# 2018

**SimSpray User Guide**

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**THIS DOCUMENT CONTAINS THE INFORMATION NECESSARY TO RUN SIMSPRAY PACKAGE.**

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**TABLE OF CONTENTS**

# 1. SimSpray Software Suite

## 1.1 Introduction

**Simulent Inc.** has developed a customized code named **SimSpray Software Suite** to study the spray and atomization process. **SimSpray** consists of several modules:

➡ Internal Flow Module for nozzle design

➡ Primary Breakup: Statistical Module

➡ Atomization Module

Simulating the spray and atomization in one step is computationally very exhausting and time consuming process. The length scale between the nozzle geometry itself and the size and location of the droplets are so different that generating number of mesh that can be handled by any solver and could represent the spray will be almost impossible.

Moreover, the jet breakup mechanism needs to be defined properly, otherwise the jet break up and droplet sizes would depend on the cell sizes and thus the results will not be accurate.

For this reason, the simulations in **SimSpray** software suite are carried on in five sequential steps, as shown in Figure (1-1). These steps are:

➢ **Pre-processing**.

In this stage the geometry of the nozzle and the inflow liquid volume are imported and volumetric uniform meshes are generated to best define the geometry. **SimMesh** module, which is a volumetric general mesh generator developed by Simulent, is used for this purpose.

➢ **Flow simulation/Nozzle Design**

In this stage, by using a volume of fluid/multi-phase algorithm the flow inside the nozzle and orifice is modeled, see Figure (1-2). **SimSpray** module is used in this stage.  In this

stage the properties of the liquid sheet exiting from the nozzle will be determined accordingly and this will eventually help designers to design a better nozzle to get the desired droplet size and velocity at the exit of the nozzle.

➢ **Primary break up**

The liquid sheet at the exit of the nozzle will break up to form spray, See Figure (1-2). The break up depends on many parameters, including the instabilities in the liquid and the surrounding gases. In this stage, by using the state of the art statistical break up models that we have access to for different types of nozzles and orifices, the average spray drop size and velocity distribution at the outlet of the nozzle is determined. This is a very important step. Without accurately predicting the average droplet size and velocity, the accurate modeling of the spray is not possible.

## Spray Modeling Suite

1- Pre-Processor
SimMesh

2- Flow simulation
SimSpray

3- Primary Breakup
SimData (Drop And Thickness Analyzer)

4- Atomization
SimSpray

5-Post Processing
TecPlot
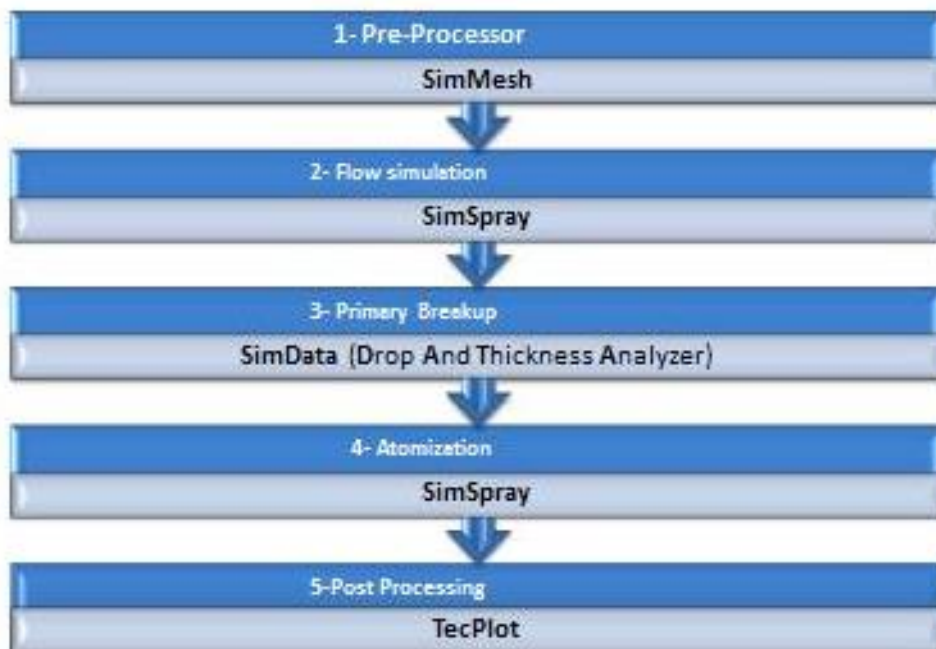
**Figure (1-1) Flow diagram for SimSpray software Suite**

> **Spray**

After the average droplet size and velocity are determined, any Lagrangian model can be used to model the atomization process, See Figure (1-2). Such alogorithm can model heat transfer with the surrounding gas, vaporization, break-up, collision, to find the spray dispersion, droplet size and velocity distributions at a far distance from the nozzle tip. Having the information of average droplet size and velocity, any commercial software can be also used to model the spray and atomization far from the nozzle tip.



**Flow simulation inside nozzle / SimSpray**

**Primary Breakup model / SimData**
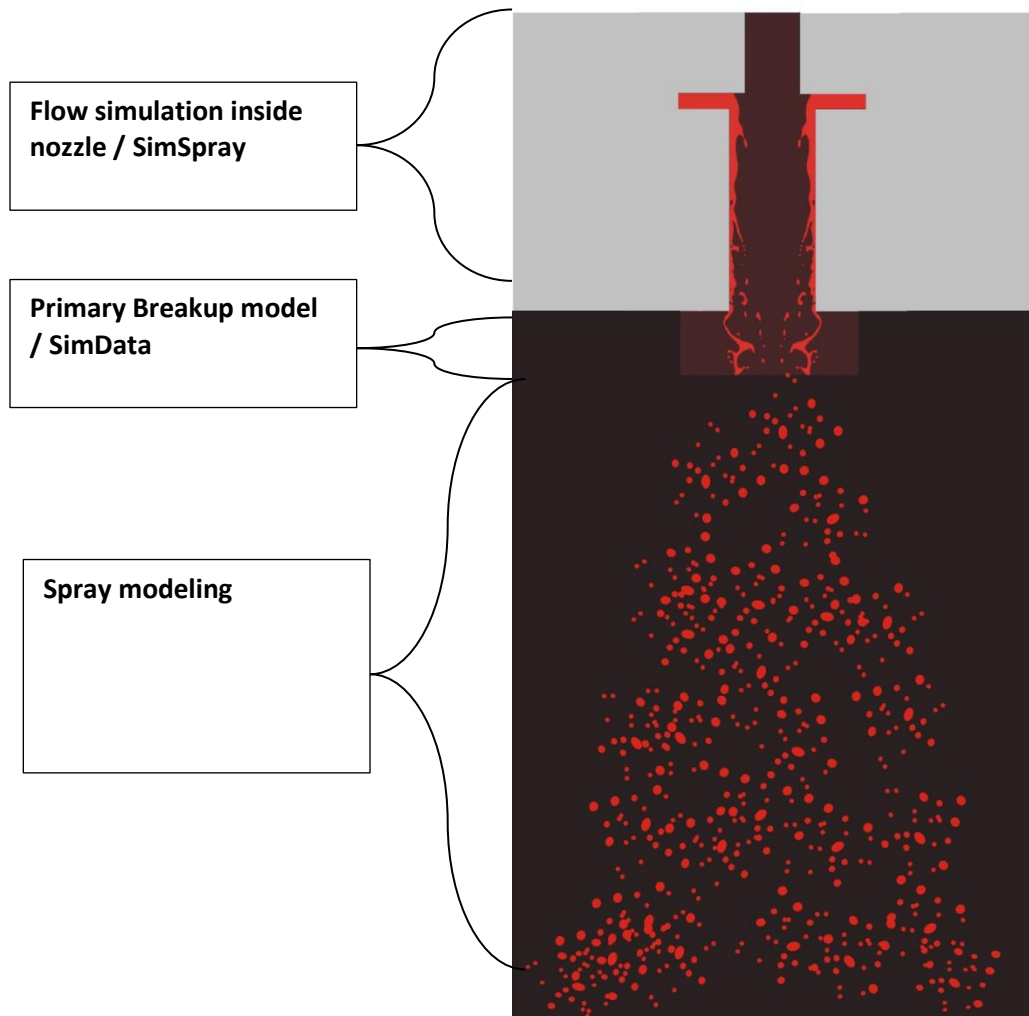
**Spray modeling**

**Figure (1-2) Complete spray & atomization modeling steps**

> ➤ **Post-Processing**

Finally, a post processing software needs to be used to process the data. SimSpray software suite uses **TecPlot** commercial software for this purpose.

## 1.2 SimSpray Advantages

— There is no commercial software tool in the market that can model the whole process of break up and atomization all together.

— SimSpray is user friendly.

— The user interface pages and the data entry are simplified based on each customer application.

— The results are accurate (they were tested and validated against available experimental results).

— Since it uses both numerical and empirical models, it is efficient.

— The experts in Simulent Inc. have the expertise and experience in dealing with spray and atomization problems both experimentally and numerically for more than 20 years.

## 1.3 SimSoray User Guide

This document is a short User Guide for SimSpray suite and is intended to explain how this software suite works and how one can benefit from the results obtained at the end of simulations.

The present document is divided into 3 main Sections: SimMesh, SimSpray, and SimData. These are three available modules that are used consequently to obtain the mean droplet size and velocity for a specific nozzle and flow condition.

This SimSpray Manual is designed to show how the fluid flow and break up model can be used for a "**pressure swirl nozzle**". For this reason most of the User Interface pages and the analytical models are developed for this type of nozzle. The SimSpray software Suite can be designed and customized to model any other single phase nozzle, including splash plate nozzles. The break up model, SimData has been customized specifically for swirl nozzles.

## 1.4 Installation

All files and folders necessary to run the flow simulation and break up model are saved in three sub directories: **SimMesh**, **SimSpray** and **SimData**. You only need to copy these folders on to your computer and double click on the executable files to run the program.

In this document, it will be shown how the nozzle geometry can be imported into SimMesh grid generator, how the mesh is imported into SimSpray module, how the results can be processed by Tecplot, and how the average droplet size and velocity at the exit of the nozzle can be determined by SimData module.

## 2. GRID GENERATION

SimMesh grid generator is a Cartesian (volumetric) uniform mesh generator that can read input geometries in **STL format**. The mesh is generated within a cube that surrounds the geometry (see Figure 2-7). Within this cube (simulation domain) the grid generator creates flags that distinguish between the solid / liquid parts of the geometry and the cells which are open for fluid movement.

In the uniform Cartesian grid, the curved boundaries of the geometry are approximated in a staircase manner. This limitation might decrease the accuracy or efficiency (since it enforces the use of a fine grid) of the numerical solution particularly for complex geometries.

### 2.1 Preparing CAD Files

Please note that for each simulation with SimSpray software, you need to generate two mesh files: One for the solid body of the nozzle and one for the liquid entering the nozzle, please see Figure 2-1. In general, the designers design the geometry (body) of the spray nozzle. This Figure shows two types of nozzles, for each nozzle a small volume of liquid at the inflow boundary is generated in addition to the nozzle geometry. Therefore, prior to generating mesh with SimMesh software, you need to prepare the following files in STL format:

- **Generate the geometry file of the nozzle in any CAD software and save it in "STL" format**. If the geometry of the nozzle consists of different parts, all parts must be merged and only one "STL" file, containing all parts of the nozzle must be saved. **Please make sure that all unwanted gaps in the geometry must be cleaned and closed before you save the file. If the cell sizes are less than the gap sizes, you may create a mesh file that leaves all these gaps open for liquid movement.**

- **Create a Liquid Volume at the Inflow Boundary. T**o perform a fluid flow simulation, we need to introduce a liquid volume at the nozzle inflow boundary. Instead of defining this volume manually in SimSpray code, you need to add a liquid volume to the object geometry using your CAD package. This liquid volume must be created at the same system of coordinates as the nozzle geometry. To do so, you need to open your nozzle geometry in your CAD package and add the liquid volume such that it conforms to the solid object interior. The extent of this liquid volume should be such that it contains 3-4 cells in the same direction as the liquid movement.

In Figure 2-1, the steps you need to take in generating two CAD files, one for the solid geometry (nozzle body) and one for initial inflow liquid volume are explained. It is important that you take these steps before starting to generate mesh with SimMesh software.

## 2.2 Software Overview

By clicking on **SimMesh** from the Start->Programs->Simulent->SimMesh menu or by double clicking on **SimMesh4-2.exe**, an informational screen will appear. Click on **OK** to close the screen and view a message to guide you to the next step, see Figure 2-2.

