

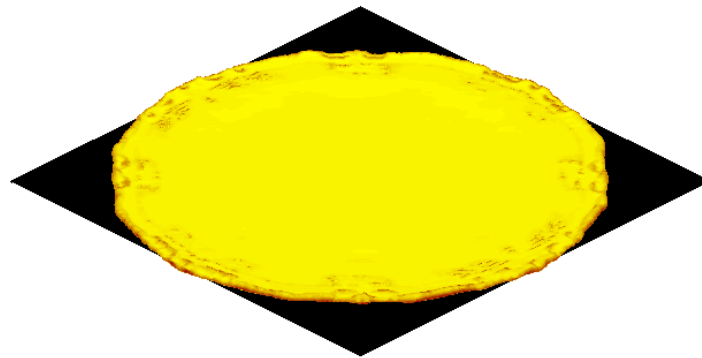
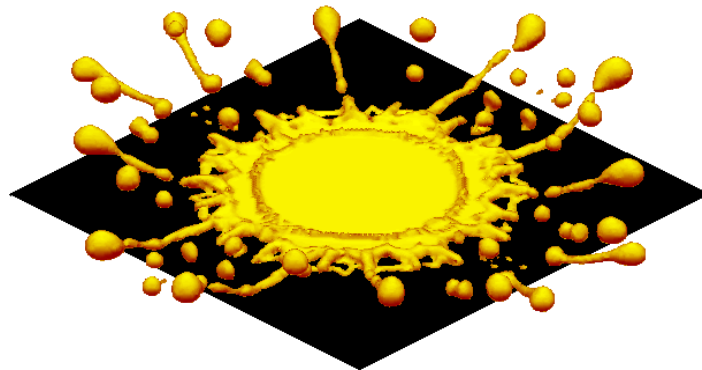
SimDrop Manual

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SimDrop 6.3

Droplet Impact & Solidification Software

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1 INTRODUCTION

SIMDROP is a user-friendly code for the simulation of the dynamics of liquid drops upon impaction on solid surfaces. This code also solves the heat transfer equations and simulates the solidification of the molten materials. SIMDROP is based on a robust, free surface modeling technique, known as Volume of Fluid (VOF) technique. The model is a three dimensional model which combines a fixed mesh discretization of the Navier-Stokes equations with a piecewise linear volume tracking algorithm to track the droplet free surface. Due to the implementation of the dynamic contact angle, the Software can simulate the liquid-solid interfaces accurately.

SIMDROP can be used to simulate the impact of a single or multiple droplets impacting on a flat or inclined surface. The initial shapes of the droplets before impact are spherical (this limitation can be removed by special request). The data-base in the present version of the Software has the information about 5 droplet materials and 3 substrate materials. However, the information about other materials can be simply given to the code.

In the next Chapter, we will present the mathematical description of the model and the numerical implementation along with the examples for the code validation. We strongly recommend that these chapters be carefully read before the program is used. Through these chapters you will be also introduced to the terms and vocabularies that are widely used throughout the Manual.

In Chapters 3 and 4 we will explain how to install the program and present an overview of the Software. In Chapter 5, we will show how to set up a droplet impact problem. The terms and

geometry that are used in this Chapter will be also used in the next Chapters. In Chapter 6 the procedure for entering the input data into the code will be explained in details. In Chapter 7, the output files and their usage will be discussed in more details. Then, in Chapter 8, several examples of droplet impact simulations will be presented. Chapter 9 deals with the possible messages that may be appeared during the execution time and the methods for overcoming the errors are presented. In the Appendices at the end of the Manual, the structures and contents of the material property files, Input and Output files can be found. In the last Appendix, a brief description of how to plot the results will be presented.

2 COMPUTATIONAL METHODOLOGY

2.1 Introduction

In this chapter we describe the computational methodology used in SIMDROP to simulate the droplet impact problems. A 3-D numerical model of droplet impact has been developed, to predict fluid deformation and possible breakup during impact onto asymmetric surfaces. The model is an Eulerian fixed-grid algorithm, utilizing a volume tracking approach to track fluid deformation. Surface tension is modeled as a volume force, acting on fluid in the vicinity of the free surface. A contact angle is specified as a boundary condition along the contact line.

The full Navier-Stokes equations in a 3D Cartesian coordinate system are solved using a finite difference scheme. The algorithm is currently written for the laminar, incompressible flows. The surface profile of the deforming interface is defined using the “fractional volume of fluid” scheme (Hirt and Nichols)¹. In this method, a scalar function f is defined whose value is equal to the fractional volume of the cell occupied by the fluid. f is assumed to be unity when a cell is fully occupied by the fluid and zero for an empty cell. Cells with values of $0 < f < 1$ contain a free surface.

Surface tension is modeled as volume force acting on fluid near the free surface. Contact angles are applied as a boundary condition at the contact line. For the impact on an inclined surface, a simple model is used to evaluate contact angle as a function of contact line velocity. The model requires values of only two contact angles, at a rapidly advancing and a rapidly receding contact line. Liquid density and surface tension are assumed to be constant. Liquid viscosity and substrate thermal properties, however, are assumed to vary with temperature.

¹ C.W. Hirt and B.D. Nichols; J. Comput. Phys. 39, 201 (1981).

2.2 Numerical Methodology & Validation

I. GOVERNING EQUATIONS

SIMDROP has a single-fluid solver for incompressible, Newtonian, and laminar flows. Equations of conservation of mass, momentum, and energy for the flow are:

$$\nabla \cdot \mathbf{V} = 0 \quad (1)$$

$$\frac{\partial \mathbf{V}}{\partial t} + \nabla \cdot (\mathbf{V}\mathbf{V}) = -\frac{1}{\rho} \nabla p + \nabla^2 \nu \mathbf{V} + \frac{1}{\rho} \mathbf{F}_b \quad (2)$$

where \mathbf{V} represents the velocity vector, p the pressure, ρ the density, ν the kinematic viscosity, and \mathbf{F}_b any body forces acting on the fluid.

Heat transfer in the droplet is modeled by solving the energy equation, neglecting viscous dissipation; densities of liquid and solid are assumed constant and equal to each other (the values for tin differ by less than 4%, which would have little influence on droplet flow):

$$\frac{\partial h}{\partial t} + (\mathbf{V} \cdot \nabla)h = \frac{1}{\rho} \nabla \cdot (k \nabla T) \quad (3)$$

where h is the enthalpy of the fluid, k the thermal conductivity, and T is the temperature.

II. BOUNDARY CONDITIONS

Flow and thermal boundary conditions are required along both the computational grid and the fluid's free surface.

FLOW BOUNDARY CONDITIONS

Calculation Domain: Assuming that the grid boundaries are rigid *walls*, two types of conditions can exist. The first type is the familiar *no-slip* condition, while the second type is called *free-slip* or *slip* and represents a plane of symmetry, or a wall with a non-adhering surface.

For all simulations the *no-slip* condition can be used for the each of the 6 boundaries of the computational grid (including the surface of impact). However, for simple cases of normal impact droplet of a single droplet on a flat surface, a plane of symmetry can be used to reduce the computational cost. It is important that computational domain sizes are chosen such that the droplet's evolution does not interact with any of the other grid boundaries (except the impact surface and the planes of symmetry, if applicable). This way, the type of boundary condition does not have any effect on the solution and the evolution of the impact process.

Free Surface: Velocity boundary conditions are applied to free surface cells by requiring that the divergence of the velocity field be zero. Various cases can exist in which a surface cell has only one empty neighboring cell or as many as six empty neighboring cells. Depending on the situation, the divergence requirement must reflect the appropriate configuration.

Also across the interface, Laplace's equation specifies the surface tension-induced jump in the normal stress p_s :

$$p_s = \gamma \kappa \quad (4)$$

where γ represents the liquid-air surface tension and κ the total curvature of the interface.

Contact Line: Finally, a boundary condition is applied at the contact line, the line at which the solid, liquid and gas phases meet. It is this boundary condition which introduces into the model information regarding the wettability of the solid surface. Although it is conceivable that one could formulate this boundary condition incorporating values of the solid surface tensions, such values are often inaccessible. Rather, we specify a “dynamic” contact angle θ_d , the apparent contact angle measured at a moving contact line, which is likely a complex function of the contact line velocity.

THERMAL BOUNDARY CONDITIONS

Calculation domain: For the grid boundaries that are rigid *walls*, three types of conditions are considered. The first type is the *adiabatic* condition and the second type is *constant temperature*. The adiabatic condition is also used for those planes that are symmetric planes. The third

condition can only be used for the impact surface and is of the *known initial temperature*. The two types of adiabatic and constant temperature conditions can also be used for substrate calculation domains.

Free surface: At the free surface of the droplet, an adiabatic boundary condition is used in this version. This condition can easily be modified to a convective or radiative boundary condition if is requested. For most cases in the droplet impact field, the dominant heat transfer is due to conduction to the substrate at the initial stages of the impact, and conduction and convection within the droplet at the later stages of the impact. Estimates of heat loss by convection from the droplet surface to the surrounding gas showed that it is three orders of magnitude lower than that the heat transfer to the substrate. Therefore, the adiabatic condition at the free surface is reasonable.

III. NUMERICAL TECHNIQUE

SIMDROP uses a 3-D fixed-grid Eulerian code written specifically for free surface flows with surface tension. Equation (1) and (2) are discretized according to typical finite volume conventions on a rectilinear grid encompassing both the volume occupied by the droplet prior to impact as well as sufficient volume to accommodate the subsequent deformation. Velocities and pressures are specified as on a traditional staggered grid: velocities at the center of cell faces, pressure at the cell center. Figure 2.1 illustrates a representative control volume in two dimensions.

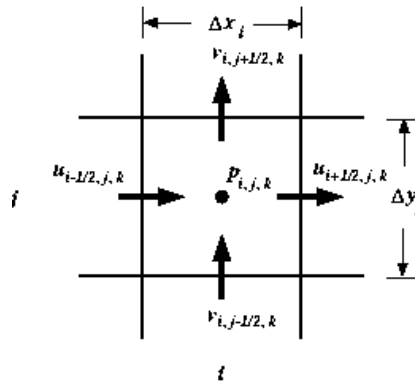


Figure 2.1. A 2D control volume, with velocities specified at cell faces, pressure at the cell center.

The choice of a fixed-grid technique was made for several reasons: the relative simplicity of implementation; the capability of a volume tracking method to model gross fluid deformation, including breakup; and the relatively small demand on computational resources. As we will demonstrate, such a model can simulate complex fluid deformation surprisingly well.

Equations (1) and (2) are solved using a two-step projection method, in which a time discretization of the momentum equation is broken up into two steps:

$$\frac{\tilde{V} - V^n}{\Delta t} = -\nabla \cdot (VV)^n + \nu \nabla^2 V^n + \frac{1}{\rho^n} F_b^n \quad (5)$$

$$\frac{V^{n+1} - \tilde{V}}{\Delta t} = -\frac{1}{\rho^n} \nabla p^{n+1}. \quad (6)$$

The superscripts n and $n+1$ refer to the previous and current time levels respectively. In the first step, Eq. (5), an interim velocity field \tilde{V} is computed explicitly from changes to the known field V^n , which result from convective, viscous and body forces acting on the fluid during the time-step δt . The explicit evaluation of these terms sets various limits on the size of δt ; the time-step chosen is the smallest of these.

In the second step, Eq. (6) is combined with Eq. (1) at time level $n+1$ to yield an implicit Poisson equation for pressure:

$$\nabla \cdot \left(\frac{1}{\rho^n} \nabla p^{n+1} \right) = \frac{\nabla \cdot \tilde{V}}{\Delta t} \quad (7)$$

Although the fluid is assumed incompressible, the density is retained within the divergence operator to account for non-zero density gradients at the liquid free surface. The resulting set of linear equations in p is symmetric and positive definite; a solution is obtained at each time-step with an Incomplete Cholesky Conjugate Gradient solver (SLATEC routine DSICCG). Finally, the new velocity field V^{n+1} is evaluated via Eq. (6).

Discretization of most boundary conditions is straightforward. No-slip conditions are applied by defining “fictitious” velocities within solid cells adjacent to fluid cells. Normal velocities at solid surfaces, and the pressure within cells empty of fluid, are simply defined as zero. Finally, the tangential stress condition at the droplet surface is implemented at cell faces between empty cells adjacent to an interface cell, by setting to zero values of $\partial u/\partial y$ and $\partial v/\partial y$.

More details about the numerical implementation can be found in Section 2.4.

IV. FREE SURFACE SIMULATION

In addition to solving the flow equations within the liquid, the numerical model must also track the location of the liquid free surface. The approach used in SIMDROP is as follows. Consider a function f defined in a continuous domain as:

$$f = \begin{cases} 1 & \text{within the liquid phase,} \\ 0 & \text{without.} \end{cases} \quad (8)$$

For a cell (I, j, k) of volume $v_{i,j,k}$ a “volume fraction” $f_{i,j,k}$ is defined as:

$$f_{i,j,k} = \frac{1}{v_{i,j,k}} \int_{v_{i,j,k}} f d v, \quad (9)$$

and a corresponding cell density $\rho_{i,j,k}$, which appears in the discretization of Eq. (7), is evaluated as:

$$\rho_{i,j,k} = \rho_f f_{i,j,k} \quad (10)$$

where ρ_f represents the (constant) value of the liquid density. Obviously, $f_{i,j,k} = 1$ for a cell filled with liquid and $f_{i,j,k} = 0$ for an empty cell. When $0 < f_{i,j,k} < 1$, the cell is deemed to contain a portion of the free surface and is termed an *interface cell*. Note that unlike f , the integrated quantity $f_{i,j,k}$ no longer contains information regarding the exact location of the interface. This is, in fact, the primary drawback of volume tracking as an interface tracking method, and becomes problematic when dealing with surface tension and contact angles, as will

be discussed. On the other hand, volume tracking is relatively simple to implement even in three dimensions, retains this simplicity regardless of the complexity of the interface geometry, conserves mass (or volume, since the fluid is incompressible) exactly, and demands only a modest computational resource beyond that required by the flow solver.

Since the function f is passively advected with the flow, f satisfies the advection equation:

$$\frac{\partial f}{\partial t} + (\mathbf{V} \cdot \nabla) f = 0. \quad (11)$$

Given the volumetric nature of $f_{i,j,k}$ and in order to maintain a sharp interface, the discretization of Eq. (11) requires special treatment. As with most other volume tracking algorithms, Youngs' algorithm consists of two steps: an approximate reconstruction of the interface followed by a geometrical evaluation of volume fluxes across cell faces.

The interface is reconstructed by locating a plane within each interface cell, corresponding exactly to the volume fraction $f_{i,j,k}$ and to an estimate of the orientation of the interface, specified as a unit normal vector $\hat{n}_{i,j,k}$ directed into the liquid phase. A discussion of the evaluation of $\hat{n}_{i,j,k}$ is left to later section. In two dimensions such an interface is simply a line crossing a cell.

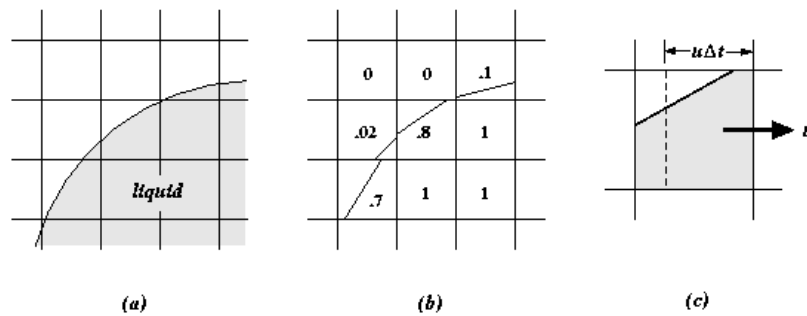


Figure 2.2. The volume tracking method in two dimensions. (a) The exact liquid interface. (b) The corresponding volume fractions and planar interfaces. (c) With velocity u positive, the shaded region to the right of the dotted line is advected into the neighboring cell during the time-step Δt .

To illustrate in two dimensions, Figure 2.2(b) portrays the volume fractions corresponding to the exact (albeit unknown) interface of Figure 2.2(a). Note that nothing guarantees that interface planes be contiguous. The position of the interface within each cell and the new velocities at the cell faces are then used to determine volume fluxes across each face during the time-step. Figure 2.2(c) illustrates such a flux across one face of a cell. Volume fluxes are evaluated one direction at a time, always followed by an interim interface reconstruction. Directional bias is minimized by alternating the order of advection from one time-step to the next.

In three dimensions the interface lines become three- to six-sided polygons, depending on how the plane slices the cell. There are five distinguish cases in a 3-D problem that are shown in Figure 2.3. These cases are triangle, tow quadrilateral types, pentagon, and hexagon faces.

“Continuum Surface Force,” or CSF, model is used in SIMDROP to include the effect of the surface tension forces in the problem. The CSF model reformulates surface tension into an equivalent volume force F^{ST} :

$$F^{st}(x) = \gamma \int_S \kappa(r) \hat{n}(r) \delta(x-r) dr \quad (12)$$

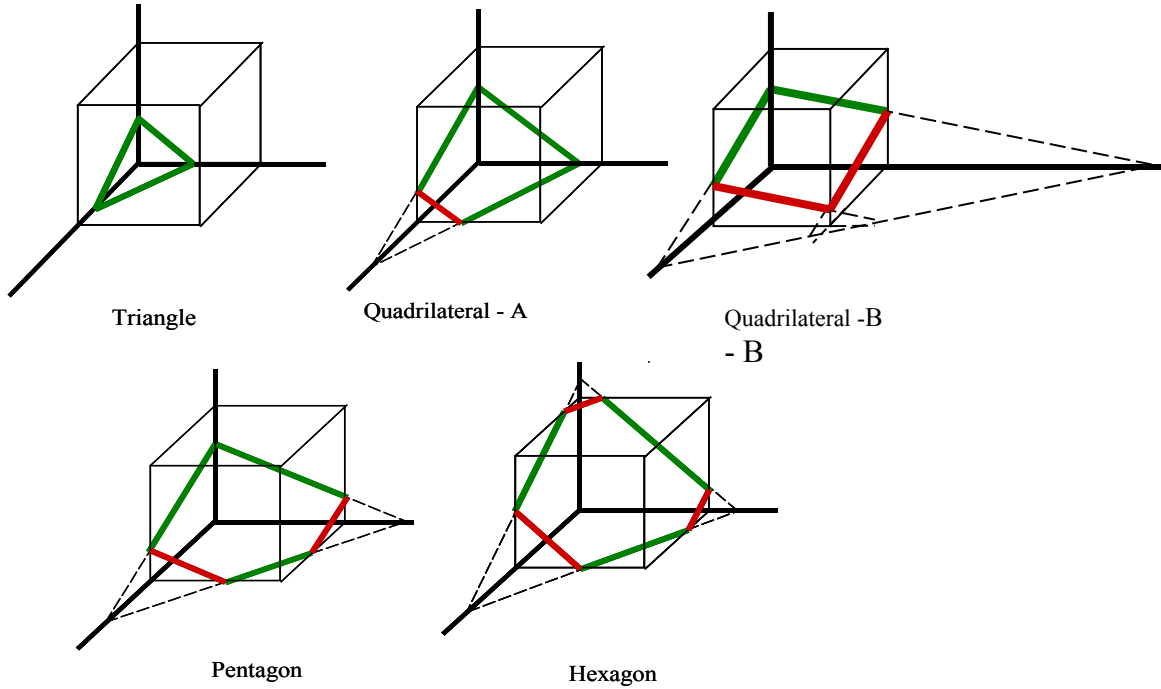


Figure 2.3. Illustration of five possible cases that may occur in implication of Young's method in a 3-D simulation.

where δ is the Dirac delta function and the integration is performed over some area of free surface S . Surface tension is then incorporated into the flow equations simply as a component of the body force F_b in Eq. (2). Discretization of Eq. (12) requires an approximation to δ which spreads the surface tension force over fluid in the vicinity of the surface. To avoid the unrealistic oscillations of fluid that might happen due to spurious fluid motion near free surfaces, Eq. (12) was discretized as follows:

Let δ_{2h} represent the kernel chosen to approximate δ , where the subscript $2h$ represents the finite radius over which δ_{2h} is non-zero. With $\delta_{2h} \approx \delta$, Eq. (11) may be written:

$$F^{ST}(x) \approx \gamma \int_S \kappa(r) \hat{n}(r) \delta_{2h}(x-r) dr \quad (13)$$

Eq. (13) is now discretized as follows. We evaluate a local volumetric surface tension force for each interface cell:

$$F_{i,j,k}^{ST} = \gamma \mathcal{K}_{i,j,k} \frac{A_{i,j,k}}{V_{i,j,k}} \hat{n}_{i,j,k}, \quad (14)$$

where $A_{i,j,k}$ is the free surface area contained within the cell, evaluated as the area of the planar interface determined by Youngs' volume tracking algorithm. $F_{i,j,k}^{ST}$ is then convolved with δ_{2h} to obtain a smoothed force field $\tilde{F}_{i,j,k}^{ST}$:

$$\tilde{F}_{i,j,k}^{ST} = g_{i,j,k} \sum_{l,m,n} F_{i,j,k}^{ST} \delta_{2h}(x_{i,j,k} - r_{l,m,n}) v_{l,m,n}. \quad (15)$$

Note the introduction of a weighting function $g_{i,j,k}$, defined as:

$$g_{i,j,k} = \frac{f_{i,j,k}}{\bar{f}}, \quad (16)$$

where $\bar{f} = 1/2$ represents the average value of f . The role of $g_{i,j,k}$ is to transform the volumetric surface tension force into a uniform body force, and consequently forces $\tilde{F}_{i,j,k}^{ST} = 0$ for empty cells.

Equation (15) is simply a summation over cells within a radius $2h$ of $\mathbf{x}_{i,j,k}$, and can be applied to any grid structure. This allows for the possibility, for example, of applying the surface tension model to an adaptively refined grid. The resulting summation in Eq. (15) will then envelope more cells in a refined region than in an unrefined region, which may allow for decreasing the radius $2h$ with grid refinement. Finally, when the grid is uniform, a more accurate Eq. (15) is possible by evaluating the kernel contribution exactly:

$$\tilde{F}_{i,j,k} = g_{i,j,k} \sum_{l,m,n} \left(F_{i,j,k}^{ST} \int_{V_{l,m,n}} \delta_{2h}(x_{i,j,k} - r_{l,m,n}) dr \right) \quad (17)$$

What remains is to evaluate $\hat{n}_{i,j,k}$, required by the volume-tracking algorithm to reconstruct the interface, and essential to the accurate evaluation of $F_{i,j,k}^{ST}$, especially since κ is evaluated as:

$$\kappa = -\nabla \cdot \hat{n} \quad (18)$$

In a continuous domain,

$$\hat{n} = \frac{\nabla f}{|\nabla f|} \quad (19)$$

But given the volumetric nature of $f_{i,j,k}$, a simple algebraic discretization of Eq. (19) leads to poor estimates of $\hat{n}_{i,j,k}$. Instead, the approach implemented in our model comes from a suggestion contained within the original CSF formulation². Analogous to spreading the surface tension force to fluid in the vicinity of the free surface, better estimates of $\hat{n}_{i,j,k}$ are obtained by evaluating the gradient of a smoothed $f_{i,j,k}$, equivalent to employing a spatially-weighted gradient operator to evaluate ∇f . In practice, we employ the same δ_{2h} for smoothing $f_{i,j,k}$ as for smoothing $F_{i,j,k}^{ST}$. $\hat{n}_{i,j,k}$ are first evaluated at cell vertices, to accommodate the evaluation of the cell-centered $\kappa_{i,j,k}$; cell-centered $\hat{n}_{i,j,k}$ are then evaluated as an average of eight vertex values. The particular δ_{2h} chosen for the model is a radially symmetric variation of a widely used kernel proposed by Peskin³:

$$\delta_{2h}(x) = \begin{cases} \left(1 + \cos\left(\frac{\pi|x|}{2h}\right)\right) / c & |x| \leq 2h, \\ 0, & |x| > 2h \end{cases} \quad (20)$$

where c normalizes the kernel:

² J. U. Brackbill, D. B. Kothe and C. Zemach; J. Comput. Phys. 100 , 335 (1992).

³ C. S. Peskin; J. Comput. Phys. 25, 220 (1977).

$$c = \frac{32}{3} h^3 (\pi^2 - 6) / \pi \quad (21)$$

The reason we modify Peskin's kernel is found in work by Aleinov and Puckett⁴, which demonstrates that radial symmetry appears to be an attractive attribute of δ_{2h} . All results presented in this work are run on a uniform grid, with $2h = 3/2\Delta x$, thereby limiting convolutions to a $4 \times 4 \times 4$ stencil. This value of $2h$, albeit arbitrary, was chosen for several reasons: the prohibitive computational cost of convolving over larger stencils; the difficulty in evaluating convolutions near solid surfaces; the minimum $2h$ is necessary to reduce noise associated with the evaluation of the curvature field, without unduly extending the surface tension force. Note too that the small stencil blurs the distinction between different δ_{2h} , thereby reducing the influence of kernel shape on model results.

To illustrate the relationship between δ_{2h} and the evaluation of ∇f , we present the expression for the x component of ∇f evaluated at the lower left vertex of the cell (i,j) illustrated in Figure 2.1:

$$f_{x_{i-\frac{1}{2},j-\frac{1}{2}}} = \frac{1}{2\Delta x} \left\{ 0.3676(f_{i,j} + f_{i,j-1} - f_{i-1,j} - f_{i-1,j-1}) + 0.1510(f_{i+1,j} + f_{i+1,j-1} - f_{i-2,j} - f_{i-2,j-1}) \right. \\ \left. + 0.0949(f_{i,j+1} + f_{i,j-2} - f_{i-1,j-2}) + 0.0281(f_{i+1,j+1} + f_{i+1,j-2} - f_{i-2,j+1} - f_{i-2,j-2}) \right\} \quad (22)$$

A corresponding equation may be written for $f_{y_{i-1/2,j-1/2}}$ the expression for ∇f in 3D is similar, but includes 64 terms with different coefficients. A different choice of δ_{2h} yields somewhat different coefficients; increasing $2h$ adds further terms to the equation.

Equation (22) may be used to evaluate \hat{n} at any vertex at least two cell widths from a solid surface. And at vertices along the boundary, normals $\hat{n}_{i,j,k}$ are imposed to reflect the contact angle θ_d boundary condition; Figure 2.4 provides an illustration. The remaining vertices, one cell width removed from a solid surface, require special treatment. The approach we take is to

⁴ I. Aleinov and E. G. Puckett; in Proceedings of the 6th International Symposium on Computational Fluid Dynamics, 1995.

assign pseudo volume fractions to solid cells adjacent to the fluid, in order to evaluate Eq. (22). In 2D, we implemented a geometric scheme to evaluate these volume fractions in a manner consistent with the value of θ_d . The influence of this scheme on global results, however, was insignificant when compared with a simpler approach of mirroring values of $f_{i,j,k}$ from fluid cells into adjacent solid cells. Since an extension of our geometric scheme to 3D appeared hopelessly complicated, the simpler scheme was adopted.

Evaluation of $\tilde{F}_{i,j,k}$ is handled the same way, by mirroring values of F^{ST} from fluid cells into adjacent solid cells. In this way, the volumetric force is conserved, in that the fraction of F^{ST} convolved out of the fluid and into the boundaries is exactly reintroduced from the boundaries into the fluid.

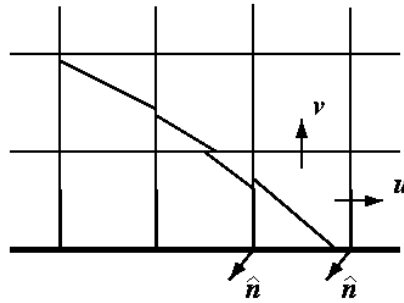


Figure 2.4. Control volumes adjacent to a solid boundary. Unit normals \hat{n} at solid boundary vertices are oriented to reflect the contact angle boundary condition. Note the u , one half-cell height above the solid surface, is the best estimate of the true contact line velocity.

Initial conditions for a droplet impact simulation are a specified droplet diameter and location to calculate an initial volume fraction field, and an impact velocity applied to all droplet fluid. The contact line treatment immediately following impact is the same as that just described, despite the short length of the contact line. The accuracy of the surface tension calculations likely suffers as a result, but this is completely offset by the insignificance of such effects at a time when inertial effects dominate.

Analytical solutions of the Navier-Stokes equations (subject to various simplifications) yield a force singularity at a contact line unless a slip condition is imposed near the line. Numerical models, which explicitly track the free surface, also require that a slip boundary condition be imposed on any contact line velocities. This turns out not to be an issue for this model, precisely because it does not explicitly track the free surface, nor does it solve for contact line velocities. Instead, since velocities are specified at cell faces, the nearest velocity to the contact line is specified one half-cell height above the solid surface. Again, Figure 2.4 provides an illustration. It is this non-zero velocity which is then used to move fluid near the contact line at each time-step.

Figure 2.5 illustrates plots of the interface reconstruction of a droplet (resolved by 10 uniform cells per radius, hereafter designated “CPR”) before and after a 7.5 diameter translation, to assess the volume tracking algorithm and calculations of \hat{n} . The figure was generated by plotting the actual polygons calculated by the advection algorithm. An exact velocity field $\mathbf{V} = (u, v, w) = (3, 2, 1)$ was imposed on a uniform grid; the translation was divided into 400 uniform time-steps, with a maximum Courant number ($\equiv u\Delta t/\Delta x$) of 0.3. Qualitatively, the only significant distortion of the droplet is a slight “squaring” along grid axes; otherwise, the algorithm advects the droplet well. Quantitatively, we evaluated an error $E_f = 0.040$ defined as:

$$E_f = \frac{\sum_{i,j,k} |f_{i,j,k} - f_{i,j,k}^e|}{\sum_{i,j,k} 1} \quad (23)$$

$f_{i,j,k}$ and $f_{i,j,k}^e$ represent calculated and expected volume fractions following translation; the summations included only cells containing (or expected to contain) fluid.

