a subclass of two-phase flows [Soo, 1967; Rudinger, 1980; Hetsroni, 1982] in which one phase consists of small particles that are solid or rigid. These particles are normally suspended and transported by the second gaseous phase (carrier gas). Gas-particle flows occur naturally in the form of smoke, haze, pollen, pollutants and volcanic ash in the atmosphere, and also in the form of sand, hail and snow storms. In industrial engineering gas-particle flows are used as fluidized beds, for particulate conveyance in pipes, and to separate particles from the carrier gas. Some common aerospace applications include the solid-propellant rocket motor, flight through a particle-laden gas, and sand erosion of helicopter blades and jet-engine compressor fans. Furthermore, gas-particle flows are inherent to grain-elevator and coal-mine explosions, and they also occur in the detonation of some heterogeneous explosives.

Some gas-particle mixtures undergo essentially equilibrium flow, that is the gas and particles move in unison at essentially the same velocity and also essentially with the same temperature, when viscous-drag (from boundary-layer shear) and heat-transfer processes are dominant over flow processes [Rudinger, 1980]. Most mixtures undergo nonequilibrium flow in which slip occurs between the gas and particle phases and when heat is transferred from the hot to cold phase, because viscous-drag and heat-transfer processes are normally slow compared to velocity and temperature changes of the gas phase, although the effects of viscosity and heat transfer always act in the direction of establishing equilibrium flow. A prime example of nonequilibrium flow is the shock-induced motion of a gas-particle mixture in accidental explosions and laboratory shock tubes.

Particles in gas-particle mixtures are frequently of different sizes, shapes and possibly material properties (e.g., a mixture of sand and soil), and they therefore move at different velocities because the viscous-drag acceleration varies with particle shape, size and density. Consequently, some neighbouring particles on collision paths undergo collisions and path deflections [Hetsroni, 1982], while some of these might simply agglomerate owing to electrostatic or other effects [Hetsroni, 1982], whereas other neighbouring particles only experience near misses and one particle passes another. Particle-particle collisions, path deflections, and passing events may be considered as another version of nonequilibrium flow.
Predictions of gas-particle flows with nonequilibrium behaviour are important to understanding flow phenomena and in providing better aerodynamic and industrial designs of equipment that may result in increased safety in the workplace. Numerical prediction models are reviewed herein with the intent of establishing a good perspective for understanding present and future computational developments for solving difficult gas-particle flow problems involving gas-particle slip, heat transfer, and particle-particle collisions. After reviewing a number of different gas-particle flow models, commencing with simple early treatments and progressing chronologically to sophisticated recent models, the objectives and scope of this study are then given.

The method of particle-trajectory tracing is reviewed first because of its simplicity, and it is one of the first models used in predicting the influence of the gas on particle motions. In some problems involving bird strikes with aircraft, large particles ingested by aircraft engines [Tabakoff & Hamed, 1989], or the separation of large particles from the carrier gas by means of a particle separator [Svarovský, 1981; Hetroni, 1982; Ogawa, 1984], and flows of particles in solid-propellant rocket motors [Carrier, Fendell, Brent, Kimbrough, Loucks, Hess, & Acosta, 1991; Sabnis, Jong, & Gibeling, 1992], only a few discrete particles normally move through a steady two- or three-dimensional flow field. Their particle trajectories are usually required to determine or control the particle impact location. The standard model for particle trajectory tracing is done in two steps. In the first step, the steady two- or three-dimensional flow without particles is computed numerically, for example by solving Euler’s continuity, momentum and energy equations

$$\frac{\partial \mathbf{F}(U_g)}{\partial x} + \frac{\partial \mathbf{G}(U_g)}{\partial y} = 0$$

for two space dimensions, for which the perfect equation of state $p_g = \rho_g R_g T_g$ is required to close these equations. In this expression the vectors are given by

$$U_g = [\rho_g \quad \rho_g u_g \quad \rho_g v_g \quad e_g]^T,$$

$$\mathbf{F}(U_g) = \begin{bmatrix} \rho_g u_g \
\rho_g (u_g^2 + p_g) \quad \rho_g u_g v_g \quad u_g (e_g + p_g) \end{bmatrix}^T,$$

$$\mathbf{G}(U_g) = \begin{bmatrix} \rho_g v_g \
\rho_g u_g v_g \quad \rho_g v_g^2 + p_g \quad v_g (e_g + p_g) \end{bmatrix}^T,$$

and $R_g$, $p_g$, $\rho_g$, $u_g$, $v_g$, $e_g = \frac{1}{\gamma - 1} p_g + \frac{1}{2} \rho_g (u_g^2 + v_g^2)$, and $T_g$ denote the gas constant, pressure, density, flow velocities in the $x$ and $y$ directions, energy per unit volume, and temperature, respectively. In the last step, particle trajectories through this computed flow field are calculated by using the known flow-field results, for the case of different trajectories originating from various starting locations. Particle-path calculations are based on flow-field properties along the particle trajectory where the equation of motion of an individual particle is used in the form

$$\dd \vec{a}_p = \frac{d\vec{u}_p}{dt} = \frac{d^2\vec{r}_p}{dt^2} = \frac{1}{m_p} [\vec{F}_{\text{drag}} + \vec{F}_{\text{grav}}],$$

where $\vec{F}_{\text{grav}} = m_p \vec{g}$ is the gravitational force on the particle and the aerodynamic drag force
on the particle is given by

\[
\vec{F}_{\text{drag}} = \frac{1}{2} C_d A_p \rho |\vec{u}_g - \vec{u}_p| (\vec{u}_g - \vec{u}_p) .
\]  

(1.4)

In the preceding equations, the vectors \( \vec{a}_p, \vec{u}_p, \) and \( \vec{F}_p \) denote particle acceleration, velocity, and position, respectively. Also, \( m_p, C_d, A_p = \pi d^2 / 4, \) and \( \vec{u}_g \) designate particle mass, coefficient of viscous drag, particle cross-sectional area where \( d \) is the diameter of the particle, and vector flow velocity. Note that \( \vec{u}_g = \hat{i}u_g + \hat{j}v_g, \) where \( \hat{i} \) and \( \hat{j} \) are the unit vectors in \( x \) and \( y \) direction, respectively; the correlation for the drag coefficient is normally given by \( C_d = 0.48 + 28 \text{Re}^{0.85}, \) where \( \text{Re} = \rho d |\vec{u}_g - \vec{u}_p| / \mu_g \) is the Reynolds number, \( d \) is the equivalent diameter of the spherical particle, and Sutherland’s approximation for the dynamic viscosity of the air is given by \( \mu_g = \mu_{go}(T/T_{go})^{0.77}, \) in which \( \mu_{go} = 1.71 \times 10^{-5} \text{N} \cdot \text{s/m}^2 \) and \( T_{go} = 273 \text{K}. \)

In this simple model of particle-trajectory tracing, the gas is treated as a continuum using Eq. (1.1), and the particles are treated as independent bodies moving through the gas using Eq. (1.3). A direct advantage is that discrete particles starting from different locations have independent trajectories through the flow field such that particles can pass one another. Another advantage is that particle-particle collisions can also be incorporated into the predictions, if the conservation of linear momentum, angular momentum, and energy with or without losses are applied as particle paths are evaluated. In addition, particle collisions with walls can be included similarly, because a wall can be considered as a large stationary particle. On the other hand, there are certain disadvantages of this simple model. There is no influence of both the particle volume and particle motion on the gas flow field, and heat transfer between the gas and particles is usually ignored. Another disadvantage is that unsteady gas-particle flows cannot normally be solved. Although this simple model of particle-trajectory tracing applies well for some applications mentioned earlier, additional models are required for other applications (e.g., for unsteady flows of dusty gases).

The method of dual gas and particle continua with negligible particle volume is reviewed next, because this more complicated model was needed historically to solve important problems involving numerous small particles in unsteady flows with viscous and heat-transfer interactions between the phases. Such flows include, for example, the migration of smoke, pollutants, and volcanic ash in the Earth’s atmosphere [Zlatev, Dimov, & Georgiev, 1994] and shock-induced dusty-gas flows in ducts and explosions [Rudinger, 1980; Miura & Glass, 1982 & 1985]. The unsteady flow equations of mass, momentum, and energy for the gas and particle phases are coupled in terms of mass transfer (if chemical reactions occur), momentum transfer (viscous drag), and heat transfer (between the gas and particle phases). These equations are given by

\[
\frac{\partial U_g}{\partial t} + \frac{\partial F(U_g)}{\partial x} + \frac{\partial G(U_g)}{\partial y} + H(U_g) = S(U_g, U_p) , \quad (1.5)
\]

\[
\frac{\partial U_p}{\partial t} + \frac{\partial F(U_p)}{\partial x} + \frac{\partial G(U_p)}{\partial y} + H(U_p) = -S(U_g, U_p) , \quad (1.6)
\]

for the case where particle volume is neglected only in the gas-phase equations. In these
equations the vectors for the gas phase are given by

\[ \mathbf{U}_g = \begin{bmatrix} \rho_g & \rho_g u_g & \rho_g v_g & e_g \end{bmatrix}^T, \]
\[ \mathbf{F}(\mathbf{U}_g) = \begin{bmatrix} \rho_g u_g & \rho_g u_g^2 & \rho_g u_g v_g & u_g(e_g + p_g) \end{bmatrix}^T, \]
\[ \mathbf{G}(\mathbf{U}_g) = \begin{bmatrix} \rho_g v_g & \rho_g u_g v_g & \rho_g v_g^2 & v_g(e_g + p_g) \end{bmatrix}^T, \]
\[ \mathbf{H}(\mathbf{U}_g) = \begin{bmatrix} 0 & \frac{\partial p_g}{\partial x} & \frac{\partial p_g}{\partial y} & 0 \end{bmatrix}^T, \]
\[ \mathbf{S}(\mathbf{U}_g, \mathbf{U}_p) = \begin{bmatrix} 0 & f_x & f_y \end{bmatrix}^T, \]

and the vectors for the particle phase are given by

\[ \mathbf{U}_p = \begin{bmatrix} \varepsilon_p \rho_p & \varepsilon_p \rho_p u_p & \varepsilon_p \rho_p v_p & \varepsilon_p e_p \end{bmatrix}^T, \]
\[ \mathbf{F}(\mathbf{U}_p) = \begin{bmatrix} \varepsilon_p \rho_p u_p & \varepsilon_p \rho_p u_p^2 & \varepsilon_p \rho_p u_p v_p & \varepsilon_p u_p(e_p + p_g) \end{bmatrix}^T, \]
\[ \mathbf{G}(\mathbf{U}_p) = \begin{bmatrix} \varepsilon_p \rho_p v_p & \varepsilon_p \rho_p v_p u_p & \varepsilon_p \rho_p v_p^2 & \varepsilon_p v_p(e_p + p_g) \end{bmatrix}^T, \]
\[ \mathbf{H}(\mathbf{U}_p) = \begin{bmatrix} 0 & \varepsilon_p \frac{\partial p_g}{\partial x} & \varepsilon_p \frac{\partial p_g}{\partial y} & 0 \end{bmatrix}^T. \]