Once the information message is closed, the main software page opens. On the top of the main window, there are 5 options: **TecPlot, Open File**, **Input**, **Mesh**, and **Exit**. The program will guide you to open different pages to give the necessary information about the geometry and the grids. At any time during the mesh generation, you may click on **Exit** to close the program.
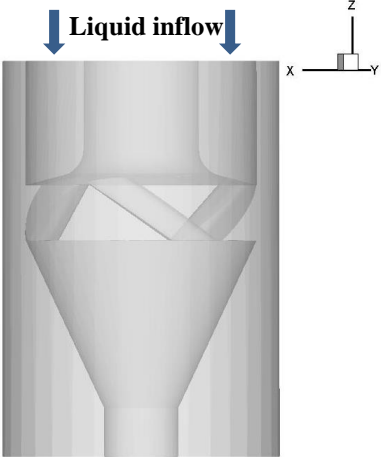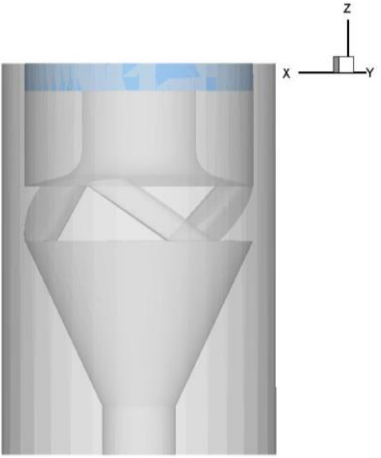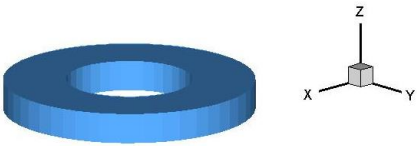
| | |
|---|---|
|  | -Generate the solid body of the nozzle, using your CAD package. Save it in STL format (ASCII or Binary).<br><br>-If the CAD geometry consist of several parts, merge all of them together and save only a single file.<br><br>-Make sure that is no unnecessary gaps/leaks between different parts of the geometry. |
|  | -While still using your CAD package, generate a volume of liquid at "inflow" boundary location.<br><br>This liquid volume must be generated within the same system of coordinates as the nozzle geometry.<br><br>- The volume of liquid must conform **tightly** to the shape of the nozzle at inflow boundary condition.<br><br>- The liquid volume must be extended into the nozzle, only to cover 3 cells (please see the next section for more information).<br><br>-**The created liquid volume must be saved separately from the nozzle body also in STL Format.** |
|  | -This is the example of the liquid volume at the boundary which was created in the CAD software and was saved in a separate file. |

**Figure 2-1. Different steps in generating files**
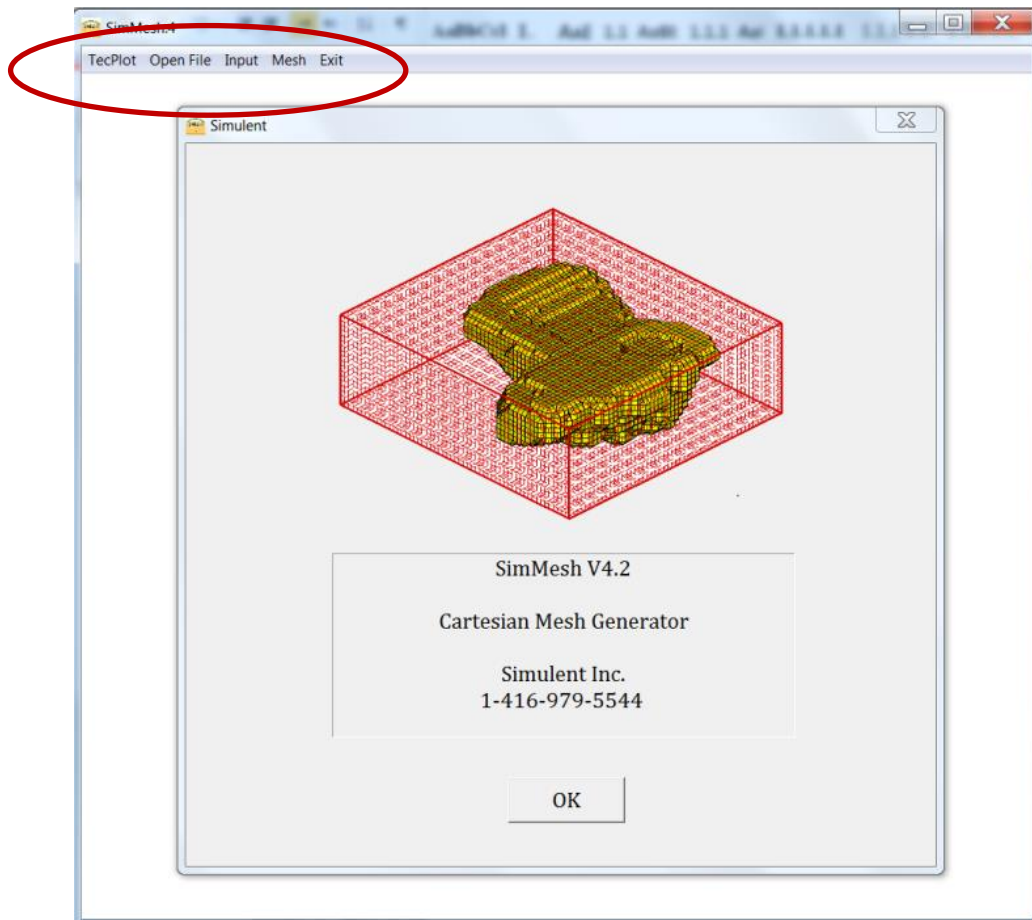
**Figure (2-2) The introduction dialog page**

**2.3 TecPlot**

This version of **SimMesh** can only import and generate mesh for geometries in "STL" format. You can check the geometry file before you start the mesh generation and after you completed the grid generation, using TecPlot post processing software.

To see the STL geometry file, follow this procedure:

- Click on TecPlot from the menu.

- When TecPlot is launched, click on File > Load Data File(s)

- A window as shown in Figure (2-3) opens. Select the first file format "3D System STL"

- Click on OK, and when prompted, browse for the "STL" file and open it.

- When the "Select Initial Plot" window opens, change the "Initial Plot Type" to "3D", as shown in Figure (2-4).

- By using the controls on the left side of TecPlot window, you can change the view of the geometry and also determine the "X", "Y", and "Z" directions of the geometry, see Figure (2-4).

Once you check the geometry, you may save the file in TecPlot format or just simply Exit from TecPlot. Close TecPlot to return to the main page of SimMesh software.
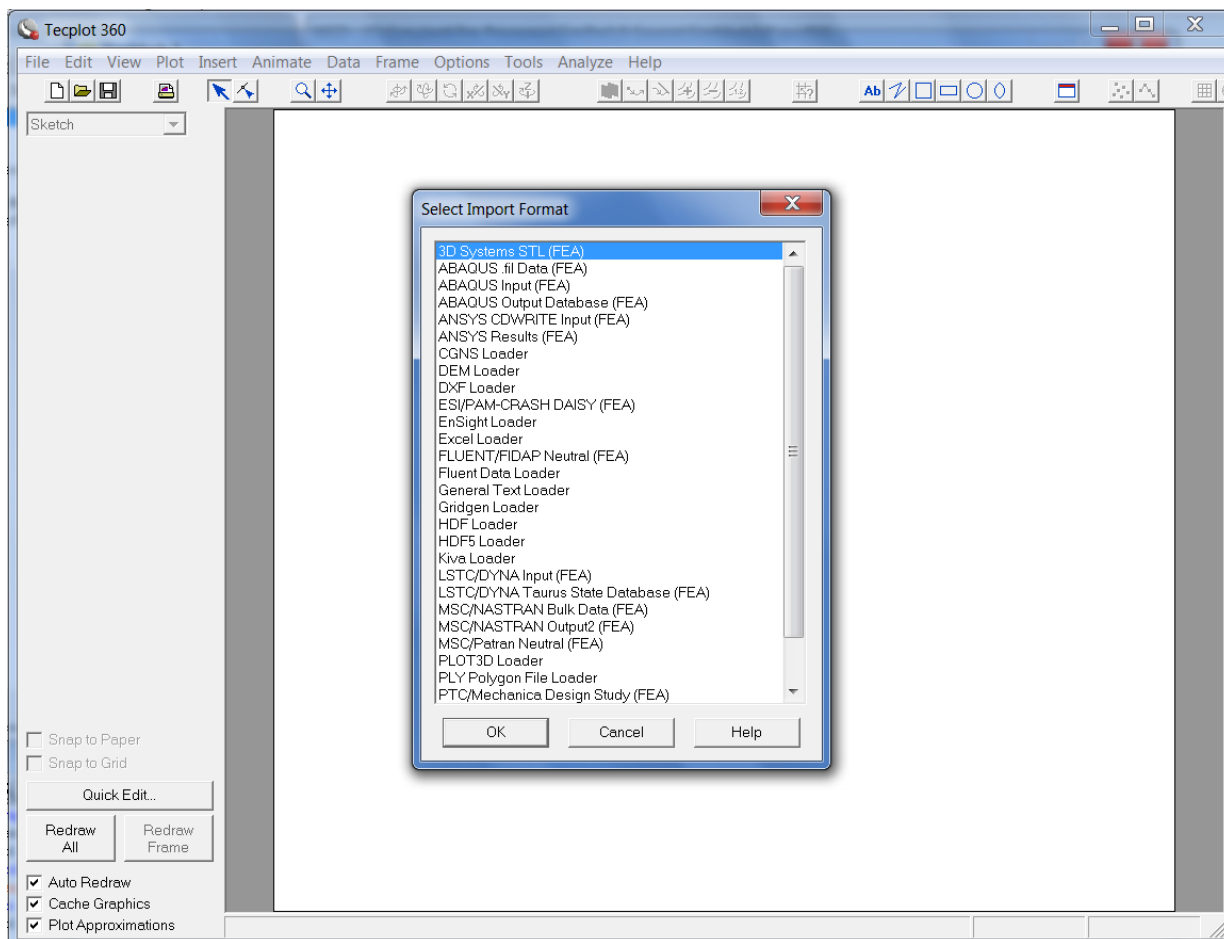


- **Figure (2-3) Loading the "STL" geometry file with TecPlot. You need to use "3D Systems STL (FEA)" option**
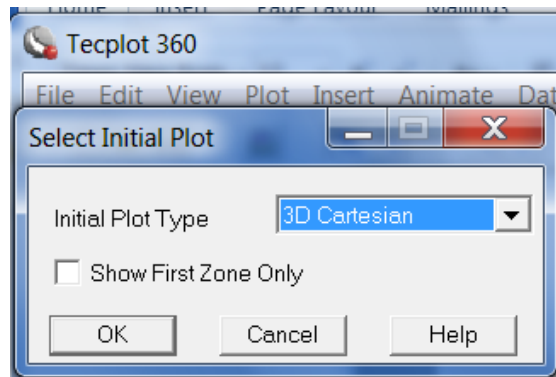
**Figure (2-4) When asked "Select Initial Plot", select "3D Cartesian"**
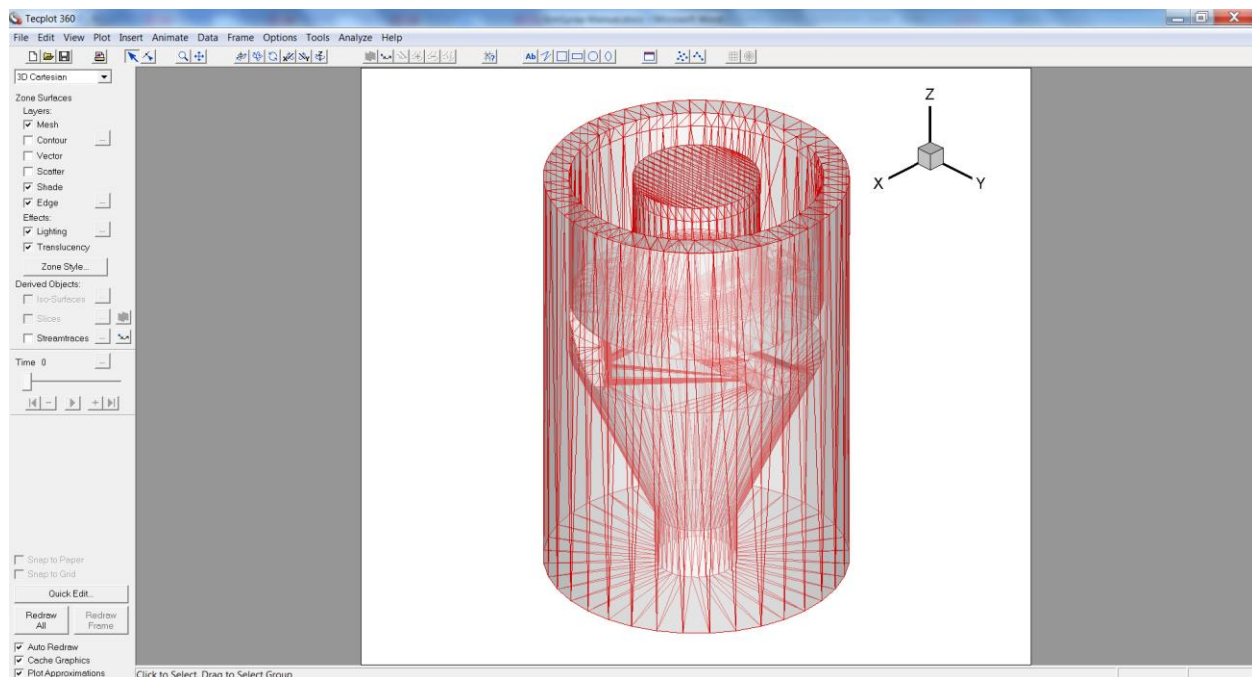


**Figure (2-5) View of the STL file by TecPlot**

### 2.4 Open File

To open the geometry file, click on "Open File" from the top menu. Locate the "STL" file and open it. Wait for the file to be read and a message that prompt you to click on "**Input**". This may take long, depending on the size of the STL file. Then, click on "Input" from the top menu to enter the meshing parameters.