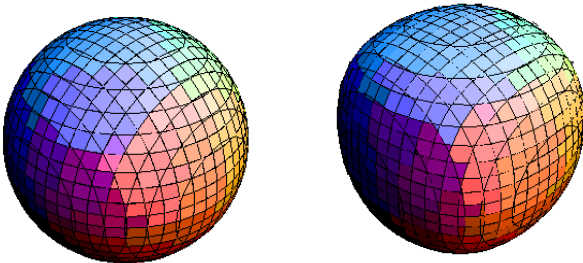


Figure 2.5. Translation test of volume advection algorithm. Plots illustrate surface reconstruction of a ten cell per radius droplet before and after a 7.5 diameter translation.

Figure 2.6 illustrates the influence of mesh refinement on the evaluation of the surface tension-induced pressure jump p_s across the surface of a static droplet. Droplets are defined at various resolutions, and for each resolution centered at five different locations within a cell. Surface tension forces are calculated and the pressure equation solved, for one time-step. The calculated pressure jump was then evaluated as:

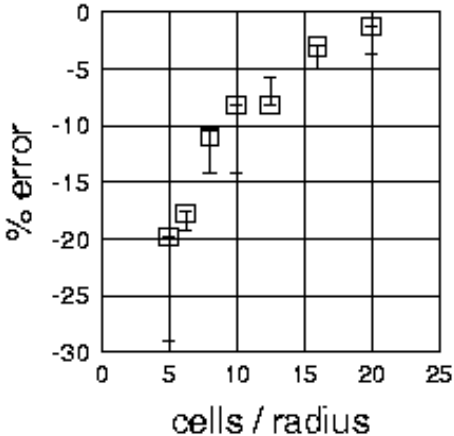


Figure 2.6. Percent errors versus grid density for the pressure jump P , across the surface of a static drop. Symbols correspond to the error evaluated for a droplet centered at a cell vertex; bars indicate the range of errors evaluated for a droplet centered at five locations within a cell.

$$p_s^c = \frac{\sum_{i,j,k} f_{i,j,k} p_{i,j,k}}{\sum_{i,j,k} f_{i,j,k}} \quad (24)$$

and an error defined as:

$$E_p = \frac{p_s^c}{4\gamma/D_0} - 1 \quad (25)$$

The symbols in Figure 2.6 indicate the error associated with a droplet centered at a cell vertex (which was the case for all simulation results presented in this paper); the corresponding bars indicate the range of errors calculated at the different cell centers. There is certain randomness to the error: as the droplet center moves, values of $f_{i,j,k}$ shift, some interface cells are filled and others created. Nevertheless, convergence varies between first and second order.

The final test examines the influence of the value of $2h$ on the uniformity of \tilde{F}^{ST} , as evidenced by the kinetic energy of the flow (so-called *parasite*) currents induced in an initially static drop as a result of noise in the surface tension forces. Results are generated for a initially static 2 mm diameter water droplet resolved by 10 cpr, with simulations run for 100 time-steps to a physical time of 1 ms. Results are illustrated in Figure 2.7. Not smoothing the F^{ST} at all, corresponding to $2h = 1/2\Delta x$, induced motion several times stronger than smoothing F^{ST} with $2h = 3/2\Delta x$. Although larger stencils yielded further incremental reductions in the kinetic energy, all subsequent simulations presented here employed $2h = 3/2\Delta x$ for the reasons mentioned above.

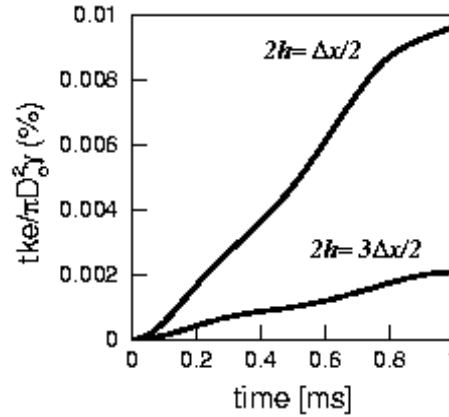


Figure 2.7. Kinetic energy (scaled by initial surface energy) versus time for static 2 mm diameter water drop defined by ten cells per radius, for smoothed ($2h = 3/2\Delta x$) and un-smoothed ($2h = 1/2\Delta x$) F^{ST} .

2.3 Heat Transfer

I. GOVERNING EQUATIONS

Simulent code includes the energy equation. In the present algorithm, the viscous dissipation terms are not included. In addition, densities of liquid and solid are assumed constant and equal to each other (the values for tin differ by less than 4%, which would have little influence on droplet flow). The energy equation solved by Simulent is the following:

$$\frac{\partial h}{\partial t} + (V \cdot \nabla)h = \frac{1}{\rho} \nabla \cdot (k\nabla T) \quad (26)$$

Since the energy equation has two dependent variables –temperature T and enthalpy h - we used the enthalpy transforming model, Cao et al.⁵, to convert the energy equation to one with only one

⁵ Cao Y., Faghri A. and Chang W. S., 1989, International Journal of Heat and Mass Transfer, Vol. 32, pp. 1289-1298.

dependent variable: the enthalpy. The main advantage of this method is that it solves energy equation for both phases simultaneously. The final form of the equation is

$$\frac{\partial h}{\partial t} + (\mathbf{V} \cdot \nabla)h = \frac{1}{\rho} \nabla \cdot (\beta \nabla h) + \frac{1}{\rho} \nabla^2 \phi \quad (27)$$

where in the solid phase:

$$h \leq 0; \quad \beta = \frac{k_s}{C_s}, \quad \phi = 0 \quad (28a)$$

at the liquid-solid interface:

$$0 < h < H_f; \quad \beta = 0, \quad \phi = 0 \quad (28b)$$

and in the liquid phase:

$$h \geq H_f; \quad \beta = \frac{k_l}{C_l}, \quad \phi = -\frac{H_f k_l}{C_l} \quad (28c)$$

where ϕ is a new source term. The energy equation now has only one dependent variable, the enthalpy h . The relationship between temperature and enthalpy is given by

$$T = T_m + \frac{1}{k}(h\beta + \phi) \quad (29)$$

where T_m is the melting point of the droplet. Heat transfer within the substrate is by conduction only. The governing equation is

$$\rho_w C_w \frac{\partial T_w}{\partial t} = \nabla \cdot (k_w \nabla T_w) \quad (30)$$

At a free surface of the droplet, we used an adiabatic boundary condition. This condition must be supplemented with the specification of enthalpy h and functions β and ϕ immediately outside the surface, where these values are needed in the finite-difference approximations for points located at the free surface. This condition can easily be modified to a convective or radiative

boundary condition. For the cases under consideration, the dominant heat transfer is due to conduction to the substrate at the initial stages of the impact, and conduction and convection within the droplet at the later stages of the impact. Estimates of heat loss by convection from the droplet surface to the surrounding gas showed that it is three orders of magnitude lower than that the heat transfer to the substrate. Therefore, the adiabatic condition at the free surface is reasonable. Thermal contact resistance between the droplet and substrate (R_c) is defined by

$$R_c = \frac{(T - T_w)_{\text{substrate}}}{q} \quad (31)$$

where q is the heat flux from the droplet to substrate. Values of R_c are provided as an input to the model. Although in principle R_c could vary with time and/or position on the interface, we used a constant value in the simulations.

II. SOLIDIFICATION

In the presence of a solid phase, computations of the velocity field have to account for the presence of a moving, irregularly shaped solidification front on which the relevant boundary conditions have to be applied. We treat the solidified regions of the domain using a modified version of the fixed velocity method. In this approach, a liquid volume fraction Θ is defined such that $\Theta = 1$ is for a cell containing only liquid, $\Theta = 0$ is for a cell containing only solid, and $0 < \Theta < 1$ is for a cell containing a portion of the solidification front. Normal and tangential velocities on the faces of cells containing only solidified material are set to zero. Based on this method, the final modified continuity and momentum equations are:

$$\nabla \cdot (\Theta \mathbf{V}) = 0 \quad (32)$$

$$\frac{\partial(\Theta \mathbf{V})}{\partial t} + (\Theta \mathbf{V} \cdot \nabla) \mathbf{V} = \frac{-\Theta}{\rho} p + \Theta \nu \nabla^2 \mathbf{V} + \frac{\Theta}{\rho} \mathbf{F}_b \quad (33)$$

$$\frac{\partial f}{\partial t} + (\Theta \mathbf{V} \cdot \nabla) f = 0 \quad (34)$$

2.4 Numerical Implementation

In this section the numerical implementation of what was presented in Sections 2.2, and 2.3 is shown.

I. COMPUTATIONAL DOMAIN

All equations are discretized using the finite difference technique. The computational domain consists of a three-dimensional Cartesian grid divided into $N_x \times N_y \times N_z$ uniform cells. A standard staggered mesh is used in which the scalar quantities (i.e. pressure and f -function) are defined at the cell centers, while the velocity components are located at the cell faces.

II. TWO-STEP PROJECTION METHOD

SIMDROP utilized the two-step projection method to solve the Navier-Stokes equations. During the first step, the velocity field is updated explicitly to reflect the convective, viscous, and surface-tension effects to yield an intermediate velocity field.

$$\frac{\tilde{u}_i^{n+1} - u_i^n}{\Delta t} = -\frac{\partial(u_i u_j)^n}{\partial x_j} + \frac{1}{\rho^n} \frac{\partial \tau_{ij}^n}{\partial x_j} + \frac{1}{\rho^n} F_i^v \quad (35)$$

where Δt is the time step and (n) is the previous time-level while $(n + 1)$ is the new time-level. The second step is used to project the intermediate velocity field, \tilde{u}_i^{n+1} onto a divergence free plane to ensure that continuity had been satisfied, thus giving the final velocity field.

$$\frac{u_i^{n+1} - \tilde{u}_i^{n+1}}{\Delta t} = -\frac{1}{\rho^n} \frac{\partial P^{n+1}}{\partial x_i} \quad (36)$$

$$\frac{\partial u_i^{n+1}}{\partial x_i} = 0 \quad (37)$$

By taking the divergence of (36) and applying (37) an equation for the new pressure as a function of the intermediate velocity field is obtained.

$$\frac{\partial}{\partial x_i} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial x_i} \right) = \frac{1}{\Delta t} \frac{\partial \tilde{u}_i^{n+1}}{\partial x_i} \quad (38)$$

This equation is often referred to as the Poisson Pressure Equation (PPE). By retaining the density inside the brackets, the non-zero density gradients at the free surface are accounted for in the final solution. The PPE is solved implicitly for the new pressure field at each time step using an incomplete Cholesky conjugate gradient solver. The final velocity is then computed by adjusting the intermediate velocity field for the pressure gradient effects.

$$u_i^{n+1} = \tilde{u}_i^{n+1} - \frac{\Delta t}{\rho^n} \left(\frac{\partial p^{n+1}}{\partial x_i} \right) \quad (39)$$

III. SPATIAL DISCRETIZATIONS

As mentioned earlier, the scalar quantities, p and f , are located at the cell's center, while the velocity components are located at the cell's faces. Specifically, the velocity component in the x-direction, u , is located at the right face, while the velocity component in the y-direction, v , and in the z-direction, w , are located on the back and top faces, respectively.

In some of the finite difference discretizations of the governing equations, occasionally the velocity components are required at *non-face* locations (i.e. cell center or cell vertex). These values were computed by applying linear interpolation.

Cell Centers:

$$u_{ijk} = \frac{1}{2} \left(u_{i+\frac{1}{2},j,k} + u_{i-\frac{1}{2},j,k} \right) \quad (40a)$$

$$v_{ijk} = \frac{1}{2} \left(v_{i,j+\frac{1}{2},k} + v_{i,j-\frac{1}{2},k} \right) \quad (40b)$$

$$w_{ijk} = \frac{1}{2} \left(w_{i,j,k+\frac{1}{2}} + w_{i,j,k-\frac{1}{2}} \right) \quad (40c)$$

Other Cell Faces:

$$u_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{u_{i+\frac{1}{2},j+1,k} \Delta y_i + u_{i+\frac{1}{2},j,k} \Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}} \quad (41a)$$

$$u_{i-\frac{1}{2},j+\frac{1}{2},k} = \frac{u_{i-\frac{1}{2},j+1,k} \Delta y_i + u_{i-\frac{1}{2},j,k} \Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}} \quad (41b)$$

$$u_{i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{u_{i+\frac{1}{2},j,k+1} \Delta z_k + u_{i+\frac{1}{2},j,k} \Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}} \quad (41c)$$

$$u_{i-\frac{1}{2},j,k+\frac{1}{2}} = \frac{u_{i-\frac{1}{2},j+1,k} \Delta z_k + u_{i-\frac{1}{2},j,k} \Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}} \quad (41d)$$

$$v_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{v_{i+1,j+\frac{1}{2},k} \Delta x_i + v_{i+1,j+\frac{1}{2},k} \Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} \quad (41e)$$

$$v_{i+\frac{1}{2},j-\frac{1}{2},k} = \frac{v_{i+1,j-\frac{1}{2},k} \Delta x_i + v_{i+1,j-\frac{1}{2},k} \Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} \quad (41f)$$

$$v_{i,j+\frac{1}{2},k+\frac{1}{2}} = \frac{v_{i,j+\frac{1}{2},k+1} \Delta z_k + v_{i,j+\frac{1}{2},k} \Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}} \quad (41g)$$

$$v_{i,j-\frac{1}{2},k+\frac{1}{2}} = \frac{v_{i,j-\frac{1}{2},k+1} \Delta z_k + v_{i,j-\frac{1}{2},k} \Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}} \quad (41h)$$

$$w_{i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{w_{i+1,j,k+\frac{1}{2}} \Delta x_i + w_{i,j,k+\frac{1}{2}} \Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} \quad (41i)$$

$$w_{i+\frac{1}{2},j,k-\frac{1}{2}} = \frac{w_{i+1,j,k-\frac{1}{2}} \Delta x_i + w_{i,j,k-\frac{1}{2}} \Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} \quad (41j)$$

$$w_{i,j+\frac{1}{2},k+\frac{1}{2}} = \frac{w_{i,j+1,k+\frac{1}{2}} \Delta y_j + w_{i,j,k+\frac{1}{2}} \Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}} \quad (41k)$$

$$w_{i,j+\frac{1}{2},k-\frac{1}{2}} = \frac{w_{i,j+1,k-\frac{1}{2}} \Delta y_j + w_{i,j,k-\frac{1}{2}} \Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}} \quad (41l)$$

IV. CONVECTIVE TERMS, $\frac{\partial(u_i u_j)}{\partial x_j}$

The conservative form of the convective terms are evaluated by integrating over the control volume and applying the discrete form of Gauss's theorem

$$\int \nabla \cdot (\vec{v} \vec{v}) dV = \sum \langle \vec{v} \rangle_s (\vec{v}_s \cdot \hat{n}_s) \delta A_s \cdot \hat{n}_s \quad (42)$$

The flux velocity is $\vec{V}_s \cdot \hat{n}_s$ and as a result, $(\vec{V}_s \cdot \hat{n}_s) \delta A_s \delta t_{adv}$ represents the flux volume. The bracketed term, $\langle \vec{V} \rangle_s$, represents the velocity to be fluxed across the control volume boundary.

Expanding the summation for the x-momentum control volume yields

$$\begin{aligned} \sum u(u_j \cdot \hat{n}_j) \delta A_j = & \left[\langle u \rangle_R u_{i+1,j,k} - \langle u \rangle_L u_{i,j,k} \right] \Delta y_j \Delta z_k + \\ & \left[\langle u \rangle_F v_{i+\frac{1}{2},j+\frac{1}{2},k} - \langle u \rangle_B v_{i+\frac{1}{2},j-\frac{1}{2},k} \right] \Delta x_{i+\frac{1}{2}} \Delta z_k + \\ & \left[\langle u \rangle_O w_{i+\frac{1}{2},j,k+\frac{1}{2}} - \langle u \rangle_U w_{i+\frac{1}{2},j,k-\frac{1}{2}} \right] \Delta x_{i+\frac{1}{2}} \Delta y_j \end{aligned} \quad (43a)$$

where the subscripts, R , L , F , B , O , U represent the right, left, front, back, over and under sides of the control volume and the non-bracketed velocities are computed using equations 41 and 42.

Similarly for the y-momentum and z-momentum equations

$$\begin{aligned} \sum v(u_j \cdot \hat{n}_j) \delta A_j = & \left[\langle v \rangle_R u_{i+\frac{1}{2},j+\frac{1}{2},k} - \langle v \rangle_L u_{i-\frac{1}{2},j+\frac{1}{2},k} \right] \Delta y_{j+\frac{1}{2}} \Delta z_k + \\ & \left[\langle v \rangle_F v_{i,j+1,k} - \langle v \rangle_B v_{i,j,k} \right] \Delta x_i \Delta z_k + \\ & \left[\langle v \rangle_O w_{i,j+\frac{1}{2},k+\frac{1}{2}} - \langle v \rangle_U w_{i,j+\frac{1}{2},k-\frac{1}{2}} \right] \Delta x_i \Delta y_{j+\frac{1}{2}} \end{aligned} \quad (43b)$$

$$\begin{aligned} \sum w(u_j \cdot \hat{n}_j) \delta A_j = & \left[\langle w \rangle_R u_{i+\frac{1}{2},j,k+\frac{1}{2}} - \langle w \rangle_L u_{i-\frac{1}{2},j,k+\frac{1}{2}} \right] \Delta y_j \Delta z_{k+\frac{1}{2}} + \\ & \left[\langle w \rangle_F v_{i,j+\frac{1}{2},k+\frac{1}{2}} - \langle w \rangle_B v_{i,j-\frac{1}{2},k+\frac{1}{2}} \right] \Delta x_i \Delta z_{k+\frac{1}{2}} + \\ & \left[\langle w \rangle_O w_{i,j,k+1} - \langle w \rangle_U w_{i,j,k} \right] \Delta x_i \Delta y_j \end{aligned} \quad (43c)$$

The bracketed velocities which represent the momentum flux across the control volume are evaluated using a combination of up-winding and central differencing. Since up-wind differencing often introduces numerical damping, while central differencing can cause numerical instability, a combination of both tends to reduce the damping error while stabilizing the solution.

For illustrative purposes, only the flux velocity entering the x-momentum control volume, (i.e. $\langle u \rangle_L$) is developed. The other bracketed velocities were similarly obtained.

$$\langle u \rangle_L = \left\{ \begin{array}{l} \tilde{u}_{i-\frac{1}{2},j,k} + \frac{1}{2} \Delta x_i \left(\frac{\partial u}{\partial x} \right)_{i-\frac{1}{2},j,k} \left[1 - \frac{|u_{i,j,k}| \Delta t_{adv}}{\Delta x_i} \right] \quad \text{if } u_{i,j,k} > 0 \\ \tilde{u}_{i+\frac{1}{2},j,k} - \frac{1}{2} \Delta x_i \left(\frac{\partial u}{\partial x} \right)_{i+\frac{1}{2},j,k} \left[1 - \frac{|u_{i,j,k}| \Delta t_{adv}}{\Delta x_i} \right] \quad \text{if } u_{i,j,k} < 0 \end{array} \right\} \quad (44)$$

The velocity gradient via up-winding at the cell face is defined to be

$$\left(\frac{\partial u}{\partial x} \right)_{i+\frac{1}{2},j,k} = \left\{ \begin{array}{l} \left(\frac{\partial u}{\partial x} \right)_{i,j,k} \quad \text{if } u_{i+\frac{1}{2},j,k} > 0 \\ \left(\frac{\partial u}{\partial x} \right)_{i+1,j,k} \quad \text{if } u_{i+\frac{1}{2},j,k} < 0 \end{array} \right\} \quad (45)$$

while its central difference formulation is:

$$\left(\frac{\partial u}{\partial x} \right)_{i+\frac{1}{2},j,k} = \frac{\Delta x_{i+1} \left(\frac{\partial u}{\partial x} \right)_{i,j,k} + \Delta x_i \left(\frac{\partial u}{\partial x} \right)_{i+1,j,k}}{\Delta x_i + \Delta x_{i+1}} \quad (46)$$

The spatial derivatives in this formulation are evaluated at the cell centers by computing a first order difference using the face velocities.

$$\left(\frac{\partial u}{\partial x}\right)_{i,j,k} = \frac{u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k}}{\Delta x_i}$$

$$\left(\frac{\partial u}{\partial x}\right)_{i+1,j,k} = \frac{u_{i+\frac{3}{2},j,k} - u_{i+\frac{1}{2},j,k}}{\Delta x_i + 1}$$

As mentioned earlier by using a combination of equations (45) and (46) the velocity gradient at the cell face is computed as follows:

$$\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j,k} = \left\{ \begin{array}{l} \left[1 + \alpha \operatorname{sgn}\left(u_{i+\frac{1}{2},j,k}\right) \right] \Delta x_{i+1} \left(\frac{\partial u}{\partial x}\right)_{i,j,k} \\ + \left[1 - \alpha \operatorname{sgn}\left(u_{i+\frac{1}{2},j,k}\right) \right] \Delta x_i \left(\frac{\partial u}{\partial x}\right)_{i+1,j,k} \end{array} \right\} / \Delta x_\alpha \quad (47)$$

where $\Delta x_\alpha = \Delta x_{i+1} + \Delta x_i + \alpha \operatorname{sgn}\left(u_{i+\frac{1}{2},j,k}\right)(\Delta x_{i+1} - \Delta x_i)$. Similarly for the derivative in the y-direction:

$$\left(\frac{\partial u}{\partial y}\right)_{i+\frac{1}{2},j,k} = \left\{ \begin{array}{l} \left[1 + \alpha \operatorname{sgn}\left(v_{i+\frac{1}{2},j,k}\right) \right] \Delta y_{j+\frac{1}{2}} \left(\frac{\partial u}{\partial y}\right)_{i+\frac{1}{2},j-\frac{1}{2},k} \\ + \left[1 - \alpha \operatorname{sgn}\left(v_{i+\frac{1}{2},j,k}\right) \right] \Delta y_{j-\frac{1}{2}} \left(\frac{\partial u}{\partial y}\right)_{i+\frac{1}{2},j+\frac{1}{2},k} \end{array} \right\} / \Delta y_\alpha \quad (48)$$

where $\Delta y_\alpha = \Delta y_{j+\frac{1}{2}} + \Delta y_{j-\frac{1}{2}} + \alpha \operatorname{sgn}\left(v_{i+\frac{1}{2},j,k}\right)(\Delta y_{j+\frac{1}{2}} - \Delta y_{j-\frac{1}{2}})$ and

$$\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{u_{i+\frac{1}{2},j+1,k} - u_{i+\frac{1}{2},j,k}}{\Delta y_{j+\frac{1}{2}}}$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+\frac{1}{2},j-\frac{1}{2},k} = \frac{u_{i+\frac{1}{2},j,k} - u_{i+\frac{1}{2},j-1,k}}{\Delta y_{j-\frac{1}{2}}}$$

And for the derivative in the z-direction:

$$\left(\frac{\partial u}{\partial z}\right)_{i+\frac{1}{2},j,k} = \left\{ \begin{array}{l} \left[1 + \alpha \operatorname{sgn}\left(w_{i+\frac{1}{2},j,k}\right) \right] \Delta z_{k+\frac{1}{2}} \left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j,k-\frac{1}{2}} \\ + \left[1 - \alpha \operatorname{sgn}\left(w_{i+\frac{1}{2},j,k}\right) \right] \Delta z_{k-\frac{1}{2}} \left(\frac{\partial u}{\partial y}\right)_{i+\frac{1}{2},j,k+\frac{1}{2}} \end{array} \right\} / \Delta z_{\alpha} \quad (49)$$

where $\Delta z_{\alpha} = \Delta z_{k+\frac{1}{2}} + \Delta z_{k-\frac{1}{2}} + \alpha \operatorname{sgn}\left(w_{i+\frac{1}{2},j,k}\right) (\Delta z_{k+\frac{1}{2}} - \Delta z_{k-\frac{1}{2}})$ and

$$\left(\frac{\partial u}{\partial z}\right)_{i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{u_{i+\frac{1}{2},j,k+1} - u_{i+\frac{1}{2},j,k}}{\Delta z_{k+\frac{1}{2}}}$$

$$\left(\frac{\partial u}{\partial z}\right)_{i+\frac{1}{2},j,k-\frac{1}{2}} = \frac{u_{i+\frac{1}{2},j,k} - u_{i+\frac{1}{2},j,k-1}}{\Delta z_{k-\frac{1}{2}}}$$

In the above equations, the coefficient α is a weighting factor (also called the van Leer limiter) which adjust the amount of upwind and central differencing present in the computation while forcing monotonicity constraints. By forcing the gradients to be monotonic, the unstable oscillations resulting from the centered difference are eliminated. Therefore, the weighting factor will satisfy $0 \leq \alpha \leq 1$ and is computed as follows

$$\alpha = \max(0, \min(\alpha_1, \alpha_2, 1))$$

where α_1 forces monotonicity from the left and α_2 forces it from the right. Each of these local weighting factors are computed as

$$\alpha_1 = \frac{u_{\max} - \min\left(u_{i+\frac{1}{2},j,k}, u_{\max}\right)}{\max\left(\varepsilon, \hat{u}_{\max} - u_{i+\frac{1}{2},j,k}\right)}$$

$$\alpha_2 = \frac{\max\left(u_{i+\frac{1}{2},j,k}, u_{\max}\right) - u_{\min}}{\max\left(\varepsilon, u_{i+\frac{1}{2},j,k} - \hat{u}_{\min}\right)}$$

The velocities, u_{\max} and u_{\min} represent the local maximum and minimum velocities, while \hat{u}_{\max} and \hat{u}_{\min} represent maximum and minimum velocities resulting from the Taylor expansions (i.e. equation 44). ε is a small number used to avoid divisions by zero.

As stated previously, similar finite difference formulations can be written for the convective terms found in both the y-momentum and z-momentum equations and for the sake of brevity are not included. At the interface or surface cells, the convective terms are computed using the non-conservative formulation. Expanding these terms for each of the momentum equations yields

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = u_{i+\frac{1}{2},j,k} \left(\frac{\partial u}{\partial x} \right)_{i+\frac{1}{2},j,k} + v_{i+\frac{1}{2},j,k} \left(\frac{\partial u}{\partial y} \right)_{i+\frac{1}{2},j,k} + w_{i+\frac{1}{2},j,k} \left(\frac{\partial u}{\partial z} \right)_{i+\frac{1}{2},j,k}$$

$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = u_{i,j+\frac{1}{2},k} \left(\frac{\partial v}{\partial x} \right)_{i,j+\frac{1}{2},k} + v_{i,j+\frac{1}{2},k} \left(\frac{\partial v}{\partial y} \right)_{i,j+\frac{1}{2},k} + w_{i,j+\frac{1}{2},k} \left(\frac{\partial v}{\partial z} \right)_{i,j+\frac{1}{2},k}$$

$$u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = u_{i,j,k+\frac{1}{2}} \left(\frac{\partial w}{\partial x} \right)_{i,j,k+\frac{1}{2}} + v_{i,j,k+\frac{1}{2}} \left(\frac{\partial w}{\partial y} \right)_{i,j,k+\frac{1}{2}} + w_{i,j,k+\frac{1}{2}} \left(\frac{\partial w}{\partial z} \right)_{i,j,k+\frac{1}{2}}$$

The derivatives are computed using upwind differencing. Since the surface cells are by definition next to a void cell (i.e. a cell without any fluid), the differencing technique must be constructed

such that only existing velocity information is used and as a result a combination of central and upwind differencing cannot be used.