The perfect equation of state \( p_g = \rho_g R_g T_g \) is required to help close this set of equations. The subscripts \( g \) and \( p \) denote the properties of gas and particle phases, respectively, and the particle energy per unit volume is \( e_p = C_{pp} T_p + \frac{1}{2} \rho_p (u_p^2 + v_p^2) \), where \( C_{pp} \) is the specific heat of the particle material. The drag-force components in \( x \) and \( y \) directions are given by \( f_x = -i \cdot \mathbf{F}_{\text{drag}} \varepsilon_p / V_p \) and \( f_y = -j \cdot \mathbf{F}_{\text{drag}} \varepsilon_p / V_p \) in units of Newtons per unit of volume, for which the centre dot designates the vector dot product and \( V_p = (1/6) \pi d^3 \) is the volume of a particle of diameter \( d \). The symbol \( \varepsilon_p \) denotes the particle-volume fraction, \( \rho_p \) is the material density of the particle which is normally considered constant [Gough, 1979]. The heat transfer per unit volume between the gas and particle phases is given by \( \dot{q} = -6 \mu_g C_{pg} \text{Nu}(T_g - T_p) / (d^2 \text{Pr}) \), where \( \text{Nu} = 2.0 + 0.6 \text{Pr}^{1/3} \text{Re}^{1/2} \) is the Nusselt number correlation, \( \text{Pr} = \mu_g C_{pg} / k_g \simeq 0.75 \) is the Prandtl number for air, \( d \) is the equivalent diameter of the spherical particle, \( \mu_g \) is the viscosity of the gas defined by a previous equation, \( C_{pg} = \frac{7}{4} R_g \) is the gas specific heat at constant pressure, and \( k_g \) is the gas thermal conductivity.

Two primary advantages of the dual gas and particle continua model are that interactions between the two phases are included within the approximation of the continuum mixture and unsteady gas-particle flows can be solved. One disadvantage is that particle volume effects on the gas phase are ignored because the gaseous volume fraction \( \varepsilon_g = 1 - \varepsilon_p \simeq 1 \); hence, the equations for the gaseous phase are valid only for sparsely populated particles. Other disadvantages are that the particle continuum prohibits realistic computations of particle-particle collisions and the passing of one particle by another.

The method of dual gas and particle continua including particle-volume effects is reviewed next, so that problems involving dense particle clouds can be solved computationally. One example is the motion of propellant grains in laboratory projectile launchers used for
studying projectile impacts on targets [Krier & Summerfield, 1979; Stiefel, 1988]. The unsteady flow equations of mass, momentum, and energy for the gas and particle phases are given by Eqs. (1.5) and (1.6), but the vectors for the gaseous phase in Eq. (1.7) are now replaced by

\[
\begin{align*}
 U_g &= [\epsilon_g \rho_g \quad \epsilon_g \rho_g u_g \quad \epsilon_g \rho_g v_g \quad \epsilon_g e_g]^T, \\
 F(U_g) &= [\epsilon_g \rho_g u_g \quad \epsilon_g \rho_g u_g^2 \quad \epsilon_g \rho_g u_g v_g \quad \epsilon_g u_g (\epsilon_g + p_g)]^T, \\
 G(U_g) &= [\epsilon_g \rho_g v_g \quad \epsilon_g \rho_g u_g v_g \quad \epsilon_g v_g^2 \quad \epsilon_g v_g (\epsilon_g + p_g)]^T, \\
 H(U_g) &= \begin{bmatrix} 0 & \epsilon_g \frac{\partial p_g}{\partial x} & \epsilon_g \frac{\partial p_g}{\partial y} & 0 \end{bmatrix}^T, \\
 S(U_g, U_p) &= \begin{bmatrix} f_x & f_y & f_x u_p + f_y v_p + \dot{q} \end{bmatrix}^T,
\end{align*}
\]

because \( \epsilon_g = 1 - \epsilon_p \) is no longer approximated as unity. The vectors for the particle phase remains as given by Eq. (1.8). The obvious advantage is that the particle volume is taken into account in the gas phase equations. This makes predictions more relevant for mixture flows when numerous particles occupy a significant volume of the two-phase flow, but particle-particle collisions are still not handled in a realistic manner. In the continuum model of particles, the concentration of particles decreases or increases in various parts of the flow field, but actual particle-particle collisions are simply not treated realistically and the possible passing of one particle by another are neglected.

The most advanced method of a gas continuum and particle non-continuum is now reviewed. The gas is treated as a continuum and particles are allowed to move as individuals. This is illustrated in the adjoining figure where particles are swept along with the flow and are also falling slowly in the flow field. Notice that flow separation and vortex shedding are shown at the rear of these spherical particles. Each particle is accelerated by both the gas pressure and viscous shear of the gas acting around its surface. If the relative velocity is supersonic, then a bow shock and other waves would also be formed. In the case of inviscid and unsteady flow, the equations of gas motion of continuity, momentum, and energy are given by

\[
\frac{\partial U_g}{\partial t} + \frac{\partial F(U_g)}{\partial x} + \frac{\partial G(U_g)}{\partial y} + H(U_g) = 0 \tag{1.10}
\]

in two space dimensions, where the vectors

\[
\begin{align*}
 U_g &= [\rho_g \quad \rho_g u_g \quad \rho_g v_g \quad \epsilon_g]^T, \\
 F(U_g) &= [\rho_g u_g \quad \rho_g u_g^2 \quad \rho_g u_g v_g \quad \epsilon_g u_g (\epsilon_g + p_g)]^T, \\
 G(U_g) &= [\rho_g v_g \quad \rho_g u_g v_g \quad \rho_g v_g^2 \quad \epsilon_g v_g (\epsilon_g + p_g)]^T,
\end{align*}
\]
The equation of state $p_g = \rho_g R_g T_g$ is required to close these equations, and slip boundary conditions need to be applied around the surface of each moving particle during computations. Because the gas flows around individual particles within the space available to the gas, $\varepsilon_g$ is unity and not needed in the equations. The motion of the particle is due to form drag, that is the integrated effects of the pressure around the particle dictate the total force and Newton's second law is normally used to calculate the movement of each particle on an individual basis. If the particle is unsymmetric in shape, then particle rotation should also be included for more credible predictions. Note that the Reynolds-averaged Navier-Stokes equations with a turbulence model for the gas flow could also be solved, and then both the form and viscous drag would be simultaneously included along with the rotation of symmetrical particles from viscous effects.

The primary advantage of the method of a gas continuum and particle non-continuum two-phase flows with a definitive gas-particle interface is that it allows more realistic computations of interactions between the gas and particle motions. For example, a bow shock and other waves are induced if the relative velocity between the gas and particle is nearly equal or larger than the sound speed, and these gas-particle interactions can be predicted accurately only if particles are represented individually. This method also allows particle-particle collisions to be computed realistically, as well as particle-particle passings to be handled according to Newton's laws of motion as individual particles moving along separate paths.

There are many difficulties in computing flow fields of gases moving around individual particles. A first difficulty is that a fine computational grid is required to resolve the flow field around small particles accurately, and this normally results in much computational effort on supercomputers. The use of grid adaption or refinement can help reduce the effort. For example, the grid subdivision method used by Colella [1985 & 1990] and Pember, Bell, Colella, Crutchfield, & Welcome [1993] illustrated in the adjacent figure is a modern approach. Where flow gradients are large and also near and at surfaces of bodies, a large rectangular cell is subdivided into two or four smaller cells for grid refinement. These small cells are further subdivided if necessary, that is when gradients of flow properties are very large. Typically up to 7 to 10 levels of cell subdivisions may be required for accurate flow representation and a significant reduction in computational effort.

A second difficulty in computing flow fields of gases moving around individual particles is that grid refinement requires locating neighbouring cells in subdivided regions, which
typically involves quad- and octal-tree data structures for two- and three-dimensional flows, respectively. Such tree structures and their usage increases the computational overhead. Bayyuk, Powell, & Van Leer [1993] conducted a detail study of the quad-tree data structure required for locating the neighbours of any particular cell. Berger & LeVeque [1989] showed how to apply such grid refinement techniques to compute flows around arbitrary shaped bodies, and Davis & Dannenhoffer [1993] developed techniques of adaptive grid refinements for Navier-Stokes equations such that viscous drag can be included in the determination of the motion of the particle.