**2.5 Input**

By clicking on "**Input**", the "**General Input**" interface is opened as shown in Figure (2-6).

> ➢ **For SimSpray code, you need to open the STL file that is saved for nozzle geometry first (solid geometry) and start generating mesh for this part (Go to Section 2.5.1).**

> ➢ **If you are generating mesh for the initial liquid volume (you have already completed the solid geometry mesh generation), open the STL file that you created for the initial liquid volume and then go to Section 2.5.2.**



**Figure (2-6) General Input interface page**

### 2.5.1   Solid Geometry Mesh

**Cell Size/Limits/Unit:**

As soon as you open the CAD geometry, the domain limits are read and are written in the spaces provided for this purpose. "Xmin", Ymin", Zmin", Xmax, Ymax, and Zmax are the geometry minimum and maximum coordination in the X, Y, and Z directions, see also Figure (2-7). These numbers are in the original units of the CAD file.

- In the first space, you need to specify the required Cell Size in the CAD file original unit. Since Simulent code uses a uniform Cartesian mesh scheme, the cell sizes in all directions are the same. Please makes sure that the cell sizes are small enough to capture the movement of the liquid and covers all details of the geometry (you can check this by using TecPlot to examine the mesh sizes, see Section 2.6). Meanwhile avoid using very small cell sizes unnecessarily, since it will increase the total number of grids and will prolong the simulation time. The default value of cell size is zero. If you forget to fill up this space and try to close the window, a warning message will ask you to change the cell size, as shown in Figure (2-9).

- The domain limits, which define the simulation domain, can be increased or decreased according to the type of the geometry or simulations. In Figure (2-7-a), the original domain that adheres to the geometry maximum and minimum are shown.  For changing the boundary limits for a spray nozzle, several facts must be considered:

  ➢ At the inflow boundary, the domain must cut/coincide with the geometry of the nozzle, as shown in Figure (2-7-b). This is because we need to define the inlet flow velocity at this boundary. So, it is recommended to reduce the limit by only one cell size at the inflow boundary.

  ➢ At the outflow boundary, the limit must be extended such that it captures the liquid sheet flowing from the nozzle exit, see Figure (2-7-b).  There is no need to

extend this domain very far; otherwise the total number of cells will be increased unnecessarily.





(a)                                            (b)
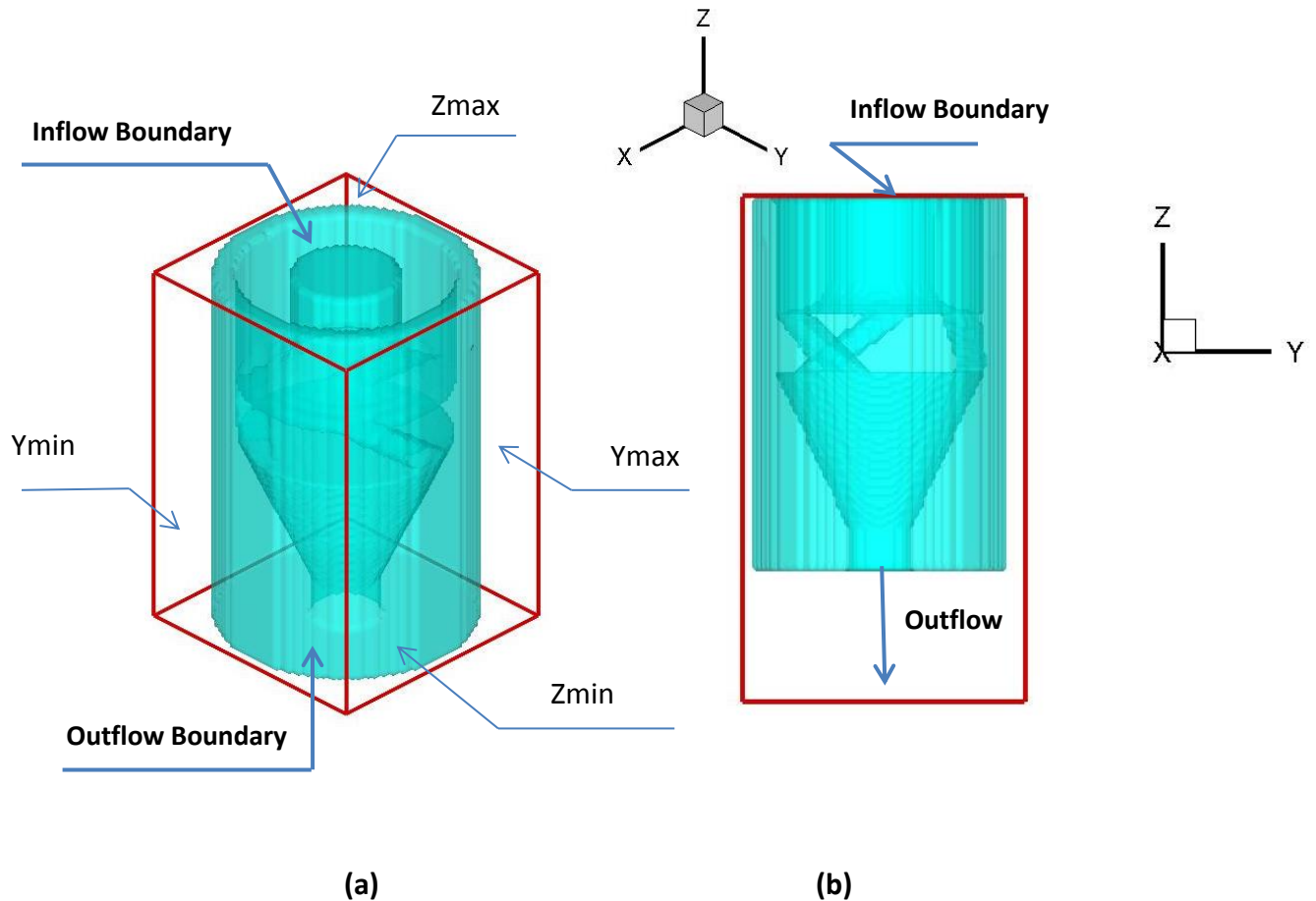
**Figure (2-7) Limit of the geometry, definition of the boundaries**

➢ For the other sides of the nozzle, where there is normally no inflow of outflow, the domains can be extended equivalent to 2-3 cells. That is to make sure that there are no open cells for the liquid to escape the geometry. Also this makes the presentation of results more realistic.

However, for those simulations with very large number of cells and If the bulk of the nozzle body has no effect on the liquid movement (no interfere between the

calculation boundaries and the liquid), the boundaries can be moved within the geometry limits to save number of cells.

➢ For those nozzles that there exists a symmetrical plane, for which only half or a quarter of the nozzle geometry is needed for simulation, the boundaries and corresponding boundary conditions may be changed as well to save the number of cells and simulation time. In these cases the domain limits can be located at the symmetric plane and boundary conditions on those planes must be changed to symmetric type (see the next Section).

**Please note that in all above situations, the <u>maximum domain limits</u> in all directions are changed slightly to accommodate the exact number of cells in each direction. So, each time you change one side of the domain, please check the changes in the other side of the domain. Once you finished changing the limits click on Apply. The number of cells in each direction will be shown in the column on the right side. Please see Figure 2-6.**

- In the next space in this section, you need to specify the length units in the original geometry file, using the drop box. Please note that all simulations and post processing results are in SI units and for this reason it is important that the original units of the geometry is defined correctly.

- In the final section, you need to specify the output file name in which the mesh data are stored. This file later will be imported by SimSpray and SimData. The default name is "Solid.DAT".  Make sure to change this name for each new simulation and when generating mesh for the Liquid volume, to prevent losing your previous data.

- At any time, you may click on "Reset", to set back the maximums and minimums to the original values.

Once the data entry is finished, click on **Apply**. By clicking on **Apply**, the number of cells in each direction will be calculated and shown under the spaces for "**Number of Cells**".

**IMPORTANT NOTES\*\*:**

1- <span style="color:red">**You may notice that the maximum limits of the geometry may change as you click on the Apply. This very important, since if your inflow boundary is at one of the "maximums", you need to change it back to the original values. This is because the boundary needs to cut the geometry limit**.</span>

2- <span style="color:red">**Before exiting this page, make a note of the final domain limits in all directions (Xmin, Xmax, Ymin, Ymax, Zmin, Zmax), as well as the total number of cells in each direction. You will need these numbers when you generate the mesh for the liquid volume (see the next section).**</span>

**Boundary Conditions**

In the second Section of this page, you need to specify the boundary conditions. Please note that the boundary conditions here refer to the conditions at the boundaries of the calculation domain, see Figure 2-7 and Figure 2-8. This domain is a cubic box that is built around the geometry. Depending on the type of simulations, the boundary conditions may be of the following types:

- **Open**: This means liquid may flow in or out of the domain (inflow or outflow boundaries).

- **Symmetric**: This is used when you want to run simulations for half of the geometry, due to symmetrical conditions.

- **Wall**: this means the liquid cannot enter or exit to/from the boundary.
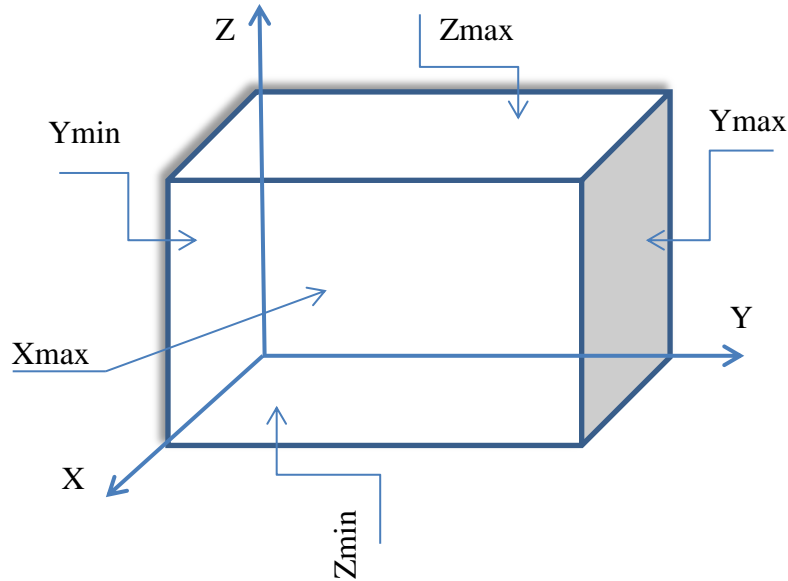
**Figure 2-8. Definitions of terms used in boundary condition flags**

For SimSpray simulation, if you have no symmetrical boundary, you can select an open boundary condition for all boundaries, since the fluid either enters the domain or exits from it.

If the mesh generation is for the nozzle geometry, solid part, you may click on "**Done**" and start generating the mesh (go to Section 2-6). An information message asks you to click on **Mesh** to start generating the mesh, see Figure (2-10).

If you are generating the mesh for the initial liquid parts, you need to continue from Section 2.5.2. **Please note once you finished generating mesh for the solid geometry, you don't need to close the software. While the main page is still open, you can open another STL file and re-start new mesh generation.**

### 2.5.2   Inflow Liquid Mesh

**Cell Size/Limits/Unit:**

As for the solid geometry mesh generation, as soon as you open the CAD geometry, the liquid domain limits are read and are written in the spaces provided for this purpose. "Xmin", Ymin",

Zmin", Xmax, Ymax, and Zmax are the liquid volume minimum and maximum coordination in the X, Y, and Z directions, see also Figure (2-7). These numbers are also in the original units of the CAD file.

- **At this point, you need to change all six limits to the exact number as the solid geometry limits you used in the last Section and click on Apply. Please check that the cell numbers in each direction are also exactly as the solid mesh and if they are not change the limits accordingly. This step is very important and must be followed carefully.**

- In the next space in this section, make sure the length units in the original geometry file is correctly selected.

- In the final section, you need to specify the output file name in which the mesh data are stored. The default name is "Solid.DAT". Make sure to change this name, for example to "Liquid.DAT", to distinguish between the Solid and Liquid mesh files.

**Boundary Conditions**

As for the Solid mesh, you need specify the boundary conditions. **For inflow liquid mesh, you need to select the same boundary conditions as you did for the Solid mesh**.

**Liquid Information**

The third section in this page asks for information about the inflow liquid location and velocity.

- First you need to confirm that this mesh generation is done for the inflow liquid volume.