V. VISCOUS TERMS, $\frac{\partial \tau_{ij}}{\partial x_j}$

For each of the three directions, the gradient of the total stresses are

$$\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \quad (50a)$$

$$\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \quad (50b)$$

$$\frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \quad (50c)$$

where each term is computed along the right, back and top cell faces for the x, y, and z-directions, respectively. As with the previous section, example differencing for only the x-direction stress, Eq. (50a) will be provided. A similar analysis for the y and z-directions was conducted to evaluate the appropriate stress gradients. First order differencing of each term in equation (50a) yields

$$\left(\frac{\partial \tau_{xx}}{\partial x} \right)_{i+\frac{1}{2},j,k} = \frac{(\tau_{xx})_{i+1,j,k} - (\tau_{xx})_{i,j,k}}{\Delta x_{i+\frac{1}{2}}} \quad (51a)$$

$$\left(\frac{\partial \tau_{xy}}{\partial y} \right)_{i+\frac{1}{2},j,k} = \frac{(\tau_{xy})_{i+\frac{1}{2},j+\frac{1}{2},k} - (\tau_{xy})_{i+\frac{1}{2},j-\frac{1}{2},k}}{\Delta y_j} \quad (51b)$$

$$\left(\frac{\partial \tau_{xz}}{\partial z} \right)_{i+\frac{1}{2},j,k} = \frac{(\tau_{xz})_{i+\frac{1}{2},j,k+\frac{1}{2}} - (\tau_{xz})_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta z_k} \quad (51c)$$

The normal stress component, τ_{xx} is computed at the cell center as follows

$$(\tau_{xx})_{i,j,k} = 2\mu \left(\frac{u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k}}{\Delta x_i} \right) \quad (52)$$

The shear stress components, τ_{xy} and τ_{xz} are evaluated at the cell vertices using the following relations

$$(\tau_{xy})_{i+\frac{1}{2},j+\frac{1}{2},k} = \mu \left[\left(\frac{u_{i+\frac{1}{2},j+1,k} - u_{i+\frac{1}{2},j,k}}{\Delta y_{j+\frac{1}{2}}} \right) + \left(\frac{v_{i+1,j+\frac{1}{2},k} - v_{i,j+\frac{1}{2},k}}{\Delta x_{i+\frac{1}{2}}} \right) \right] \quad (53a)$$

$$(\tau_{xz})_{i+\frac{1}{2},j,k+\frac{1}{2}} = \mu \left[\left(\frac{u_{i+\frac{1}{2},j,k+1} - u_{i+\frac{1}{2},j,k}}{\Delta z_{k+\frac{1}{2}}} \right) + \left(\frac{w_{i+1,j,k+\frac{1}{2}} - w_{i,j,k+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} \right) \right] \quad (53b)$$

VI. POISSON PRESSURE EQUATION

Expanding the Poisson Pressure equation (38) for three dimensions yields

$$\underbrace{\frac{\partial}{\partial x} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial x} \right)}_{LHS1} + \underbrace{\frac{\partial}{\partial y} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial y} \right)}_{LHS2} + \underbrace{\frac{\partial}{\partial z} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial z} \right)}_{LHS3} = \frac{1}{\Delta t} \underbrace{\left(\frac{\partial \tilde{u}^n}{\partial x} + \frac{\partial \tilde{v}^n}{\partial y} + \frac{\partial \tilde{w}^n}{\partial z} \right)}_{RHS} \quad (54)$$

Expressing the LHS terms as a function of the cell centered variables yields:

{LHS1}

$$\left\{ \frac{\partial}{\partial x} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial x} \right) \right\}_{i,j,k} = \frac{1}{\Delta x_i} \left\{ \frac{1}{\rho_{i+\frac{1}{2},j,k}} \left(\frac{\partial p}{\partial x} \right)_{i+\frac{1}{2},j,k}^{n+1} - \frac{1}{\rho_{i-\frac{1}{2},j,k}^n} \left(\frac{\partial p}{\partial x} \right)_{i-\frac{1}{2},j,k}^{n+1} \right\} \quad (54a)$$

{LHS2}

$$\left\{ \frac{\partial}{\partial y} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial y} \right) \right\}_{i,j,k} = \frac{1}{\Delta y_j} \left\{ \frac{1}{\rho_{i,j+\frac{1}{2},k}} \left(\frac{\partial p}{\partial y} \right)_{i,j+\frac{1}{2},k}^{n+1} - \frac{1}{\rho_{i,j-\frac{1}{2},k}^n} \left(\frac{\partial p}{\partial y} \right)_{i,j-\frac{1}{2},k}^{n+1} \right\} \quad (54b)$$

{LHS3}

$$\left\{ \frac{\partial}{\partial z} \left(\frac{1}{\rho^n} \frac{\partial p^{n+1}}{\partial z} \right) \right\}_{i,j,k} = \frac{1}{\Delta z_k} \left\{ \frac{1}{\rho_{i,j,k+\frac{1}{2}}} \left(\frac{\partial p}{\partial z} \right)_{i,j,k+\frac{1}{2}}^{n+1} - \frac{1}{\rho_{i,j,k-\frac{1}{2}}^n} \left(\frac{\partial p}{\partial z} \right)_{i,j,k-\frac{1}{2}}^{n+1} \right\} \quad (54c)$$

where the pressure derivatives are computed using first order differencing.

$$\left(\frac{\partial p}{\partial x} \right)_{i+\frac{1}{2},j,k}^{n+1} = \frac{p_{i+1,j,k}^{n+1} - p_{i,j,k}^{n+1}}{\Delta x_{i+\frac{1}{2}}}$$

$$\left(\frac{\partial p}{\partial x} \right)_{i-\frac{1}{2},j,k}^{n+1} = \frac{p_{i,j,k}^{n+1} - p_{i-1,j,k}^{n+1}}{\Delta x_{i-\frac{1}{2}}}$$

$$\left(\frac{\partial p}{\partial y} \right)_{i,j+\frac{1}{2},k}^{n+1} = \frac{p_{i,j+1,k}^{n+1} - p_{i,j,k}^{n+1}}{\Delta y_{j+\frac{1}{2}}}$$

$$\left(\frac{\partial p}{\partial y} \right)_{i,j-\frac{1}{2},k}^{n+1} = \frac{p_{i,j,k}^{n+1} - p_{i,j-1,k}^{n+1}}{\Delta y_{j-\frac{1}{2}}}$$

$$\left(\frac{\partial p}{\partial x}\right)_{i,j,k+\frac{1}{2}}^{n+1} = \frac{p_{i,j,k+1}^{n+1} - p_{i,j,k}^{n+1}}{\Delta z_{k+\frac{1}{2}}}$$

$$\left(\frac{\partial p}{\partial x}\right)_{i,j,k-\frac{1}{2}}^{n+1} = \frac{p_{i,j,k}^{n+1} - p_{i,j,k-1}^{n+1}}{\Delta z_{k-\frac{1}{2}}}$$

Re-writing the RHS term yields

$$\left(\frac{\partial \tilde{u}}{\partial x} + \frac{\partial \tilde{v}}{\partial y} + \frac{\partial \tilde{w}}{\partial z}\right) = \frac{\tilde{u}_{i+\frac{1}{2},j,k} - \tilde{u}_{i-\frac{1}{2},j,k}}{\Delta x_i} + \frac{\tilde{v}_{i,j+\frac{1}{2},k} - \tilde{v}_{i,j-\frac{1}{2},k}}{\Delta y_j} + \frac{\tilde{w}_{i,j,k+\frac{1}{2}} - \tilde{w}_{i,j,k-\frac{1}{2}}}{\Delta z_k} \quad (54d)$$

Substitution of these equations (54a-d) into equation (54) yields a set of linear algebraic equations for the new pressure field.

$$-A[p_{i+1,j,k}] - B[p_{i-1,j,k}] - C[p_{i,j+1,k}] - D[p_{i,j-1,k}] - E[p_{i,j,k+1}] - F[p_{i,j,k-1}] + G[p_{i,j,k}] = -\frac{\nu_{cell}(\nabla \cdot \tilde{V})}{\Delta t}$$

where the coefficients, $A \dots G$, are functions of the grid spacing and face densities. The density at the cell faces are computed using linear interpolation and for the right, back and top faces are computed as follows

$$\rho_{i+\frac{1}{2},j,k} = \frac{\rho_{i,j,k}\Delta x_{i+1} + \rho_{i+1,j,k}\Delta x_i}{\Delta x_i + \Delta x_{i+1}}$$

$$\rho_{i,j+\frac{1}{2},k} = \frac{\rho_{i,j,k}\Delta y_{j+1} + \rho_{i,j+1,k}\Delta y_i}{\Delta y_j + \Delta y_{j+1}}$$

$$\rho_{i,j,k+\frac{1}{2}} = \frac{\rho_{i,j,k}\Delta z_{k+1} + \rho_{i,j,k+1}\Delta z_j}{\Delta z_k + \Delta z_{j+1}}$$

For the cells without any fluid, the coefficients, $A \dots F$, are null while the G coefficient is taken to be a very large number. These equations are symmetric, sparse and positive definite allowing the solution for $p_{i,j,k}^{n+1}$ to be obtained using an incomplete Cholesky conjugate gradient (ICCG) solver.

VII. BOUNDARY CONDITIONS

Boundary conditions are required along both the computational grid and the fluid's free surface. Assuming that the grid boundaries are rigid walls, two types of conditions can exist. The first type is the familiar no-slip condition, while the second type is called free-slip or slip and represents a plane of symmetry, or a wall with a non-adhering surface.

GRID BOUNDARY CONDITIONS

As an example, the following relations are used to represent the *slip* condition along the left wall of the computational grid. The conditions at the other walls are similarly computed.

$$f_L = f_{L+1}$$

$$p_L = p_{L+1}$$

$$u_L = 0$$

$$v_L = v_{L+1}$$

$$w_L = w_{L+1}$$

For the same left wall, the following values can be used for the *no-slip* condition.

$$f_L = f_{L+1}$$

$$p_L = p_{L+1}$$

$$f_L = f_{L+1}$$

$$u_L = 0$$

$$v_L = -v_{L+1}$$

$$w_L = -w_{L+1}$$

FREE SURFACE BOUNDARY CONDITIONS

Velocity boundary conditions are applied to free surface cells by requiring that the divergence of the velocity field be zero. Various cases can exist in which a surface cell has only one empty neighboring cell or as many as six empty neighboring cells. Depending on the situation, the divergence requirement must reflect the appropriate configuration.

VIII. COMPUTATIONAL CYCLE

In summary the following algorithm represents the steps to compute the complete solution during one time step.

1. Compute the intermediate velocity components using equation (35).
2. If the energy equations are solved:
 - a. Given the droplet enthalpy and substrate temperature fields, solve Eqs. (27) and (30) implicitly to obtain the new enthalpy field in the droplet and the new temperature field in the substrate. Calculate the temperatures in the droplet from Eq. (29).
 - b. Calculate the new values of the liquid volume fraction Θ from the enthalpy field in the droplet by using Eq. (28a-c) in conjunction with an algorithm described by Voller and Cross⁶. In this algorithm, while a change of phase is occurring in the sub-region of a computational cell, the rate of change in the cell enthalpy equals the velocity of the phase change front across the sub-region multiplied by the latent heat of fusion.

⁶ Voller V. and Cross M., 1983, International Journal of Heat and Mass Transfer, Vol. 26, pp. 147-150.

3. Update the flow boundary conditions for both the computational grid and the free surface.
4. If energy equations are solved:
 - a. Impose the thermal boundary conditions on the free surface, at the solidification front, and the boundaries of the computational domain. Apply the thermal contact resistance at the droplet-substrate interface by using Eq. (31) to calculate the heat flux from the droplet. Use this value of q to update temperature boundary conditions along the bottom surface of the droplet and the upper plane of the substrate.
5. Compute the new pressure field by implicitly solving equation (38).
6. Obtain the final velocities using equation (36).
7. Update the flow and thermal boundary conditions for the free surface.
8. Advect the fluid via VOF.
9. Update the boundary conditions for both the computational grid and the free surface.
10. Increment time and Repeat steps 1-9 until done.

3 SIMDROP 4.1 INSTALLATION

3.1 System Requirements

SIMDROP version 4.1 is the PC version of the program. The minimum requirements are:

OS: Windows 7 or 10.

RAM: 1 GB minimum.

Hard Drive: 1 GB Minimum.

3.2 Installation

1. Find the **setup.exe** file in package you received online. Then follow the installation procedure from the screen. Make sure that you have enough space on your hard drive. For typical runs (without solidification), you may need at least 100 MB space to save the output files. This number is highly dependent on the grid resolution, calculation domain, and the number of the output files.
2. The default directory for SimDrop installation is “C:/Program Files/Simulent/Drop/”. However, you can change this path during installation. Note that the directory that is created on the computer during installation, which contains the executable file **Drop.exe**, is called the **root directory** throughout this Manual.
3. First time you run the code, the subdirectory **Data** will be created in the root directory. Make sure this directory is properly created. Most of the output files are written in the *data* subdirectory.
4. Follow the Sentinel Hardware Lock Installation Guide that is included in the package.

4 SOFTWARE OVERVIEW

By clicking on **SimDrop** from the Start->Programs->Simulent->SimDrop>SimDrop menu or by double clicking on **simdrop4-1x64.exe**, an informational screen will appear. Click on **OK** to close the screen, see Figure 1.

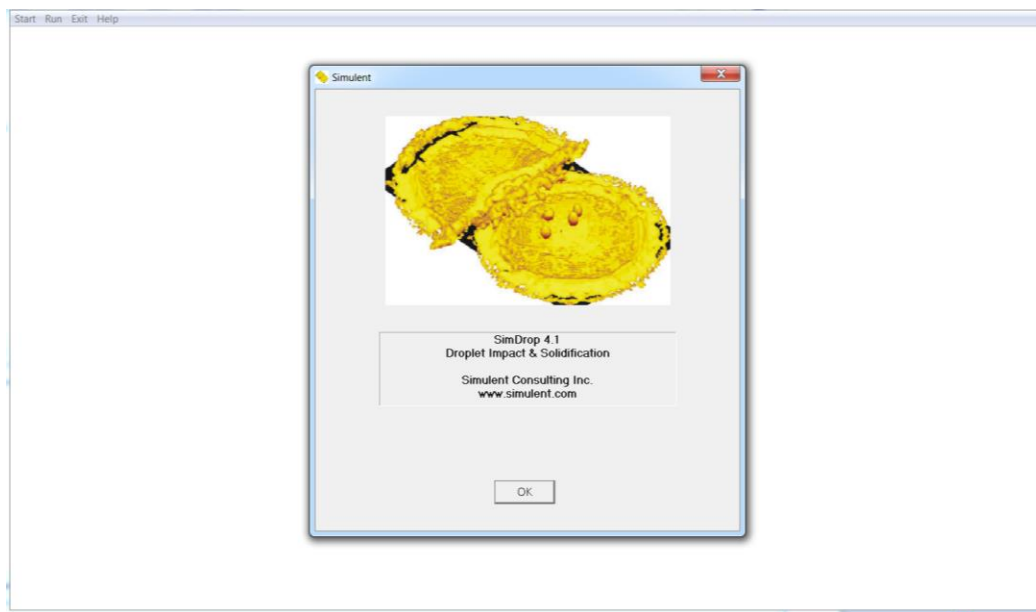


Figure 4.1. The introduction dialog page

4.1 Main Screen

There is a menu in the upper part of the main screen. By clicking on **Start**, a dialogue page appears that introduces the program. From this dialogue page an automatic screen forwarding procedure helps you to fill-up the other dialogue pages through the “Next” buttons. Each dialog page is used to accept parts of input data. These pages are: **General**, **Type of Surface**, **Drop material Properties**, **Single Drop Information**, **Multiple Drop Impact**, **Interface Properties**, **Substrate Material Properties**, **Boundary Conditions**, **Thermal Boundary Conditions**, and **Grids**. Depending on the option selected by you in the **Start** page, all or some of the above dialogue pages are opened for the user.

In addition, there are three more buttons on the main screen: **Run**, **Exit**, and **Help**. After filling up all the dialogue pages, you can click on **Run** to start the calculations. You can click on **Start**

again to repeat the data entry and make modifications as necessary. At any time in this step you can click on **Exit** button to terminate the program.

All of the information given as input to the program is stored in a file named *Input*. Note that each time you run the program the input data from the most recent calculations are appeared in the input dialog pages. This will save a great amount of time when you want to repeat a series of similar calculations. Figure 4.2 shows the flow chart of the program structure.

4.2 Monitoring Windows

After program starts, a window opens that shows a plot of *Spread factor* or *Substrate Temperature* versus time as the calculations proceeds. Figure 4.3 shows a typical monitoring window showing the spread factor versus time. If you decide not to solve the energy equations (isothermal impact), see Section 6.1 in this Manual, the plot of spread factor appears. Spread factor is the ratio of the maximum spread droplet size along the x -axis to the initial droplet diameter. This measure can be used to determine the degree of splash or recoil as the program is executed. In case of solving the energy equations, the plot of the substrate temperature appears. This temperature is calculated at the center of the substrate. At any time during execution, you may click on **Exit** button (upper left of the window) to stop the program. All results up to that time are saved in the *output* files. Please note that for large programs that need extensive memory, the procedure of stopping the program from the monitoring window and also resizing the monitoring window itself may take time.

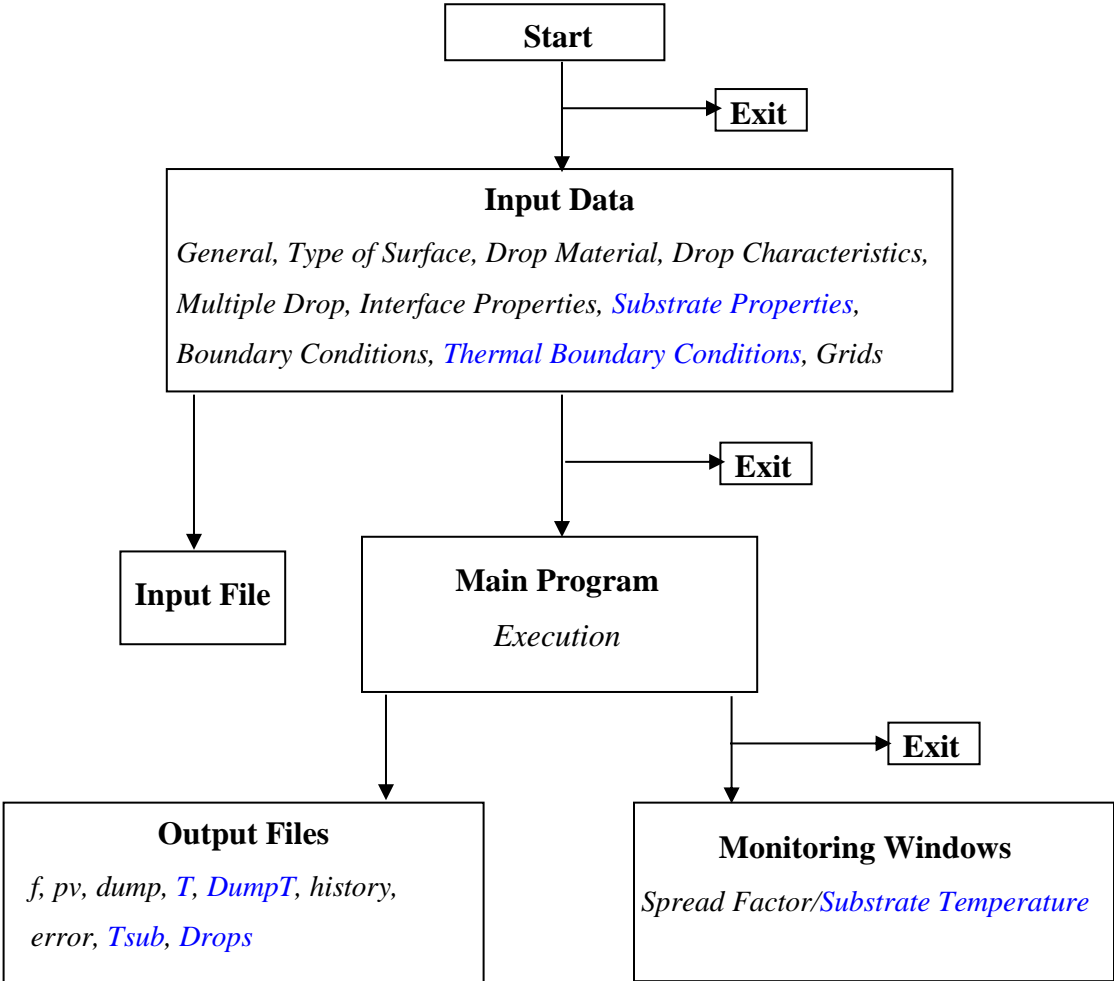


Figure 4.2. Structure of SIMDROP Code. The features with blue color only appear if energy equations are solved in the Start Dialogue Page.

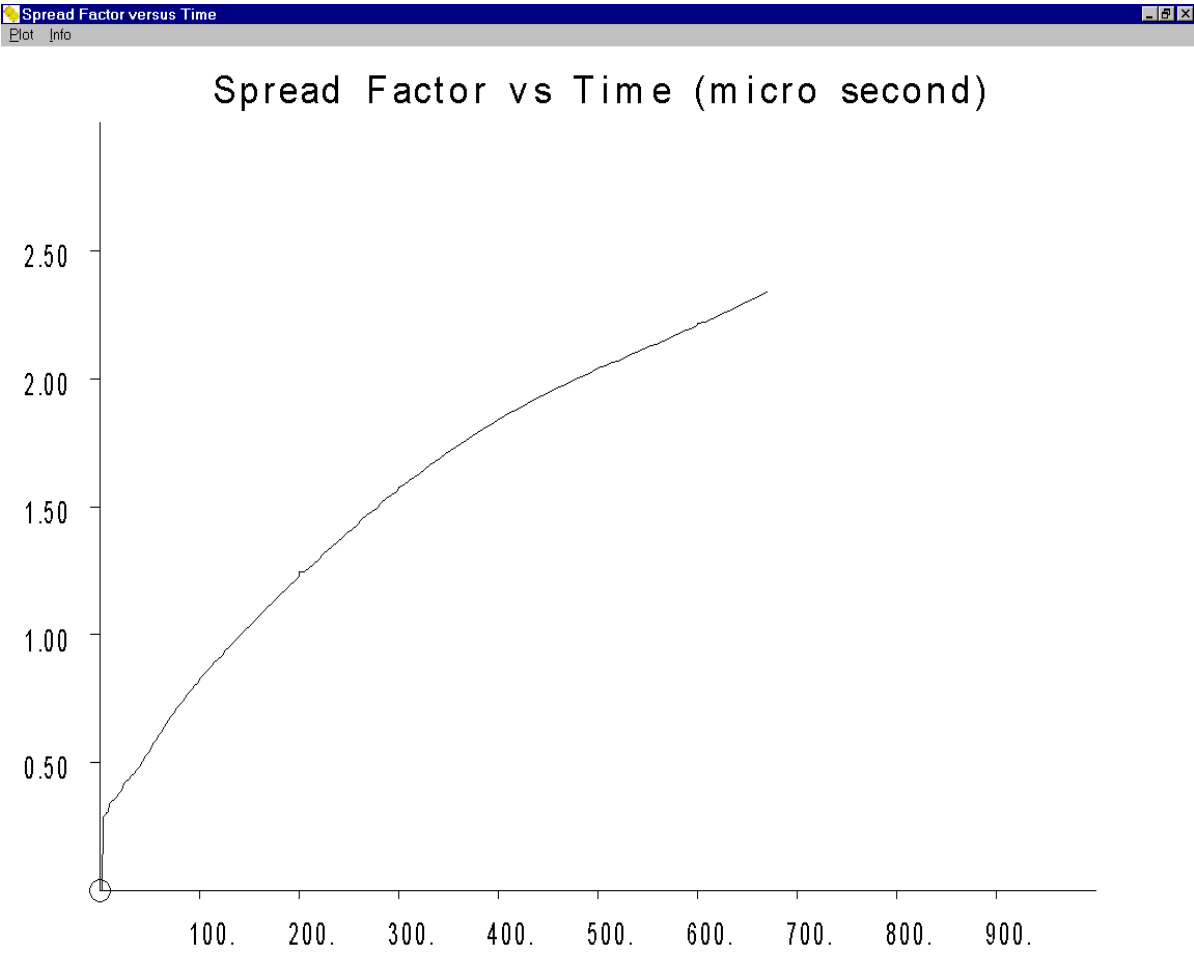


Figure 4.3. The monitoring window which appears during run time

5 SETTING-UP THE PROBLEM

It is always a good practice to set up the problem before starting the SIMDROP Code. First make a sketch of the droplet and the Cartesian system of coordinates. Note that SIMDROP builds up the calculation domain starting from the center of coordinates. Due to the nature of the impact, the length of the calculation domains in x , and y directions must be long enough to include any spread of the droplet without exceeding the boundaries. In the z direction this length must be always greater than $(Z_{\text{center}} + \text{Droplet Radius})$, see Figure 5.2. Here four sample cases of setting up the problem is illustrated:

1. In a case of normal impact of a single droplet where the surface of the impaction is flat there is only one velocity component in the z direction. For this case the center of droplet can be initially located on the z -axis and the calculations can be performed for a quarter of the droplet. This case is shown in Figure 5.1. The results may later be mirrored to show the behavior of the whole droplet.

Note that in this case the x - z and y - z planes are the symmetric planes and the boundary conditions for the calculation domain at these planes must be defined as *Slip* Type condition.

2. In the case of a single droplet with velocity vector in the y or x direction, or multi droplets impaction, or when the surface is inclined, the program shall be set up as illustrated in Figure 5.2. **The boundary conditions for the calculation domain are all *No-Slip* type.**

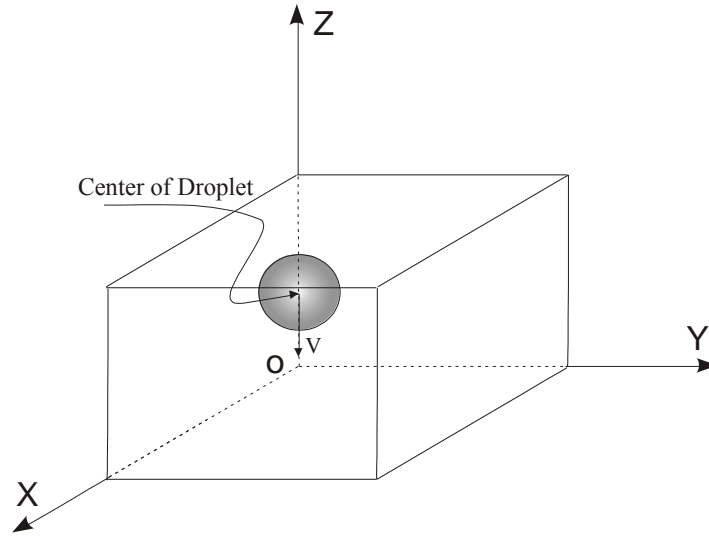


Figure 5.1. Illustration of the system of coordinates, the calculation domain, and the initial position of the droplet for a symmetric case.

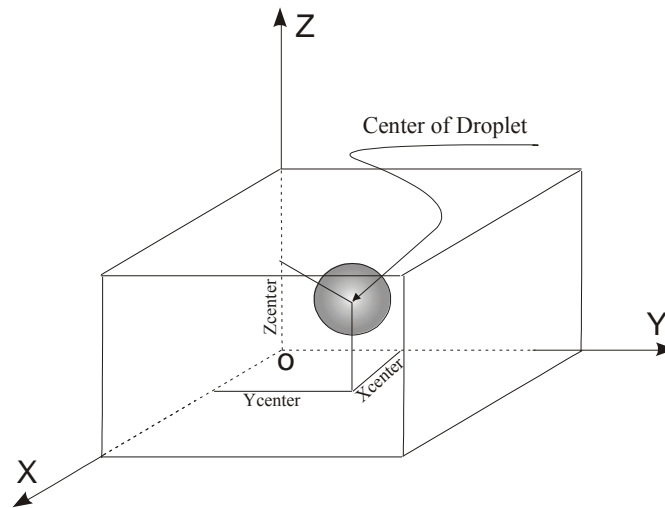


Figure 5.2. Illustration of the system of coordinates, the calculation domain, and the initial position of the droplet, when the center of the droplet is not on the z-axis.

3. When the surface of impact is inclined:

- First define the surface and the system of coordinates as shown in Figure 5.3. Note that the surface is located such that the inclination angle Φ is defined in the x - z plane. This is the angle that must be specified in Section 6.4, when defining the type of surface.

- Then rotate the system of coordinates around the y-axis such that the x-y plane is located on the surface, see Figure 5.4. Note that by doing this transformation, the specific gravity vector is no longer perpendicular to the new x-y plane. SIMDROP will calculate the components of the specific gravity vector for the new system of coordinates.

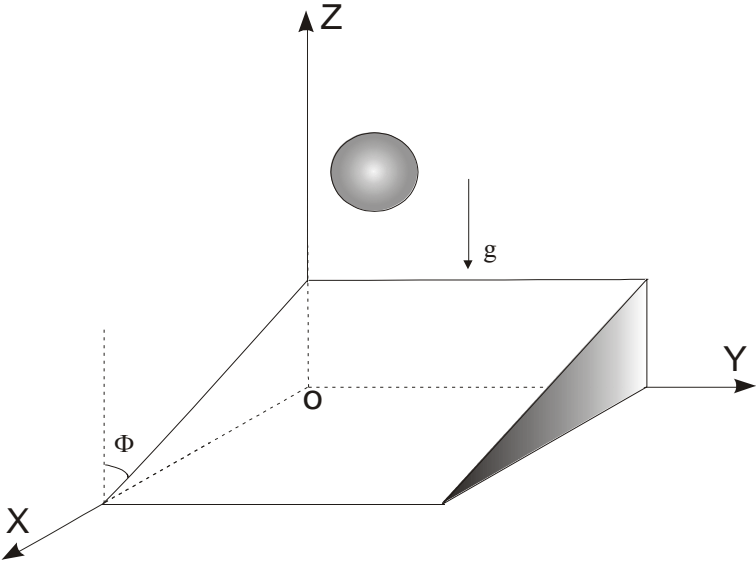


Figure 5.3. Definition of an inclined surface.

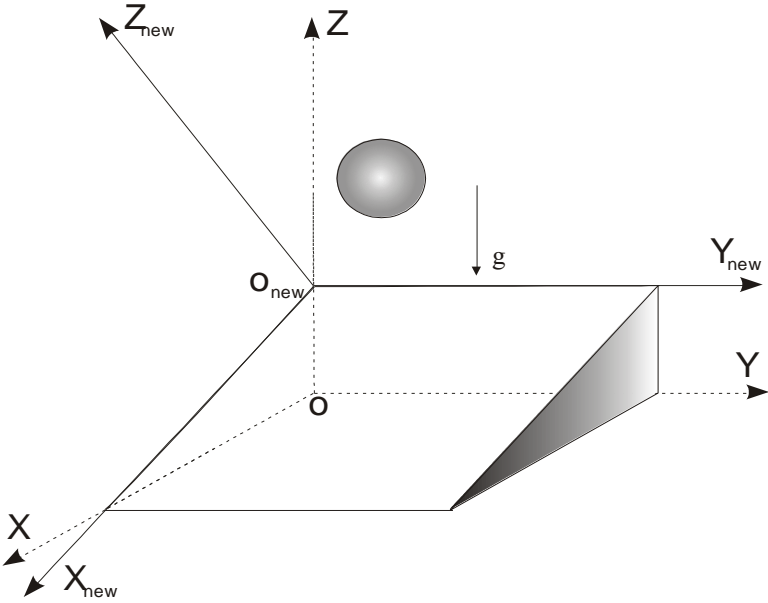


Figure 5.4. Rotation of the system of coordinates.