A third difficulty in computing flow fields of gases moving around individual particles is that the piece of a cell not overlapped by a particle (the shaded piece in the adjacent figure) can cause a reduction in the time step based on the Courant-Friedrichs-Lewy (CFL) criterion. In updating the gas flow properties of all cells, the common time step for all cells is limited by the shortest exposed side of all cells partly covered by particles. For complicated flows there is at least one exposed cell with an arbitrarily small exposed side; hence, the time step is correspondingly arbitrarily small.

The limiting time-step problem can usually be overcome by two methods. One method is that of cell merging and unmerging, which is illustrated in the adjacent figure. This is sometimes called local h-refinement [Powell, Roe, & Quirk, 1993]. In this h-refinement method, cells partly covered by particles are treated as specially shaped cells when all sides of an exposed cell are longer than one-half of their respective lengths. The overlapped particle surface is normally replaced by a straight line joining the two intersection points of the particle and cell boundaries. This special cell can have three, four, or five sides. In the other case when a particle covers more than one half the length of any cell side, the exposed part of the cell is merged with a neighbouring cell.

Another method of overcoming this limiting time-step problem is that of changing or adjusting cell corners. Needham [1994] implemented this scheme in solving defence problems involving the fracturing and dispersion of materials (e.g., concrete bulker walls) from explosions. This scheme is illustrated in the adjacent figure. In this case, the cell corners are adjusted to lie on the particle surface. Hence, these special cells all have four sides but these sides are normally not rectangular, and they therefore require special computational effort.

A fourth difficulty in computing flow fields of gases moving around individual particles occurs when two particles collide and many adjacent cells (e.g., part of a column of cells) are covered simultaneously, and when two particles separate and uncover many adjacent cells simultaneously. Cell merging and unmerging and cell corner alternations required additional corrections (fixups) such that the gas mass, momentum, and energy is neither created nor destroyed, and anomalous pressure excursions (zero or infinity) are not introduced.
A fifth difficulty in computing flow fields of gases moving around individual particles is that realistic handling of multiple particle collisions for flows with numerous particles. In numerical predictions, firstly, one must keep track of the boundaries of all the individual particles in the flow field and ensure that no overlapping of particles occurs. Secondly, if two particles have an impending collision then this collision process must be handled in a special manner such that they make contact and either rebound elastically or inelastically (or simply stick together). Triple or even multiple particle collisions pose additional difficulties in modelling. Note that cell mergings, corner alternations, and particle-particle collisions required complicated algorithm and computational overhead to implement. Typically, 5% to 15% of the cells in two-phase flow problems are simultaneously affected and need special computational care.

The present study introduces and assesses a new method of computing two-phase gas-particle flows with gas-particle interactions and particle-particle collisions. This method of computing two-phase flows introduces slightly smoothed interfaces between the phases, and this helps overcome most of the previous difficulties but introduces very few others. The interfaces between the gas and each solid-phase particle are slightly distributed in space and the two phases overlap at their common interface. For example, the particle-volume fraction $\varepsilon_p$ decreases rapidly at the body surface from unity within the body to zero outside the body. This is shown in the adjacent diagram for a spherical particle, where the thickness of the distributed particle surface is exaggerated greatly for illustration proposes. The gas-volume fraction $\varepsilon_g = 1 - \varepsilon_p$ decreases rapidly at its distributed interface with the particle from unity in the pure gas region to zero inside the solid particle. In addition to solving conventional gas-particle flow problems, this new method can also be used to solve other problems such as gas flows around airfoils (see the adjoining figure), but the primary advantage is obtained when solving two-phase flows with numerous moving particles that have a variety of shape and sizes.

The motion of the gas is computed throughout the entire flow field as flow through a mixture of free space (outside particles) and moving porous media (inside interfaces and particles). Euler's equations given by Eqs. (1.5) and (1.9) are used, in which $f_x$ and $f_y$ denote the viscous-flow resistances in $x$ and $y$ directions, respectively. Note that $\varepsilon_g = 1$ for the gas flow outside particles and $\varepsilon_g$ varies inside the distributed interfaces of particles and possibly also inside particles (e.g., $\varepsilon_g$ is set to a minimum value such as $10^{-4}$). Within interfaces and inside particles, large viscous forces are introduced such that gas-particle slip causes retarding interaction forces that helps diminish slip rapidly to zero as $\varepsilon_g$ becomes very small. The distributed interface eliminates the need for cell merging and unmerging, and
it also regularizes the computations for cells into a standard unified procedure. However, a suitable viscous-force function is needed to achieve this goal with sophistication.

The integrated effect of distributed viscous forces and gas pressure within the interface about a particle can be used as the driving forces in Newton’s laws to predict the motion of a particle. During particle-particle collisions the distributed surfaces of these particles are allowed to overlap. However, overlapping porosity distributions are then used to invoke repulsive forces which slow down the collision process and also repel the particles. A repulsive force model needs to be proposed to achieve this behaviour. Note that particle collisions with walls can be handled similarly by slightly distributing the wall surface; the wall is simply considered as a large stationary particle.

Grid adaption is still required to increase computational accuracy with reduced computational effort. Cell subdivision is now performed only where high gradients of flow properties and volume fraction occur in the flow field. No special grid subdivisions are required to help define particle surfaces as in previous methods. However, strong source terms involving the viscous and repulsive forces are introduced into Euler’s equations, and these cause difficulties in obtaining numerical solutions.

The primary objective of this study is to assess the advantages and difficulties of applying this newly proposed method of distributed interfaces between phases in gas-particle flows. One-dimensional flow problems involving (a) the reflection of a moving shock wave at a closed duct end and (b) the launching of a projectile by a high-pressure gas are solved for this propose. This is a preliminary step before solving more complicated two- and three-dimensional problems, because algorithms for the viscous forces and particle-particle collisions can be proposed, tested and refined by using these simple problems.

The governing equations of motion of gas-particle flow with distributed interfaces are introduced and discussed in chapter 2. The computational solution procedure is then described in chapter 3, and this is followed by a presentation of test-problem results. These test problems involve the reflection of a shock wave at a closed duct end and the launching of a projectile by a high-pressure gas in chapter 4. The thesis ends with concluding remarks in chapters 5 and reference follow.
Chapter 2

Model for Gas-Particle Flows with Distributed Phase Interfaces

2.1 Governing Equations for Gas Flows

Euler's continuity, momentum, and energy equations for unsteady, one-space-dimensional, compressible, inviscid flow of the continuum gaseous phase of a two-phase flow can be written in the form

\[
\begin{align*}
\frac{\partial}{\partial t} \begin{bmatrix}
\varepsilon_g \rho_g \\
\varepsilon_g \rho_g u_g \\
\varepsilon_g e_g
\end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix}
\varepsilon_g \rho_g u_g \\
\varepsilon_g \rho_g u_g^2 \\
\varepsilon_g u_g (e_g + p_g)
\end{bmatrix} + \begin{bmatrix}
0 \\
\varepsilon_g \frac{\partial p_g}{\partial x} \\
\frac{\partial \varepsilon_g}{\partial t}
\end{bmatrix} = \begin{bmatrix}
0 \\
f_{\text{visc}} \\
f_{\text{visc}} u_p
\end{bmatrix}
\end{align*}
\] (2.1)

with viscous losses due to gas flow through a porous medium. These equations have been adapted from Gough [1979] for the present case of gas-particle flows with distributed phase interfaces and viscous losses therein. The gas- and particle-volume fractions are denoted by \( \varepsilon_g \) and \( \varepsilon_p = 1 - \varepsilon_g \), respectively. The viscous-flow resistance \( f_{\text{visc}} \) has units of Newtons per unit of mixture volume and stems from the relative motion between the gas and porous medium in the distributed phase interface. Also, \( u_p \) is the velocity of the particle material, \( e_g = \rho_g C_v T_g + \frac{1}{2} \rho_g u_g^2 \) is the gas energy per unit volume, and \( f_{\text{visc}} u_p \) is the work done per unit mixture volume by the gas on a moving particle. There are no source terms for mass and energy in the continuity and energy equation because mass transfer and its corresponding energy transfer between the two phases are not considered in this work. Furthermore, heat transfer between the phases is not included in this preliminary study, so a heat transfer term does not occur as a source term in the energy equation.

The form of the term \( \varepsilon_g \frac{\partial p_g}{\partial x} \) in the momentum equation and the presence of the term \( p_g \frac{\partial \varepsilon_g}{\partial x} \) in the energy equation are both important. The term \( \varepsilon_g \frac{\partial p_g}{\partial x} \) gives the correct pressure force around a particle, whereas \( \frac{\partial (e_g p_g)}{\partial x} \) does not. The term \( p_g \frac{\partial \varepsilon_g}{\partial t} \)
is required to balance a similar term $p_g \partial \epsilon_p / \partial t$ in the particle equations such that the work between the moving phase boundaries is treated properly. Both terms are included correctly in the work of Gough [1979].

Equations (2.1) can be written in vector notation as

$$\frac{\partial U_g}{\partial t} + \frac{\partial F(U_g)}{\partial x} + H(U_g) = S(U_g, U_p)$$  \hspace{1cm} (2.2)

for brevity, where

$$U_g = \begin{bmatrix} \epsilon_g \rho_g \\ \epsilon_g \rho_g u_g \\ \epsilon_g e_g \\ 0 \end{bmatrix}, \quad F(U_g) = \begin{bmatrix} \epsilon_g \rho_g u_g \\ \epsilon_g \rho_g u_g^2 \\ \epsilon_g u_g \left( \epsilon_g + p_g \right) \end{bmatrix},$$

$$H(U_g) = \begin{bmatrix} \epsilon_g \frac{\partial p_g}{\partial x} \\ \epsilon_g \frac{\partial e_g}{\partial t} \\ p_g \frac{\partial e_g}{\partial t} \end{bmatrix}, \quad S(U_g, U_p) = \begin{bmatrix} 0 \\ f_{\text{visc}} \\ f_{\text{visc}} u_p \end{bmatrix}$$  \hspace{1cm} (2.3)

are the vectors.