- Next you need to specify the inflow boundary location. This is done by considering Figures (2-7) and (2-8). Make sure that you are selecting the correct plane for inflow condition. For example in Figure (2-7), the inflow boundary is at **Zmax** location.

- Considering the location of the inflow plane, you also need to specify three components of the inflow liquid velocity. Please note that it is assumed that the velocity is constant all across the surface of the liquid entry.

Once the data entry is completed click on OK. A message warns you to click on **Mesh** on the top menu to generate mesh, see Figure (2-10).

Please note that two mesh files for Solid geometry and inflow liquid have the same format. However, in liquid mesh file there is an additional line (first line) that contains a number to indicate the location of the inflow boundary, and three components of the liquid velocity.
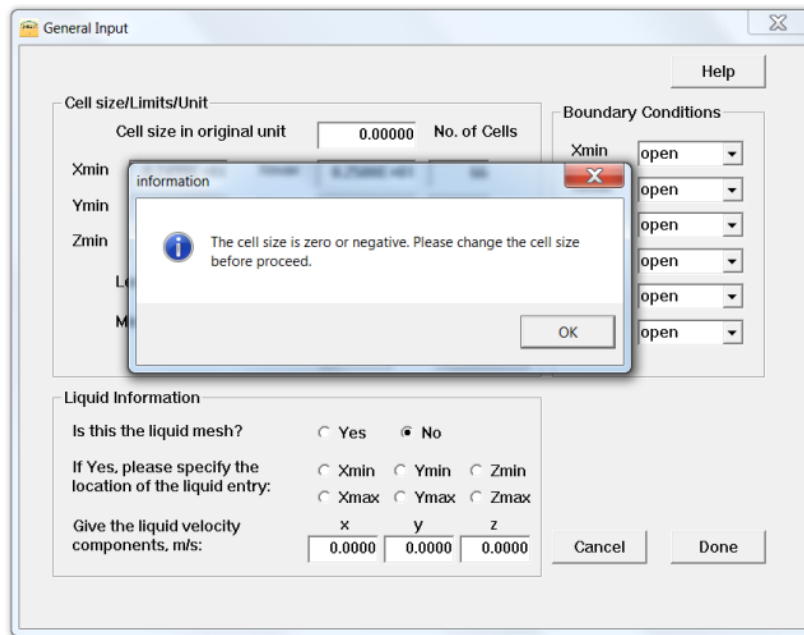


**Figure (2-9) Warning message to change the cell size**
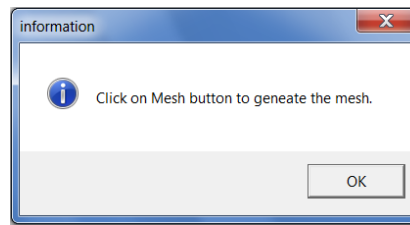
**Figure (2-10) Information message to start mesh generation**

## 2.6 Mesh generation

By clicking on the **Mesh**, the mesh generation starts. When the mesh generation is complete (this may take some time, depending on the size of the geometry and the number of cells), you will be notified of the completion, see Figure (2-11).  At this point you can examine the quality of the mesh by using TecPlot.

**Please note once you finished generating mesh for the solid geometry, you don't need to close the software. While the main page is open, you can open another STL file and re-start the mesh generation.**
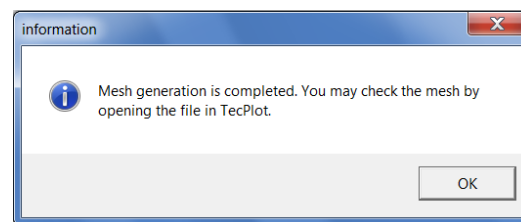


**Figure (2-1) Completion of mesh generation**

**2.7 Checking mesh quality**

When you see the message of the mesh completion, you can open TecPlot again to check the quality (and the quantity) of the Cartesian uniform mesh:

- In TecPlot, click on File > Load Data File(s).

- Then, select "TecPlot Data Loader", as shown in Figure (2-10)

- The mesh generator creates a mesh file in TecPlot format with name "**PLT.plt**". When asked, please select this file. This file is located where you copied the executable files (root directory).

- When file is opened, you only see the grids. From the left side menu, select "Iso Surfaces". The geometry also appears at this time.

- You may check if the generated mesh covers the area you are interested in. Also by magnifying different parts of the geometry, check if the mesh size is enough to capture different parts of the geometry. **Please note that you need at least two grids for each location of the geometry or liquid parts that is open to liquid movement, in order the simulation returns correct result and there would be no" leak".**

- If you need to change to domain sizes or the cell sizes, you must exit from Tecplot first, then from the main menu click on "Input" and change the information. Then generate the mesh again and examine the meshes again. You can repeat this procedure, without any need to exit the program and start again.

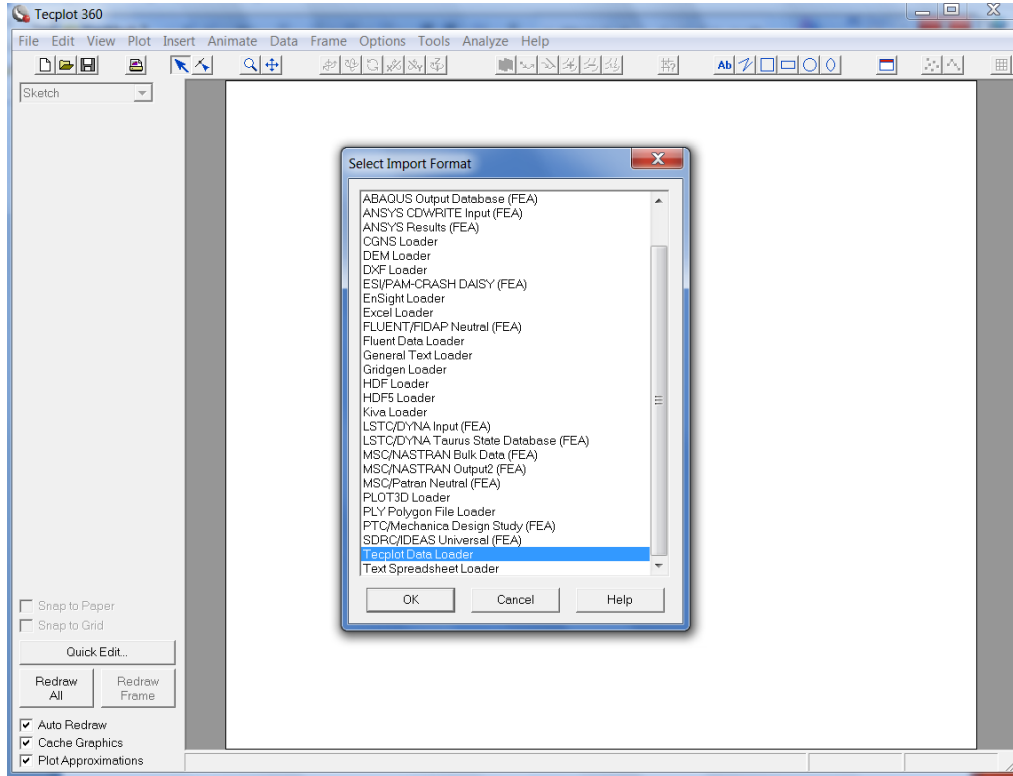- **Do not try to open the Geometry again at this point, since it is already loaded.**

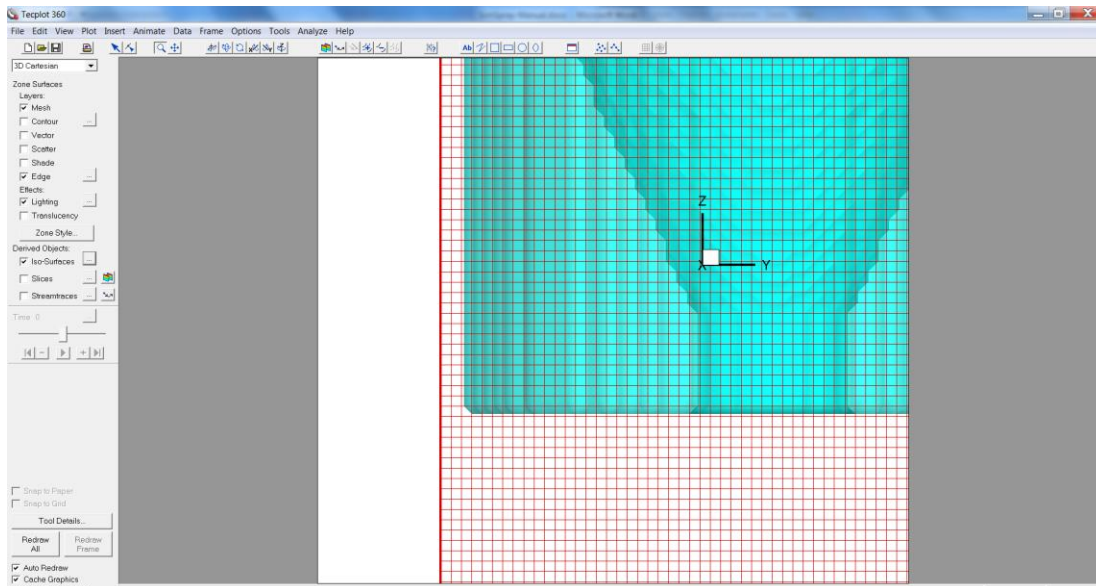**Figure (2-12) Loading the mesh file into TecPlot**.



**Figure (2-13). Examining the mesh quality and quantity by TecPlot.**

**2.8 SimMesh Output Files**

There three types of output files generated by SimMesh grid generator, each time you run the code:

1- **PLT.PLT**

   This file is written in binary TecPlot format. It can be used to visualize the generated mesh and to check if the grid resolution has been enough to capture all sections of the geometry. Please see Section 2.5. **Each time you run the mesh generation, this file is overwritten. Thus, if you want to keep a copy of the file for any future use, you need to rename it or move it to your specific location**.

2- **BC.DAT**

   This file contains the domain size in each direction, number of cells and the type of boundary conditions. This file is also overwritten each time you generate a new mesh. Therefore, you may rename it for each mesh generation or move it. Please note that for each spray nozzle geometry and inflow liquid mesh generation, the BC.DAT file should be unique.

   This file is read by all Simulent codes. **Make sure that this file is copied to the working directory of the simulations you are expecting to perform with SimSpray software, once you completed the mesh generation.**

3- **Mesh Files (Solid.DAT, Liquid.DAT,….)**

   These files, in ASCII format, contain the location (in terms of I, J, K) of those cells that are either solid, for solid geometry mesh, or liquid, for inflow liquid mesh, as well as information about the domain and cell sizes. When generated for inflow liquid mesh, they also contain the flag to show the location of the inflow boundary and the velocity components.

   **These files must be also copied into the directory created for your SimSpray project.**

## 3. SIMSPRAY

SimSpray is a commercial code for simulating the liquid film formation and its breakup in an industrial spay nozzle. The model predicts the liquid film characteristics of a nozzle as a function of its geometrical design, operating conditions, and fluid properties. The model combines the solution of continuity and momentum equations with an algorithm for free surface tracking in presence of an arbitrary nozzle shape. The model simulates the swirling flow inside the injector chamber and predicts the formation of a conical liquid film at the exit of the nozzle.

Fluid flow in the injector nozzle is modeled using a finite volume solution of the Navier-Stokes equation in a 3D Cartesian coordinate system, assuming laminar, incompressible, Newtonian flow. The surface profile of deforming liquid is defined using the "fractional volume of fluid", VOF scheme using a free surface flow model is an Eulerian fixed-grid algorithm that utilizes a volume tracking approach to track fluid deformation. The 3D fixed-grid Eulerian method was written specifically for free surface flows with surface tension.

More technical information about the code and complete governing equation can be found in reference shown below[1]:

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[1] - M.P. Fard, N. Ashgriz, J. Mostaghimi, L.A. Prociw and T.C.J. Hu, "Modeling Liquid Film Formation and Breakup in an Industrial Spray Nozzle", in the proceedings of the 15th Annual Conference on Liquid Atomization and Spray Systems, Dearborn, MI, May 2002.

- M.P. Fard, N. Ashgriz, J. Mostaghimi, D.M. Levesque and S. Morrison, "Film Thickness and Velocity Distribution in a Splash-Plate Atomizer: Comparison between Simulations and Experiments", Proceedings of the 9th International Conference on Liquid Atomization and Spray Systems, Sorrento, Italy, July 2003.

- D.Levesque, S. Morrison, M.P. Fard and J. Mostaghimi, "Simulation of the Spray Characteristics of Black Liquor", PAPTAC 89th Annual Meeting (Pulp and Paper Technical Association of Canada), Montreal, January 2003.