- Now you can define the position of the droplet center and the calculation domain with respect to the *new* system of coordinates as shown in Figure 5.2. Note that the position of the droplet and the velocity vector have not changed to this point. For this reason, the velocity components must be redefined (if necessary) with respect to the new system of coordinates, see Example 2 for more details.
4. In case of a single droplet impacting on an inclined surface, you can define the system of coordinates such that the center of the droplet locates on the *New* x - z plane, see Figure 5.5. This way the calculations will be performed for only half of droplet. **The boundary condition type for the x - z plane then would be of Slip type since the x - z plane is the symmetric plane. For other boundaries of the calculation domain the *No-Slip* type should be used.**

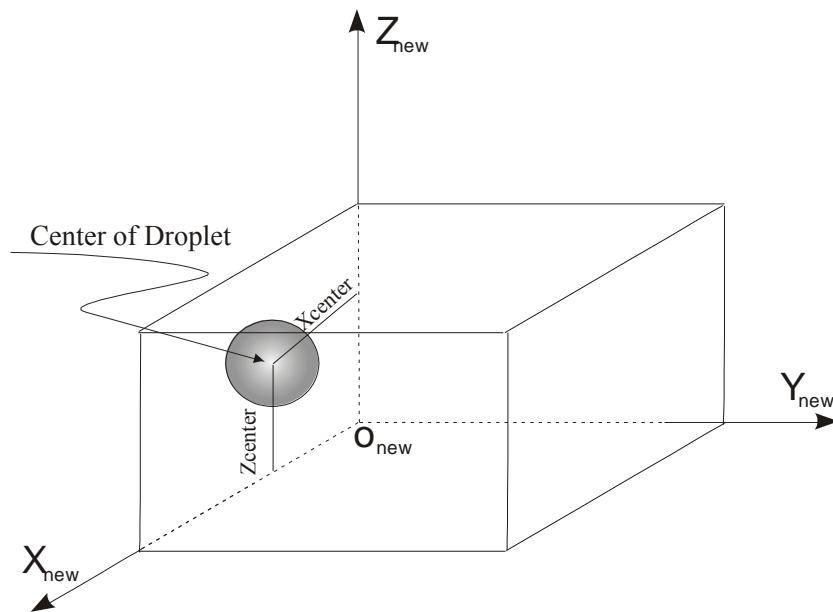


Figure 5.5. Problem set up for calculating half droplet.

6 HOW TO ENTER THE INPUT DATA

In the main screen of the program click on the *Start* button at the upper left of the menu bar. The Start Dialogue page will pop up. This is the starting point of the data entry.

6.1 Start Dialogue page

You can use the subsequent dialogue pages to record all necessary information for running the program. However, you may also use an existing data file to read the information. The default name for this file is "Input" and the sub-directory for saving the out-put files is "Data", both located in the root directory of Simulent Drop.

You may also browse to select the input file you have already created (see Appendix B: to follow the correct format) and to specify a new path for the directory you want to save the result files. In the Directory Name tab you may also enter a path corresponding to a folder in which you wish your data being recorded in. It is recommended to keep the input file and data directory in the same folder, this way it is easier to keep track of your results with respect to your input file, and you can also easily paste the path for the input file in the Directory Name tab avoiding any possible errors.

Note that in either case you need to open all dialogue pages before you can run the program, See Figure 6.1.

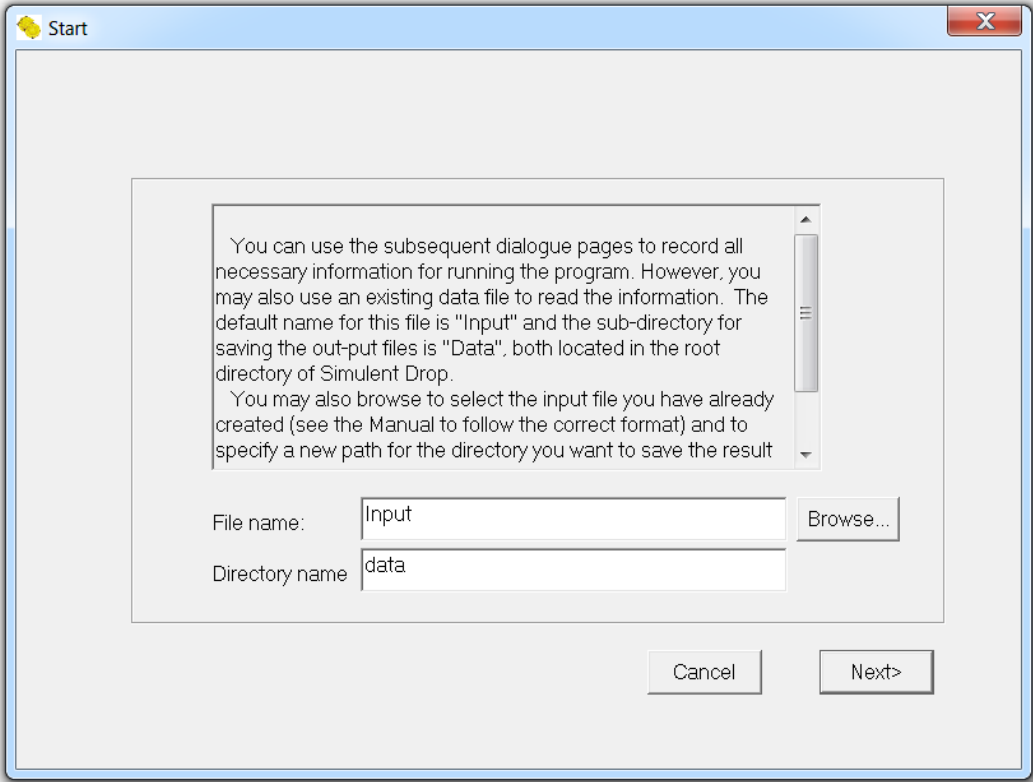


Figure 6.1. The Start Page

6.2 Energy Dialogue page

This Dialogue page helps you to decide whether the energy equations (or solidification) have to be solved or not, See Figure 6.2.

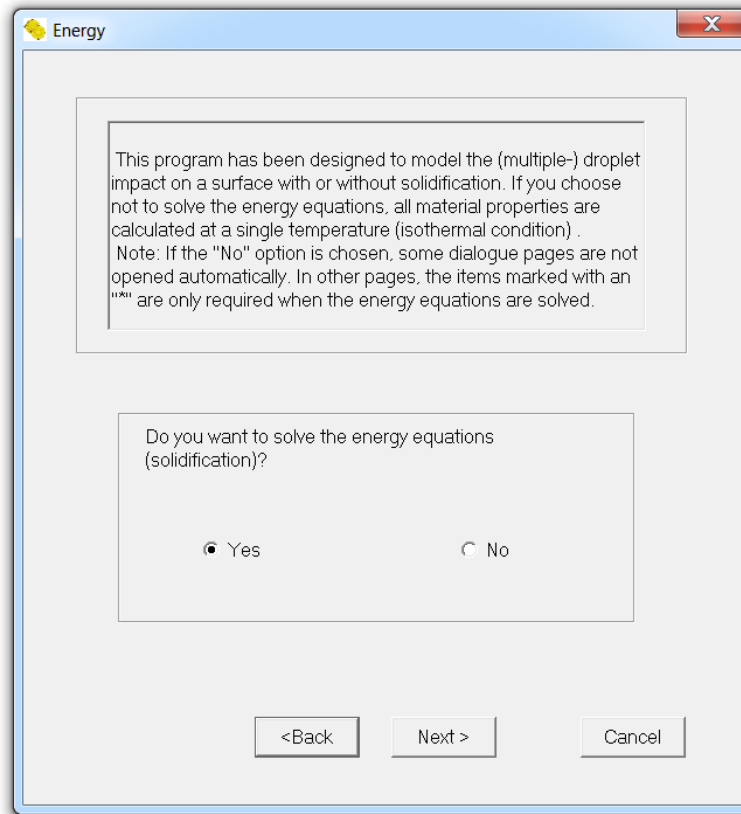


Figure 6.2. The Energy Page

SimDrop can simulate the droplet impaction depending on the selection of “*Yes*” or “*No*” option, all or some of the data entry dialogue pages are opened for the user.

6.3 General Dialogue Page

1. Is this a fresh start:

The code can start calculations as a fresh start. In this case the answer is *Yes*. Otherwise, it will use the information about the flow and thermal fields from a previous set of calculations, option *No*.

2. If you want to re-start from a previous run, give the dump file:

You have the option of using the flow field and temperatures from the previous calculations. In this case you must specify the file names that contain such information. These files should be one of the "dump.xxxx" and "dumpt.xxxx" files. Note that both files must have the same extensions, i.e., both files should have been written at the same time. You can use the "Browse" button to locate these files., see Chapter 7 Note that in any case, all other information about the droplet and the interface must be given to the code.

3. Give the following time periods:

- 3.1. The maximum time step, Delt (Δt): This is the initial time step for calculating droplet impact. The actual time step is determined during the execution time based on the factors presented in Section 2.2. The time step can be estimated from $\Delta t < (R_0 / CPR) / V_0$, where R_0 and V_0 are the initial radius and velocity of the droplet. *CPR* stands for Cell Per Radius which is an indication of the grid size and its definition can be found in Section 6.12.

Note that the initial time step Δt , is used in the code to determine the minimum allowable time step.

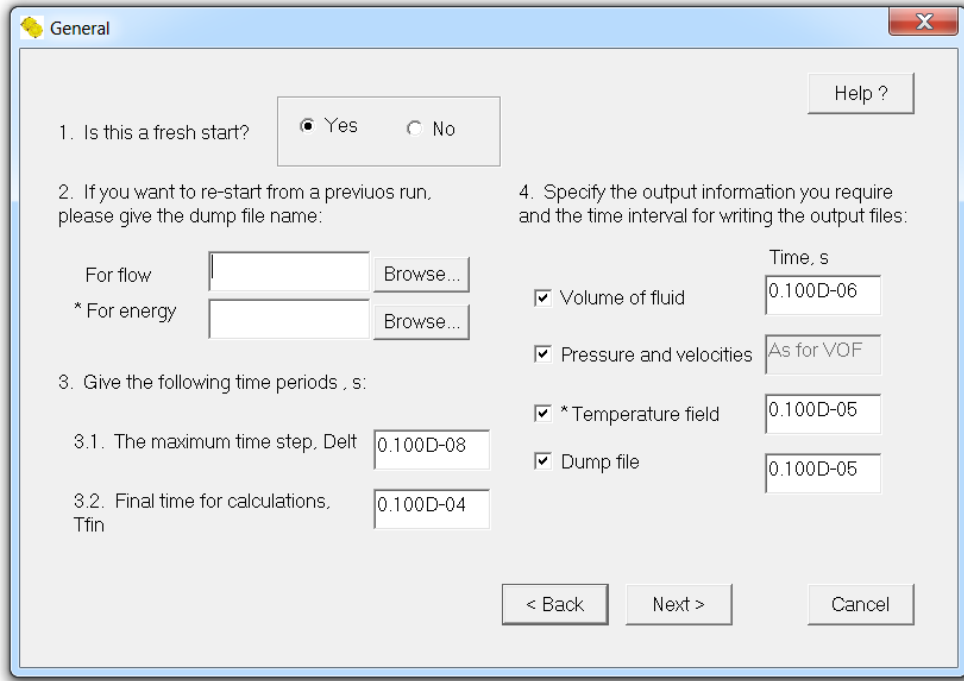


Figure 6.3. The Dialogue page for General information

3.2. **Tfin** is the total time for terminating the calculations. This time can be estimated by considering the droplet velocity and radius. Note that the spread factor versus time is plotted on the screen as the program is executing. You may stop the program from the menu bar at any time during the calculations.

4. Specify the output information you require and the time interval for writing the output files:

There are several types of output files that can be used for obtaining the simulation results. More information about these files can be found in Chapter 7. Since these files usually have a large size, you have the option to asking for all of these files to be created or only some of them.



Volume of Fluid

Time interval (Tpol)

If you check this item, the “*f*” files are created that have information about the volume of fluid of the liquid phase and the solid phase (if the solidification is happening) of the impact droplet. You must also specify the time interval at which these files are created. These files may be used to plot the calculation results at a specific time. If you want to make a movie from the results, it's recommended that the time interval, **Tplot**, be chosen such that: $T_{plot} \leq \frac{0.1 D_0}{V_0}$, where D_0 is the initial diameter of the droplet. By default this option is checked.

Pressure and velocities Time interval (as for the VOF time)

If you check this item, the “*pv*” files are written which contain the values of the velocity components and the pressure at each grid cell. The time interval for writing these files is the same as the VOF files. Therefore, even if you choose not to write the “*f*” files, if you want to have “*pv*” files, you must specify the time interval for the VOF files.

Temperature field Time interval

You can check this item if you solve the energy equations and you want to have the temperature field inside the droplet and the substrate. These data are stored in “*T*” files. Since these files are generally large in size, it is recommended you check this item only if you need the temperature field. The time interval for writing these files must also be specified.

Dump files Time interval

By checking this item, the “*dump*” and “*dumpT*” (only if the energy equations are solved) files are created. The time interval you specify in the box will be used for writing both two files. These files are used when you want to re-start the program from the previous results, (see section 2. in this page). The *dump* and *dumpT* files are stored in subdirectory *data* in the main directory.

6.4 Type of Surface Dialogue page

In this page the type of surface and its geometry is specified, see Figure 6.4. In order to determine the position of the droplet with respect to the impact surface and the system of coordinates, you must first set-up the system as described in Chapter 5

Figure 6.4. The Dialogue for Type of Surface

1. Specify the geometry of the surface: SimDrop code can be used to simulate the droplet impact on a flat or inclined surface. In this section you specify whether the surface is flat or inclined.
2. If the surface is inclined, please give the angle of inclination, Φ : When the surface is flat, the only body force is in the z direction. However, if the surface is inclined, based

on the angle of the inclination, Φ , the components of the gravitational acceleration in other directions are calculated. To specify the inclination angle, see Figure 6.5.

Please note:

- **When the surface is inclined, the system of coordinates is rotated such as the z -axis becomes perpendicular to the surface of impaction. In this case, you must recalculate the components of the velocity vector in the new x , y , and z directions in Section 6.6.2. Please also see Example 2.**
- **Always rotates the impact surface with respect to the y -axis. Therefore, the gravitational acceleration has components in z and x directions. Please also see Example 2.**

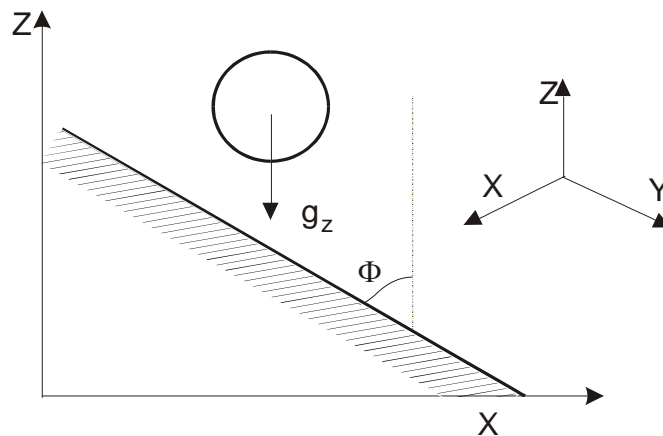


Figure 6.5. Illustration of the droplet impact on an inclined surface

3. The surface of the impact can be smooth or rough. Please note that due to the numerical limitations, the minimum size of the roughness, in any direction, is limited to the grid (cell) size.
4. When the surface is rough, three parameters would specify the characteristics of the surface, see Figure 6.6. These parameters can be introduced in microns. :

4.1 Peak to Valley height.

4.2 Peak to peak distance.

4.3 Width of the tooth.

Please note:

- **It is assumed that all three parameters are uniform throughout the surface.**

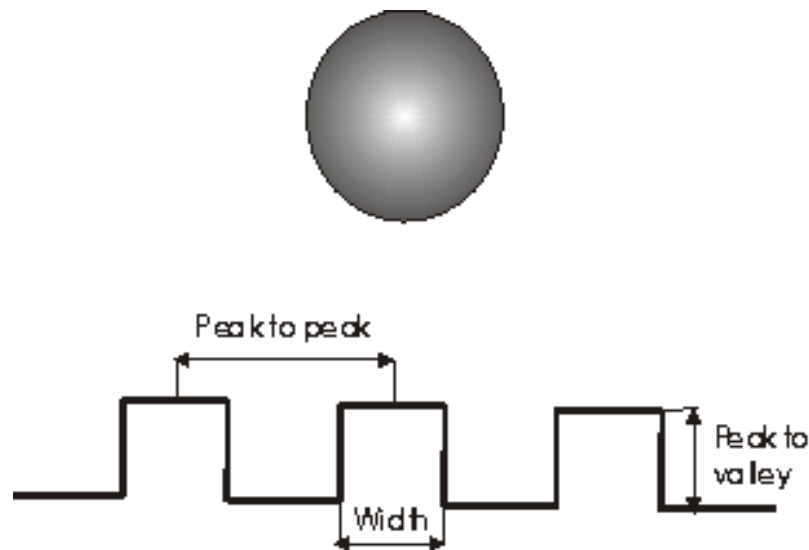


Figure 6.6. Illustration of the surface roughness parameters

5. There is an option in the code that allows users to consider a rotating substrate. Please check if you want to use this option. Click on “Yes” or “No”.

Please note:

Before starting to complete the information in this page, you must set up your problem as shown in Figure 6.7 to do so, you can follow these steps:

- **First define the initial position of the droplet such that it locates in the top right quadrant of the substrate, with center of rotation in the middle of it (assuming substrate is a round plate.)**

- Define the calculation domain (in the x and y directions), especially the (0,0) point, to be within this quadrant.
- Make sure that the positions of the “x” and “y” axis are defined as the close up shown in Figure 6.8.

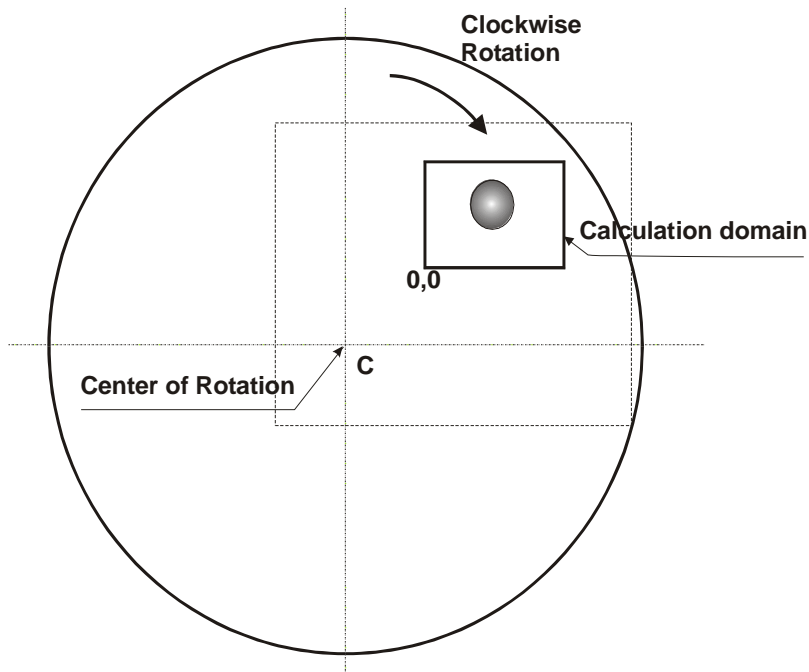


Figure 6.7. Illustration of a rotating substrate.

6. Direction of rotation when looking from the top of the substrate: The direction of the rotation can be clockwise or counter clockwise when looking from the top on the "XY" plane, see Figure 6.7.
 - 4.1. Rotational speed, rpm. Specify the rotational speed in round per minute.
 - 4.2. X- position of center of rotation, m: Give the position of the center of rotation, XDR, in the x direction. This center is defined with respect to the center of coordinates for the calculation domain, see Figure 6.8.
 - 4.3. Y- position of center of rotation, m: Give the position of the center of rotation, YDR, in the y direction. This center is defined with respect to the center of coordinates for the calculation domain, see Figure 6.8.

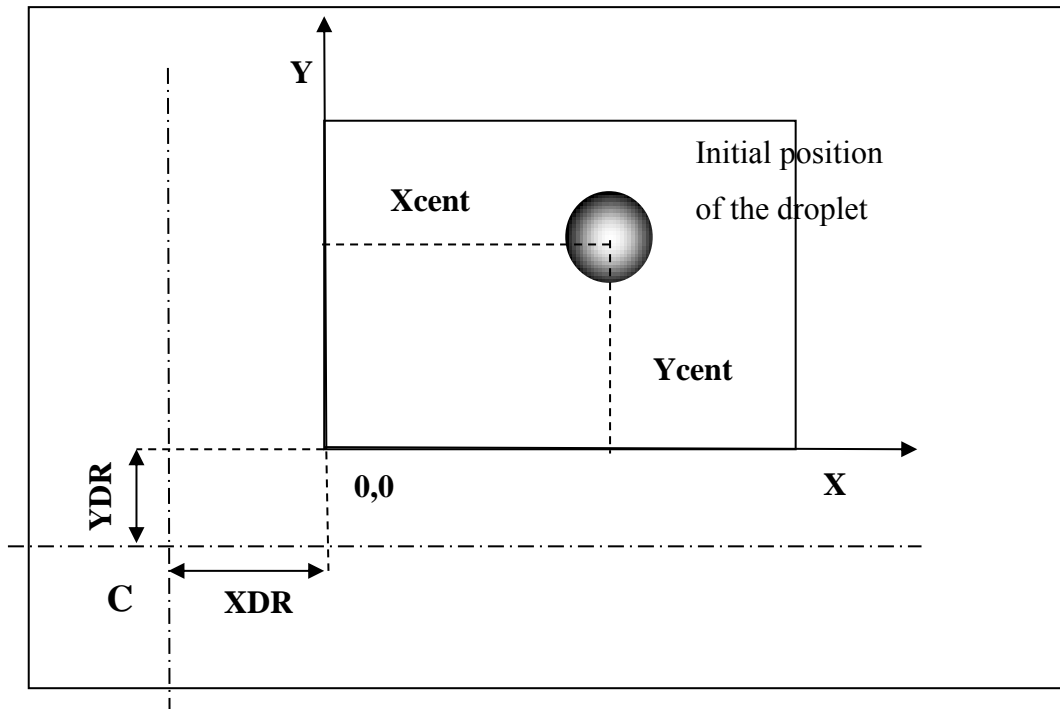


Figure 6.8. Close up the calculation domain and its location with respect to the center of rotation, see Figure 6.7.

Tips: Please note that in order to see the effect of the substrate rotational speed, the average tangential velocities of different points of the substrate must be in the same order as the droplet velocity. This average velocity can be calculated at the initial center of the droplet (X_{cent} , Y_{cent}) and divided by the initial velocity of the droplet. This parameter is calculated when the program has finished importing the data and is indicated in the “Inputw” file, as “Ratio”.

6.5 Drop Material Dialogue Page

In this page the information about the drop material is needed, see Figure 6.9.

1. The initial drop temperature in °C: This temperature is used for calculating the droplet properties. Note that in case of a molten droplet impact, this temperature must be equal or greater than the melting point of the drop material.
2. Specify the droplet material: There is a material list box in this page. You can choose the drop material from the list. Once you selected the material, a property file name appears in the window box below the list. SIMDROP reads the physical properties from this file. The property files, located in the root directory, are listed in Table 1. These files contain the information about density, liquid phase kinematic viscosity, thermal conductivity, specific heat, surface tension; solid phase thermal conductivity, and specific heat; melting point, and heat of fusion (solidification) for the drop material. All temperatures are in °C. More details about these files, format, and units can be found in Appendix B: Drop Property Files.

Note: If you want to use another material or to change the values of properties, the “User Defined” option can be selected from the list box. In this case before you start the program, first create a property file with the same format presented in Appendix B:, and **then write its name in the window box**. Maximum 80 characters can be used for the file name.

Table 1. Property files for materials used in the program

Material Name	File name
Nickel	Nickel.dat
Alumina	Alumina.dat
Tin	Tin.dat
Molybdenum	Molyb.dat
Water	Water.dat
Zirconia	Zirconia.dat

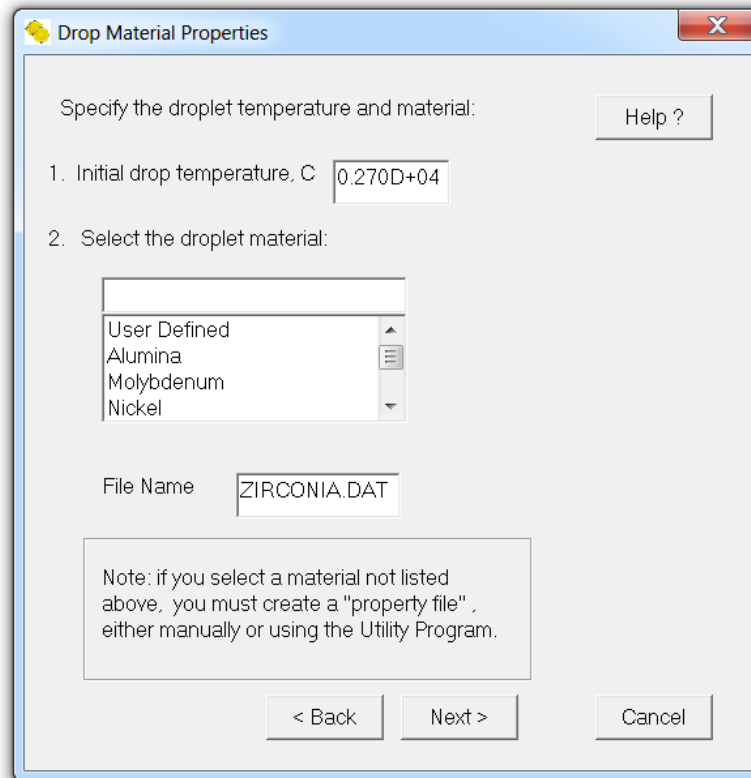


Figure 6.9. Dialogue page for drop material properties.

6.6 Single/First Drop Characteristics Dialogue Page

In this page the information about the single drop (single drop impact), or the first drop (multiple drop impact) is required, see Figure 6.10.

1. **The initial radius of the drop (in meters):** Enter the initial droplet radius in this section. Note that all dimensions in this code are in terms of meters. It's assumed that the drop is spherical before impact.
2. **Initial drop velocities, m/s:** Enter the initial velocity components of the droplet in x , y , and z directions. Note that:
 - If the droplet is impacting the surface perpendicularly, only the velocity component, in z direction exists. Based on the definition of the system of coordinates, the velocity in z direction is always negative (see Figure 6.11).

- In case of an inclined impact surface, the velocity components must be recalculated according to the new system of coordinates, see Example 2.
3. Location of the drop center at initial time, m: Give the location of the center of the droplet at time equal zero. This location is indicated with respect to the surface of impaction and the center of coordinates. The vertical distance of the drop center (in z direction) must be equal or greater than the droplet Radius. Two other coordinates, i.e., x, and y, are required when the center of the drop is not the same as the center of coordinates, e.g., when surface is inclined. See Chapter 5 for more details.

Note that the Center of droplet and the boundary condition types for the calculation domain must be specified accordingly (see Section 6.10).

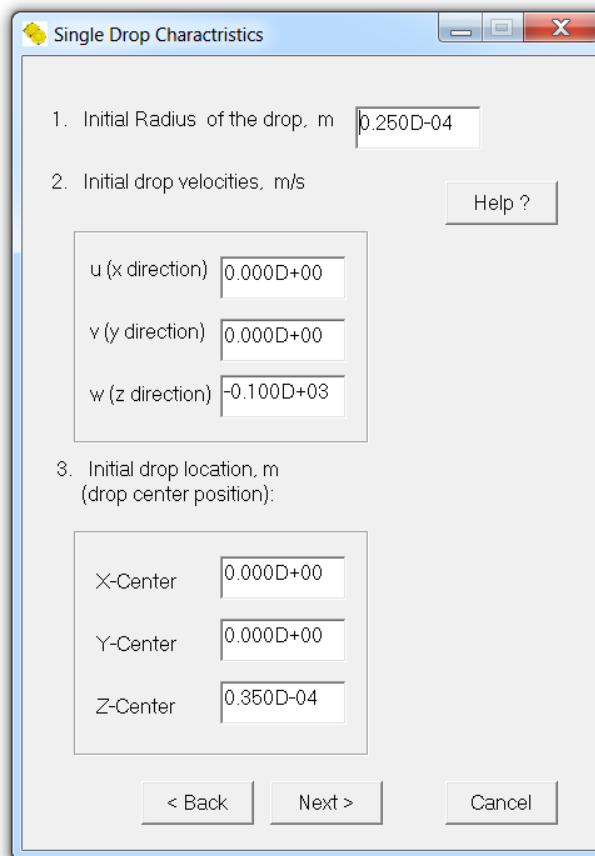


Figure 6.10. The Dialogue for Drop Information

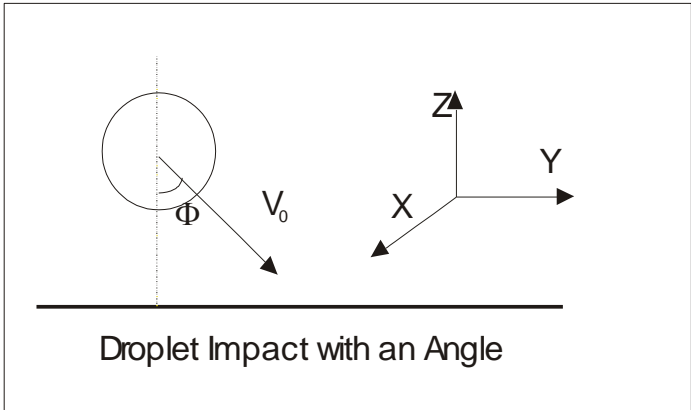


Figure 6.11. Illustration of droplet impacting with an angle on a flat surface.

6.7 Multiple Droplet Impact Dialogue Page

In this Dialogue page the information about the multiple drop impact is needed, see Figure 6.12.