The thermally perfect equation of state $p_g = \rho_g R_g T_g$ is used to help close the previous gas-flow equations. The variables $R_g$, $p_g$, $\rho_g$, and $T_g$ designate the gas constant, pressure, density, and temperature, respectively. Expressions given later for $f_{\text{visc}}$, and other results obtained from solving the equations of motion of the other phase for $\epsilon_p = 1 - \epsilon_g$ and $u_p$ complete the closure of the preceding equations. Note that the energy of the gas can be expressed as $e_g = \rho_g C_{p_g} T_g + \frac{1}{2} \rho_g u_g^2 = \frac{1}{1 - \epsilon_g} p_g + \frac{1}{2} \rho_g u_g^2$.

It is important to distinguish the difference between the density and partial density of both phases in a gas-particle mixture. The density $\rho_g$ of a gas is defined as the gas mass divided by the gas volume and the particle density $\rho_p$ (constant) is defined as the particle mass divided by the volume it occupies. On the other hand, the partial densities (or concentrations) $\sigma_g = \epsilon_g \rho_g$ and $\sigma_p = \epsilon_p \rho_p$ are defined as the gas mass and particle mass divided by the volume of the mixture, respectively. Similarly, the partial gas- and particle-phase momenta are defined by $\epsilon_g \rho_g u_g$ and $\epsilon_p \rho_p u_p$, respectively, and partial gas- and particle-phase energies are defined by $\epsilon_g e_g$ and $\epsilon_p e_p$, respectively. Note that $e_p = \rho_p C_{p_p} T_p + \frac{1}{2} \rho_p u_p^2$, in which $C_{p_p}$ and $T_p$ is the specific heat and temperature of the particle material, respectively.

2.2 Governing Equations for Particle Motions

Euler’s equivalent continuity, momentum, and energy equations for unsteady, one-dimensional, compressible, inviscid flow of the continuum particle phase of a two-phase flow
can be expressed in the form

\[
\frac{\partial}{\partial t} \begin{bmatrix}
  \varepsilon_p \rho_p \\
  \varepsilon_p \rho_p u_p \\
  \varepsilon_p e_p
\end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix}
  \varepsilon_p \rho_p u_p \\
  \varepsilon_p \rho_p u_p^2 \\
  \varepsilon_p e_p u_p (\varepsilon_p + p_g)
\end{bmatrix} + \begin{bmatrix}
  0 \\
  \varepsilon_p \frac{\partial \rho}{\partial x} \\
  p_g \frac{\partial e_p}{\partial t}
\end{bmatrix} = \begin{bmatrix}
  0 \\
  -f_{\text{visc}} \\
  -f_{\text{visc} u_p}
\end{bmatrix}
\] (2.4)

with viscous losses due to gas flow through a porous medium. These equations have been adapted from Gough [1979] for the present case of gas-particle phase interfaces and viscous flow losses therein. The viscous flow losses \(-f_{\text{visc}}\) in these particle-phase equations are identical but opposite in sign to that in the gaseous equations, because these are the interaction effects occurring between the two phases. The term \(p_g \frac{\partial e_p}{\partial t}\) in the energy equation is important. Without this term the temperature of the particle would change even though there is no heat transfer to cause this effect.

The conservation equations (2.4) can be expressed in vector notation as

\[
\frac{\partial \mathbf{U}_p}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U}_p)}{\partial x} + \mathbf{H}(\mathbf{U}_p) = -\mathbf{S}(\mathbf{U}_g, \mathbf{U}_p)
\] (2.5)

for convenience, where

\[
\mathbf{U}_p = \begin{bmatrix}
  \varepsilon_p \rho_p \\
  \varepsilon_p \rho_p u_p \\
  \varepsilon_p e_p
\end{bmatrix}, \quad \mathbf{F}(\mathbf{U}_p) = \begin{bmatrix}
  \varepsilon_p \rho_p u_p \\
  \varepsilon_p \rho_p u_p^2 \\
  \varepsilon_p u_p (\varepsilon_p + p_g)
\end{bmatrix},
\]

\[
\mathbf{H}(\mathbf{U}_p) = \begin{bmatrix}
  0 \\
  \varepsilon_p \frac{\partial \rho}{\partial x} \\
  p_g \frac{\partial e_p}{\partial t}
\end{bmatrix}, \quad \mathbf{S}(\mathbf{U}_g, \mathbf{U}_p) = \begin{bmatrix}
  0 \\
  f_{\text{visc}} \\
  f_{\text{visc} u_p}
\end{bmatrix}
\] (2.6)

are the vectors. Note that mass and heat transfer between the phases are absent as source terms because these effects are not included in this study.

The previous equations describe the motion of the particle phase as a continuum. In this study, this assumption of a continuum is relaxed and the motions of non-continuum independent particles are considered. This change in methodology is achieved by making the assumption that each particle is both incompressible and rigid. The effects of these changes is illustrated below.

Firstly, consider the continuity equation \(\frac{\partial (\varepsilon_p \rho_p)}{\partial t} + \frac{\partial (\varepsilon_p \rho_p u_p)}{\partial x} = 0\) for the particle phase. The material density \(\rho_p\) is constant (incompressible) and the velocity \(u_p\) is spatially constant within each particle (rigid and \(\partial u_p/\partial x = 0\)). The continuity equation reduces to

\[
\frac{\text{D}\varepsilon_p}{\text{D}t} = \frac{\partial \varepsilon_p}{\partial t} + u_p \frac{\partial \varepsilon_p}{\partial x} = 0
\] (2.7)
Hence, the particle-volume fraction \( \varepsilon_p \) for each particle is constant along its path through space with time, and independent particles can have their own \( \varepsilon_p \) distributions and move at their own velocities.

Secondly, consider the momentum equation
\[
\frac{\partial (\varepsilon_p \rho_p u_p)}{\partial t} + \frac{\partial (\varepsilon_p \rho_p u_p^2)}{\partial x} + \varepsilon_p \frac{\partial p_g}{\partial x} = -f_{\text{visc}}.
\]
For particles that are incompressible (constant \( u_p \)) and rigid (\( \partial u_p / \partial x = 0 \)), this equation reduces to
\[
\rho_p \varepsilon_p \frac{D u_p}{D t} + \varepsilon_p \frac{\partial p_g}{\partial x} + u_p \frac{D \varepsilon_p}{D t} = -f_{\text{visc}},
\]
with the last term \( u_p D \varepsilon_p / D t \) being zero by virtue at the earlier continuity equation. By integrating over a mixture volume that includes an entire particle (i.e., \( \int \cdots \, dV_m \)), and letting \( dV_m = A_m \, dx \) for one-dimensional flows and using Newton's second law, the acceleration of a particle in the gas flow is given by
\[
a_p = \frac{D u_p}{D t} = -\frac{A_m}{m_p} \int_{\text{particle}} \varepsilon_p \frac{\partial p_g}{\partial x} \, dx - A_m \int_{\text{particle}} f_{\text{visc}} \, dx,
\]
where \( A_m \) is the mixture cross-sectional area for a one-dimensional flow. This equation governs the velocity of a particle along its trajectory from the influence of the forces from both the flow pressure gradient and viscous-flow losses in the distributed phase interface around the particle.

Thirdly, the energy equation
\[
\frac{\partial (\varepsilon_p e_p)}{\partial t} + \frac{\partial (\varepsilon_p (e_p + p_g))}{\partial x} + p_g \frac{\partial e_p}{\partial x} = -f_{\text{visc}} u_p
\]
can be reduced to the following form
\[
\frac{D T_p}{D t} = 0,
\]
by using the assumptions of particle incompressibility and rigidity and previous results from the continuity and momentum equations. The above equation illustrates that the temperature \( T_p \) of a particle remains constant along its path. This result should be expected because heat transfer and external work are not included in the energy equation.

### 2.3 Equations for Smoothly Distributing an Interface

Smoothly distributed interfaces between the gas and particle phases are introduced such that the thickness of the interface is small compared to particle size dimensions and the average distance between particles in which the gas flows. In these thin interfaces the porosity of the solid is rapidly changed from a particle-volume fraction \( \varepsilon_p \) of zero outside the particle to unity within the particle. The gas-volume fraction \( \varepsilon_g = 1 - \varepsilon_p \) changes correspondingly from unity in the gaseous phase to zero within the solid-particle phase. The thickness of phase interface is problem dependent, and the numerical modeller or computer-code user must set this thickness for the particular problem being solved. In this section, a convenient transition shape function is suggested for smoothly distributing \( \varepsilon_p \) and \( \varepsilon_g \) with distance at the periphery of the particle. Note that variations in gas flow properties (e.g.,
pressure, density, gas-flow velocity) through the distributed interface are the outcome of the flow computations that depend on the viscous-flow losses within the interface.