- D. Levesque, M.P. Fard, S. Morrison; "*BLSpray: Understanding the effect of black liquor properties and splash plate nozzle configuration on Spray Characteristics*"; Pulp & paper Canada; 106:10 (2005), pp 198-203

### 3.1 Preparations

Before you start simulation with SimSpray, make sure that you have generated mesh files for the nozzle geometry and inflow liquid volume. Figure (3-1) shows a sample of meshes generated for a nozzle and the inflow liquid.
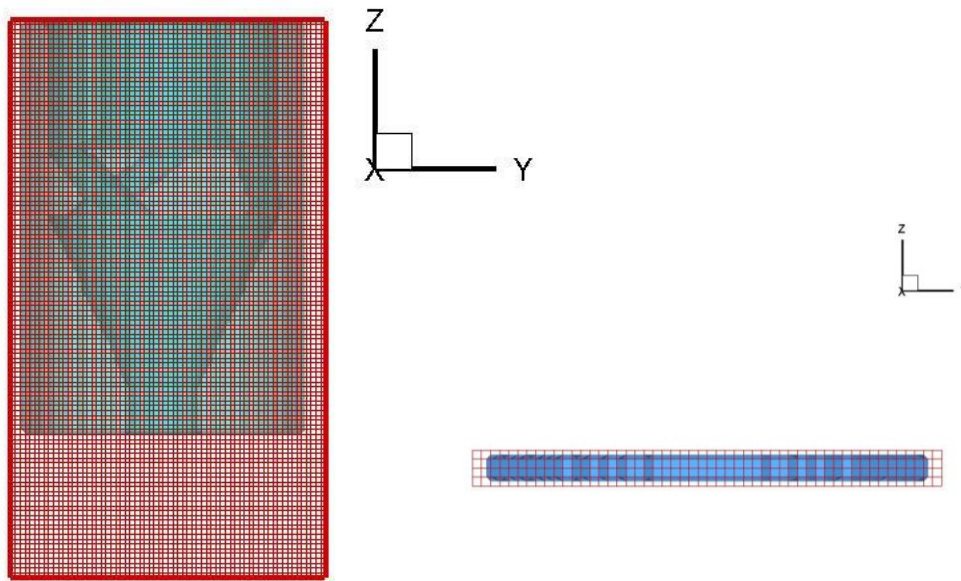


**Figure (3-1). Sample of mesh generated for solid geometry and inflow liquid for a nozzle.**

At this point you must to have three mesh files:

- Solid mesh file, e.g.: SOLID.DAT

- Inflow liquid file, e.g.: LIQUID.DAT

- Boundary conditions file: BC.DAT

It is recommended that you create a folder to save your input files and simulation results for each simulation.  Copy all mesh and BC files, as well as all TecPlot Macro files (*.mcr) into this folder.  The macro files are the files that are used to facilitate visualization of the simulation results using TecPlot. These files are:

- Extract-fav.mcr
- Extract-obs.mcr

These file would extract the necessary information for plotting and generating the "plt" files.

**3.2 Software Overview**

Click on the "Simspray-3.exe" to start running the program. The User Interface and the introduction page will be open, as shown in Figure (3-2). By clicking on the **OK**, the introduction page will close.

On the top menu bar of the main pages, there are 4 options: **Input**, **Start**, **TecPlot**, and **Exit**. By clicking on **Exit** at any time, you close terminate the program.

Click on **Input** to open the data entry page.
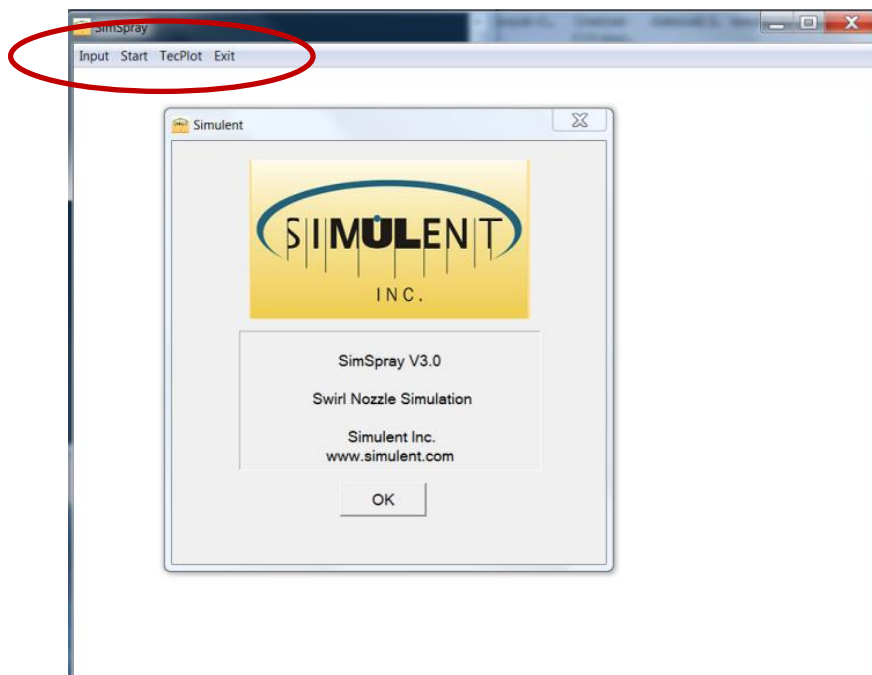


**Figure (3-2) Introduction Page in SimSpray V3.0**

## 3.3 General Input Page

The General Input Page, as shown in Figure (3-3), is used to enter the necessary data and parameters used by SimSpray.
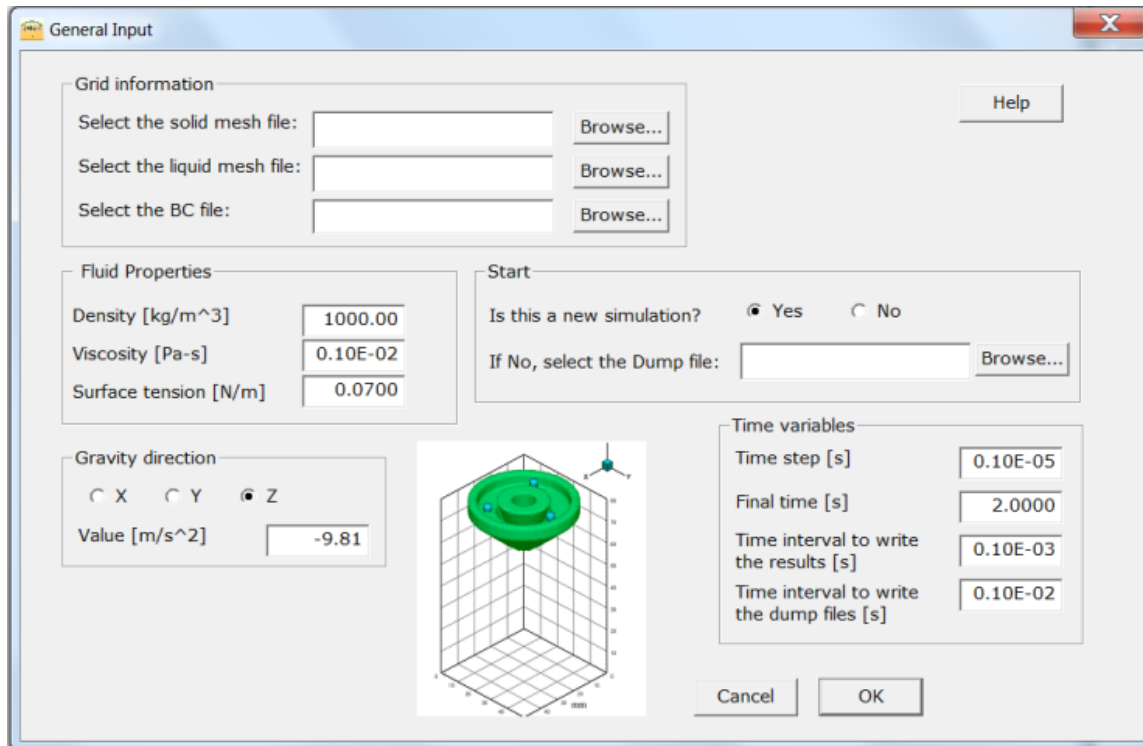


**Figure (3-3) Input Page for SimPray-V3**

### 3.3.1   Grid Information:

In the Section of the Input page, you are asked to open the mesh file for Solid, Liquid, and Boundary conditions. You can use the **Browse** to find the files and open them. If you forget to open a file and try to close the page, a warning message would remind you to open the missing file.

### 3.3.2   Fluid Properties

In this Section, you can specify the density, viscosity and surface tension for the liquid. The common liquid properties for water are already specified and used as default numbers. If your numbers are different, simply replace these numbers with the new ones.

### 3.3.3   Gravity Direction

In this section, you need to specify the direction of the gravity force and its magnitude. Please note that the direction of the gravity is defined based on how the orientation of the nozzle in the coordinate system and the direction of the inflow liquid, see the picture on the interface.

Also, the sign of the gravity magnitude indicates whether it is towards the positive or negative side of that direction. For example, if the inflow boundary is at Zmax and liquid is moving toward the negative direction, the value of the gravity acceleration is "-9.81". The default magnitude of the gravity acceleration is 9.81 m/s$^2$.

### 3.3.4   Start

You have the option to start a new simulation from time zero or you can re-start an old simulation that for any reason has been terminated. In the first line you will specify if this is a new simulation "Yes" (default option) or it is a continuation of the previous simulation "No". If the answer is "No", you need to specify the name of the "dump.xxxx" file that must be used for reading the information. (For the definition of the output file names, please Section 3.6). This is usually the last dump file that was created in the previous simulation. Simply use the **Browse**, find the file name, and click on Open, see Figure (3-4). The file name will appear in the small window besides the Dump File name.

### 3.3.5   Time Variables

In the Time variable section, you need to specify the initial time step for calculations, Final time for terminating the simulations, Time interval between writing the output files (f.xxxx, and fav.xxxx files, please see Section 3.6 for file name definition), and Time interval for writing the Dump files (dump.xxxx). The dump files are generated in larger time intervals and contain all information about the liquid. They can be used when the simulations needed to be re-started. The last Dump file is also used in SimData module to predict the primary breakup parameters.

In this page, there is also a "**Help**". At any time by clicking on it a help page, as shown in Figure (3-5), will be opened. This help page can be used while filling up the Input Page.
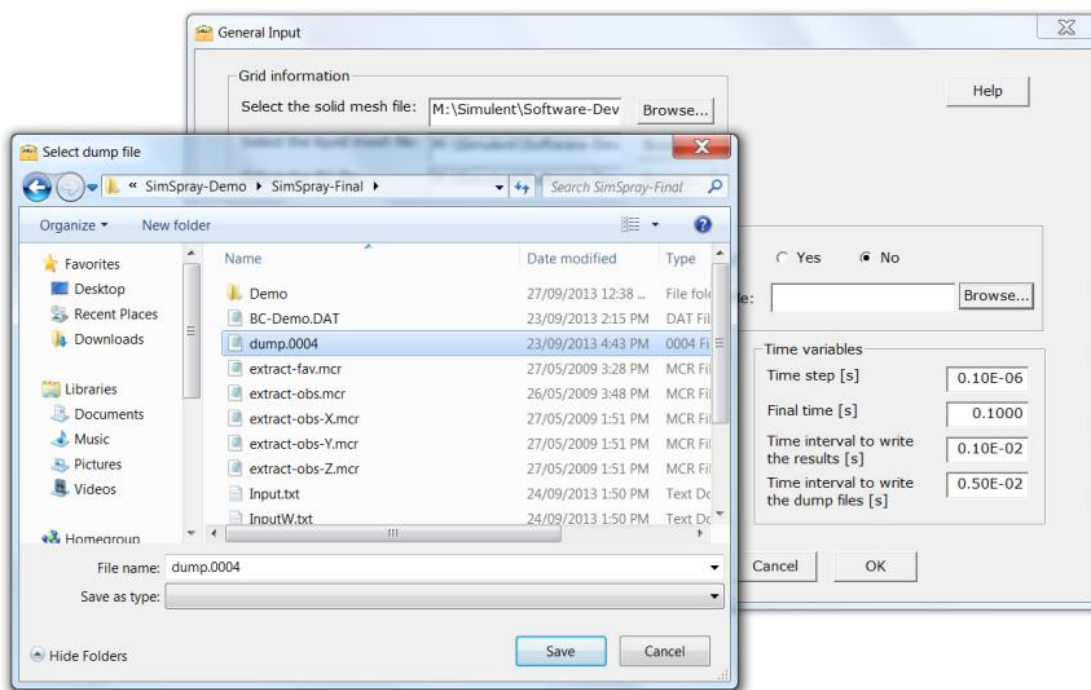


**Figure (3-4) Dump File Selection page**

Once you click on the **OK** from the Input page, you are directed to start the simulations, see Figure (3-6) and asked to select the working directory. This is the directory in which most of the Output files are saved, please see Figure (3-7) and also Section 3-6.
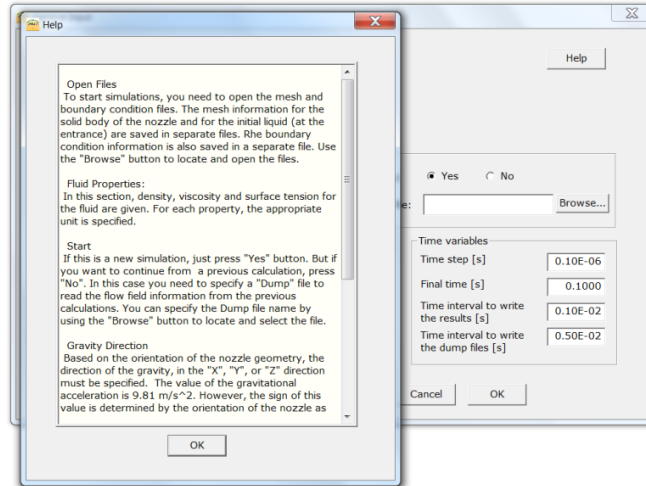
**Figure (3-5) Help Page for SimSpray**
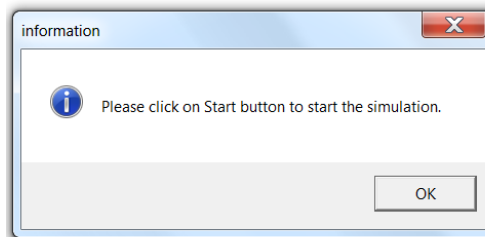


**Figure (3-6) Starting the simulation in SimSpray**

**3.4 Start**

Once you click on **Start**, a Dos Window opens and the simulations will start, see Figure (3-7). You can stop the simulations at any time by closing this Window, as well.