1. Do you want to have a multiple impact simulation: By answering *Yes* to this question, SIMDROP will look for information about the additional droplets. The default option is “*No*”. In case of a single drop impact, you can proceed to the next dialogue page

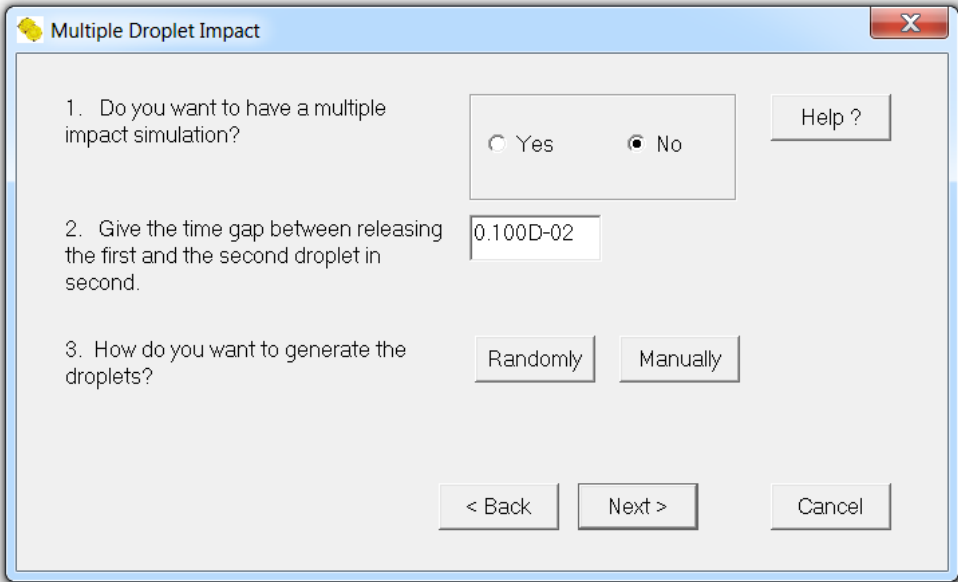


Figure 6.12. Multiple Drop Impact dialogue page.

2. Give the time gap between releasing the first and second droplet, second: In a case of simulating a multiple impact scenario, you must give the time at which the second droplet is released in this box. Note that if this time is larger than the final time of the calculation, T_{fin} , the program automatically considers a single droplet impact. In other words, in case of a multiple drop impact, T_{fin} , must be large enough to allow for releasing all droplets.
3. How do you want to generate the droplets: The information about the additional droplets can be generated randomly or manually. By pressing on *Randomly*, SIMDROP will use a random generation subroutine to determine the specification and number of the additional droplets. You have no control on these parameters other than specifying the ranges for the information. If you press on *Manually*, you must give the information about the additional droplets as well as the number of the released droplets. By clicking on each button, a different dialogue page appears as follows:

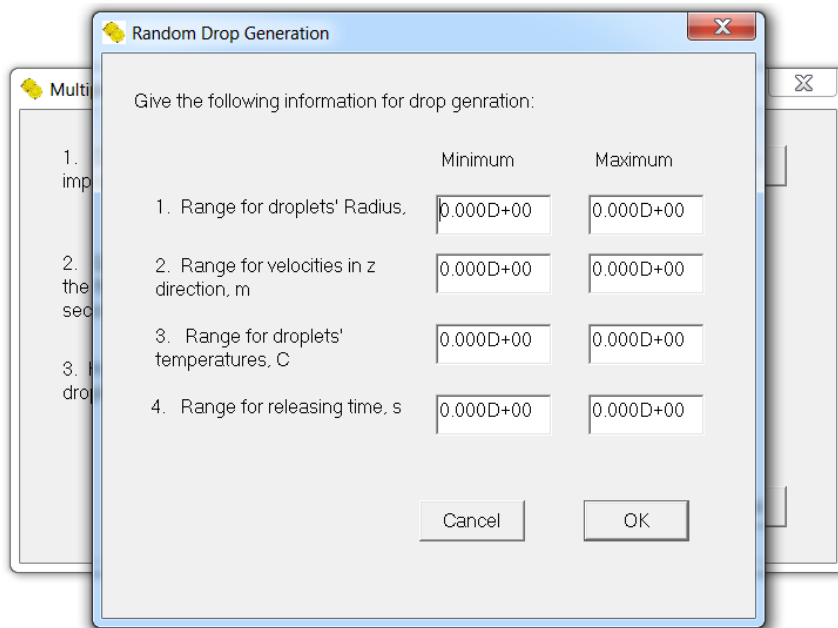
6.7.1 Random Drop Generation

The Random Drop Generation page appears after clicking on “Randomly” button, See Figure 6.13. If this option is selected, program uses a random pick subroutine to obtain the radius, normal velocity, initial temperature, and releasing time for the next drop for each droplet. The program stops generating additional drops, when the random releasing time exceeds the final time, T_{fin} . You can control the droplet characteristics by specifying the ranges at which the above-mentioned parameters are generated. Note that all additional droplets have the same material and furthermore it is assumed that they only have one velocity component in the z direction.

1. The range for the droplets’ radius: Enter the minimum and maximum droplet radius in these windows. The generated droplets will have radii in this range.
2. The range for velocities in the z direction, m/s: Enter the minimum and maximum values for normal velocities. Note that since in a normal drop impact problem, the normal

velocity is always negative, the absolute value of the minimum velocity is larger than the absolute value of the maximum velocity. For example if the range for absolute drop velocity is between 2 and 5 m/s, the minimum velocity should be specified as -5 m/s and the maximum velocity as -2 m/s.

3. Range for initial drop temperatures in $^{\circ}\text{C}$: Enter the minimum and the maximum values for the initial drop temperatures.
4. Range for releasing time: Enter the minimum and the maximum values for the time gap between releasing two subsequent droplets in second. Note that the number of droplets is determined through the program based on the releasing time and the final time T_{fin} .



	Minimum	Maximum
1. Range for droplets' Radius,	0.000D+00	0.000D+00
2. Range for velocities in z direction, m	0.000D+00	0.000D+00
3. Range for droplets' temperatures, C	0.000D+00	0.000D+00
4. Range for releasing time, s	0.000D+00	0.000D+00

Figure 6.13. Random Drop Generation Page

6.7.2 Manual Drop Generation

The manual Drop Generation page appears after clicking on “Manually” button, See Figure 6.14. If this option is selected you must specify the characteristics for each additional droplet (the information about the first droplet is already known). Note that each time the page is opened a

text notifying the number of the additional droplet appears in the window box designed for this purpose. After filling up the appropriate window boxes in this page, you must click on “Ok” button. By clicking on “Ok”, the page is closed and returns to the Multiple Drop Impact page. For additional droplets, click again on the Manually button and repeat this procedure until the information for all droplets is completed.

The information to be given for each additional droplet in this page, as appear on the page, are: Radius in meters; The location of the center of droplet by specifying the X-center, Y-center, and Z-center in meters (please refer to Section 6.6 for more details); Velocity components in the Y direction, v , and the Z direction, w ; The initial drop temperature; And the time gap for releasing the next droplet. Note that the final time, T_{fin} must be estimated based on the information of this page, i.e., $T_{fin} > \sum_{i=1}^N \Delta T_i$, where N is the total number of the droplets and ΔT_i is the releasing time gap specified for droplet “ i ”.

Manual Drop Generation

Note:
After writing each data set, please press on "OK". The dialog page returns to the "Multiple Droplet Impact" page. For more droplets, press the "Manually" button again and repeat this process until you add the information for all droplets.

Give the following information for the droplet:

Radius, m	<input type="text" value="0.000D+00"/>	v (y direction), m/s	<input type="text" value="0.000D+00"/>
X-center, m	<input type="text" value="0.000D+00"/>	w (z direction), m/s	<input type="text" value="0.000D+00"/>
Y-center, m	<input type="text" value="0.000D+00"/>	Temperature, C	<input type="text" value="0.000D+00"/>
Z-center, m	<input type="text" value="0.000D+00"/>	Time gap for releasing the next droplet, s	<input type="text" value="0.000D+00"/>

OK
Cancel

Figure 6.14. Manual Drop Generation Page

6.8 Interface Properties Dialogue Page

In this page the information about the interface is required, see Figure 6.15.

1. What type of contact angle you use: Contact angles are required for determining the “unit normal” vectors at the liquid-solid boundaries, see Chapter 2. You have the choice of using a *Static* or a *Dynamic* contact angle. The *Static* contact angle shall be used if:

- The droplet material is a metal and the impact condition is isothermal.
- The drop velocity is high enough such that $We \gg \sqrt{Re}$, where:⁷

$$\text{Weber No. } We = \frac{\rho D_0 V_0^2}{\gamma}$$

$$\text{Reynolds No. } Re = \frac{D_0 V_0}{\nu}$$

For all other cases it is recommended a *Dynamic* contact angle to be used. This means that the contact angle depends on the contact line velocity and the code will use a simple model to find the relation between the contact line velocity and the contact angles at advancing and trailing edges.⁸

2. For a static contact angle, you may choose the contact condition from the menu: You may choose type of a particular liquid-solid system from the list box. The default *Static* contact angle for that system then will pop up in Section 3. This contact angle is the advancing contact angle measured for the specific liquid-solid. If you want to use contact angles other than those listed, select the *User defined* option.
3. For User Defined option, specify the static contact angle between the drop and the surface [degrees]: If you select *User defined* option from the list box, you must enter the desired contact angle in this window box (a good estimate for most high speed spray coating conditions is 90 °).

⁷ Pasandideh-Fard, M., Bhola, R. Chandra, S. and Mostaghimi, J. , 1998a, International Journal of Heat and Mass Transfer, Vol. 41, pp. 2929-2945.

4. For dynamic contact angles, you may choose the contact condition from this menu: If you have selected the *Dynamic* contact angle option, you may choose a particular liquid-solid system from the list box. The default *advancing* and *receding* contact angles for that system then will pop up in Section 5. If you want to use contact angles other than those listed, select the *User defined* option.
5. If you choose the *User defined* option in the list box, you must enter the desired contact angles in these window boxes.

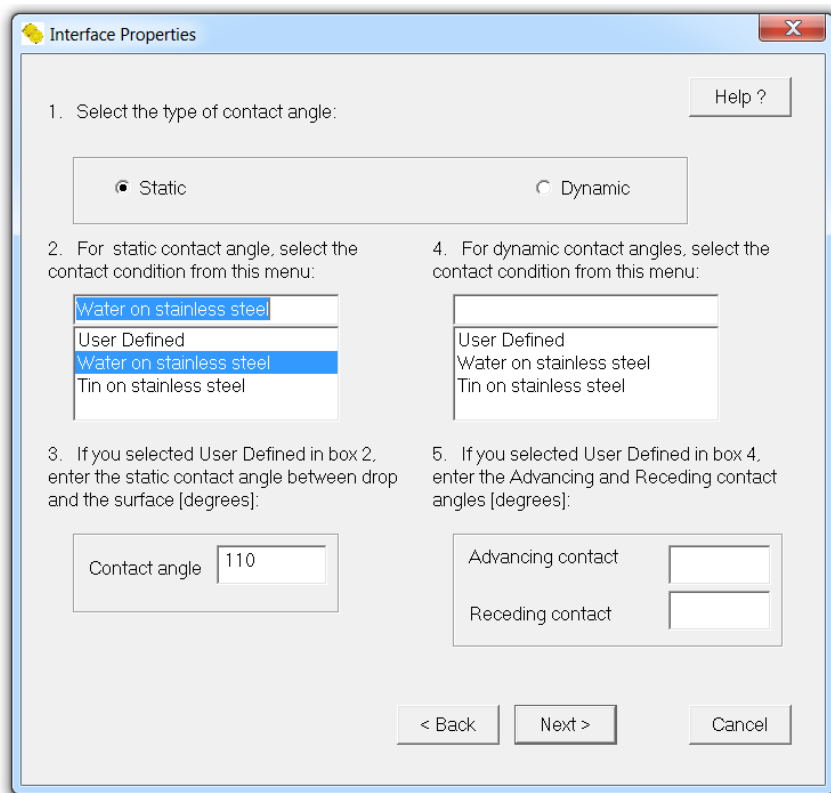


Figure 6.15. The Dialogue page for Interface Properties

6.9 Substrate properties Dialogue Page

This page is opened only if you selected to solve the energy equation in **Start** Dialogue Page. In this page the information related to the substrate is needed, see Figure 6.16.

1. **Initial substrate temperature in °C:** Enter the initial substrate temperature in this window.
2. **The thermal resistance between the solid phase and the substrate, K-m²/W:** This is a thermal property that affects the heat transfer between the substrate and the droplet. Although this property could vary with time and/or position on the interface, a constant value is used throughout the simulation. In principal the value of the thermal contact resistance depends on the substrate temperature. In thermal spray processes its value is typically between 1×10^{-7} m²-K/W (for room temperature substrates) to 1×10^{-6} m²-K/W (for higher temperature substrates).⁹ Enter the value for the thermal resistance in this window.
3. **Specify the substrate material:** There is a material list box in this page. You can choose the substrate material from the list. Once you selected the material, a property file name appears in the window box below the list. SIMDROP reads the physical properties from this file. The property files, located in the root directory, are listed in Table 2. These files contain the information about Substrate density, thermal conductivity, and specific heat for the substrate material. All temperatures are in degree centigrade. More details about these files, format, and units can be found in Appendix C.; Substrate Property Files. For each property, maximum 20 data sets are permitted. If you want to use another material or to change the values of properties, the “User Defined” option shall be selected from the list box. In this case before you start the program, first create a property file with the same format presented in Appendix C.; then put its name in the window box. Maximum 80 characters can be used for the file name.

⁹ Pasandideh-Fard, M., Pershin V., Thomson I., Chandra S., and Mostaghimi J., “*Splat Shapes in a Thermal Spray Coating Process: Simulation and Experiments*”

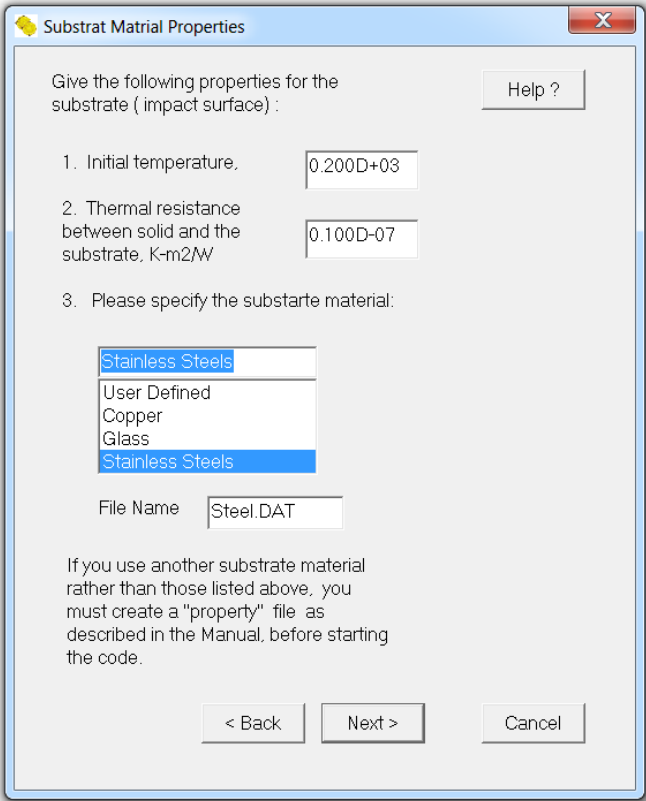


Figure 6.16. Substrate Properties Dialogue Page.

Table 2. Material Property files

Material	Property File
Stainless Steels	Steel.dat
Glass	Glass.dat
Copper	Copper.dat

6.10 Boundary Conditions Dialogue Page

In this page the information about the flow boundary conditions is required, see Figure 6.17.

1. **Select the Flag Numbers for Flow Boundary Conditions:** After you set up the problem based on what is presented in Chapter 5, the boundary conditions of the calculation domain (computational grid) are known. In this page, you specify the flag numbers that are assigned for this purpose. Assuming that the calculation boundaries are rigid “walls”, there are basically two types of boundary conditions. The first type is the so-called “*no-slip*” condition and the second type is a free-slip of “*slip*” condition. This latter one represents a plane of symmetry or a wall with a non-adhering surface. The flag number for the “*slip*” boundary condition is 1 and for the “*no-slip*” condition is 2. The six boundaries of the calculation domains are distinguished as follows (see also Figure 6.18):

- **Kleft** refers to the boundaries on the z - y plane.
- **Kright** refers to the boundary on the surface parallel to z - y plane.
- **Kback** refers to the boundary on the x - z plane.
- **Kfront** refers to the boundary on the surface parallel to x - z plane.
- **Kunder** refers to the boundary condition on the impact surface.
- **Kover** refers to the boundary condition on the surface parallel to the impact surface, i.e., x - y plane.

The boundary conditions for surfaces with free flow movement (including the impact surface) must be of the “*No-Slip*” type.

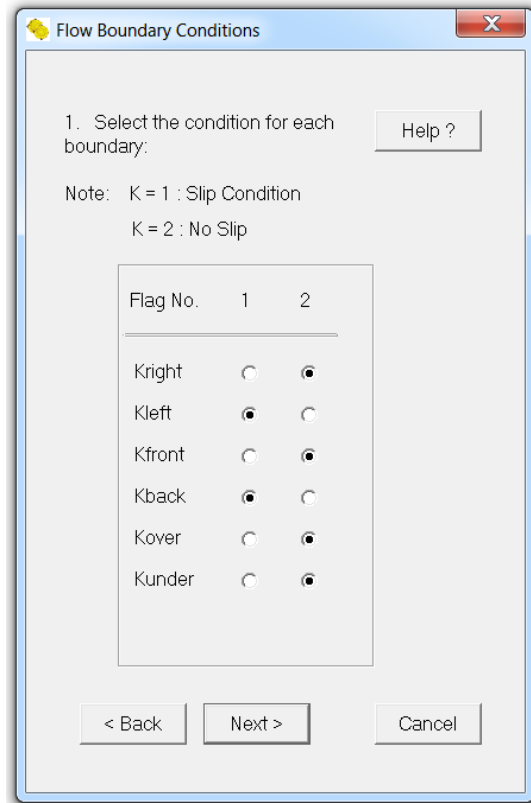


Figure 6.17. The Dialogue page for Boundary Conditions

Note that:

- **With the exception of impact surface, the calculation domain must be chosen large enough such that at no time the droplet touches the boundaries with *No-Slip* condition.**
- **The boundary condition type and the location of the center of the droplet (see Chapter 5) must be specified accordingly.**

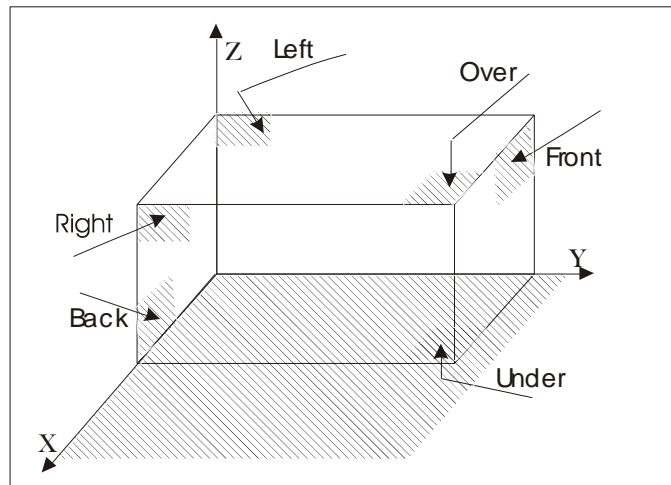


Figure 6.18. Definitions of terms used in boundary condition flags

6.11 Thermal Boundary Conditions Dialogue Page

This page is opened only if you choose to solve the energy equations through **Start** Dialogue Page. In this page the thermal boundary condition types are required, see Figure 6.20.

In SIMDROP, two types of thermal boundary conditions for the flow and the substrate calculation domains are defined (except for the impact surface which there is a third type). First is the adiabatic condition which is used for the symmetry planes and/or if the calculation grid boundary is isolated. The second type is the constant temperature condition. This condition is used for the grid boundaries which are “far” enough, i.e., the real droplet boundaries are far from the grid boundaries. For the impact surface there is another boundary type which is the “known initial temperature”. This is a typical boundary condition for the droplet impact simulations.

As for the flow boundaries, the flag numbers for specifying thermal boundary condition types refer to the boundaries for the calculation domain. See Figure 6.18 for flow and Figure 6.19 for the substrate boundaries.

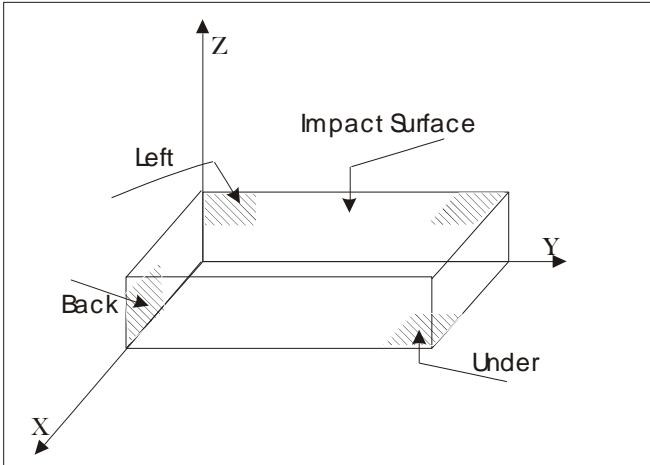


Figure 6.19. Definitions of terms used in substrate thermal boundary condition flags.

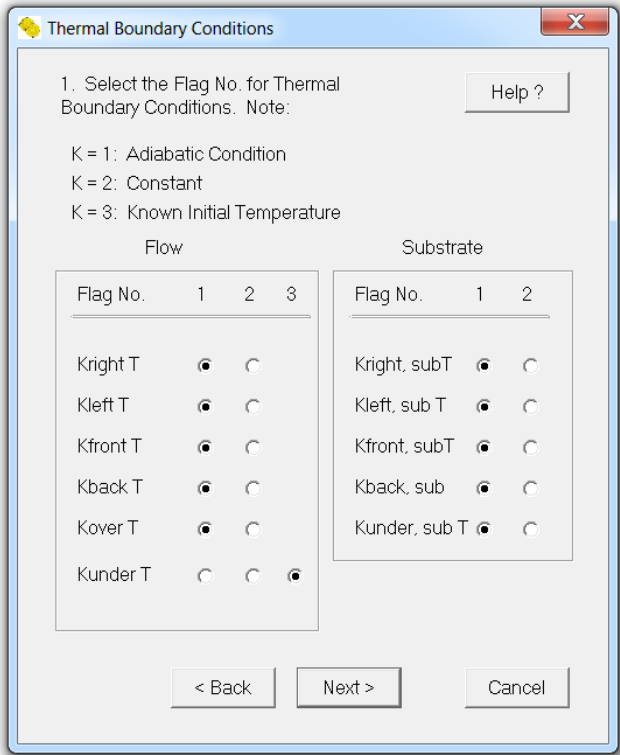


Figure 6.20. Thermal Boundary Conditions Dialogue Page.

1. Select the Flag No. for Thermal Boundary Conditions: For thermal boundary conditions, the definitions of the boundary locations are the same as in Section 6.10, i.e., :

- **KleftT** refers to the boundaries on the z - y plane.
- **KrightT** refers to the boundary on the surface parallel to z - y plane.
- **KbackT** refers to the boundary on the x - z plane.
- **KfrontT** refers to the boundary on the surface parallel to x - z plane.
- **KunderT** refers to the boundary condition on the impact surface.
- **KoverT** refers to the boundary condition on the surface parallel to the impact surface, i.e., x - y plane.

The notation “*T*”, refers to thermal and “*sub*” indicates the substrate. The thermal boundary conditions for both flow and for the substrate calculation domains share the same impact surface. Since the thermal boundary condition for the impact surface is specified, “**KunderT**”, there is no need to specify the substrate “**over**” (impact surface) boundary condition.

6.12 Grids Dialogue Page

In this page the information about the calculation domain is required, see Figure 6.21.

1. Specify the desired length of Grids for the calculation domain in each direction: Here you enter the length of the calculation domain [in meter] in three directions of x -, y -, and z - axis as indicated. Note that due to the nature of the impact, the length of the calculation domains in x , and y directions must be long enough to include any spread of the droplet without exceeding the boundaries. In the z direction this length must be $> Z_{center} + Drop\ Radius$. Otherwise, a warning message appears to let you to correct the domain length.
2. Select one of the following options for determining the grid numbers in each direction. Note that Option 1 is used when you know the grid numbers in one direction and Option 2 is used when you know the resolution.

In this section the number of grids in the x , y , and z directions are determined. Note that there are two options for specifying these numbers:

- **Option 1:** You may choose this option when you want to use a specific number of grids in one direction. After you specified the direction and the number of grids in that direction, click on **Calculate** button. The number of grids in the other two directions will be calculated automatically and appeared at the boxes provided for this purpose. Note that the grid numbers are determined based on a uniform grid size in all directions
- **Option 2:** You may use this option when you want to use a specific resolution. Resolution is defined by specifying the number of grids (Cells) per initial droplet Radius (CPR). The larger this number, the higher is the resolution. **It is recommended that the number of Cells per droplet Radius, CPR, be at least 10 (the optimum number of CPR is 15). This number can be calculated for each calculation domain from:**

$$\text{CPR} = \frac{\text{Radius}}{\text{Calculation Domain}} \times \text{Number of Grids}$$

After entering the value of CPR in the box, click on the **Calculate** button. The number of grids in the x , y , and z directions will be calculated and appeared in the boxes provided for this purpose.

Note that if the CPR is less than 10, a warning message appears. You have the choice to leave the information as it is or to return to the Grid dialogue page to change the grid numbers.

If you have chosen to not solve the energy equation, the procedure of data entry is completed at this point.

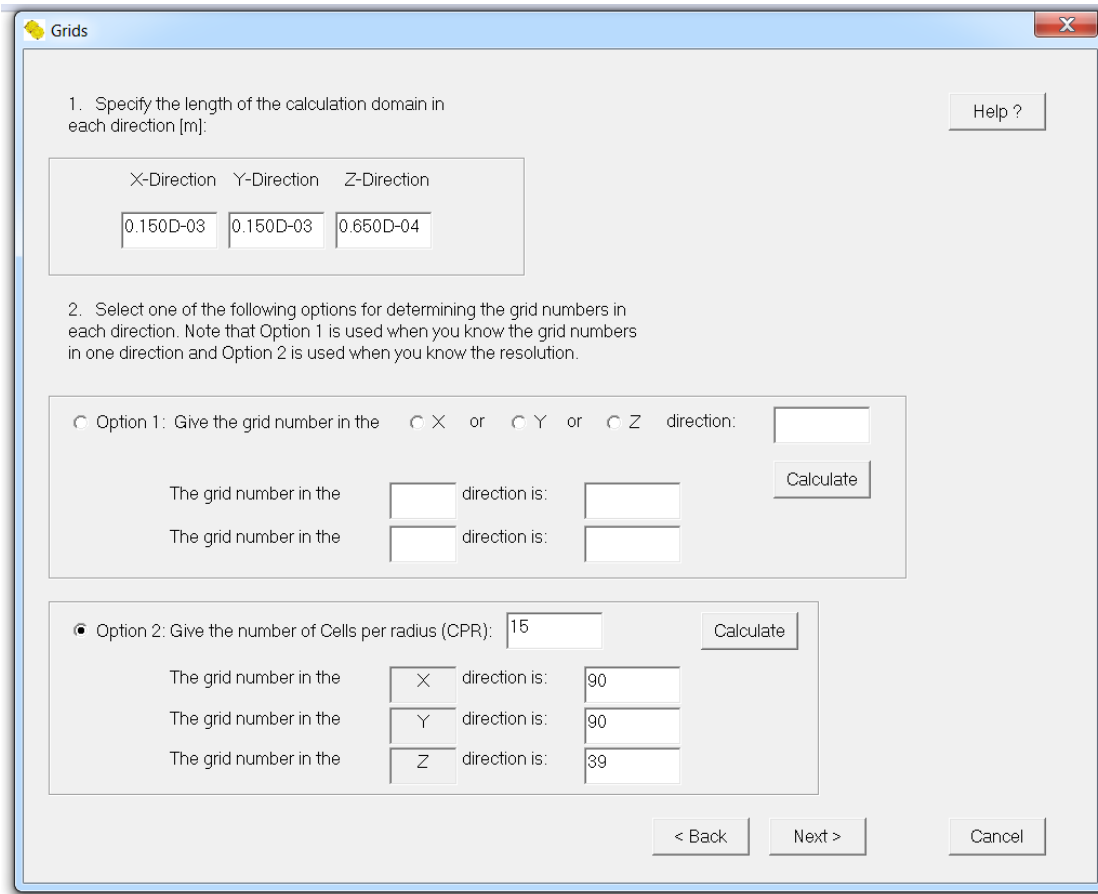


Figure 6.21. The Dialogue for Grid specification

6.13 Substrate Grids Dialogue Page

This page is opened only if you choose to solve the energy equations through the **Start** Dialogue Page. In this page the information about the substrate calculation domain is required, see Figure 6.22.

1. **Give the number of Grids and Depth for the substrate:** You can specify the substrate calculation domain and the grid resolution in this page. Here you are asked to give the length and the grid numbers in the z direction. Note that length and the grid sizes in the substrate in the x and y directions are the same as in the flow calculation domain.

- 1.1 **Length, m:** The length of calculation domain in the substrate the z direction is required.
 - 1.2 **Number of grids:** The number of grids in the z direction in the substrate domain is given.
2. If the density of grids has to be different in part of the substrate, please specify the followings: It is possible that you chose a non-uniform mesh in the substrate. This is recommended for those cases where the substrate material has a low thermal conductivity. In this case, the mesh density in the z direction close to the impact surface, can be higher than the rest of the substrate. Note that in any case the grid sizes in the substrate in the x and y directions are the same as in the flow calculation domain. To have a non-uniform mesh in the substrate, the following information is required:

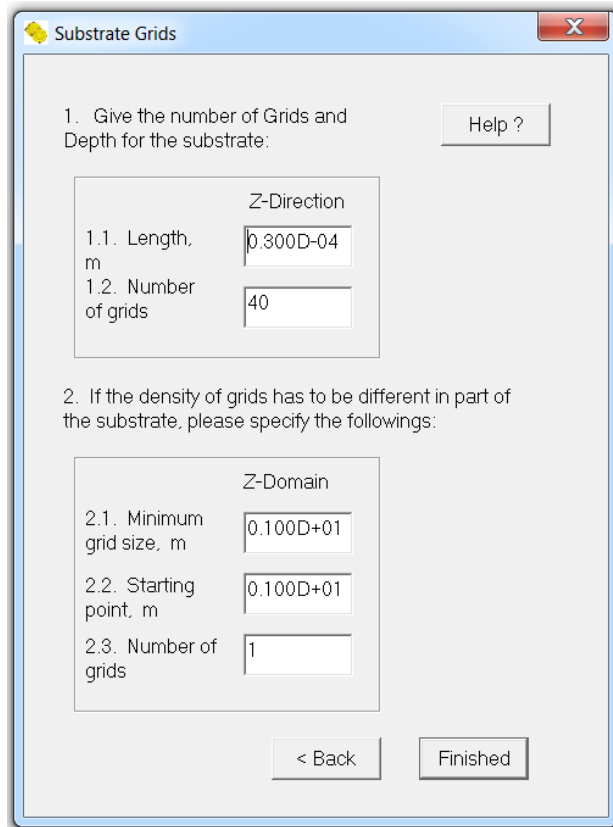


Figure 6.22. The Dialogue page for substrate calculation domain.