A Bézier's cubic polynomial [Sarfraz, 1994] is used to simultaneously distribute smoothly the particle- and gas-volume fractions \( \varepsilon_p \) and \( \varepsilon_g \) through the distributed phase interface. A convenient parametric representation is given below for both \( \varepsilon_g \) and \( \varepsilon_p \) as

\[
\begin{align*}
\varepsilon_g &= \varepsilon_{g1} + 3(\varepsilon_{g2} - \varepsilon_{g1})\eta(1 - \eta)^2 + 3(\varepsilon_{g3} - \varepsilon_{g1})\eta^2(1 - \eta) + (\varepsilon_{g4} - \varepsilon_{g1})\eta^3, \\
\varepsilon_p &= \varepsilon_{p1} + 3(\varepsilon_{p2} - \varepsilon_{p1})\eta(1 - \eta)^2 + 3(\varepsilon_{p3} - \varepsilon_{p1})\eta^2(1 - \eta) + (\varepsilon_{p4} - \varepsilon_{p1})\eta^3, \\
x &= x_1 + 3(x_2 - x_1)\eta(1 - \eta)^2 + 3(x_3 - x_1)\eta^2(1 - \eta) + (x_4 - x_1)\eta^3,
\end{align*}
\]

for which the free parameter \( \eta \) has the range \( 0 \leq \eta \leq 1 \). This Bézier curve begins at the \( \varepsilon_{g1} = 1, \varepsilon_{p1} = 0 \), and \( x = x_1 \) when \( \eta = 0 \), changes smoothly as \( \eta \) increases, and ends at the location \( \varepsilon_{g4} = 0, \varepsilon_{p4} = 1 \), and \( x = x_4 \) when \( \eta = 1 \). The shape is controlled by specifying two control coordinates \( \varepsilon_{g2} \) or \( \varepsilon_{p2} \) at \( x_2 \) and \( \varepsilon_{g3} \) or \( \varepsilon_{p3} \) at \( x_3 \). For a symmetrically shaped interface with zero slopes for \( \varepsilon_g \) and \( \varepsilon_p \) at both ends, we set \( x_2 - x_1 = x_4 - x_3, \varepsilon_{g2} = 1 \) or \( \varepsilon_{p2} = 0 \) and \( \varepsilon_{g3} = 0 \) or \( \varepsilon_{p3} = 1 \). In this study we also set \( x_2 - x_1 = x_4 - x_3 = \frac{3}{10}(x_4 - x_1) \).

The interfacial variation of \( \varepsilon_g \) and \( \varepsilon_p \) versus normalized distance are both illustrated on the adjacent figure for interest. The four coordinates defining the \( \varepsilon_g \) curve are indicated by black dots and the corresponding coordinates for the \( \varepsilon_p \) curve are shown as open circles.

### 2.4 Equations for Viscous-Flow Resistance

The viscous-flow resistance is specified in the form

\[
f_{\text{visc}} = -C_{\text{visc}}B(x) \left[ \frac{1}{2} c_{\text{visc}} \alpha_g (u_g - u_p) + \frac{1}{2} \rho_g (u_g - u_p) |u_g - u_p| \right]
\]

for the present work. The coefficient \( C_{\text{visc}} \) is set to a value of 0.52. The coefficient \( c_{\text{visc}} \) in the “linear dynamic-slip pressure” term is set to a value of about \( 3.02 \times 10^{-2} \), and in this term \( \alpha_g \) is the sound speed (normally set to a constant value of \( 331.32 \text{ m/s} \)). The last term in the viscous-flow resistance is the “quadratic dynamic-slip pressure”. The variable \( B(x) \) denotes the function which depends on \( x \); it is zero where particle material is absent (\( \varepsilon_p = 0 \)) and it rises to a maximum value where particle material occupies the entire mixture volume (\( \varepsilon_p = 1 \)). \( B \) versus \( x \) is shown in the adjoining figure (below). The parametric equations for
setting up $B(x)$ are given by

\begin{align}
B(x) &= B_1 + 3(B_2 - B_1)\zeta(1 - \zeta)^2 + 3(B_3 - B_1)\zeta^2(1 - \zeta) + (B_4 - B_1)\zeta^3, \quad (2.15) \\
x &= x_b + 3(x_b - x_{b1})\zeta(1 - \zeta)^2 + 3(x_{b3} - x_{b1})\zeta^2(1 - \zeta) + (x_{b4} - x_{b1})\zeta^3, \quad (2.16)
\end{align}

where $\zeta$ is a parameter with $0 \leq \zeta \leq 1$ and $(x_{b1}, B_1)$ are four control points for which $(x_{b1}, B_1) = (0, 0), (x_{b2}, B_2) = (1, 0), (x_{b3}, B_3) = (0.5, 1.0), \text{ and } (x_{b4}, B_4) = (1, 1)$. This function $B(x)$ is related to the particle-volume fraction $\varepsilon_p$ via Eqs. (2.12) and (2.13). Hence, $B(x)$ is directly related to the particle-volume fraction in this sense. $B$ versus $\varepsilon_p$ is shown in the adjoining figure (below).
Chapter 3

Computational Solution Procedure

The computational procedure outlined in this chapter begins by defining the grid and cells used in the numerical computations. Then the method of estimating fluxes into and out of cells by means of solving Riemann problems is described. Godunov's scheme for solving the partial differential equations for the motion of the gaseous phase of the two-phase mixture is introduced next. The gas motion is solved independently of the particle-phase motion by using a special integration software package called VODE. A description of this commercially available package and its use is presented next. After outlining the solution procedure using the VODE software for the gaseous motion, the description of the method of solving the motion of the particle phase is finally presented.

3.1 Grid for Numerical Computations

The grid used for the present numerical computations consists of equally sized cells in one space dimension, and nodes are located at the centres of each cell. This node-centered grid is illustrated in the following figure. The nodes are numbered from 1 to N and the cell width is equal to $\Delta x$.

3.1.1 Flux Estimations

Flux evaluation at cell boundaries consists of solving a Riemann problem, and the Riemann problem is now discussed. It is a problem which deals with the fluid's behaviour
at a discontinuity. The adjoining figure shows a typical wave pattern of a Riemann problem. The average conservative variables in a cell (e.g., $\epsilon_g \rho_g$, $\epsilon_g \rho_g u_g$, and $\epsilon_g e_g$) are indicated by a dash line. Average variables in adjoining cells may be different and this produces a discontinuity at the cell boundaries. The discontinuity at the boundary ($i - 1/2$) produces a shock wave ($S$) that travels to the left and a rarefaction wave ($R$) that travels to the right. A contact surface ($C$) is also produced and it is shown as travelling to the left. To obtain the states between various waves in the Riemann problem, a Riemann solver is required. The Riemann solver of Gottlieb & Groth [1988] for unsteady, one-dimensional, compressible, inviscid flow of perfect gases is used. It is important to notice that their Riemann solver does not apply directly to solving the conservation equation (2.1) because it does not include the effects of gas-volume fraction $\epsilon_g$ and all source terms directly in its solution. However, the application of this Riemann solver is used to estimate the solution of the Riemann problem and then extract the flux at the cell boundary.

3.2 Godunov’s First-Order Scheme

The gas-phase conservation equations were given previously by Eq. (2.2) as

$$\frac{\partial \mathbf{U}_g}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U}_g)}{\partial x} + \mathbf{H}(\mathbf{U}_g) = \mathbf{S}(\mathbf{U}_g, \mathbf{U}_p)$$

(3.1)

where the vectors follow in Eq. (2.3), but are redefined slightly below:

$$\mathbf{U}_g = \begin{bmatrix} \epsilon_g \rho_g \\ \epsilon_g \rho_g u_g \\ \epsilon_g e_g \end{bmatrix}, \quad \mathbf{F}(\mathbf{U}_g) = \begin{bmatrix} \epsilon_g \rho_g u_g \\ \epsilon_g (\rho_g u_g^2 + p_g) \\ \epsilon_g u_g (e_g + p_g) \end{bmatrix}.$$

1The Riemann solver applies directly to the one-dimensional compressible, inviscid, flow of perfect gases for which the conservation equations are given by

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho_g \\ \rho_g u_g \\ e_g \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \rho_g u_g \\ \rho_g u_g^2 + p_g \\ u_g (e_g + p_g) \end{bmatrix} = 0$$

without change in flow area.
To solve this set of partial differential equations, Godunov's first-order scheme is used because it deals directly with the physics of fluid motions from one cell to the next. Also it is one of the simplest to apply in its first-order form. In Godunov's first-order scheme, the spatial derivatives at the $i$th cell are written in terms of the fluxes at the cell boundaries as

$$\frac{\partial F(\hat{U}_g)}{\partial x} \approx \frac{F\left[\mathcal{R}\left(\hat{U}_{g_{i-1/2}}^{-}, \hat{U}_{g_{i+1/2}}^{+}\right)\right] - F\left[\mathcal{R}\left(\hat{U}_{g_{i-1/2}}^{-}, \hat{U}_{g_{i+1/2}}^{+}\right)\right]}{\Delta x},$$

where

$$\hat{U}_g = \begin{bmatrix} \rho_g \\ \rho_g u_g \\ e_g \end{bmatrix}, \quad F(\hat{U}_g) = \begin{bmatrix} \rho_g u_g \\ \rho_g u_g^2 + p_g \\ u_g(e_g + p_g) \end{bmatrix} \quad (3.4)$$

are the vectors. In the above equations, $F\left[\mathcal{R}\left(\hat{U}_{g_{i-1/2}}^{-}, \hat{U}_{g_{i+1/2}}^{+}\right)\right]$ denotes the flux evaluated at the left boundary $(i-1/2)$ from the Riemann solution $\mathcal{R}\left(\hat{U}_{g_{i-1/2}}^{-}, \hat{U}_{g_{i+1/2}}^{+}\right)$ between states $\hat{U}_{g_{i-1/2}}^{-}$ and $\hat{U}_{g_{i+1/2}}^{+}$. Notice that $\hat{U}_{g_{i-1/2}}^{-}$ denotes the state on the left side of the left boundary $(i-1/2)$ and $\hat{U}_{g_{i+1/2}}^{+}$ denotes the state on the right side of the left boundary $(i-1/2)$. Similarly, $F\left[\mathcal{R}\left(\hat{U}_{g_{i+1/2}}^{-}, \hat{U}_{g_{i+1/2}}^{+}\right)\right]$ denotes the flux evaluated at the right boundary $(i+1/2)$ from the Riemann solution $\mathcal{R}\left(\hat{U}_{g_{i+1/2}}^{-}, \hat{U}_{g_{i+1/2}}^{+}\right)$ between states $\hat{U}_{g_{i-1/2}}^{-}$ and $\hat{U}_{g_{i+1/2}}^{+}$. Notice that $\hat{U}_{g_{i+1/2}}^{-}$ denotes the state on the left side of the right boundary $(i+1/2)$ and $\hat{U}_{g_{i+1/2}}^{+}$ denotes the state on the right side of the right boundary $(i+1/2)$. For Godunov's first-order scheme we use