As shown in this Figure, the first line that appears on the screen indicates the location (or plan) at which the liquid enters the nozzle. In this specific case, the line reads: "6- Liquid entering from Zmax". This line can be checked to make sure that the inflow liquid is positioned correctly. The Flag number and positions are as follows:
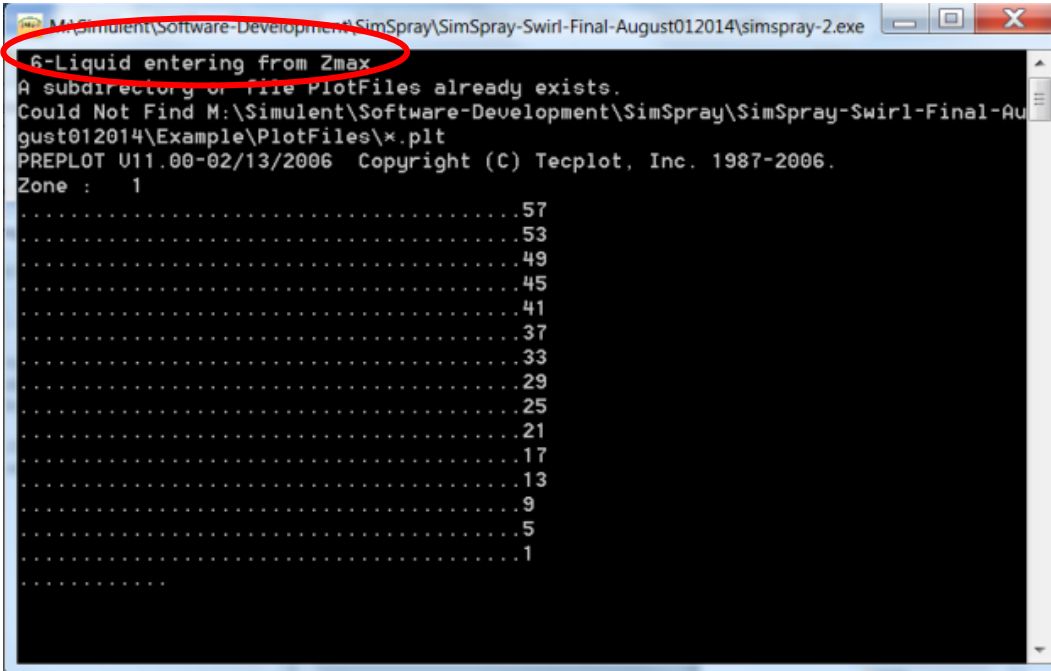
- - 1- Liquid entering from Xmin
- - 2- Liquid entering from Xmax
- - 3- Liquid entering from Ymin
- - 4- Liquid entering from Ymax

- 5- Liquid entering from Zmin

- 6- Liquid entering from Zmax
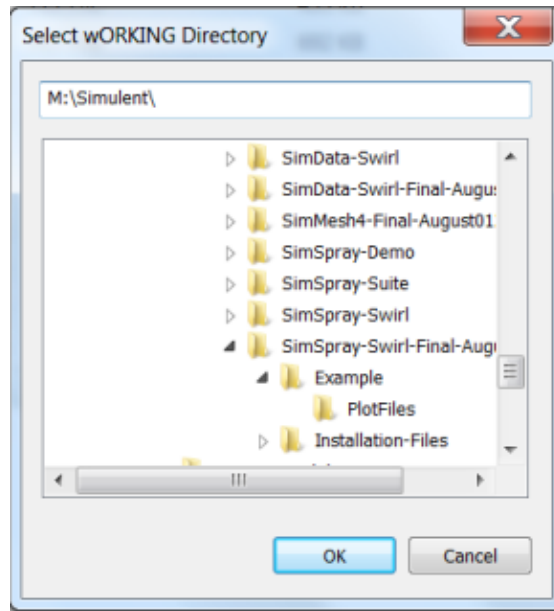


**Figure (3-7) Selecting the Working Directory**

Following this message, the initial TecPlot files are created, followed by simulation progress. During the simulation, there are 5 columns of data are written on the screen. These columns are, see also Figure (3-8):
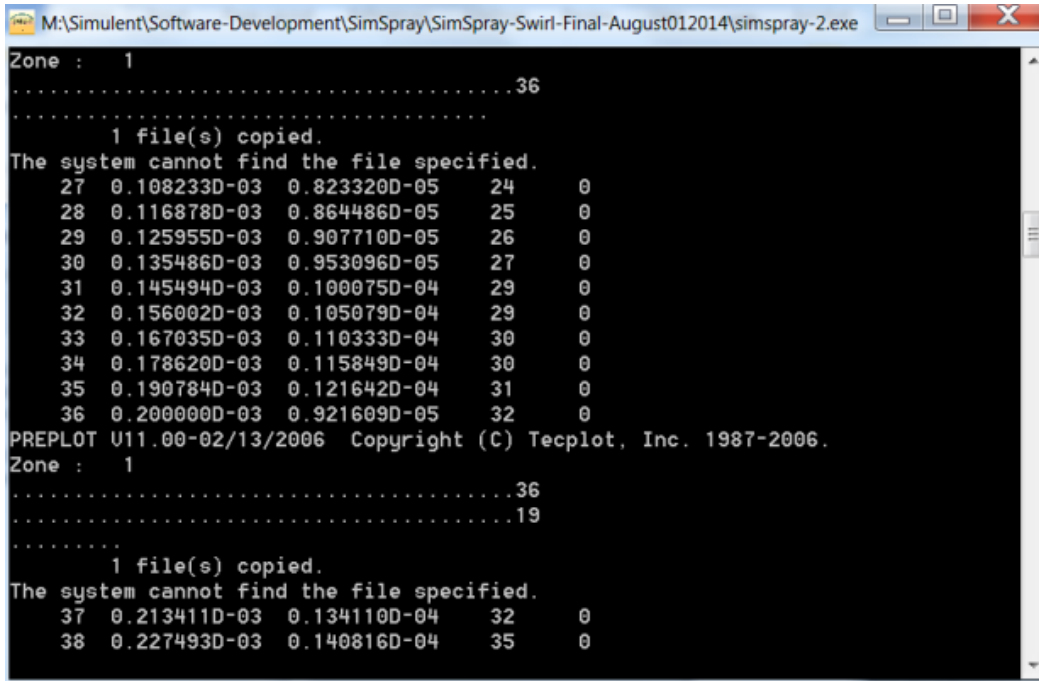
**Figure (3-7) Monitoring Dos Window**

- **Column 1:** The first colum shows the number of cycles during simulation. Each cycle is an indication of one time step forward.

- **Column 2:** The second column shows the total time of simulation. (SimSpray is a time dependent algorithm to simulate the fluid flow proceeding inside the spray nozzle.)

- **Column 3:** The third column shows the current time step. Please note that the time steps change during the simulation. For more information, please see the References introduced at the beginning of present Chapter. When the time step is decreasing monotonically, it could be some instability in simulations.

- **Column 4:** In this column the total number of iterations in pressure solver is shown. The maximum allowed iteration is 1000.

- **Column 5:** The number shown in this column is an error number to indicate if the simulation is error free or if there is an error.  Number "0" indicates the simulations are performed correctly. Any other number indicates a problem in simulations.



**Figure (3-8) Output Formats on DOS screen**

### 3.5 TecPlot

When simulations are completed, you are asked to click on TecPlot to post process the data. You may do it while you are still in the program environment or you may exit the program and run the post processing later. If you close the Dos window during the execution of the program to terminate the simulation, the main SimSpray window will be closed as well.

### 3.6  Output Files

SimSpray software generates different output files that are saved in two locations. The majority of files are saved in the folder that is selected by User before starting the simulation, see Section 3.3.4.   We call this folder as the "**Working Directory**". Some of the files will be saved in subfolder **Plotfiles**, which is generated when the simulation starts. This subfolder is located in Working Directory.

### 3.6.1   Working Directory

This is the list and functions for all output files that are saved in this folder:

- **Inputw.txt**: This is the summary of the input data that are given to the code. You may check this file to confirm the input data is correct.

- **Obstacle.plt & Obstacle-iso.plt**: This file that can be post process by TecPlot shows the complete geometry of the nozzle.

- **f.xxxx.plt** : These output files are generated in time sequences based on the value of time interval (we name it: PLTDT) entered in the Input Page. The files are named *f.0000.plt* (corresponding to Time=0), *f.0001.plt* (corresponding to Time=PLTDT), *f.0002.plt* (corresponding to Time=2 PLTDT), and so on.

  These files include all information regarding the flow in the computational cells: location of each cell, liquid volume fraction, velocity in three directions, and pressure and will be used for post processing purpose by TecPlot. The files are first written in ASCII format and during the execution of the code are transformed automatically to TecPlot Binary format. This is done in order to save the disc space and also because loading files into TecPlot would be much faster with the Binary format.

- **Dump.xxxx**: These output files are generated in time intervals based on the values you specified in Input page for "Time interval to write the dump files". The files are

named: *dump.0000* (corresponding to Time=0), *dump.0001* (corresponding to the first time interval), *dump.0002* (corresponding to the second time interval), and so on. The files are in ASCII format and include all necessary information to re-start a simulation or later in SimData module.  Since they are not used for post processing, the time intervals you specify for these files can be much larger than the *f.xxxx* files. Usually you need the last dump file generated by SimSpray to run the SimData module.

- **Error**: Most of the warning and error messages during the program execution are written in this file. This file can be reviewed for diagnostic purposes if a crash happens during the run time.

- **Out**: This is an ASCII file that shows the grid information for simulation. Also all output information that is written in the DOS window is recorded in this file as well.

### 3.6.2   PlotFiles Folder

This is the list and functions for all output files that are saved in the PlotFiles folder:

- **Fav.xxxx.plt:** The "f.xxxx" files generated in the previous step include data for the whole liquid volume. To only display the shape of the liquid free surface and the nozzle body, the iso-surfaces from the volume fraction files for both liquid and solid volumes are extracted and save separately.

  To make this process automatic, two TecPlot macro files are provided with the code (*extract-obs.mcr* and *extract-fav.mcr*). The first macro file, "*extract-obs.mcr*", is called at the beginning of the program to make an iso-surface of the nozzle body. This file is called "Obstacle-iso.plt" which is saved in the Working Directory.

  The second macro file, "*extract-fav.mcr*", however, is called by the code each time an output file (*f.0000.plt*, *f.0001.plt*, etc.) is generated in the main directory. When the macro files are running, you will see Tecplot commands and working process on

the *DOS* window. The iso-surface display files are named *fav.0000.plt*, *fav.0001.plt*, *fav.0002.plt*, etc., written at the same time as for files *f.0000.plt*, *f.0001.plt*, *f.0002.plt*, etc,. These files show the combined iso-surface images of the spray nozzle geometry and the liquid and are mostly useful for presentation purposes.

***Note: In case the "fav.xxxx" files are not created automatically, once the simulations are completed, open TecPlot and play "make-fav.mcr". The macro creates "fav.xxxx.plt" files. This macro must be located in the working directory, where all "f.xxxx.plt" are located.***

## 4. SIMDATA

This Chapter is a short Manual of SimData, Module to analyze the SimSpray software results and predicts the primary break up at the exit of the splash plate nozzle.

The results of **SimSpray** computer program include all necessary information regarding the liquid location, velocity and pressure in the whole computational domain. In order to get specific data from these results such as the distribution of film thickness, film velocity and spray flow, Simulent Inc. has developed another computer program module that automatically provides this information from **SimSpray** output files. The developed program module for predicting the primary break up is called **SimData** (**Sim**Spray **D**rop **A**nd **T**hickness **A**nalyzer)**.**

In this module the mean droplet size and velocity of the spray are predicted from the results of SimSpray code, using analytical models for the prediction of the droplet sizes that use the local liquid sheet thickness and velocity. The analytical models used is based on the empirical models suggested by different researchers for pressure swirl nozzles.