- 2.1 **Minimum grid size, m:** Give the minimum grid size in the z direction in the substrate. If this value is larger than the calculation domain, a uniform grid is created throughout the substrate domain.
- 2.2 **Starting point, m:** Give the starting point where the non-uniform mesh has to be started. Note that if you specify this value equal the minimum mesh size (section 2.1 the non-uniform mesh is started from the impact surface. If this value is larger than the calculation domain, a uniform grid is created throughout the substrate domain.
- 2.3 **Number of grids:** Give the number of grids in the calculation domain before this non-uniform domain starts. To have the domain starts from the impacting surface, enter “1” for this number.

7 OUTPUT FILES

There are several types of output files in this code.

- The “*f.xxxx*” files contain the values of the volume fraction of the droplet. If the simulation is an isothermal case, *f* shows the volume fraction of *liquid phase*. If the case involves solidification, *f* shows the volume fraction of *liquid phase* and *solid phase* together and *s* shows the volume fraction of the *solid phase* only. The 4-digit extension stands for the time intervals at which the files are created (see Section 6.3). For example *f.0000* is the first file created at the start of the calculations. At each time interval, another file is created and the extensions are increased accordingly, i.e., *f.0001*, *f.0002*,... Note that you can write a total of 10000 files during each calculation. At the present time the “*f*” files are written in **ASCII** format with a header that can be loaded by **TecPlot®** Software. A sample of an “*f*” file is presented in Appendix D: **By creating a sequence of iso-surface plots from these files, you can see the evolution of the droplet with time.** These files are saved in the subdirectory “*data*”.
- The “*pv.xxxx*” files contain the values of the velocity components *u*, *v*, and *w*, and the liquid pressure at different locations. These files are created at the same time intervals as for the *f.xxxx* files if requested by you. The extension numbers and format for these files are similar to the “*f*” files. These files are also saved in the subdirectory “*data*”.
- The “*T.xxxx*” files store the values of the droplet and substrate temperatures at different locations. These files are created at time intervals specified by you, only if the energy equations are solved. The extension numbers and format for these files are similar to the “*f*” files. These files are located in the subdirectory “*data*”.
- The “*dump*” files contain information used by the program including the values of velocities, pressure and also volume of fluid at each point in the calculation domain. These files with name *dump.xxxx*, are also created during execution at time intervals

as specified in General Dialogue Page (see section 6.3). These files are useful when you want to re-start a new set of calculations using the results from a previous run. This happens for instance when the assigned calculation time, T_{fin} (see Section 6.3) is not long enough to show the complete impact of the droplet. Then, you can use the latest *dump.xxxx* file to re-start the calculations with a longer calculation time. These files are also saved in the subdirectory “*data*”.

- The “*dumpT*” files, which contain thermal information of the droplet and the substrate. These files have the form of *dumpT.xxxx* and are stored at the same time intervals as *dump.xxxx* files. These files are saved in the subdirectory “*data*”.
- File “*TcSub*”, which contains the information about substrate temperature at the center. This file is written only if the energy equation is solved and is saved in the root directory.
- File “*Drops*”, which contains information about additional drops generated during a multi-drop impact simulation. This file is saved in the root directory.
- File “*Error*”, contains the messages coming from the code during execution time. This file is saved in the root directory. More information about the contents of this file can be found in Chapter 9
- File “*history*”, which contains information about the history of the calculations. This file is saved in the root directory. More details about the contents of this file can be found in Chapter 9

It's recommended that you rename or remove any existing files before starting a new set of calculations, otherwise the files are overwritten and the information can be lost.

8 EXAMPLES

In this Chapter the procedure of data entry for four different droplet impact cases and the simulation results are shown. We start with a simple case of the normal impact of a single water droplet on a flat surface. Then we repeat the simulation for the same droplet but impacting on an inclined surface. In Examples 3 we show the simulation for a molten nickel droplet impacting on a cold surface. This would be a simulation in which the energy equation is solved and the solidification happens. In Example 4, the impact of two molten nickel droplets on a flat surface is simulated.

Note that since the SIMDROP code is written in double precision, all numbers in the data entry pages and the output files are in double precision.

8.1 Example 1: Single Drop Impact.

In the first example we consider the vertical impact of a 1 mm radius water droplet on a stainless steel plate with a velocity of 2 m/s. The input data given to the program is as follows. Note that for each dialogue page we use the same item number.

8.1.1 Start

Since we are simulating a water drop impact, the solidification is not considered. So the selection must be “*No*”.

8.1.2 General

1. This is a fresh start, so you must click on the “*Yes*” button.
2. There is no need to specify anything in these boxes.
3. The time periods for this example are:

3.1. $\Delta t = 1.D-6$ sec

3.2. $T_{fin} = 1.D-3$ sec

3. For this case we need only information about “ f ” function.

Volume of Fluid Time interval = $1.D-4$ sec

Dump File $T_{dump} = 1.D-4$ sec

8.1.3 Type of Surface

1. Type of surface is “*Flat*”.
2. Since the surface is flat, “*Phi*” is equal to zero.

8.1.4 Drop Material Properties

1. The initial drop temperature is assumed to be 25°C (room temperature)
2. The drop material is “Water”.

8.1.5 Single Drop Characteristics

1. Initial Radius of Droplet = $1.D-3$ m
2. Since droplet impacts on the surface perpendicularly, it only has a velocity component in z direction, w . Then, $w = -2$ m/s.
3. Since the impact occurs on a flat surface, the calculations can be performed for one quarter of droplet. Therefore, X_{center} and Y_{center} are equal to zero (i.e., z axis is the symmetric axis). $Z_{center} = 1.2D-3$ m (slightly larger than the droplet radius).

8.1.6 Multiple Drop

1. This is a case with only a single droplet; therefore the answer is “*No*”. Note that by default the answer to this question is “*No*”.

2. and 3. When the answer to the above question is “No”, you may ignore these two sections.

8.1.7 Interface Properties

1. In this page, you decide what type of the contact angle is to be used in the simulation and based on the answer, options 2 and 3, or, 4 and 5 are activated.

For the conditions of this example:

$$We = \frac{1000 \times 2 \times 10^{-3} \times 2^2}{7.4 \times 10^{-2}} = 108.1$$

$$Re = \frac{2 \times 2 \times 10^{-3}}{1 \times 10^{-6}} = 4000$$

Therefore, $We > \sqrt{Re} = 63.25$. We choose the option of *Dynamic* contact angle for this case.

2. Not applicable.
3. Not applicable.
4. By choosing the “Water on Stainless Steel” from the list box, the advancing and receding contact angles are appeared in the boxes provided in Section 5.
5. The advancing angle of 110 and the receding contact angle of 40 degree are the default values for the impact of water on the stainless steel surface.

8.1.8 Substrate Properties

Since the energy equations are not solved, this page is not opened.

8.1.9 Boundary Conditions

1. Because the problem is solved for $\frac{1}{4}$ of droplet the flags for boundary conditions are:

$$K_{right} = 2 \qquad K_{left} = 1$$

$$K_{front} = 2 \qquad K_{back} = 1$$

$$K_{over} = 2 \qquad K_{under} = 2$$

8.1.10 Thermal Boundary Conditions

This page is not opened.

8.1.11 Grids

1. Based on the drop velocity and radius, the size of calculation domain can be specified. The domains in x , y , and z directions start from the center of origin. Therefore, one must pay attention to choose these domains such that the drop does not touch the boundaries at any time. To save calculation time and computer space for the first estimate one may choose the domains in x and y direction about three times the drop radius (or diameter, depending on the boundary condition types). If during the calculation time you find that the drop has touched the boundaries, the calculations can be restarted with one of the correct dump files with larger calculation domain. **Note that in this case the number of grids must be such that the grid sizes remain exactly the same as the first run.**

In this case since calculations are performed for a quarter of the droplet, the domain has been chosen to cover three times the droplet radius, i.e., $3.6D-3$ meter in each direction. However in z direction, due to the nature of impact, the z -domain can be chosen slightly larger than the drop diameter. This must be also done considering the drop center location in z direction. In this case since the drop center is equal to drop radius, the z -domain is given as $2.6D-3$ m.

After choosing the calculation domain, one must choose the number of grids in each direction. A good estimate of this number is 15 Cells per Radius. This number means that 15 cells exist per radius of droplet. To obtain to total Number of grids in each direction, e.g. x direction, one can use the following calculations:

$$\text{Total number of grids in x direction} = \frac{x_{domain}}{Radius} \times 15$$

The above calculations must be repeated for each domain. **Note that it's highly recommended the cell size in all directions be the same to obtain better smoothing process during the calculations.** In this example the following number grids are used:

$$\text{Total number of grids in } x \text{ direction} = \frac{3.6 \times 10^{-3}}{1.0 \times 10^{-3}} \times 15 = 54$$

$$\text{Total number of grids in } y \text{ direction} = \frac{3.6 \times 10^{-3}}{1.0 \times 10^{-3}} \times 15 = 54$$

$$\text{Total number of grids in } z \text{ direction} = \frac{2.6 \times 10^{-3}}{1.0 \times 10^{-3}} \times 15 = 39$$

NOTE: The Numbers given here are different from what the program gives.

8.1.12 Results

The following pictures, Figure 8.1, show the development in droplet impact of Example 1. The plots are created by TecPlot® and show the iso-surface plot of the droplet created from the “*f*” files. Also a clip of what the simulation will look like is available to you by clicking on the following link, [DROP 1](#).

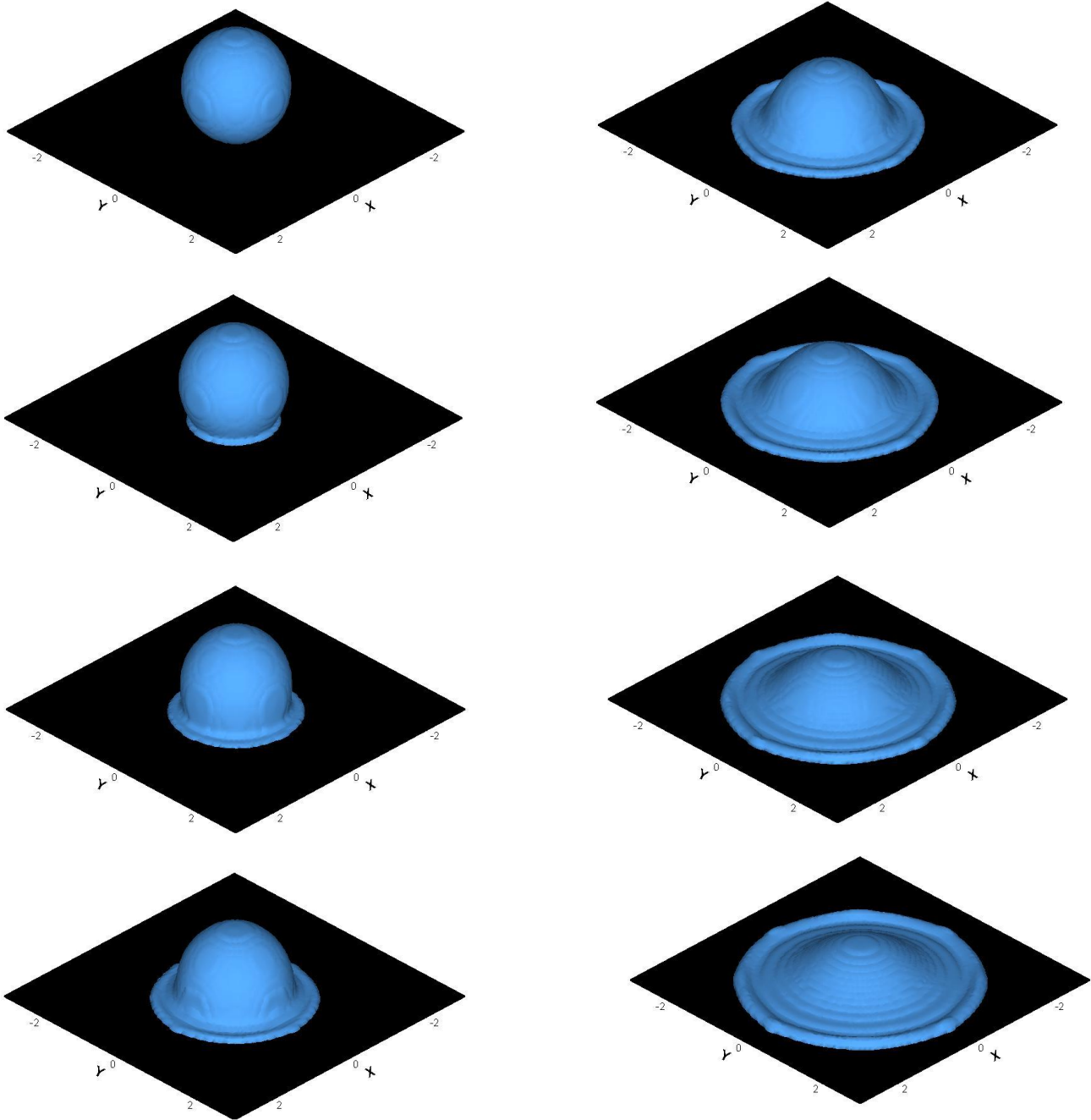


Figure 8.1. Example 1., the isometric view of droplet impact on the surface at different times.

8.2 Example 2: Impact on Inclined Surfaces

In the second example we consider the impact of the same droplet (1 mm radius water droplet) on an inclined stainless steel plate. The initial velocity is 1 m/s and is in the same direction as the gravitational acceleration, see Figure 8.2. The input data given to the program is as follows. Note that for each dialogue page we use the same item number.

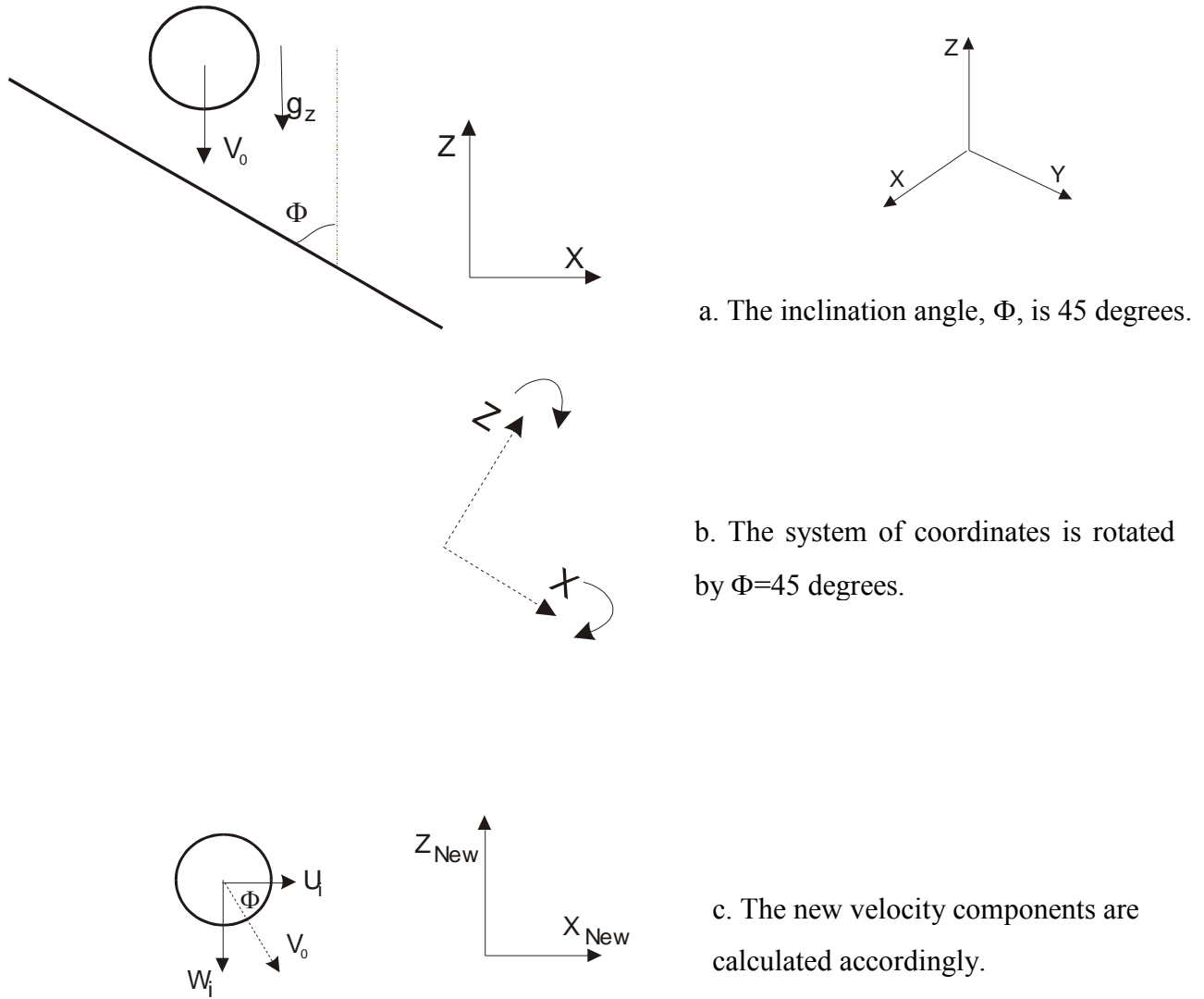


Figure 8.2. Illustration of a droplet impact on an inclined surface, a. the original system of coordinates; b. System of coordinates is rotated such that the new z-axis is perpendicular to the surface; c. with the new system of coordinates, the velocity components are determined.

8.2.1 Start

The same as Example 1.

8.2.2 General

1. This is a fresh start, so you must click on the “Yes” button.
2. There is no need to specify anything in these boxes.
3. The time periods for this example are:
 - 3.1. $\Delta t = 1.D-6$ sec
 - 3.2. $T_{fin} = 1.D-2$ sec
4. For this case we need only information about “ f ” function.

Volume of Fluid Time interval = 1.D-3 sec

Dump File $T_{dump} = 1.D-2$ sec

8.2.3 Type of Surface

1. Type of surface is “*Inclined*”.
2. The inclination angle, “*Phi*”, is 45 degrees.

8.2.4 Drop Material Properties

As in Example 1.

8.2.5 Single Drop Characteristics

1. Initial Radius of Droplet = 1.D-3 m
2. Since droplet impacts on the surface with an angle, you must calculate the velocity components:

$$U_i = 0.707 \text{ m/s}$$

$$V_i = 0 \text{ m/s}$$

$$W_i = -0.707 \text{ m/s}$$

3. Since the impact occurs on an inclined surface, the calculations must be performed at least for half of the droplet. Therefore, although Y_{center} can be chosen to be zero,

X_{center} must be far enough from the center of the origin to include the spread of the droplet. Here we consider $X_{center} = 2.5D-3$ m, $Y_{center} = 0.0$ m, and $Z_{center} = 1.0D-3$ m.

8.2.6 Multiple Drop

As in Example 1.

8.2.7 Interface Properties

1. Since the impact surface is inclined, a *Dynamic* contact angle is recommended.
2. Not applicable.
3. Not applicable.
4. Same as in Example 1.
5. Same as in Example 1.

8.2.8 Boundary Conditions

1. Since the problem is solved for 1/2 of droplet the flags for boundary conditions are:

$$\begin{array}{ll} K_{right} = 2 & K_{left} = 2 \\ K_{front} = 2 & K_{back} = 1 \\ K_{over} = 2 & K_{under} = 2 \end{array}$$

8.2.9 Grids

1. Since calculations are performed for 1/2 of droplet, the domain has been chosen accordingly. In the x direction, the domain length will be approximately $9.D-3$ meter. For this length, number of grids with a CPR of 15 is:

$$\text{Number of grids in the } x \text{ direction: } \frac{9 \times 10^{-3}}{1 \times 10^{-3}} \times 15 = 135$$

In the y direction by choosing the domain to be $3.6D-3$ m long, the number of grids will be:

$$\text{Number of grids in the } y \text{ direction: } \frac{3.6 \times 10^{-3}}{1 \times 10^{-3}} \times 15 = 54$$

The z domain is given as $2.4D-3$ m, therefore the number of grids is:

Number of grids in the z direction: $\frac{2.4 \times 10^{-3}}{1.0 \times 10^{-3}} \times 15 = 36$

8.2.10 Results

The following pictures, Figure 8.3, show the development in droplet impact of Example 2. The plots are created by TecPlot® and show the iso-surface plot of the droplet. Also a clip of what the simulation will look like is available to you by clicking on the following link, [DROP 2](#).

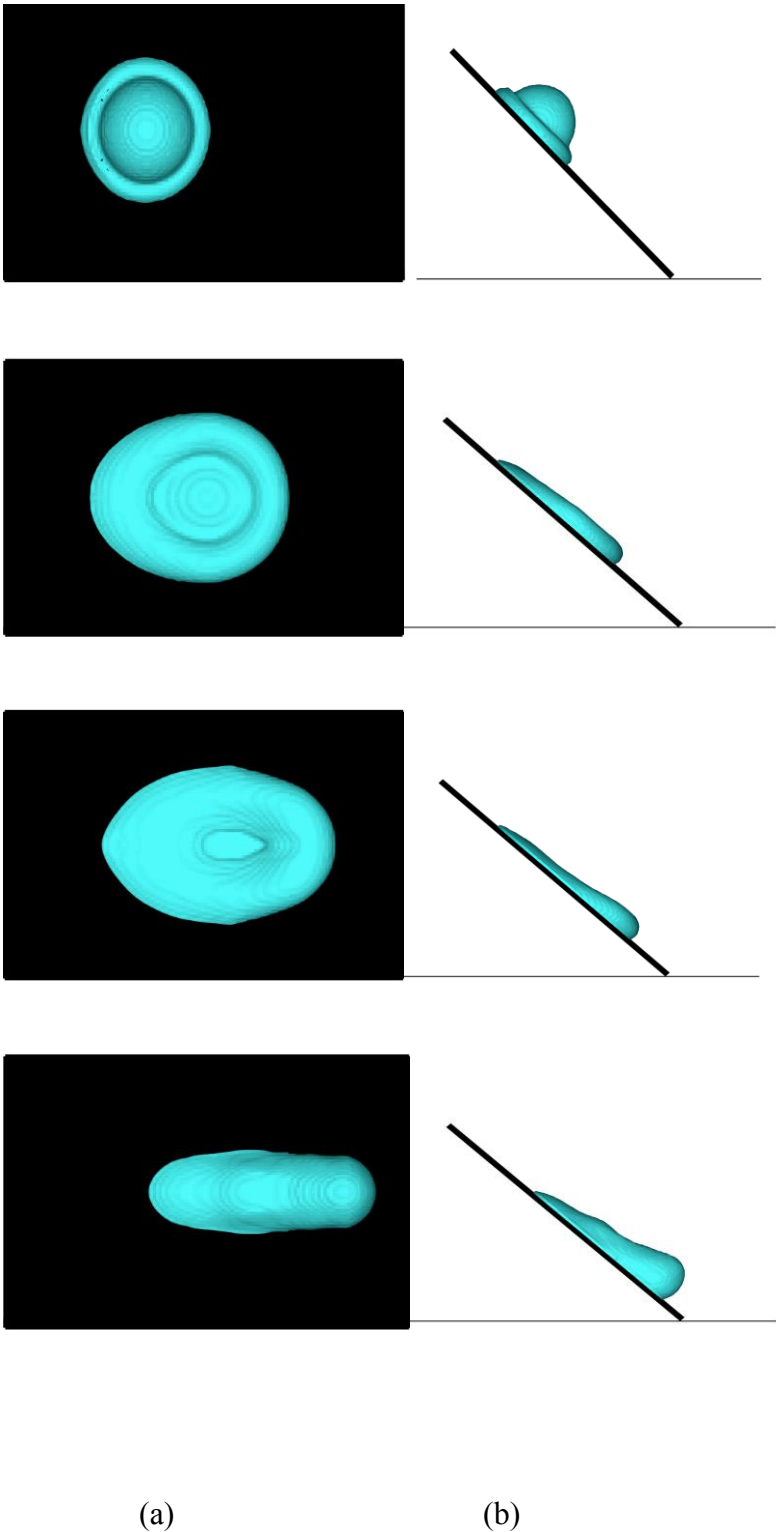


Figure 8.3. Example 2., the top (a) and side (b) views of droplet impact on an inclined surface at different times.

8.3 Example 3: Molten Drop Impact

In this example we consider the vertical impact of a 30 μm molten nickel droplet on a hot stainless steel plate with a velocity of 70 m/s. This is a typical scenario in a thermal spray process. The input data given to the program are as the follow. Note that for each dialogue page we use the same item number:

8.3.1 Start

Since we are simulating a molten drop impact, the energy transfer and solidification is considered. So the answer is “Yes”.

8.3.2 General

1. This is a fresh start, so you must click on the “Yes” button.
2. There is no need to specify anything in these boxes.
3. The time periods for this example are:
 - 3.1 Delt = 1.D-9 sec
 - 3.2 Tfin = 5.D-6 sec
4. For this case we need information about “*f*” function and temperature field.

Volume of Fluid	Time interval = 0.5D-7 sec
Temperature field	Time interval = 1.D-7
Dump File	Tdump = 1.D-7 sec

8.3.3 Type of Surface

1. Type of surface is “Flat”.
2. Since the surface is flat, “Phi” is equal to zero.

8.3.4 Drop Material Properties

1. The initial drop temperature is assumed to be 1600 °C (higher than melting point).
2. The drop material is “Nickel”.

8.3.5 Single Drop Characteristics

1. Initial Radius of Droplet = 3.0×10^{-5} m
2. Since droplet impacts on the surface perpendicularly, it only has a velocity component in z direction, w . Then, $w = -70$ m/s.
3. Since the impact occurs on a flat surface, the calculations can be performed for one quarter of droplet. Therefore, X_{center} and Y_{center} are equal to zero (i.e., z axis is the symmetric axis). $Z_{center} = 4.0 \times 10^{-5}$ m (slightly larger than the droplet radius).

8.3.6 Multiple Drop

1. This is a case with only a single droplet; therefore the answer is “No”. Note that by default the answer to this question is “No”.
2. and 3. When the answer to the above question is “No”, you may ignore these two sections.

8.3.7 Interface Properties

1. Since the impact velocity is high, the contact angle does not play an important role. Therefore, you may choose a “Static” contact angle.
2. In the case of a high-speed impact velocity, the User Defined option is preferred.
3. A contact angle of 90 degrees can be used in the calculation.
4. Not applicable.
5. Not applicable.

8.3.8 Substrate Properties

1. The initial substrate temperature is 200 °C.
2. A typical thermal resistance under these conditions is 1.0×10^{-7} K- m^2 /W
3. The substrate material is “Stainless Steels”.

8.3.9 Boundary Conditions

1. Because the problem is solved for a quarter of droplet the flags for boundary conditions are:

$$\begin{array}{ll} K_{\text{right}} = 2 & K_{\text{left}} = 1 \\ K_{\text{front}} = 2 & K_{\text{back}} = 1 \\ K_{\text{over}} = 2 & K_{\text{under}} = 2 \end{array}$$

8.3.10 Thermal Boundary Conditions

The thermal boundary conditions can be set up as follows:

$$\begin{array}{ll} K_{\text{right}} T = 1 & K_{\text{left}} T = 1 \\ K_{\text{front}} T = 1 & K_{\text{back}} T = 1 \\ K_{\text{over}} T = 1 & K_{\text{under}} T = 3 \\ K_{\text{right,sub}} T = 1 & K_{\text{left,sub}} T = 1 \\ K_{\text{front,sub}} T = 1 & K_{\text{back,sub}} T = 1 \\ K_{\text{Under,sub}} T = 1 & \end{array}$$

8.3.11 Grids

1. In this case since calculations are performed for $\frac{1}{4}$ of droplet, the domains in the x and y directions are chosen more than five times the droplet radius to cover any splashing, i.e., $1.65D-4$ m. In the z direction, domain can be $7.5D-5$ m.

To obtain to total number of grids in each direction, e.g. x direction, we follow the same rule, i.e., $\frac{\text{domain length}}{\text{Radius}} \times 15$. This gives us 83, 83, and 38 number of grids in x , y , and z direction, respectively.

8.3.12 Substrate Grids

1. For the substrate in the z direction, we choose total grid number of 20, with a length of $4.0D-5$ m.

2. Not applicable in this example.

2.1 To make sure that the program creates a uniform grid in the substrate, we put the minimum grid length to be 1.D+0 m which is much higher than the calculation domain.

2.2 The same as above.

2.3 The default number is zero.

8.3.13 Results

Figure 8.4 show the sample results for a single drop impact. Also a clip of what the simulation will look like is available to you by clicking on the following link, [DROP 3](#).