$$\hat{U}_{g_{i-1/2}}^{-} = \hat{U}_{g_{i-1}}, \quad \hat{U}_{g_{i+1/2}}^{+} = \hat{U}_{g_i},$$

$$\hat{U}_{g_{i+1/2}}^{-} = \hat{U}_{g_{i}}, \quad \hat{U}_{g_{i+1/2}}^{+} = \hat{U}_{g_{i+1}},$$

because state extrapolations to the boundaries is not incorporated. Then Euler's equations (2.2) for the $i$th cell can be expressed as

$$\frac{\partial \mathbf{U}_g}{\partial t} = \mathbf{S}(\mathbf{U}_g, U_p) - \mathbf{H}(\mathbf{U}_g) - \frac{F\left[\mathcal{R}(\mathbf{U}_{g_{i-1}}, \mathbf{U}_{g_i})\right] - F\left[\mathcal{R}(\mathbf{U}_{g_{i}}, \mathbf{U}_{g_{i+1}})\right]}{\Delta x} \quad (3.7)$$

in vector form.

The term $p_g \partial e_g / \partial x$ in the vector $\mathbf{H}(\mathbf{U}_g)$ in the conservation equation (3.7) is approximated by a second-order central-difference formula

$$p_g \left(\frac{\partial e_g}{\partial x}\right)_i \approx p_g \frac{e_{g_{i+1}} - e_{g_{i-1}}}{2\Delta x} \quad (3.8)$$

where the subscript $i$ denotes the $i$th cell. The term $p_g \partial e_g / \partial t$ is ignored in the present work.
3.3 Variable-Coefficient ODE Solver

The heart of the solution procedure for solving the partial differential equations for the gaseous phase is the usage of a double-precision variable-coefficient ordinary differential equation solver called VODE. The primary reason for using this solver is that the conservation equations (2.2) contains strong source terms. Strong source terms produce large changes in the flow variables during a flow time step; hence, sub time steps are required to properly integrate into the solution in the influence of the source terms with more accuracy and to even maintain solution stability. The VODE subroutine treats the set of partial differential equations (PDEs) as if they were a set of ordinary differential equations (ODEs) for the purpose of integration.

3.3.1 System of ODEs

The set of partial differential equations for the gaseous phase can be written in the form

\[
\frac{\partial \mathbf{V}}{\partial t} = \mathbf{T}(\mathbf{V}), \quad (3.9)
\]

for solution by the VODE subroutine, where

\[
\mathbf{V} = \begin{bmatrix}
\mathbf{\tilde{U}}_1 \\
\vdots \\
\mathbf{\tilde{U}}_{i-1} \\
\mathbf{\tilde{U}}_i \\
\vdots \\
\mathbf{\tilde{U}}_{i+1} \\
\vdots \\
\mathbf{\tilde{U}}_{N-1} \\
\mathbf{\tilde{U}}_N
\end{bmatrix}, \quad \mathbf{T}(\mathbf{V}) = \begin{bmatrix}
0 \\
\mathbf{\tilde{S}}_2 \\
\vdots \\
\mathbf{\tilde{S}}_{i-1} \\
\mathbf{\tilde{S}}_i \\
\vdots \\
\mathbf{\tilde{S}}_{i+1} \\
\vdots \\
\mathbf{\tilde{S}}_{N-1} \\
0
\end{bmatrix} - \frac{1}{\Delta x} \begin{bmatrix}
0 \\
\mathbf{\tilde{G}}_2 \\
\vdots \\
\mathbf{\tilde{G}}_{i-1} \\
\mathbf{\tilde{G}}_i \\
\vdots \\
\mathbf{\tilde{G}}_{i+1} \\
\vdots \\
\mathbf{\tilde{G}}_{N-1} \\
0
\end{bmatrix}, \quad (3.10)
\]

with

\[
\mathbf{\tilde{U}}_i = \begin{bmatrix}
\mathbf{U}_{gi} \\
\varepsilon_{gi}
\end{bmatrix}, \quad \mathbf{\tilde{S}}_i = \begin{bmatrix}
\mathbf{S} \left( \mathbf{U}_{gi}, \mathbf{U}_{pi} \right) - \mathbf{H} \left( \mathbf{U}_{gi} \right) \\
\frac{\partial \varepsilon_{gi}}{\partial t}
\end{bmatrix}, \quad (3.11)
\]

\[
\mathbf{\tilde{G}}_i = \begin{bmatrix}
\mathbf{F} \left[ \mathbf{R} \left( \mathbf{U}_{gi}, \mathbf{U}_{gi+1} \right) \right] - \mathbf{F} \left[ \mathbf{R} \left( \mathbf{U}_{gi-1}, \mathbf{U}_{gi} \right) \right] \\
0
\end{bmatrix}.
\quad (3.12)
\]

Notice that each \( \mathbf{\tilde{U}}_i \), for \( 1 \leq i \leq N \), contains three conservative variables \( \varepsilon_{gi}, \rho_{gi}, \varepsilon_{gi}, \rho_{gi}, \varepsilon_{gi} \), and \( \varepsilon_{gi}, \varepsilon_{gi} \) for the gas. The gas-volume fraction \( \varepsilon_{gi} \) is the fourth entry for the \( i^{th} \) cell, such
that the dimension of \( \vec{V} \) is \( 4N \times 1 \). The source vector \( \vec{S}_i \) of the \( i \)th cell consists of \( S(U_g, U_P) \) and \( H(U_g) \) in Eq. (3.2) and with a fourth entry

\[
\left( \frac{\partial s_i}{\partial t} \right)_i \approx \frac{\varepsilon_{gi}^{\text{new}} - \varepsilon_{gi}^{\text{old}}}{\Delta t},
\]

is a first order approximation of the time derivative of the gas-volume fraction. \( \vec{G}_i \) is a \( 4 \times 1 \) vector consists of three entries that are an approximation of the spatial derivative of the flux vector given by the Riemann solution and the last entry is zero. Each entry inside the square bracket in Eq. (3.10) is a \( 4 \times 1 \) vector and \( \vec{O} \) is a \( 4 \times 1 \) null vector.

The first and the last cell in the source terms of the ODE system in Eq. (3.10) are forced to be zero, which is equivalent to having zero time derivative for the conservative variables in the first and last cells of the grid. These is stem from the application of non-reflecting boundary conditions at the grid ends. However, this is only half of the picture. The other step in applying non-reflecting boundary conditions [Gottlieb, Zhang, & Groth, -] is that the states at the first and last cells are set equal to the states at their adjacent cell. Hence, no wave can be reflected back into the flow field.

### 3.3.2 Jacobian Matrix for the ODE System

The Jacobian for the ODE system is a banded matrix given by

\[
\frac{\partial T(V)}{\partial V} = \\
\begin{bmatrix}
\frac{\partial T_1}{\partial U_1} & \frac{\partial T_1}{\partial U_2} & 0 & \cdots & \cdots & 0 \\
\frac{\partial T_2}{\partial U_1} & \frac{\partial T_2}{\partial U_2} & \frac{\partial T_2}{\partial U_3} & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \frac{\partial T_3}{\partial U_2} & \frac{\partial T_3}{\partial U_3} & \frac{\partial T_3}{\partial U_4} & 0 & \cdots \\
0 & \cdots & 0 & \frac{\partial T_{N-2}}{\partial U_{N-3}} & \frac{\partial T_{N-2}}{\partial U_{N-2}} & \frac{\partial T_{N-2}}{\partial U_{N-1}} \\
0 & \cdots & \cdots & 0 & \frac{\partial T_{N-1}}{\partial U_{N-2}} & \frac{\partial T_{N-1}}{\partial U_{N-1}} \\
0 & \cdots & \cdots & \cdots & 0 & \frac{\partial T_N}{\partial U_{N-1}} & \frac{\partial T_N}{\partial U_N}
\end{bmatrix}
\]

\[ (3.14) \]
Because of the definitions of V and T(V) in Eq. (3.10), there are a major diagonal, 7 upper, and 7 lower sub-diagonals in the Jacobian. The Jacobian is evaluated internally by the VODE subroutine.