These analytical models are coupled with **Simspray**, such that the local liquid sheet thickness and velocity is directly fed into the analytical model, and a mean droplet size is provided.

### 4.1 Linear Instability Analysis

The analytical models used in this module are mostly based on the linear instability analysis, suggested by many researches, such as Senecal et al[2]. A linear stability analysis is presented for a liquid sheet that includes the effects of the surrounding gas, surface tension and the liquid

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[2] - P.K. Senecal, D.P. Schmidt, I. Nouar, C.J. Rutland, R.D. Reitz, M.L. Corradini; "Modeling High Speed Viscous Liquid Sheet Atomization"; International Journal of Multiphase Flow 25 (1999) 1073-1097

viscosity on the wave growth process. It is, then, useful to have an overview of this model before we start explaining the software.

In order to model the drop formation process, one must postulate a mechanism of sheet breakup and pose a mathematical formulation of this mechanism. Many researchers have speculated that the drop sizes may be correlated with the wavelengths that grow on the surface of the sheet. They identified the wavelength with the largest growth rate and assumed that this wave broke up the sheet at half wavelength intervals into ligaments. One of the explanations is that the ligaments break up into droplets, according to Weber's theory for a cylindrical liquid column, as shown in Figure (4-1).
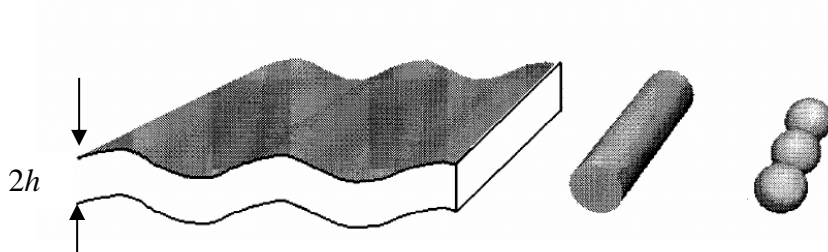


**Figure (4-1)  Schematic of the sheet disintegration and drop formation processes as proposed by Dombrowski and Johns (1963)**

Based on an inviscid model equation and the critical Weber number for the transition from long to short wave growth, it has shown that the long wave regime is dominant for low-speed sheet atomization, while short waves are responsible for breakup in the case of high-speed sheets. According to Senecal et al, this critical Weber number, $W_e$, is 1.68. The Weber number in this case is calculated from:

$$W_e = \frac{\rho_G U^2 h}{\sigma}$$

Where $\rho_G$ is the density of the gas, $U$ is the relative velocity between the liquid sheet and the surrounding gas, $h$ is the half thickness of the sheet (see Figure 4-1), and $\sigma$ is the surface tension between the gas and the liquid.

The simplified wave growth rate, $\omega_r$, for the sinuous mode is given by:

$$\omega_r = -\frac{2v_l k^2 \tanh(kh)}{\tanh(kh)+Q} + \frac{\sqrt{4v^2_l k^4 \tanh^2(kh) - Q^2 U^2 k^2 - [\tanh(kh)+Q](-QU^2 k^2 + \sigma k^3 / \rho_l)}}{\tanh(kh)+Q}$$

Where, $v_l$ is the kinematic viscosity of the liquid, $k$ is the wave number, $\rho_l$ is the liquid density, and $Q = \rho_G / \rho_l$ is the density ratio of the gas to the liquid. Furthermore, if short waves are assumed for high-speed sheets and in the limit of $Q \ll 1$ the above equation reduces to:

$$\omega_r = -2v_l k^2 + \sqrt{4v^2_l k^4 + QU^2 k^2 - \sigma k^3 / \rho_l}$$

For the above equations, the most unstable wave number, $K_S$, at which the growth rate is maximum, $\Omega_S$, can be obtained either algebraically or numerically.

According to Senecal for short waves the sheet will break up at a length, $L_b$, given by:

$$L_b = \frac{V}{\Omega_S} F_A$$

Where, $V$ is the absolute velocity of the liquid sheet at break up point and $F_A$ is an empirical parameter. Different values for this quantity have been offered by many researchers, depending on the Reynolds number. In this work we have used a quantity that was offered by Ashgriz et al which also depends on the nozzle diameter and jet velocity in the nozzle.

Furthermore, ligaments are assumed to form from the sheet fragments at the point of breakup and their diameter can be obtained from a mass balance. For the case of short waves it is

assumed that the ligaments are formed from tears in the sheet once per wavelength, and the resulting diameter, $d_L$ is, thus, given by

$$d_L = \sqrt{\frac{16h}{K_S}}$$

For long waves though, the sheet break up length, $L_b$, can be obtained from:

$$L_b = V(3F_A)^{2/3} \left( \frac{J\sigma}{Q^2 U^4 \rho_l} \right)^{1/3}$$

Where $J$ is a constant that can be obtained from $h = J/t$, knowing the sheet thickness at any given time, $t$. $V$ and $U$ are once again the absolute sheet velocity and liquid/gas relative velocity, respectively. In addition, the most unstable wave number, $K_S$, for long waves is given by:

$$K_S = \frac{\rho_G U^2}{2\sigma}$$

The ligament diameter for long wave growth can be obtained from:

$$d_L = \sqrt{\frac{8h}{K_S}}$$

In both cases, long and short waves, the drop diameter can be obtained from:

$$d_D = 1.88 d_L (1 + 3 Ohh)^{1/6}$$

where $Oh$ is the Ohnesorge number.

## 4.2 Preparations

Before you start modeling the primary break-up with SimData models, you have to completed a simulation with SimSpray module and have the following files:

- One of the last "dump.xxxx" files form SimSpray simulation. This file must correspond to the time that the fluid flow inside the nozzle is basically fully developed and steady.

- Nozzle geometry mesh file, e.g., SOLID.DAT.

- Boundary conditions file, BC.DAT.

It is recommended that you save all above files (correspond to the same nozzle and simulations) in a specific folder to avoid mixing up the output files.

## 4.3 Software Overview

In the working directory of SimData module, double click on SimData2-1.exe. By clicking on the executable file a welcoming page, as shown in Figure (4-2), opens. On the top menu of the main page, you can see **Input**, **Start**, **Results**, **TecPlot**, and **Exit**.
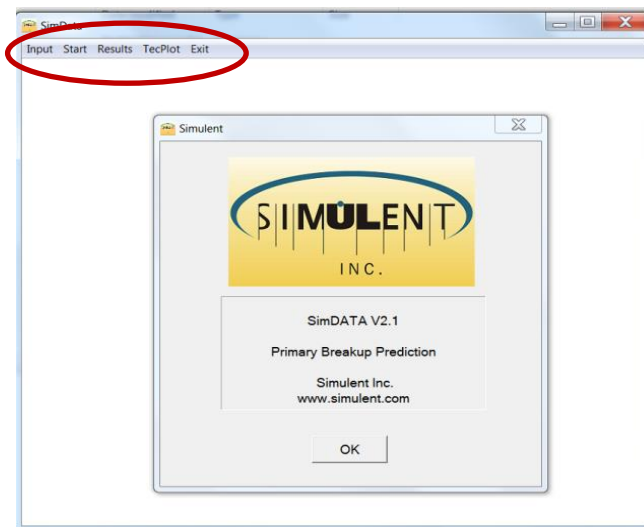


**Figure (4-2) Welcome window for SimData Module**

You can then click on "**Input**" to start data entry. By clicking on the **OK**, this introductory window is closed. At any time, you calick on **Exit** to close the program.

**4.4 Input Page**

From Input Page, as shown in Figure (4-3), you can enter the parameters and files used by the code. All the information entered through this page is saved in a file: Input-Drop.txt. A default copy of this file exists in the Root directory. Each time you run the Module, a new version of this file, containing input information for each project will be saved. The second copy of this file will be saved in your working directory.
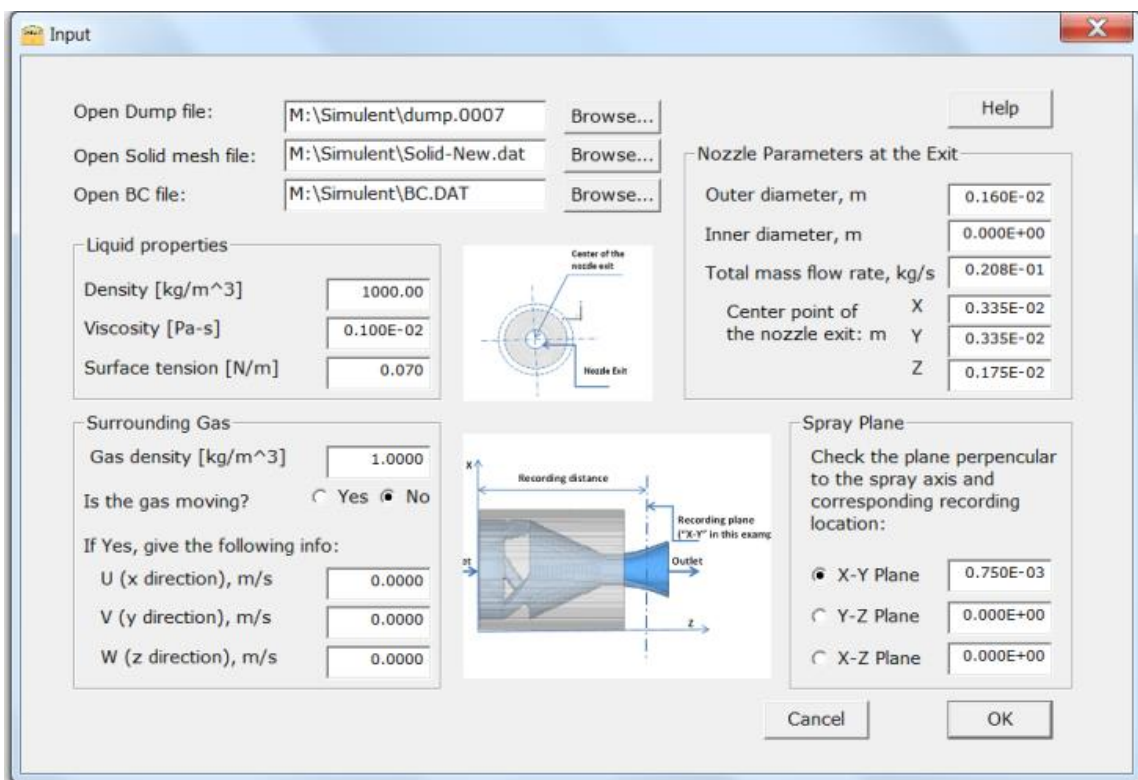


**Figure (4-3) Input interface page for SimData Module**

**4.4.1   Open Files**

In this section, you are prompt to open the following files:

- Last dump file created by **SimSpray** module,

- The solid mesh file (here Solid.dat) and;

- The boundary conditions file (BC.dat).

Browse for these files that you have already copied them in your working directory.

### 4.4.2 Liquid Properties

You need to also specify the liquid properties here. Use the same liquid properties that you used in **SimSpray** simulation. These properties are: the density, viscosity and surface tension for the liquid.

### 4.4.3 Surrounding Gas:

If your spray nozzle is spraying liquid within an environment with moving gases (like a boiler), few information about the gas flow inside the boiler is also required. These are:

- First you need to specify if you have surrounding gas or not. If the answer is **Yes**, the effect of the gas velocity in the boiler on the break up mechanism will be considered in the modeling.

- Gas density of the gas, $kg/m^3$.

- Gas velocity component in the "x" direction, m/s.

- Gas velocity component in the "y" direction, m/s.

- Gas velocity component in the "z" direction, m/s.

### 4.4.4   Nozzle Parameters at the Exit

In this section the specifications of the swirl nozzle is given to the code. In Figure (4-4), an example of such nozzle and the definitions are presented.

- Nozzle outer diameter at the exit. Depending on the type and design of the nozzle, the exit of the nozzle can be a complete circle, see Figure (4-4) or it could be an annular shape. In case of a complete circle, the diameter of the circle must be given here. For annular shape, the outer diameter is given here.

- Nozzle inner diameter. For a complete circle, this diameter must be given zero. For an annular circle, the inner diameter is given in this section.

- In the third section, the total mass flow rate of the liquid (kg/s) is given.