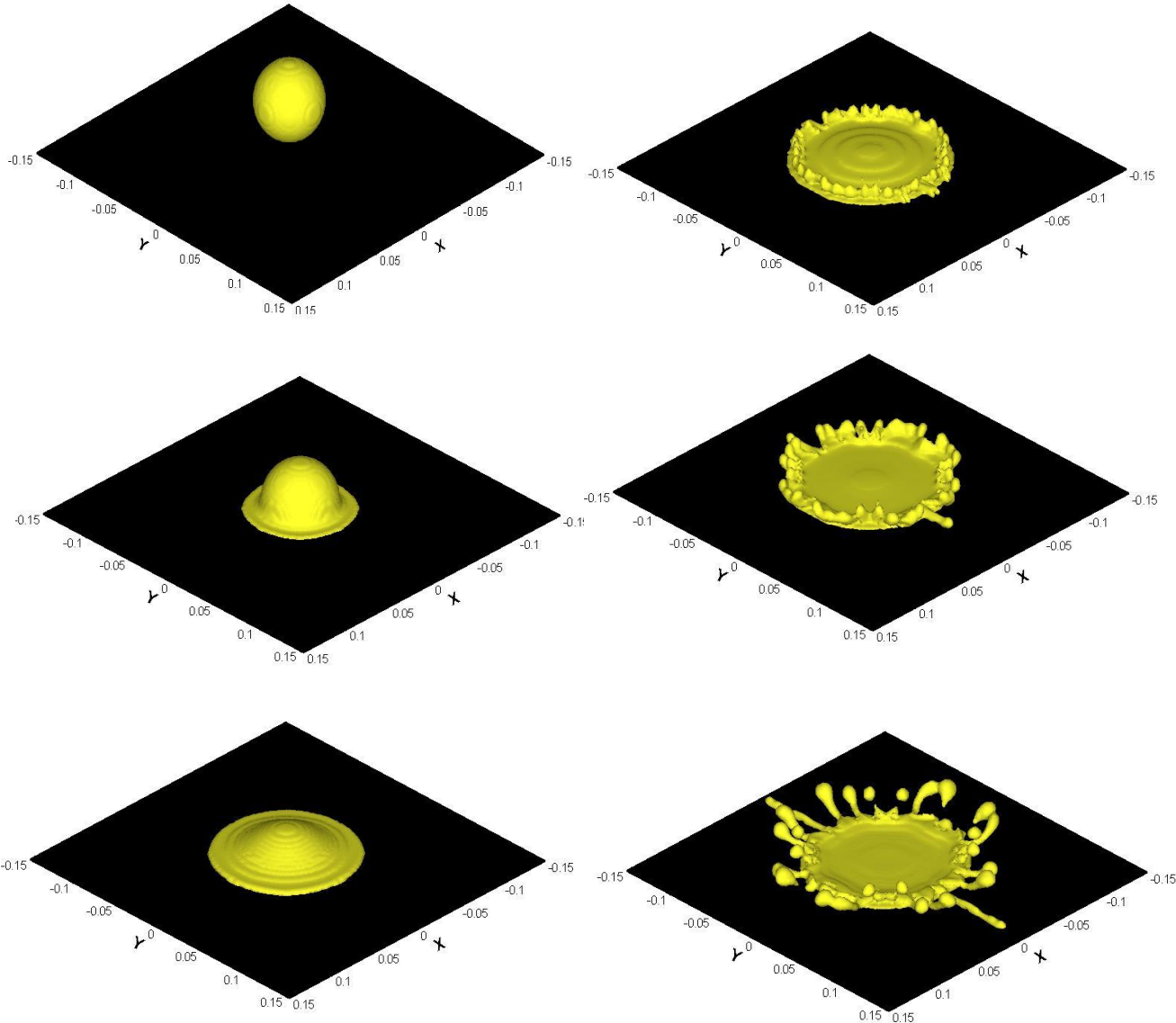


Figure 8.4. The results for the impact of a single nickel droplet on a stainless steels plate. The plots show the isometric view of the impaction. All other conditions are stated in Example 3.

8.4 Example 4: Two-Drop Impact

In this example we consider the vertical impact of two molten nickel droplets on a cold stainless steel plate. The input data given to the program are as the follow. Note that for each dialogue page we use the same item number:

8.4.1 Start

Since we are simulating a molten drop impact, the energy transfer and solidification is considered. So the answer is “*Yes*”.

8.4.2 General

1. This is a fresh start, so you must click on the “*Yes*” button.
2. There is no need to specify anything in these boxes.
3. The time periods for this example are:
 - 3.1 $\Delta t = 1.D-9$ sec
 - 3.2 $T_{fin} = 6.D-5$ sec
4. For this case we need information about “*f*” function and temperature field.

Volume of Fluid Time interval = 1.D-7 sec

Temperature field Time interval = 1.D-6

Dump File Tdump = 1.D-5 sec

8.4.3 Type of Surface

1. Type of surface is “*Flat*”.
2. Since the surface is flat, “*Phi*” is equal to zero.

8.4.4 Drop Material Properties

1. The initial temperature for the first drop is assumed to be 1500 °C.
2. The material for both drops is “*Nickel*”.

8.4.5 First Drop Characteristics

Note that the following information is for the *first* droplet.

1. Initial Radius of Droplet = $3.D-5$ m.
2. Since droplet impacts on the surface perpendicularly, it only has a velocity component in z direction, w . Then, $w = -60$ m/s.
3. In the case of the multiple drop impact, the calculations must be performed for the complete domain. In this example we choose:

$$X_{center} = 1.5D-4 \text{ m}$$

$$Y_{center} = 1.5D-4$$

$$Z_{center} = 5.0D-5$$

8.4.6 Multiple Drop

1. In this section the answer is “Yes”.
2. The time at which the second droplet is released is $3.D-6$ second.
3. In this example we select the “Manual” drop generation. By clicking on this button, another page is opened. Note that in the upper window in this page, you are asked to give the information for the *second* droplet:

$$\text{Radius} = 4.D-5 \text{ m}$$

$$\text{Velocity in the } y \text{ direction, } v = 0.0D \text{ m/s}$$

$$X_{center} = 2.5D-4 \text{ m}$$

$$\text{Velocity in the } z \text{ direction, } w = -40 \text{ m/s}$$

$$Y_{center} = 2.5D-4 \text{ m}$$

$$\text{Initial drop temperature} = 1600 \text{ }^\circ\text{C}$$

$$Z_{center} = 0.5 D-4 \text{ m}$$

$$\text{Time gap for releasing the next drop} = 6.D-5 \text{ s.}$$

Note that the last information is the time-step at which the third droplet may be released. This time is measured from the time step at which the second droplet is release and so on. In this example with only two droplets to be released, we chose this time gap large enough (larger than the final time for calculation). This way the code will not look for the information about the third droplet.

8.4.7 Interface Properties

1. Since the impact velocity is high, the contact angle does not play an important role. Therefore, you may choose a “Static” contact angle.
2. In the case of a high-speed impact velocity, the User Defined option is preferred.
3. A contact angle of 90 degrees can be used in the calculation. This contact angle will be used for all droplets.
4. Not applicable.
5. Not applicable.

8.4.8 Substrate Properties

1. The initial substrate temperature is 20 °C.
2. We choose the thermal resistance to be 1.0D-7 K-m²/W
3. The substrate material is “*Stainless Steels*”.

8.4.9 Boundary Conditions

Because the problem is solved for the whole domain the flags for boundary conditions are:

Kright = 2	Kleft = 2
Kfront = 2	Kback = 2
Kover = 2	Kunder = 2

8.4.10 Thermal Boundary Conditions

The thermal boundary conditions can be set up as follows:

Kright T = 1	Kleft T = 1
Kfront T = 1	Kback T = 1
Kover T = 1	Kunder T = 3
Kright,subT = 1	Kleft, subT = 1
Kfront, subT = 1	Kback, subT = 1
KUnder, subT = 1	

8.4.11 Grids

1. The x and y calculation domain are chosen to be 4.D-4 m each. In the z direction we use a 1.D-4 m domain.

To obtain to total number of grids in each direction, we choose a CPR of 10 to save the calculation time and memory usage. Therefore, Number of grids = $\frac{\text{domain length}}{\text{Radius}} \times 10$.

This gives us 134, 134, and 33 as the number of grids in x, y, and z direction, respectively.

8.4.12 Substrate Grids

1. For the substrate in the z direction, we choose a total grid number of 20, with a length of 4.0D-5 m.
2. Same as Example 3.

8.4.13 Results

Figure 8.5 shows the sample results of the multiple impact simulation. Also a clip of what the simulation will look like is available to you by clicking on the following link, [DROP 4](#).

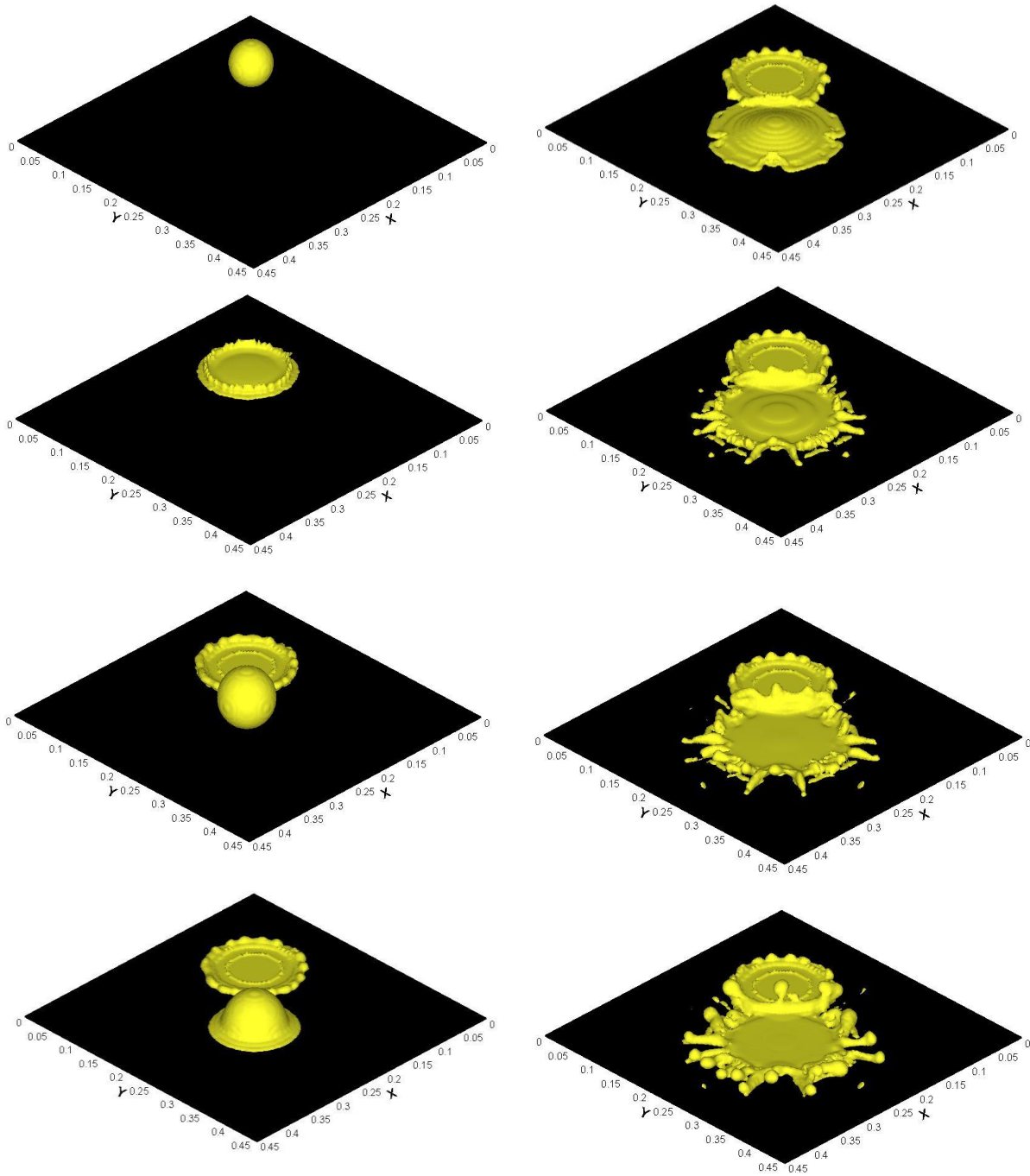


Figure 8.5. The isometric view for a multiple droplet Impact simulation. Note that at time = 3 μ sec, the second droplet is released. While the yellow patterns show the molten nickel splashed on the surface, the dark spots show the solid nickel as the result of the solidified.

9 MESSAGES AND TROUBLESHOOTING

The most common problems that may be seen during the execution of the SIMDROP program are:

- The shortage of memory. This will cause the program to stop at the very beginning of the execution. Therefore, it is recommended that a memory (RAM) of at least 512MB be used for this program.
- Program crashes with the error message referring to the “bc” subroutine. This happens if the spread droplet has reached the boundaries. Please check the last output file. You may re-run the program using the latest “Dump” file as described in Section 6.3.
- If you are running the Software on Windows 2000, you may notice that each time you minimize or resize the Monitoring Window, the plot axis disappears. This has no effect on the simulation and you can still have control over menu bar.

Most of the warning and error messages during the execution time are written in a file named “error”. The location of this file is in the root directory of the software. You can monitor this file during the run time to see the messages. Also when an abnormal termination of the program occurs, you may find the error message in this file.

9.1 Error messages

Table 3 shows are the list of the error messages that are possibly appeared in the “error” file, the causes for the error and the recommended remedy solution to solve the problem. Note that all the listed error messages in this Table cause the program to stop. If you cannot solve the problem by implementing the solution method, it is recommended that the “error”, “input”, and “out” files be sent to **Simulent Inc.** (infosim@simulent.com) for more investigation.

Table 3. List of error messages.

	Error message	Reason	What to do
1	<i>DELT less than DTEND on cycle</i>	The time step in that particular cycle is less than the minimum time step set by the program.	1- Check “Input” file to see that the given information are correct. 2- Increase the “Delt”, see Section 6.3, by one order of magnitude.
2	<i>Too many VOF advection failures</i>	VOF function convection limit has reached.	Check “Input” file to see the information are given correctly.
3	<i>Too many pressure iteration failures</i>	Pressure convergence failures.	Check “Input” file to see the information are given correctly.
4	<i>DLY error 1</i>	VOF advection error occurs.	1- Check “Input” file to see the information are given correctly. 2- Check if the Boundary Conditions are given correctly with respect to the calculation domain.
5	<i>DLY error 2</i>	VOF advection error occurs.	1- Check “Input” file to see the information are given correctly. 2- Check if the Boundary Conditions are given correctly with respect to the calculation domain.
6	<i>M0,M1,M2,M3,"M MISMATCH</i>	The definition of free surfaces failed in Young’s method.	1- Check “Input” file 2- Check if the meshes are defined uniformly. 3- Check the Boundary Conditions.
7	<i>Triangle anomaly</i>	The same as above.	The same as above.
8	<i>Quad A anomaly</i>	The same as above.	The same as above.
9	<i>Pentagon anomaly</i>	The same as above.	The same as above.
10	<i>Pen DIAG problem</i>	The same as above.	The same as above.
11	<i>Hex DIAG problem</i>	The same as above.	The same as above.

12	<i>Quad B problem</i>	The same as above.	The same as above.
13	<i>M0,M1,M2,M3 problem in AREA:</i>	The same as above.	The same as above.
14	<i>NVERTS problem in AREA:</i>	The same as above.	The same as above.
15	<i>The program is in PROPERT subroutine FK(IJK) has become zero</i>	The adiabatic thermal boundary condition on the surface is not applied.	1- Check “Input” file to see all information are correct. 2- Check Thermal Boundary Conditions.
16	<i>The program is in ENTHALPY subroutine FK(IJK) has become zero</i>	The adiabatic thermal boundary condition on the surface is not applied.	1- Check “Input” file to see all information are correct. 2- Check Thermal Boundary Conditions.

9.2 Warning Messages

Table 4 shows a list of warning messages that might be appear in the “error” file. Normally theses warnings do not stop the program and can be ignored. However, in some cases if they repeat in certain cycle, they might lead to an error listed in Table 3 which then it will stop the program.

Table 4. List of warning messages

	Warning message	Reason	Caution
1	<i>IMPLCTP pressure solution for cycle ‘ ‘ time did not converge after ‘ ‘ iterations</i>	Pressure iteration is not converging. If this repeats it may lead to Error No. 3.	Check “Input” file to see all information are correct.
2	<i>VOF advection error</i>	If repeated it leads to Error No. 2.	Check “Input” file to see all information are correct.
3	<i>The program is in BCT subroutine FK(IJK) is still zero</i>	The adiabatic boundary condition has problem. If not corrected in the program, leads to Errors Nos. 15 and 16.	Check thermal boundary conditions.
4	<i>DSICCG -IC factorization broke down-diagonal was set to unity and factorization proceeded</i>	This is a warning message from the pressure solver. It causes the IERR number become 5 or 6 (see Section 9.3).	Check “Input” file and Boundary Conditions.

5	<i>DSICS - A and EL data structure mismatch</i>	If this warning message is repeated, it may lead to either of Errors Nos. 3, 4, and 5.	Check “Input” file and Boundary Conditions.
---	---	--	---

9.3 “History” File

During the execution of the program, a “history” file is created which is located in the root directory of the software. This file contains the information about the number of cycles, time steps, time and error flags come from the solver. There are 5 columns in this file:

First column: This column shows the number of cycles as the program proceeds. At each cycle the time is increased by a time step.

Second column: This column shows the instantaneous time at that cycle.

Third column: This column indicates the time-step used at that specific cycle. The time-step could be different at each cycle, because the program adjusts the time step based on the advection limit, viscosity limit, and surface tension limit (for more information see Chapters 2). This time step gives a good indication of how the program is working. If it is decreasing constantly at each cycle, it may be an indication that there is a problem in the simulation. This may lead to a stop caused by Error No. 1. In the other hand, an almost constant value time step is an indication of a problem free solution.

Forth column: This column is the number of iteration that pressure solver performs to solve the problem at each time step.

Fifth column: Column number five shows the Error number, IERR, returning from the pressure solver at each cycle. The solver is a Preconditioned Conjugate Gradient Sparse Solver routine to solve a symmetric positive definite linear system $A X = B$ using the Preconditioned Conjugate Gradient method. The numbers are:

- IERR = 0 => All is going well.

- IERR = 1 => Insufficient space allocated for the Solver. This error message should not appear at any time, since the code automatically takes care of it.
- IERR = 2 => Method failed to converge.
- IERR = 3 => Error in user input. This error message should not appear at any time, since the code automatically takes care of it.
- IERR = 4 => User error tolerance set too tight. This error message should not appear at any time, since the code automatically takes care of it.
- IERR = 5 => Preconditioning matrix, is not positive definite. The code usually fixes this problem.
- IERR = 6 => Matrix A is not positive definite. The program usually corrects itself. If that continues, it causes the code to stop. You must check the Input data to verify the physical conditions are correct.

Appendix A: “INPUT” FILE FORMAT

Here a sample of an “*Input*” file is presented. Notice that each new “*Input*” file is created after starting the program. In the other words, all input data entered through the dialogue pages are stored in this file for future reference. Also each time a new program is started, the data from this file are used as the default values in the dialogue pages. You must be sure that an “*Input*” file exists all the time in the root directory. Otherwise, if the code cannot find such a file, it will crash. In front of each line a brief description and the corresponding Section in the Manual is added. Note that symbols “&start” and “&end” are the indication of the beginning and ending of each section and must be remained in the file.

Table 5. Sample of an *Input* file.

<i>Input File</i>	Description	Manual
&start		
SLVENG = .FALSE.,	Indication of energy equation solver. “TRUE” means the solidification and energy equations are solved. “FALSE” means an isothermal condition is solved.	6.1
&end		
&general		
Istart = 0 ,	Istart equal zero indicates a fresh start. If this number is one, it means a start using previous calculation results.	6.3
Dumpname = dump.0001 ,	Name of dump file containing flow information.	6.3
DumpTname = dumpt.0001,	Name of dump file containing thermal information.	6.3
Deltc = 0.100D-06 ,	Starting value for time step.	6.3
Twfinc = 0.100D-01 ,	Final calculation time.	6.3
Ivof = 1	Ivof equal to zero means no “ <i>f</i> ” file is written.	6.3
IVP = 1 ,	Ivp equal to zero means no “ <i>PV</i> ” file is written.	6.3
Pltdtc = 0.500D-04 ,	Time interval at which an “ <i>f</i> ” or “ <i>PV</i> ” file is created.	6.3
Itemp = 0 ,	Itemp equal to zero means no “ <i>T</i> ” files is written.	6.3

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	Itemp equal one means the temperature files are required.	
Tfilec = 0.200D-04	This is a time interval at which a “T” file is created.	6.3
ITdump = 1 ,	ITdump equal to zero means no “dump” file is written.	6.3
Dumpdtc = 0.500D-05 ,	Time interval at which dump files are written.	6.3
&end		
&surface		
Gxc = 0.694D+01 ,	This is the “x” component of specific gravity calculated by the code.	6.4
Gyc = 0.000D+00 ,	This is the “y” component of specific gravity calculated by the code.	6.4
Gzc = -0.694D+01 ,	This is the “z” component of specific gravity calculated by the code.	6.4
Phic = 45.0 ,	This is the inclination angle of the impact surface.	6.4
Iflat = 0 ,	If iflat is equal to one, the surface is flat.	6.4
Ismooth = 0 ,	If ismooth is euqual to zero, the surface is smooth.	6.4
DVc = 0.000D+00	DV is peak to valley height in microns.	6.4
DPc = 0.000D+00	Dp is the peak to peak distance in microns.	6.4
EPc = 0.000D+00	Ep is the width of the tooth.	6.4
Irotate = 1 ,	If Irotate is equal to one, the substrate is rotating	6.3
NFLAG = 1 ,	If NFLAG = 1, the rotation is clockwise If NFLAG = 2, the rotation is clockwise	6.3
OMEGAc = 0.100D+04 ,	This is the rotational speed of the substrate	6.3
XDC = 0.200D+01 ,	This is the X-position of the center of rotation with respect to the center of coordinates of the calculation domain.	6.3
YDC = 0.300D+01 ,	This is the Y-position of the center of rotation with respect to the center of coordinates of the calculation domain.	6.3
Inclined = .TRUE.	If inclined is True, the surface is inclined.	6.4
&end		
&Liquid		
Dropname = WATER.DAT,	The file name for liquid properties.	6.5
Rhofc = 0.765D+03 ,	Density for the liquid drop.	Appendix B:
Tidropc = 0.250D+02 ,	Initial drop temperature.	6.5

SimDrop

NVA = 1 ,	As described in Drop Property Files	Appendix B:
VA1C = 0.2500D+02,	As described in Drop Property Files	Appendix B:
VA2C = 0.1004D-04,	As described in Drop Property Files	Appendix B:
NVB = 1 ,	As described in Drop Property Files	Appendix B:
VB1C = 0.2500D+02,	As described in Drop Property Files	Appendix B:
VB2C = 0.7500D+02,	As described in Drop Property Files	Appendix B:
NVC = 1 ,	As described in Drop Property Files	Appendix B:
VC1C = 0.2500D+02,	As described in Drop Property Files	Appendix B:
VC2C = 0.4179D+04,	As described in Drop Property Files	Appendix B:
NVD = 1 ,	As described in Drop Property Files	Appendix B:
VD1C = 0.0000D+00,	As described in Drop Property Files	Appendix B:
VD2C = 0.3500D-01,	As described in Drop Property Files	Appendix B:
&end		
&Solidp		
Tmeltc = 0.000D+00 ,	Melting temperature of the drop material.	Appendix B:
Hfusnc = 0.000D+00 ,	Heat of fusion of the drop material.	Appendix B:
NVE = 1 ,	As described in Drop Property Files	Appendix B:
VE1C = 0.0000D+00,	As described in Drop Property Files	Appendix B:
VE2C = 0.0000D+00,	As described in Drop Property Files	Appendix B:
NVF = 1 ,	As described in Drop Property Files	Appendix B:
VF1C = 0.0000D+00,	As described in Drop Property Files	Appendix B:
VF2C = 0.0000D+00,	As described in Drop Property Files	Appendix B:
&end		
&DI		
Radiusc = 0.700D-04 ,	Initial radius of the drop (first drop).	6.6
Uic = 0.000D+00 ,	Initial velocity component in the x direction of the	6.6

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	drop (first drop).	
Vic = 0.000D+00 ,	Initial velocity component in the y direction of the drop (first drop).	6.6
Wic = -0.800D+01 ,	Initial velocity component in the z direction of the drop (first drop).	6.6
Xcentc = 0.100D-02 ,	Initial position of the drop center in the x direction.	6.6
Ycentc = 0.950D-03 ,	Initial position of the drop center in the y direction.	6.6
Zcentc = 0.180D-03 ,	Initial position of the drop center in the z direction.	6.6
&end		
&Multip		
Multiple = .FALSE.	If Multiple is True, a multiple impaction is solved.	6.7
Manualp = .TRUE.	If Manualp is .True., the specifications for additional droplets must be given manually. If Manualp is .False., the program uses a Random generator routine.	6.7
Dropdte = 0.500D-03 ,	This is the realizing time gap for the <i>second</i> droplet.	6.7
NDROPC = 1 ,	Total number of the droplets.	
VDROPC = 0.000D+00, ...,	Depending on the number of additional droplets, there would be (NDROPC-1) lines starting with VDROPC name. See Note * .	6.7.2
RADminc = 0.000D+00 ,	If the random generation routine is used, this is the minimum range for the drop initial radius.	6.7.1
RADmaxc = 0.000D+00 ,	If the random generation routine is used, this is the maximum range for the drop initial radius.	6.7.1
WIminc = 0.000D+00 ,	If the random generation routine is used, this is the minimum range for the drop initial normal velocity.	6.7.1
WImaxc = 0.000D+00 ,	If the random generation routine is used, this is the maximum range for the drop initial normal velocity.	6.7.1
TIDminc = 0.000D+00 ,	If the random generation routine is used, this is the minimum range for the drop initial temperature.	6.7.1

* **Note:** Each line starting with “VDROPC = “ contains information about individual droplets. These are: the initial position of the drop center in the x direction, the initial position of the drop center in the y direction, the initial position of the drop center in the z direction, the initial drop radius, the initial velocity component in the y direction, the initial velocity component in the z direction, the initial drop temperature, and the time gap for releasing the next droplet, respectively.

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TIDmaxc = 0.000D+00 ,	If the random generation routine is used, this is the maximum range for the drop initial temperature.	6.7.1
DDTminc = 0.000D+00 ,	If the random generation routine is used, this is the minimum range for the time gap between releasing two consequent droplets.	6.7.1
DDTmaxc = 0.000D+00	If the random generation routine is used, this is the maximum range for the time gap between releasing two consequent droplets.	6.7.1
&end		
&IP		
Dynam = .TRUE.	If Dynam is .TRUE., a dynamic contact angle concept is implemented. If Dynam is .False., a static contact angle is used.	6.8
Thetaac = 110.0 ,	This is the advancing contact angle if Dynam = .TRUE.	6.8
Thetarc = 40.0 ,	This is the receding contact angle if Dynam = .TRUE.	6.8
Cangleuc = 110.0	This is the Static contact angle, if Dynam = .FALSE.	6.8
&end		
&SUB		
Subname = Steel.DAT,	This is the name for substrate property file.	6.9
Tiwallc = 0.200D+03 ,	This is the initial substrate temperature.	6.9
Rsubc = 0.790D+04 ,	This is the density of the substrate.	Appendix C:
Rclsc = 0.100D-08 ,	This is the thermal resistance between the droplet and the substrate.	6.9
NVG = 6 ,	As described in Substrate Property Files	Appendix C:
VG1C = 0.1270D+03, ...,	As described in Substrate Property Files	Appendix C:
VG2C = 0.1660D+02, ...,	As described in Substrate Property Files	Appendix C:
NVH = 6 ,	As described in Substrate Property Files	Appendix C:
VH1C = 0.1270D+03, ...,	As described in Substrate Property Files	Appendix C:
VH2C = 0.5150D+03, ...,	As described in Substrate Property Files	Appendix C:
&end		
&GRID		
Imaxc = 240 ,	Maximum number of grids in the x direction.	6.12
Jmaxc = 240 ,	Maximum number of grids in the y direction.	6.12

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Kmaxc = 31 ,	Maximum number of grids in the z direction.	6.12
Kmaxwc = 2 ,	Maximum number of grids in the z direction in the substrate.	6.12
Xec = 0.200D-02 ,	The length of calculation domain in the x direction.	6.12
Yec = 0.200D-02 ,	The length of calculation domain in the y direction.	6.12
Zec = 0.260D-03 ,	The length of calculation domain in the z direction.	6.12
Zewc = 0.100D-04 ,	The length of calculation domain in the z direction in the substrate.	6.12
Dzmnwc = 0.100D+01 ,	The minimum grid size of the <i>non-uniform</i> domain in the substrate in the z direction.	6.12
Zmnwc = 0.100D+01 ,	The starting point of the <i>non-uniform</i> domain in the substrate in the z direction.	6.12
Nzmnwc = 1	The number of grids before the <i>non-uniform</i> domain in the substrate is started.	6.12
&end		
&BC		
KRc = 2 ,	Right side boundary condition flag.	6.10
KLc = 2 ,	Left side boundary condition flag.	6.10
KFc = 2 ,	Front side boundary condition flag.	6.10
KBc = 2 ,	Back side boundary condition flag.	6.10
KOc = 2 ,	Over side boundary condition flag.	6.10
KUc = 2 ,	Under side boundary condition flag.	6.10
KRTc = 1 ,	Right side thermal boundary condition flag.	6.11
KLTe = 1 ,	Left side thermal boundary condition flag.	6.11
KFTc = 1 ,	Front side thermal boundary condition flag.	6.11
KBTe = 1 ,	Back side thermal boundary condition flag.	6.11
KOTc = 1 ,	Over side thermal boundary condition flag.	6.11
KUTc = 3 ,	Under side thermal boundary condition flag.	6.11
KRTWc = 2 ,	Right side thermal boundary condition flag in the substrate.	6.11
KLWc = 1 ,	Left side thermal boundary condition flag in the substrate.	6.11
KFTWc = 2 ,	Front side thermal boundary condition flag in the substrate.	6.11
KBTWc = 1 ,	Back side thermal boundary condition flag in the substrate.	6.11

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KUTWc = 2	Under side thermal boundary condition flag in the substrate.	6.11
&end		

Appendix B: DROP PROPERTY FILES

In this appendix the property files used for the droplet materials are presented. You may change these files or create one based on the desired information. However the format of these files **must be kept** as it is. The definitions of the terms used in these files are as follows:

- RHOF is the liquid density of the drop in kg/m^3 . Throughout the calculation a single density is used for both liquid and solid phases of the drop. This density is the liquid phase density.
- LIQUIDVIS section is used for presenting the liquid phase kinematic viscosity of the material at different temperatures. The general form of this section is:

$$\mathbf{NVA} = n,$$

$$\mathbf{VA1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VA2} = \nu_1, \nu_2, \dots, \nu_n$$

where **NVA** is the total number of the paired data sets, **VA1** is the array of temperatures (in $^{\circ}\text{C}$), and **VA2** is the array of kinematic viscosities at corresponding temperatures (in m^2/s).