3.3.3 VODE Usage

Inputs of the VODE subroutine consist of both standard and optional inputs, input constants, and variables. Specific values are listed below:

\[
\begin{align*}
\text{NEQ} &= 2004, \\
T &= 0.0, \\
\text{TOUT} &= 0.0, \\
\text{ITOL} &= 1, \\
\text{RTOL} &= 1.0 \times 10^{-5}, \\
\text{ATOL} &= 1.0 \times 10^{-6}, \\
\text{ITASK} &= 1, \\
\text{ISTATE} &= 1, \\
\text{IOPT} &= 1, \\
\text{LRW} &= 62146, \\
\text{LIW} &= 2034, \\
\text{ML} &= 7, \\
\text{MU} &= 7, \\
\text{MF} &= -25, \\
\text{RPAR} &= 0.0, \\
\text{IPAR} &= 0, \\
\text{H0} &= 0.0, \\
\text{HMAX} &= 0.0, \\
\text{HMIN} &= 0.0, \\
\text{MAXORD} &= 0, \\
\text{MXSTEP} &= 10000, \\
\text{MXHNIL} &= 20.
\end{align*}
\]

To use the VODE package, in addition to the setting up input parameters, one needs to decide which differencing method is used, the corresponding sizes of double-precision variables and integer work-arrays in LRW and LIW, the size of the upper and lower sub-diagonals of the Jacobian in ML and MU, etc. Please refer to the internal documentation of the VODE package for more details. Also, see Byrne & Hindmarsh, 1975; Jackson & Sacks-Davis, 1980; Hindmarsh, 1983; Byrne & Hindmarsh, 1987; Brown, Byrne, & Hindmarsh, 1989; and Byrne, 1992.
### 3.4 Particle Motion

The acceleration of a particle was given by Eq. (2.9) as

\[
a_p = -\frac{A_m}{m_p} \int_{\text{particle}} \rho_p \frac{\partial p_g}{\partial x} \, dx - A_m \int_{\text{particle}} f_{\text{visc}} \, dx ,
\]

for which the integration is over the entire particle. This integration is done by using finite differencing, and

\[
a_p^{\text{new}} \simeq -\frac{A_m}{m_p} \sum_i \rho_p \frac{p_{g,i+1} - p_{g,i-1}}{\Delta x} - A_m \sum_i f_{\text{visc},i} \Delta x
\]

is used in the computer code. The superscript 'new' is used because the variables in the above equation are the updated flow properties from the last time level. Hence, the displacement and velocity of a particle with distributed interface are given by

\[
x_p^{\text{new}} = x_p^{\text{old}} + u_p^{\text{old}} \Delta t + \frac{1}{2} a_p^{\text{old}} \Delta t^2 ,
\]

\[
u_p^{\text{new}} = u_p^{\text{old}} + a_p^{\text{old}} \Delta t ,
\]

where \(x_p, u_p,\) and \(\Delta t\) denote the particle displacement, velocity, and time step between the last time level (the superscript 'old') and the current time level (the superscript 'new'). In particular, \(a_p^{\text{old}}\) is the particle acceleration evaluated in Eq. (3.16) in which the gas properties in that equation are obtained from the last time level.
Chapter 4

Test Problems

In this chapter, two test problems are discussed and results are shown by applying the concept of distributed phase interfaces between the gas and particles. The first problem is the numerical prediction of the reflection of a moving shock wave by a stationary closed duct end that has a distributed interface with the gas. The second problem is the numerical prediction of the motion of a projectile by a high-pressure gas on one side and a low-pressure gas on the other. Each problem is first defined, followed by a discussion of the known analytical solution, and the required application of initial conditions. The computational results for each problem are then discussed.

4.1 Shock Reflection at a Distributed Interface

4.1.1 Problem Definition

As a first trial of the concept of distributed phase interface, an unsteady one-space-dimensional prediction of the interaction between perfect gases and a stationary distributed interface is completed, so that the effects of the gas-volume fraction and the viscous-flow resistance as sources in the Euler's equations can be studied. This prediction involves the reflection of a shock wave by a distributed interface in a constant area duct with compressible, inviscid flows of perfect gases. Three assumptions are made. Firstly, the end of the constant area duct is slightly distributed over a number of cells while the side surface of the duct remains well-defined. Secondly, there is no heat transfer between the gas and the constant area duct. Thirdly, the distributed interface of the duct end is non-deformable. The
reflection of a shock wave by a duct end shown in the adjoining figure (top) is solved analytically. The solution of this problem is well known, and it can be predicted theoretically by using gasdynamic theory [Zucrow, 1976; Anderson, 1982]. The interface of the duct end and the gas is slightly distributed in the adjoining figure (bottom). Notice that both figures are aligned at the average end of the duct and the exaggerated length of shading illustrated the distributed phase interface for illustration purposes only. A number of numerical predictions are completed by applying Godunov's first order scheme with VODE to the appropriate Euler's equations.

4.1.2 Analytical Solution

The analytical solution of the one-dimensional reflection of a shock wave by a duct end is well known and can be obtained via gasdynamic theory [Zucrow, 1976; Anderson, 1982].

\[
\frac{p_2}{p_1} = \frac{2\gamma M_i^2}{\gamma + 1} - \frac{\gamma - 1}{\gamma + 1}, \quad (4.1)
\]

\[
\frac{\rho_2}{\rho_1} = \frac{\gamma + 1}{2} \left( 1 + \frac{\gamma - 1}{2} M_i^2 \right), \quad (4.2)
\]

\[
u_2 \frac{a_1}{a_1} = \frac{2 M_i^2 - 1}{\gamma + 1} M_i, \quad (4.3)
\]

\[
\left( \frac{a_2}{a_1} \right)^2 = \frac{p_2}{p_1} \left[ \frac{\gamma - 1}{\gamma + 1} + \frac{2}{(\gamma + 1) M_r^2} \right]. \quad (4.4)
\]

Knowing that the gas flow velocity \( u_3 \) behind the reflected shock is zero, one can determine the shock Mach number \( M_r \) of the reflected shock from the following quadratic equation,

\[
M_r^2 + \frac{\gamma + 1}{2} \frac{u_2}{a_2} M_r - 1 = 0. \quad (4.5)
\]
Notice that for the above quadratic equation, one root is positive while the other one is negative because the product equals $-1$. The positive solution is dropped because the reflected shock is moving to the left. Thus,

$$M_r = -\frac{1}{2} \left[ \frac{\gamma + 1}{2} \frac{u_2}{a_2} + \sqrt{\left(\frac{\gamma + 1}{2} \frac{u_2}{a_2}\right)^2 + 4} \right]. \quad (4.6)$$

Hence, the state after the reflected shock is given by

$$\frac{p_3}{p_2} = \frac{2\gamma}{\gamma + 1} M_r^2 - \frac{\gamma - 1}{\gamma + 1}, \quad (4.7)$$

$$\frac{\rho_3}{\rho_2} = \frac{\frac{\gamma + 1}{2} M_r^2}{1 + \frac{\gamma - 1}{2} M_r^2}, \quad (4.8)$$

$$u_3 = 0, \quad (4.9)$$

$$(\frac{a_3}{a_2})^2 = \frac{p_3}{p_2} \left[ \frac{\gamma - 1}{\gamma + 1} + \frac{2}{(\gamma + 1)M_r^2} \right], \quad (4.10)$$

where the subscripts 1, 2, and 3 refer to the gaseous state in front of and behind the incoming shock, and the gaseous state behind the reflected shock, respectively. Notice that the subscript $g$ is dropped in the above equations.

### 4.1.3 Initial Conditions

In the numerical prediction of shock moves into a perfect gas at atmospheric conditions. A grid of 200 evenly distributed nodes are used. The full length of the grid is 10 m such that each cell is 0.05 m in width. From $x = 0$ m to $x = 2.5$ m, the grid is in the gas phase where $\varepsilon_g = 1$. The distributed phase interface of the closed duct end starts at $x = 2.5$ m to $x = 7.5$ m and $\varepsilon_g$ is defined via the method described in section 2.3. From $x = 7.5$ m to $x = 10$ m, the grid is in the solid phase where $\varepsilon_g = \varepsilon_{g_{\text{min}}}$.

The initial conditions for the gas properties are as follows. In front of the shock, the pressure is 101.3 kPa, 1.293 kg/m$^3$ in the density, 0 m/s in flow velocity, 287 J/kg-K in gas constant, and 1.4 in ratio of specific heats.

Initially, the incoming shock is located at $x = 1$ m. The shock Mach number is 2 in one trial and 4 in a different trial. The gas properties behind the incoming shock are evaluated by using the shock relations from Eq. (4.1) to Eq. (4.4).

### 4.1.4 Results

In solving this problem, numerous results are obtained with different parameters. In this report, some of the best are shown. In the following results, there is a 0.5 millisecond
difference in time between successive profiles shown.

In Fig. 4.1, the gas-volume fraction profile is shown. The distributed phase interfaces starts at $x/\Delta x = 50$ and ends at $x/\Delta x = 150$. The minimum of the gas-volume fraction is given by $\varepsilon_{\text{gmin}} = 10^{-4}$. Notice that the four control points used to generate the profile are shown as hollow squares. In Fig. 4.2, the second-order central-differencing of the spatial derivative $\partial \varepsilon_\text{g}/\partial x$ and the term in the viscous-flow resistance $B(x)$ are shown. Notice that the four control points used to generate the profile are shown as hollow squares. From Fig. 4.3 to Fig. 4.6, the gas pressure, density, sound speed, and flow Mach number are shown, respectively, for the case of $M_\text{i} = 2$. The incoming and reflected shock wave can be easily identified and a dashed line is shown as the incoming starts to interact with and reflected by the distributed phase interface. Notice that the theoretical prediction of state after the reflected shock wave is marked by a horizontal line. In Fig. 4.3, the pressure after the reflected shock is slowly rising to the theoretical prediction.

In Figs. 4.7 and 4.8, the pressure and density profile are shown for the incoming shock Mach number at 4, respectively. The pressure and density rises more rapidly, but a larger overshoot also occurs. This is illustrated in the Fig. 4.7.

From Figs. 4.9 to 4.11, the minimum of gas-volume fraction is given by $\varepsilon_{\text{gmin}} = 10^{-2}$ which is two orders in magnitude larger than before. The pressure and density profile are shown in Figs. 4.10 and 4.11, respectively. It is interesting to notice that there are smaller overshoots in this setup compared to previous results.
4.2 Projectile Acceleration

4.2.1 Problem Definition

The second problem involves the interactions between the compressible, inviscid, flow of a perfect gas and the launching projectile with distributed phase interfaces in one space dimension. Four assumptions are made for this numerical prediction. Firstly, the projectile is of the shape of a cylinder, and the frontal and rear surfaces of the projectile are slightly distributed. Secondly, the projectile fits perfectly inside the constant area duct. Thirdly, there is neither heat transfer nor friction between the duct and the projectile. Finally, the projectile and the constant area duct are non-deformable. The motion of a projectile in the adjacent figure (top) can be predicted with a rarefaction wave at the back and a compression wave at the front of the projectile by using gasdynamic theory. The frontal and rear surfaces of the projectile are distributed artificially in the adjoining figure (bottom), where the form of the distribution is pre-defined. Notice that in both figures the projectile are aligned at the average of the projectile surface. A number of numerical predictions are completed by applying Godunov's first-order scheme with VODE, a variable-coefficient ODE solver.