- LIQUIDCON section is used for presenting the liquid phase thermal conductivity of the material at different temperatures. The general form of this section is:

$$\mathbf{NVB} = n,$$

$$\mathbf{VB1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VB2} = K_1, K_2, \dots, K_n$$

where **NVB** is the total number of the paired data sets, **VB1** is the array of temperatures (in $^{\circ}\text{C}$), and **NB2** is the array of thermal conductivities at corresponding temperatures (in W/m-K).

- LIQUIDSPH section is used for presenting the liquid phase specific heat of the material at different temperatures. The general form of this section is:

$$\mathbf{NVC} = n,$$

$$\mathbf{VC1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VC2} = C_1, C_2, \dots, C_n$$

where **NVC** is the total number of the paired data sets, **VC1** is the array of temperatures (in °C), and **NC2** is the array of specific heats at corresponding temperatures (in Joule/kg-K).

- LIQUIDSURF section is used for presenting the liquid phase surface tension of the material at different temperatures. The general form of this section is:

$$\mathbf{NVD} = n,$$

$$\mathbf{VD1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VD2} = \gamma_1, \gamma_2, \dots, \gamma_n$$

where **NVD** is the total number of the paired data sets, **VD1** is the array of temperatures (in °C), and **ND2** is the array of the surface tensions at corresponding temperatures (in kg/s²).

- SOLIDCON section is used for presenting the solid phase thermal conductivity of the material at different temperatures. The general form of this section is:

$$\mathbf{NVE} = n,$$

$$\mathbf{VE1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VE2} = K_{S1}, K_{S2}, \dots, K_{Sn}$$

where **NVE** is the total number of the paired data sets, **VE1** is the array of temperatures (in °C), and **NE2** is the array of thermal conductivities at corresponding temperatures (in W/m-K).

- SOLIDSPH section is used for presenting the solid phase specific heat of the material at different temperatures. The general form of this section is:

$$\mathbf{NVF} = n,$$

$$\mathbf{VF1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VF2} = C_{S1}, C_{S2}, \dots, C_{Sn}$$

where **NVF** is the total number of the paired data sets, **VF1** is the array of temperatures (in °C), and **NF2** is the array of specific heats at corresponding temperatures (in Joule/kg-K).

- TMELT is the melting point of the material in °C.
- HFUSN is the heat of fusion (latent heat of transformation) of the material in Jouls/kg.

Table 6. Property file for nickel

Properties for "Nickel"

&DENSITY

RHOF = 7.9D3
&END

&LIQUIDVIS

NVA = 6,
VA1 = 1453.D0, 1477.D0, 1527.D0, 1577.D0, 1627.D0, 1727.D0,
VA2 = 6.7D-7, 6.4D-7, 6.0D-7, 5.7D-7, 5.4D-7, 5.0D-7
&END

&LIQUIDCON

NVB = 1,
VB1 = 1453.D0,
VB2 = 45.D0
&END

&LIQUIDSPH

NVC = 1,
VC1 = 1453.D0,
VC2 = 444.D0
&END

&LIQUIDSURF

NVD = 1,
VD1 = 1453.D0,
VD2 = 1.78D0
&END

&SOLIDCON

NVE = 4,
VE1 = 527.D0, 727.D0, 927.D0, 1227.D0,
VE2 = 67.6D0, 71.8D0, 76.2D0, 82.6D0
&END

&SOLIDSPH

NVF = 4,
VF1 = 527.D0, 727.D0, 927.D0, 1227.D0,
VF2 = 530.D0, 562.D0, 594.D0, 616.D0
&END

&THERMAL

TMELT = 1453.D0
HFUSN = 3.1D3
&END

Table 7. Property file for alumina

Properties for "Alumina"

&DENSITY

RHOF = 3.0D3

&END

&LIQUIDVIS

NVA = 1,

VA1 = 2200.D0,

VA2 = 1.026D-5

&END

&LIQUIDCON

NVB = 1,

VB1 = 2050.D0,

VB2 = 6.D0

&END

&LIQUIDSPH

NVC = 1,

VC1 = 2050.D0,

VC2 = 1300.D0

&END

&LIQUIDSURF

NVD = 1,

VD1 = 2050.D0,

VD2 = 0.69D0

&END

&SOLIDCON

NVE = 1,

VE1 = 2050.D0,

VE2 = 6.D0

&END

&SOLIDSPH

NVF = 1,

VF1 = 2050.D0,

VF2 = 1273.D0

&END

&THERMAL

TMELT = 2050.D0,

HFUSN = 1.075D6

&END

Table 8. Property file for tin**Properties for "Tin"**

&DENSITY

RHO_F = 6.97D3

&END

&LIQUIDVIS

NVA = 1,

VA1 = 240.D0,

VA2 = 2.75D-7

&END

&LIQUIDCON

NVB = 1,

VB1 = 240.D0,

VB2 = 33.6D0

&END

&LIQUIDSPH

NVC = 1,

VC1 = 240.D0,

VC2 = 244.D0

&END

&LIQUIDSURF

NVD = 1,

VD1 = 240.D0,

VD2 = 0.526D0

&END

&SOLIDCON

NVE = 1,

VE1 = 240.D0,

VE2 = 62.2D0

&END

&SOLIDSPH

NVF = 1,

VF1 = 240.D0,

VF2 = 243.D0

&END

&THERMAL

TMELT = 232.D0,

HFUSN = 6.09D4

&END

Table 9. Property file for molybdenum

Properties for "Molybdenum"

&DENSITY

RHOF = 9.34D3

&END

&LIQUIDVIS

NVA = 1,

VA1 = 2620.D0,

VA2 = 2.14D-7

&END

&LIQUIDCON

NVB = 2,

VB1 = 2620.D0, 2800.D0,

VB2 = 75.D0, 74.D0

&END

&LIQUIDSPH

NVC = 1,

VC1 = 2620.D0,

VC2 = 530.D0

&END

&LIQUIDSURF

NVD = 1,

VD1 = 2620.D0,

VD2 = 2.25D0

&END

&SOLIDCON

NVE = 6,

VE1 = 527.D0, 727.D0, 927.D0, 1227.D0, 1727.D0, 2227.D0,

VE2 = 118.D0, 112.D0, 105.D0, 98.D0, 90.D0, 86.D0

&END

&SOLIDSPH

NVF = 6,

VF1 = 527.D0, 727.D0, 927.D0, 1227.D0, 1727.D0, 2227.D0,

VF2 = 285.D0, 295.D0, 308.D0, 330.D0, 380.D0, 459.D0

&END

&THERMAL

TMELT = 2620.D0,

HFUSN = 2.93D5

&END

Table 10. Property file for water***Properties for "Water"**

&DENSITY

RHO = 1.0D3

&END

&LIQUIDVIS

NVA = 1,

VA1 = 25.D0,

VA2 = 1.0037D-6

&END

&LIQUIDCON

NVB = 1,

VB1 = 25.D0,

VB2 = 0.6055D0

&END

&LIQUIDSPH

NVC = 1,

VC1 = 25.D0,

VC2 = 4179.D0

&END

&LIQUIDSURF

NVD = 1,

VD1 = 0.D0,

VD2 = 7.4D-2

&END

&SOLIDCON

NVE = 1,

VE1 = 0.D0,

VE2 = 0.D0

&END

&SOLIDSPH

NVF = 1,

VF1 = 0.D0,

VF2 = 0.D0

&END

&THERMAL

TMELT = 0.D0,

HFUSN = 0

&END

*. Note that if the droplet is water, no energy equation is solved and therefore only the liquid properties are needed.

Table 11. Property file for Zirconia¹⁰**Properties for "Zirconia"**

&DENSITY

Rhof = 5600.00

&END

&LIQUIDVIS **

NVA = 6 ,

VA1 = 0.1000D+04, 0.1200D+04, 0.1500D+04, 0.2000D+04, 0.2500D+04, 0.3000D+04,

VA2 = 0.3740D-03, 0.1380D-03, 0.5080D-04, 0.1870D-04, 0.1030D-04, 0.6890D-05,

&END

&LIQUIDCON

NVB = 1 ,

VB1 = 0.2727D+04,

VB2 = 0.2000D+01,

&END

&LIQUIDSPH

NVC = 1 ,

VC1 = 0.2727D+04,

VC2 = 0.9628D+03,

&END

&LIQUIDSURF

NVD = 1 ,

VD1 = 0.1000D+04,

VD2 = 0.5000D+00,

&END

&SOLIDCON

NVE = 1 ,

VE1 = 0.2000D+04,

VE2 = 0.2000D+01,

&END

&SOLIDSPH

NVF = 3 ,

VF1 = 0.7270D+03, 0.1027D+04, 0.1727D+04,

VF2 = 0.6838D+03, 0.7315D+03, 0.8307D+03,

&end

&THERMAL

Tmelt = 0.269D+04 ,

Hfusn = 0.708D+06

&end

**¹⁰ Please note that the data for liquid viscosity of Zirconia is not extensively available. The data in this File can be modified based on new and more accurate information.

Table 12. Property file for Zirconia¹¹

```

"Properties for " Zirconia "
&DENSITY
  Rhof= 5600.0000
&END
-----
&LIQUIDVIS **
NVA = 6 ,
  VA1 = 0.2500D+02, 0.2695D+04, 0.275D+04, 0.2800D+04, 0.2900D+04, 0.300D+04
  VA2 = 1.330D-05, 7.5D-06, 7.5D-06, 7.4D-06, 7.20D-06, 7.14D-06
&END
-----
&LIQUIDCON
NVB = 1 ,
  VB1 = 0.2695D+04,
  VB2 = 0.2700D+01,
&END
-----
&LIQUIDSPH
NVC = 1 ,
  VC1 = 0.2695D+04,
  VC2 = 0.9628D+03,
&END
-----
&LIQUIDSURF
NVD = 2 ,
  VD1 = 0.3D+02, 0.2695D+04,
  VD2 = 0.5000D+00, 0.5D+0
&END
-----
&SOLIDCON
NVE = 2 ,
  VE1 = 25.D0, 0.2692D+04,
  VE2 = 0.912D0, 1.3500D+00,
&END
-----
&SOLIDSPH
NVF = 3 ,
  VF1 = 0.2500D+02, 0.1027D+04, 0.2695D+04,
  VF2 = 0.4538D+03, 0.7315D+03, 0.1000D+04,
&end
-----
&THERMAL
  Tmelt = 0.2695D+04 ,
  Hfusn = 0.708D+06
&end
-----

```

****¹¹** Please note that the data for liquid viscosity of Zirconia is not extensively available. The data in this File was taken from: In situ measurement system for deformation and solidification phenomena of yttria-stabilized zirconia droplets impinging on quartz glass substrate under plasma-spraying conditions. Kentaro Shinoda, Yoichi Kojima, Toyonobu Yoshida, [Journal of Thermal Spray Technology](#), December 2005, Volume 14, [Issue 4](#), pp 511–517

Appendix C: SUBSTRATE PROPERTY FILES

In this appendix the property files used for the substrate materials are presented. You may change these files or create one based on the desired information. However the format of these files **must be kept** as it is. The definitions of the terms used in these files are as follows:

- **RSUB** is the density of the substrate in kg/m^3 .
- **SUBCON** section is used for presenting the thermal conductivity of the substrate at different temperatures. The general form of this section is:

$$\mathbf{NVG} = n,$$

$$\mathbf{VG1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VG2} = C_{\text{sub}1}, C_{\text{sub}2}, \dots, C_{\text{sub}n}$$

where **NVG** is the total number of the paired data sets, **VG1** is the array of temperatures (in $^{\circ}\text{C}$), and **VG2** is the array of thermal conductivities at corresponding temperatures (in W/m-K).

- **SUBSPH** section is used for presenting the substrate specific heat at different temperatures. The general form of this section is:

$$\mathbf{NHE} = n,$$

$$\mathbf{VH1} = T_1, T_2, \dots, T_n,$$

$$\mathbf{VH2} = K_{\text{sub}1}, K_{\text{sub}2}, \dots, K_{\text{sub}n}$$

where **NHE** is the total number of the paired data sets, **VH1** is the array of temperatures (in $^{\circ}\text{C}$), and **NH2** is the array of specific heats at corresponding temperatures (in Joule/kg-K).

Table 13. Property file for stainless steels

Properties for "Stainless Steels"

&DENSITYS

RSUB = 7.9D3

&END

&SUBCON

NVG = 6,

VG1 = 127.D0, 327.D0, 527.D0, 727.D0, 927.D0, 1227.D0,

VG2 = 16.6D0, 19.8D0, 22.6D0, 25.4D0, 28.0D0, 31.7D0

&END

&SUBSPH

NVH = 6,

VH1 = 127.D0, 327.D0, 527.D0, 727.D0, 927.D0, 1227.D0,

VH2 = 515.D0, 557.D0, 582.D0, 611.D0, 640.D0, 682.D0

&END

Table 14. Property file for glass

Properties for "Glass"

&DENSITYS

RSUB = 2.5D3

&END

&SUBCON

NVG = 1,

VG1 = 27.D0,

VG2 = 1.4D0

&END

&SUBSPH

NVH = 1,

VH1 = 27.D0,

VH2 = 750.D0

&END

Table 15. Property file for copper

Properties for "Copper"

&DENSITYS

RSUB = 8.933D3

&END

&SUBCON

NVG = 5,

VG1 = 127.D0, 327.D0, 527.D0, 727.D0, 927.D0,

VG2 = 393.D0, 379.D0, 366.D0, 352.D0, 339.D0,

&END

&SUBSPH

NVH = 5,

VH1 = 127.D0, 327.D0, 527.D0, 727.D0, 927.D0,

VH2 = 397.D0, 417.D0, 433.D0, 451.D0, 480.D0,

&END

Appendix D: OUTPUT FILES

D.1. “f” Files

In this section a sample of an “f” file is presented. The first three lines of the file are headings which are written for TecPlot® Graphic Software. You can modify the heading if it is necessary.

These three lines are:

1st line: Indicates the name and location of the file.

2nd line: Defines the titles for the variables as appear in the columns from line 4 to the end of the file, as follows:

- The first column shows the “X” positions of the center of each grid cells, in **mm**.
- The second column shows the “Y” positions of the center of each grid cells, in **mm**.
- The third column shows the “Z” positions of the center of each grid cells, in **mm**.
- The forth column shows the values of the volume of fluid, f , for the liquid phase which are calculated at the center of the grid cells. The value of the f is between zero (no liquid) to 1 (inside the liquid). Other values between one and zero indicate an interface cell.
- The fifth column shows the values of the volume of fluid, s , for the solid phase which are calculated at the center of the grid cells. The value of the s is between zero (no solid) to 1 (inside the solid). Other values between one and zero indicate an interface cell. This column is added to the file only if the energy equation and solidification are solved.

3rd line: is used by TecPlot.

SimDrop

0.38333333D-01	0.50000000D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.41666667D-01	0.50000000D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.45000000D-01	0.50000000D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.48333333D-01	0.50000000D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.51666667D-01	0.50000000D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.55000000D-01	0.50000000D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.00000000D+00	0.83333333D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.16666667D-02	0.83333333D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
0.50000000D-02	0.83333333D-02	0.83333333D-02	0.00000000D+00	0.00000000D+00	0.00000000D+00
....					
....					
....					
....					

D.2. “T” File

In this section a sample of a “T” file is presented. This file has two sections. The first section contains the information about the droplet and flow calculation grids. The second part, which immediately follows the first part, has the information about the substrate, see the sample file. The second section is separated from the first section by a line starting with “ZONE”. This line and the first three lines of the file are headings which are written for **TecPlot®** Graphic Software.

You can modify the heading if it is necessary. These three lines are:

- 1st line: Indicates the name and location of the file.
- 2nd line: Defines the titles for the variables as appear in the columns from line 4 to the end of the file, as follows:
- The first column shows the “X” positions of the center of each grid cells in **mm**.
 - The second column shows the “Y” positions of the center of each grid cells, in **mm**.
 - The third column shows the “Z” positions of the center of each grid cells, in **mm**.
 - The forth column shows the values of the temperatures, T , in °C for the droplet which are calculated at the center of the grid cells. The values of temperature at some grid points are set to be zero or -1 by the code. These cells are outside the boundaries of the droplet and do not contain any material.
- 3rd line: is used by TecPlot®.

Sample of a “T” file

TITLE=data/T.0000

VARIABLES="X","Y","Z","T"

ZONE F=POINT,I= 34 ,J= 34 ,K= 15

0.00000000D+00 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.37313433D-04 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.16169154D-03 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.38557214D-03 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.70895522D-03 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.11318408D-02 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.16542289D-02 0.00000000D+00 0.14407025D+00 -0.10000000D+01
...
...
...
0.15684080D-01 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.17500000D-01 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.19415423D-01 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.21430348D-01 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.23544776D-01 0.00000000D+00 0.14407025D+00 -0.10000000D+01
0.25758706D-01 0.00000000D+00 0.14407025D+00 0.00000000D+00
0.28072139D-01 0.00000000D+00 0.14407025D+00 0.00000000D+00
0.30485075D-01 0.00000000D+00 0.14407025D+00 0.00000000D+00
0.32997512D-01 0.00000000D+00 0.14407025D+00 0.00000000D+00
...
...
...
0.47052239D-01 0.38557214D-03 0.15105372D+00 0.00000000D+00
0.50161692D-01 0.38557214D-03 0.15105372D+00 0.00000000D+00
0.53370647D-01 0.38557214D-03 0.15105372D+00 0.00000000D+00
0.00000000D+00 0.70895522D-03 0.15105372D+00 0.12500000D+04
0.37313433D-04 0.70895522D-03 0.15105372D+00 0.12500000D+04

0.16169154D-03 0.70895522D-03 0.15105372D+00 0.12500000D+04
0.38557214D-03 0.70895522D-03 0.15105372D+00 0.12500000D+04
0.70895522D-03 0.70895522D-03 0.15105372D+00 0.12500000D+04
0.11318408D-02 0.70895522D-03 0.15105372D+00 0.12500000D+04
0.16542289D-02 0.70895522D-03 0.15105372D+00 0.12500000D+04
0.22761194D-02 0.70895522D-03 0.15105372D+00 0.12500000D+04

...

...

...

ZONE F=POINT,I= 101 ,J= 101 ,K= 3

0.00000000D+00 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.37313433D-04 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.16169154D-03 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.38557214D-03 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.70895522D-03 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.11318408D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.16542289D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.22761194D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.29975124D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.38184080D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.47388060D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.57587065D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.68781095D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.80970149D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.94154229D-02 0.00000000D+00 -0.50000000D-04 0.25000000D+02
0.10833333D-01 0.00000000D+00 -0.50000000D-04 0.25000000D+02

...

...

...

D.3. “*pv*” Files

In this section a sample of “*pv*” file is presented. The first three lines of the file are headings which are written for **TecPlot®** Graphic Software. You can modify the heading if it is necessary.

These three lines are:

- 1st line: Indicates the name and location of the file.
- 2nd line: Defines the titles for the variables as appear in the columns from line 4 to the end of the file, as follows:
- The first column shows the “*X*” positions of the center of each grid cells, in **mm**.
 - The second column shows the “*Y*” positions of the center of each grid cells, in **mm**.
 - The third column shows the “*Z*” positions of the center of each grid cells, in **mm**.
 - The forth, fifth, and sixth columns show the values of the velocity components in the *x*, *y*, and *z* directions which are calculated at the center of the grid cells. These components are shown by *u*, *v*, and *w* and have the units of **m/s**.
 - The seventh column shows the values of the pressure, *p*, for the droplet which are calculated at the center of the grid cells in **Pa**. This column does not show the actual pressure, but it shows the difference between the initial pressure inside the droplet and the pressure at the time this file is created.
- 3rd line: is used by TecPlot®.

Sample of a “pv” file

TITLE=data/PV.0001
VARIABLES="X","Y","Z","U","V","W","P"
ZONE F=POINT,I= 12 ,J= 11 ,K= 21

0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.41666667D-02	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.1250000D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.20833333D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.29166667D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.3750000D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.45833333D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.54166667D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.6250000D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.70833333D-01	0.0000000D+00	0.0000000D+00	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
...				
...				
...				
0.41666667D-02	0.70833333D-01	0.29354839D-01	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.1250000D-01	0.70833333D-01	0.29354839D-01	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.20833333D-01	0.70833333D-01	0.29354839D-01	0.0000000D+00	0.0000000D+00
0.0000000D+00	0.0000000D+00			
0.29166667D-01	0.70833333D-01	0.29354839D-01	0.55569622D-02	0.55569622D-02
0.75886240D-01	0.0000000D+00			
0.3750000D-01	0.70833333D-01	0.29354839D-01	0.55569622D-02	0.55569622D-02
0.75886240D-01	0.0000000D+00			
0.45833333D-01	0.70833333D-01	0.29354839D-01	0.84475391D-02	0.84475391D-02
0.34008157D-01	0.0000000D+00			
0.54166667D-01	0.70833333D-01	0.29354839D-01	0.84475391D-02	0.84475391D-02
0.0000000D+00	0.0000000D+00			
...				
...				
...				

Appendix E: POST-PROCESSING THE RESULTS

As mentioned earlier, the SIMDROP output files have a format that can be downloaded by TecPlot® Software for post-processing. In this Appendix the procedure for making a simple iso-surface plot with this software will be presented. The information presented here will show you the overall procedure that can be used to plot a set of data. For more detailed information you must refer to TecPlot® Menu. Also a sample Macro that is written for this purpose will be shown. The macro files will be used when there are number of plots to be created from similar data files. Note that all instruction and the macro file are based on TecPlot Version 9, Revision 2.

E.1. Iso-Surface Plotting

In order to plot an iso-surface from the result, you can use one of the *f.xxxx* files. First launch the TecPlot® software and then follow the steps shown below:

1. From the TecPlot® menu bar, click on “FILE” and then click on “LOAD DATA FILE(S)”. In the window that is opened next, select the “*f*” file that you want to plot. By doing so, the calculation domain and the grid lines appear on the screen.
2. Now click on the “PLOT” from the menu and then select the “ISO-SURFACE”. In the window that appears, select “Show Iso-Surfaces”. Now you can select many options in this window. You may use the following procedure to obtain a good quality image:
 - a. In “Draw iso-Surfaces at” box, select “1 Specifies Value”. This way the iso-surfaces with one value is drawn. Consequently in “Value 1” box, enter number “0.5”. Then only the iso-surfaces with value 0.5 are shown.
 - b. Disable “Show Contour Flood” and select “Show Shade”.

- c. Then from the “Color” menu, choose the desirable color for your plot.
 - d. In “Use Lighting Effect” menu, select “Gouraud”. With this selection, you will have a smooth surface for your plot.
 - e. If you like to have the transparency effect in your plot, select “Use Surface Translucency” and select the degree of the transparency effect. By using this option, you will be able to see not only the surface of the plot, but also inside the liquid.
 - f. Now you may close the Window and from the menu at the left of the screen, disable “Mesh” and “Boundary”, if you want.
 - g. At any time you may select again the “3D Iso-Surfaces Details” from the “FIELD” menu and change all the settings.
3. At this time, you must have an iso-surface plot of your results. The next steps presented here are optional and they just polish the final result.
4. You can change the appearance of the axis, add more information, or even delete the axis by clicking on the “PLOT” from the menu bar and then selecting the “AXIS”. In the window that appears, you can customize the information about each axis, as you like.
5. If you need to mirror your results in any direction, you can click on “DATA” from the menu. Then select “CREATE ZONE” and then “MIRROR”. In the window that appears, select the zones you want to mirror. Usually you only need to mirror the zones that start with “ISO:”. Highlight that zone and then from the option menu, select with respect to which plane you want the data to be mirrored. Then click on “CREATE” and after the mirroring has finished, click on OK.
6. If you made all desirable changes in your plot, you can save your work. To save your plot, click on “FILE” and then “SAVE LAYOUT AS” and save your file in the desired directory you choose. The TecPlot® files have the “.lay” extension. You may be advised that since “ the data attached to frame “Frame xxx” has changed, give a file name for the

data set”. This new file will have the information about all changes that you have made in the previous steps. Change the file name, if you wish. It is recommended that you change the file name in order to keep the original data for future use.

7. For plotting the second “*f*” file, while the first plot is still on the screen click on “FILE” from the menu bar and select “LOAD DATA FILE(S)”. A window appears that gives you three options. Select the option: “REPLACE DATASET AND RETAIN PLOT STYLE” and then choose the data file name. The second iso-surface plot will be replaced with the first plot with the same plot styles. After you completed the second plot, you can save and/or export the plot as mentioned in the previous steps.

You may also plot a slice (section) of the results by selecting “3D Slice Details” from the “Field” menu. In this option you can specify the location of the slice in the *x*, *y*, or *z* direction.

E.2. Making a movie

You can also export your plot in a desirable format from TecPlot®. The “EXPORT” option in “FILE” menu is usually used for creating movies. If you want to create a movie starting from the first frame, while the frame is on the screen, select “Export” from the “File” menu. Then select the “AVI” format. By doing so the “AVI EXPORTER” window appears. You may choose the speed of the animation in this window and then click on OK. Then you are asked to give a file name for the movie that is created.

The “Record Animation File” windows remains on the screen while you are creating next frames. Upon finishing each frame, click on “Record Next Image” and continue working. At the end, Click on “Finish Animation”, and the animation will be completed.

E.3. TecPlot® Macros

When plotting a number of data files that all have the same styles and information, you may use the “Macro” feature that is offered by TecPlot 9.0®. In this case, you can RECORD the macro while created a plot (to have more information about this feature, please refer to TecPlot 9.0®

Manual). After writing the macro for few plots, you can stop the recording. Then, using a text editor, copy and paste the macro for each file for the number of files that you want to plot. You can then play the macro in TecPlot 9.0® to created all iso-surface plots and/or movie from the result. A sample of such macro is presented here.

A Sample Macro for Tecplot 9.0:

This is a Sample macro file that is written for creating a series of iso-surface plots and making an animation. To do so, first a plot of one set of results was created and saved by the name “Drop.lay”. This file was then used to create the other plots and the animation result was saved as “Drop.avi”. This file can be used as a guide and the file names, the paths, and some other settings must be changed accordingly.

```
-----  
-  
#!MC 900  
$!VarSet |MFBD| = 'E:\Simulent-Drop\data'  
$!PICK SETMOUSEMODE  
    MOUSEMODE = SELECT  
$!OPENLAYOUT "E:\ Simulent-Drop\data \drop.lay"  
$!REDRAWALL  
$!EXPORTSETUP EXPORTFORMAT = AVI  
$!EXPORTSETUP BITDUMPREGION = ALLFRAMES  
$!EXPORTSETUP ANIMATIONSPEED = 3  
$!EXPORTSETUP IMAGEWIDTH = 722  
$!EXPORTSETUP USEMULTIPLECOLORTABLES = YES  
$!EXPORTSETUP EXPORTFNAME = 'E:\ Simulent-Drop\data \drop.avi'  
$!PromptforTextString |NumFiles|  
    Instructions = "How many Files do you have?"  
$!EXPORTSTART  
$!LOOP |NumFiles|  
$!IF |Loop| > 99  
    $!VARSET |FNAME| = (|LOOP|*5)  
    $!READDATASET "'|MFBD|\f.0|LOOP|.plt" '  
        READDATAOPTION = NEW  
        RESETSTYLE = NO  
        INCLUDETEXT = NO  
        INCLUDEGEOM = NO  
        INCLUDECUSTOMLABELS = NO  
        VARLOADMODE = BYNAME  
        VARNAMELIST = ' "X" "Y" "Z" "F" "U" "V" "W" "P" '  
$!FIELDLAYERS SHOWMESH = NO  
$!REDRAWALL  
$!ENDIF  
$!IF |Loop| > 9  
    $!IF |Loop| <= 99  
        $!VARSET |FNAME| = (|LOOP|*5)
```

```
    $!READDATASET  '|MFBD|\f.00|LOOP|.plt" '
    READDATAOPTION = NEW
    RESETSTYLE = NO
    INCLUDETEXT = NO
    INCLUDEGEOM = NO
    INCLUDECUSTOMLABELS = NO
    VARLOADMODE = BYNAME
    VARNAMELIST = '"X" "Y" "Z" "F" "U" "V" "W" "P"'
$!FIELDLAYERS SHOWMESH = NO
$!REDRAWALL
$!ENDIF
$!ENDIF
$!IF |Loop| <= 9
    $!VARSET |FNAME| = (|LOOP|*5)
    $!READDATASET  '|MFBD|\f.000|LOOP|.plt" '
    READDATAOPTION = NEW
    RESETSTYLE = NO
    INCLUDETEXT = NO
    INCLUDEGEOM = NO
    INCLUDECUSTOMLABELS = NO
    VARLOADMODE = BYNAME
    VARNAMELIST = '"X" "Y" "Z" "F" "U" "V" "W" "P"'
$!FIELDLAYERS SHOWMESH = NO
$!REDRAWALL
$!ENDIF
$!PICK ADD
    X = 2.55231884058
    Y = 6.55579710145
$!PICK CLEAR
$!ATTACHTEXT
    XYPOS
    {
        X = 11.5700483092
        Y = 20.3985507247
    }
    TEXT = 'T = |FNAME|  micro second'
$!PICK ADD
    X = 3.33753623188
    Y = 7.19144927536
$!REDRAWALL
$!EXPORTNEXTFRAME
$!ENDLOOP
$!EXPORTFINISH
$!RemoveVar |MFBD|
$!RemoveVar |NumFiles|
```