4.2.2 Analytical Solution

The equation of motion of the projectile in a constant-area duct is given by the Newton’s second law

\[ a_p = \frac{du_p}{dt} = \frac{d^2x_p}{dt^2} = \frac{1}{m_p} (F_{\text{front}} + F_{\text{back}}) , \]

where \( a_p, u_p, x_p, \) and \( m_p \) designate the particle acceleration, velocity, displacement, and mass, respectively. The variables \( F_{\text{front}} \) and \( F_{\text{back}} \) denote the force acting on the projectile. The forces can be derived by using gasdynamic theory. At the frontal surface of the projectile, a compression wave is formed. By crossing this compression wave using the method of characteristics [Zucrow, 1976; Anderson, 1982], the force acting on the frontal surface of the projectile is given by

\[ F_{\text{front}} = -A_p p_r \left( 1 + \frac{\gamma_r - 1}{2a_{gr}} u_p \right)^{\frac{\gamma_r}{\gamma_r - 1}} \]

as the forces on the frontal surface of the projectile. The symbol \( A_p \) denotes the cross-sectional area of the projectile and the subscript \( r \) designates the gaseous properties on the right side of the projectile. Notice that this force has a minus sign because the direction is
to the left. Similarly, the force acting on the back of the projectile can be determined by assuming a rarefaction wave is formed at the back of the projectile. The force acting on the back of the projectile is given by

\[ F_{\text{back}} = A_p p_{\text{gi}} \left( 1 - \frac{\gamma_i - 1}{2a_{\text{gi}}} u_p \right)^{\frac{2\gamma_i}{\gamma_i - 1}}. \]  

(4.13)

Hence, the projectile velocity can be written as an ordinary differential equation

\[ \frac{du_p}{dt} = \frac{A_p}{m_p} \left[ p_{\text{gi}} \left( 1 - \frac{\gamma_i - 1}{2a_{\text{gi}}} u_p \right)^{\frac{2\gamma_i}{\gamma_i - 1}} - p_{\text{gr}} \left( 1 + \frac{\gamma_r - 1}{2a_{\text{gr}}} u_p \right)^{\frac{2\gamma_r}{\gamma_r - 1}} \right], \]  

(4.14)

which is solved numerically for \( u_p \). The displacement and acceleration of the projectile are then calculated according to Eq. (4.11).

### 4.2.3 Initial Conditions

In this problem a projectile with a diameter of about 5 inches and mass of about 40 kg (steel, 7860 kg/m\(^3\)) is moved from one end of the grid of 4 meters long by high-pressure gas. The state at the high-pressure end of the projectile is 25 MPa in pressure, 249.5 kg/m\(^3\) in density, 0 m/s in flow velocity, 287 J/kg\cdot K in gas constant, and 1.4 in ratio of specific heats. The state at the other side of the projectile is 101.3 kPa in pressure, 1.293 kg/m\(^3\) in density, 0 m/s in flow velocity, 287 J/kg\cdot K in gas constant, and 1.4 in ratio of specific heats.

Due to the fact that the projectile moves very fast after a short time, which makes the time step very small and slows down the prediction, the gas quantities at the high pressure end of the projectile are "relaxed" such that it is 1013.0 kPa in pressure, 12.93 kg/m\(^3\) in density, 0 m/s in flow velocity, 287 J/kg\cdot K in gas constant, and 1.4 in ratio of specific heats at the high-pressure end. Notice that in section 4.2.4, the first set of initial condition denotes the relaxed one while the second set denotes the original one.

In this numerical prediction, an equally spaced 250-node grid is used. With 0.005 m as the width of the cells, the total length of the grid is then 1.25 m. The first 40 cells denotes a space of length 0.2 m before the projectile inside the gun tube for the propellant. The total length of the projectile is 0.6 m or 120 cells, and divided into three regions of equal length. The first region denotes the distributed interface at the rear of the projectile while the last region denotes the distributed interface at the frontal surface of the projectile, and the middle section denotes the body of the projectile.

To set up the above initial conditions for this problem, the following is done. Knowing that if the projectile is held stationary and let the gas flow through it, the steady state solution can be obtained, which is having a linear profile for pressure and density inside the projectile. With this steady-state profile, the projectile will then let go and begin the numerical prediction.
4.2.4 Results

In this study, many results are obtained for this problem but only a few are shown here. Two sets of results are shown in this report for the numerical prediction of the launching of a projectile. From Fig. 4.12 to Fig. 4.15, the "relaxed" initial condition is used, whereas from Fig. 4.16 to Fig. 4.18, the realistic initial conditions are used.

In Fig. 4.12, the gas-volume fraction \( \varepsilon_g \) profile, spatial derivative of the gas-volume fraction \( \partial \varepsilon_g / \partial x \), and the term \( B(x) \) is shown. Notice that the four control points in generating the profile via Bézier's polynomials are shown as hollow squares. In Figs. 4.13, 4.14, and 4.15, the acceleration, velocity, and displacement of the projectile are shown, respectively. Notice that in the percentage difference in acceleration illustrated in Fig. 4.13, the error first rises as the projectile starts picking up speed, and eventually drops to a finite value before it rises linearly. It is interesting to notice that there are small sudden drops in the percentage difference wherever the boundaries of the distributed phase interface crosses a cell boundary, and the crossings of boundaries at the high pressure end are responsible for the larger drops whereas the crossings of boundaries at the low pressure end are responsible to the smaller drops.

From Fig. 4.16 to Fig. 4.18, the realistic setup for the problem of launching a projectile is used. In Fig. 4.16, the projectile acceleration is over-predicted by about 7% at the end of 10 milliseconds which is very large compare to the case where a "relaxed" initial condition is used. Similar conclusion can be drawn from the projectile velocity and displacement profile.
Chapter 5

Concluding Remarks

A new model of distributing phase interfaces in predicting two-phase flows of gas and particles was introduced. Two one-space-dimensional problems were solved numerically using this new model; they are the reflection of a shock wave at a distributed phase interface (closed duct end) and the acceleration of a projectile for which the surfaces were distributed.

The study of the computational fluid dynamics (CFD) solution procedure and the implementation of the VODE software package took a lot of effort. The primary difficulty was accurately handling the strong source terms in Euler’s equations, for which the VODE subroutine was incorporated. Also, the problem became extremely time consuming to solve computationally. This appeared to be the results of the strong source terms, but may also be the result of the initial setups of the equations or possibly improper software usage. If one-dimensional flow problems are solved for real times that are short but take hours to solve on a modern workstation, then realistic two- and three-dimensional flow problems are impractical to solve by the VODE software.

Very few definitive conclusions can be made from the present preliminary work for the following reasons. Firstly, the VODE subroutine package took too long computationally to give meaningful flow solutions over realistic flow times. Secondly, a first-order scheme may not have been sufficiently high-order to produce accurate results, and high order solutions may help reduce run time using the VODE software. Thirdly, the terms $p_g \partial \epsilon_g / \partial t$ and $p_g \partial \epsilon_p / \partial t$ in the gas and particle energy equations were not used in solving the projectile problem, as they are not used in many computations of gas-particle flows, because they were brought to the attention to the author in the writing of this thesis. Including such terms may improve the accuracy of predictions, but they would not solve the long run time using the VODE software. Fourthly, the partial decoupling of the gas and particle equations may have resulted in degraded accuracy of the numerical predictions, but they would not solve the long run time using the VODE software. Fifthly, the Riemann solver used in this study to estimate the fluxes at cell boundaries is only a first-order scheme and this also contribute to the inefficiency of the VODE software but this is questionable.

The present study, however, does identify specific problems and difficulties that must be overcome in order to determine if the concept of distributed phase interface is worthwhile.
The following are recommend by the author on what should be done in the future. Firstly, either the VODE software package has to be made more efficient or another solution procedure must be used. Secondly, a second- or even higher-order numerical scheme should be developed to increase the solution accuracy. Thirdly, the conservation equations should be studied such that all terms are to be included in future predictions. Fourthly, a fully coupled gas- and particle-phase solution procedure should be incorporated to increase accuracy. Fifthly, a more relevant Riemann solver should be incorporated for calculating fluxes at cell boundaries, and the generalized Riemann problem of Matania Ben-Artiz might provide such solution.
Bibliography


Figure 4.1: Gas-volume fraction profile with $M_i = 2.0$, $e_{g_{\text{min}}} = 10^{-4}$. 
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Figure 4.3: Pressure profile with $M_t = 2.0$, $\varepsilon_{g_{\min}} = 10^{-4}$.
Figure 4.4: Density profile with $M_i = 2.0$, $\varepsilon_{\text{min}} = 10^{-4}$. 

\[ \rho \text{ [kg/m}^3] \] 

\[ \frac{x}{\Delta x} \]
Figure 4.5: Sound speed profile with $M_i = 2.0$, $\epsilon_{\text{gmin}} = 10^{-4}$. 
Figure 4.6: Flow mach number profile with $M_i = 2.0$, $\varepsilon_{\text{min}} = 10^{-4}$. 
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Figure 4.9: Terms in viscous-flow resistance with $M_i = 2.0$, $\varepsilon_{\text{min}} = 10^{-2}$.
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Figure 4.17: Projectile velocity for the realistic setup.
Figure 4.18: Projectile position for the realistic setup.