- Finally, the coordination of the center of the nozzle exit must be given. To get this information, you can open the "**Obstacle.plt**" file from the **SimSpray** simulation by TecPlot and then obtain the "X", "Y", and "Z" location of the center.
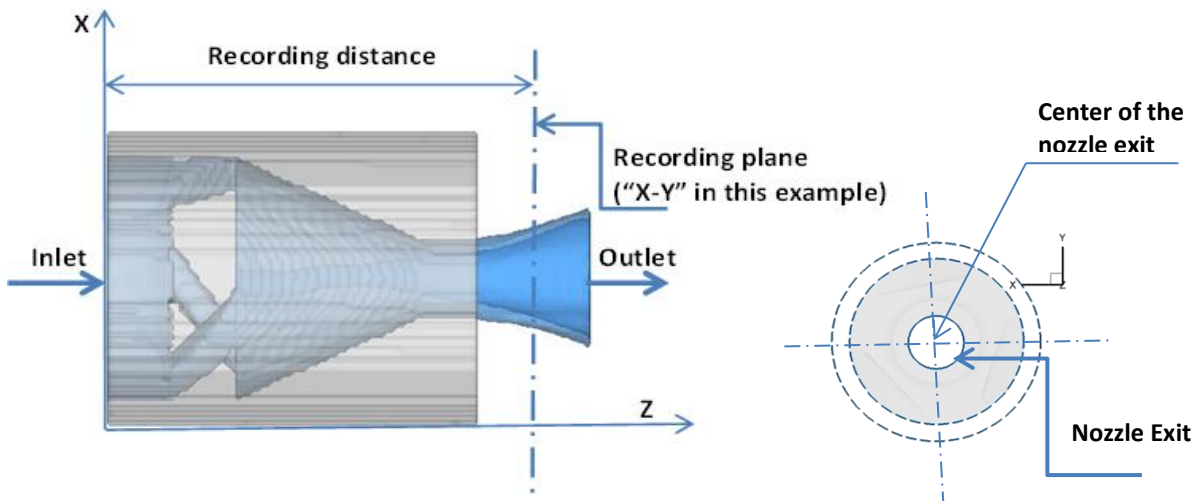


**Figure (4-4) Sample of a pressure swirl nozzle and used definitions. The right image shows the exit of the nozzle which is not to scale.**

### 4.4.5   Spray Plane

The liquid sheet thickness of the spray is measured in a plane perpendicular to the spray axis. The location of this plane is arbitrary, but should not be very far from the nozzle exit (it is in order of millimetres).

- Based on the geometry of the nozzle and the simulation results from SimSpray, this plane needs to be specified here, please see Figure (4-4).  For example in this Figure, the plane at which the sheet thickness is measured is perpendicular to the Z axis, i.e., X-Y plane.

- Next the distance of this plane from the center of the origin must be given. You may use TecPlot to examine one of the lasts files (**f.xxxx.plt**) along with the geometry file (**Obstacle.plt**), to determine the location of the measurement. Or one of the last "**fav.xxxx.plt**" files that contain both files may be examined for this purpose.

### 4.5 Start

Once you finished data entry, click on **OK**.  You are then asked to click on **Start** and select the working directory to store the data.  By selecting the working directory calculation starts and a message soon tells you that it is completed.

At any time while you are on the main page, you can click on **TecPlot** to examine the geometry and other TecPlot files.

### 4.6 Results

From the main page, you can click on **Results** to check the average Drop sizes based on different models or check the mass flow distribution in the liquid sheet, see Figure (4-5). Please note that on the plane perpendicular to the spray outlet, the area is divided to 36 equal segments (each segment 10 degrees) to cover the whole spray area. The locations are moving anti clockwise, with respected to view direction, see Figure (4-6).  Therefore, for each type of data/parameter there would be 36 sets of data.
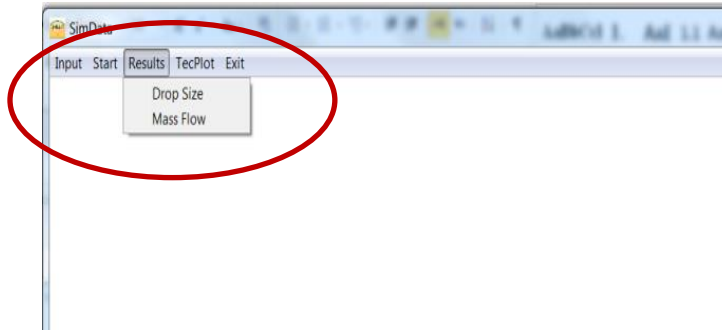
**Figure (4-5) Open the Results files.**
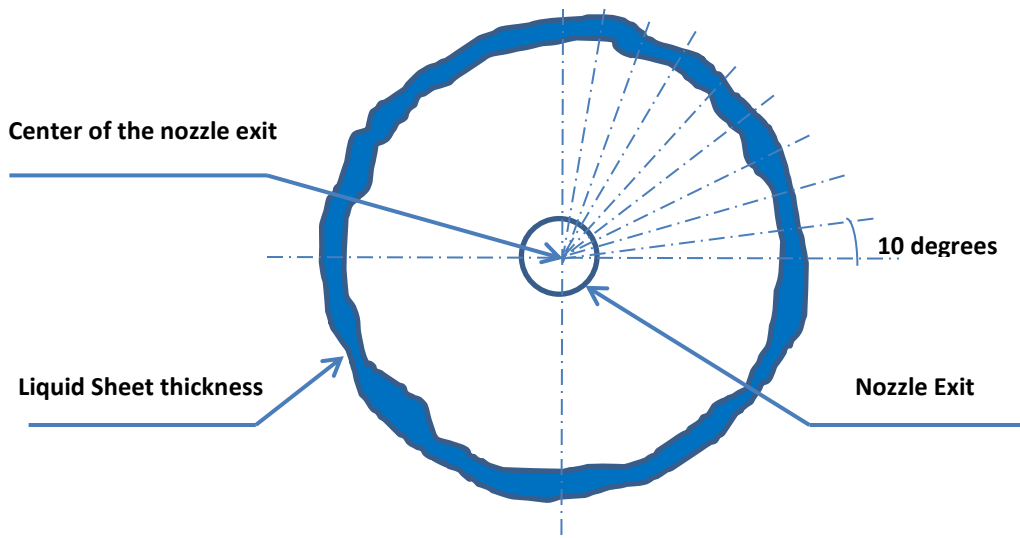


**Figure (4-6) Nozzle exit, sheet thickness and drop size distribution locations.**

### 4.6.1 Drop Size Distribution

By selecting Drop Size option, the file "Drop-Size.DAT" will be opened which has the general format as shown in Figure (4-6). The first line indicates which plane the data has been recorded. In this example since the spray nozzle axis is the "Z" axis, the recording data is done in X-Y plane. The second line is heading with nine columns and the rest of the data are divided in these nine columns.

- The first and second columns indicate the starting and ending angles of the segments.

- The third column shows the average velocity of the liquid sheet within that segment (Film velocity), in m/s.

- The forth column shows the average liquid film thickness in that segment, in mm

- Columns 5 to 9 show the calculation results for the average drop size within that segment, based on different theories, all in mm:

  ➢ Column 5 is the average $D_{30}$ (volumetric) drop size for inviscid liquids for Weber Number << 1, based on Squire model[3]. Weber Number is calculated as $\sigma/(\rho\ V^2\ t)$. Where $\sigma$ is the surface tension, V is the relative velocity between gas and liquid, and t is the half thickness of the sheet. When Weber Number is greater than one, the drop size is recorded as zero.

  ➢ Column 6 is average $D_{30}$ drop size for inviscid liquids for Webber Number >>1, based on York et al. model[4].  When Weber Number is less than one, the drop size is recorded as zero.

  ➢ Column 7 is average $D_{30}$ drop size for viscous liquids, based on Senecal et al. model[5].

  ➢ Column 8 is average $D_{30}$ drop size for viscous liquids, based on Clark and Dombrowski model[6], which is dependent on the Reynolds number of the liquid as well.

  ➢ Column9 is average $D_{30}$ drop size for viscous liquids, based on Dombrowski and Johns model[7], who developed a correlation for dominant wave length from a set of experiments with conical sprays.

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[3] H.B. Squire; British Journal of Applied Physics, 1953, **4-**167.

[4] J.L. York, H.E.  Stubbs, M.R.  Tek; Transactions of the ASME, 1953, 1279.

[5] P.K. Senecal, D.P. Schmidt, I. Nouar, C.J. Rutland, R.D. Reitz, M.L. Corradini; International Journal of Multiphase Flow, 1999, **25-**1073.

[6] C.J. Clark, N. Dombrowski; Proceeding of Royal Society of London A; 1972, **329-**467.

[7] N. Dombrowski, W.R. Johns; Chemical Engineering Science, 1963, **18-**203.

The cross section is in X-Y Plane

| ANGLE1 | ANGLE2 | VFILM [m/s] | TFILM [mm] | D30_SQUIR [mm] | D30_YORK [mm] | D30_SEN [mm] | D30_CLARK [mm] | D30_DOM [mm] |
|---|---|---|---|---|---|---|---|---|
| 0.0 | 10.0 | 17.592 | 0.194 | 2.473 | 0.000 | 0.374 | 0.645 | 1.039 |
| 10.0 | 20.0 | 17.332 | 0.185 | 2.498 | 0.000 | 0.383 | 0.648 | 1.039 |
| 20.0 | 30.0 | 16.987 | 0.117 | 2.047 | 0.000 | 0.327 | 0.541 | 0.907 |
| 30.0 | 40.0 | 16.231 | 0.223 | 2.983 | 0.000 | 0.395 | 0.656 | 1.162 |
| 40.0 | 50.0 | 16.854 | 0.226 | 2.735 | 0.000 | 0.375 | 0.647 | 1.117 |
| 50.0 | 60.0 | 18.824 | 0.093 | 1.472 | 0.000 | 0.261 | 0.473 | 0.756 |
| 60.0 | 70.0 | 17.741 | 0.183 | 2.196 | 0.000 | 0.305 | 0.555 | 0.986 |
| 70.0 | 80.0 | 17.555 | 0.187 | 2.150 | 0.000 | 0.313 | 0.574 | 0.986 |
| 80.0 | 90.0 | 16.890 | 0.184 | 2.083 | 0.000 | 0.326 | 0.596 | 0.986 |
| 90.0 | 100.0 | 16.180 | 0.089 | 1.409 | 0.000 | 0.264 | 0.476 | 0.778 |
| 100.0 | 110.0 | 15.881 | 0.141 | 1.713 | 0.000 | 0.315 | 0.578 | 0.902 |
| 110.0 | 120.0 | 15.481 | 0.091 | 1.340 | 0.000 | 0.261 | 0.480 | 0.779 |
| 120.0 | 130.0 | 15.064 | 0.207 | 2.012 | 0.000 | 0.335 | 0.629 | 1.032 |
| 130.0 | 140.0 | 15.745 | 0.220 | 1.985 | 0.000 | 0.329 | 0.632 | 1.024 |
| 140.0 | 150.0 | 17.783 | 0.090 | 1.109 | 0.000 | 0.233 | 0.465 | 0.698 |
| 150.0 | 160.0 | 17.029 | 0.169 | 1.477 | 0.000 | 0.263 | 0.542 | 0.865 |
| 160.0 | 170.0 | 16.038 | 0.178 | 1.588 | 0.000 | 0.279 | 0.561 | 0.912 |
| 170.0 | 180.0 | 14.955 | 0.205 | 1.812 | 0.000 | 0.330 | 0.643 | 0.998 |
| 180.0 | 190.0 | 14.714 | 0.090 | 1.214 | 0.000 | 0.264 | 0.499 | 0.765 |
| 190.0 | 200.0 | 14.831 | 0.155 | 1.577 | 0.000 | 0.332 | 0.635 | 0.912 |
| 200.0 | 210.0 | 15.144 | 0.115 | 1.333 | 0.000 | 0.304 | 0.580 | 0.815 |
| 210.0 | 220.0 | 14.912 | 0.186 | 1.727 | 0.000 | 0.343 | 0.660 | 0.967 |
| 220.0 | 230.0 | 16.171 | 0.206 | 1.725 | 0.000 | 0.337 | 0.668 | 0.957 |
| 230.0 | 240.0 | 17.649 | 0.203 | 1.594 | 0.000 | 0.299 | 0.619 | 0.904 |
| 240.0 | 250.0 | 18.753 | 0.191 | 1.476 | 0.000 | 0.269 | 0.574 | 0.854 |
| 250.0 | 260.0 | 18.916 | 0.202 | 1.580 | 0.000 | 0.301 | 0.628 | 0.880 |
| 260.0 | 270.0 | 19.037 | 0.105 | 1.186 | 0.000 | 0.251 | 0.505 | 0.716 |
| 270.0 | 280.0 | 19.415 | 0.153 | 1.451 | 0.000 | 0.309 | 0.617 | 0.809 |
| 280.0 | 290.0 | 19.299 | 0.189 | 1.690 | 0.000 | 0.340 | 0.670 | 0.884 |
| 290.0 | 300.0 | 19.093 | 0.147 | 1.558 | 0.000 | 0.321 | 0.615 | 0.828 |
| 300.0 | 310.0 | 17.853 | 0.232 | 2.161 | 0.000 | 0.357 | 0.675 | 1.018 |
| 310.0 | 320.0 | 18.684 | 0.256 | 2.212 | 0.000 | 0.360 | 0.693 | 1.028 |
| 320.0 | 330.0 | 20.801 | 0.138 | 1.496 | 0.000 | 0.282 | 0.556 | 0.785 |
| 330.0 | 340.0 | 19.747 | 0.175 | 1.898 | 0.000 | 0.294 | 0.563 | 0.900 |
| 340.0 | 350.0 | 18.772 | 0.270 | 2.568 | 0.000 | 0.364 | 0.676 | 1.088 |
| 350.0 | 360.0 | 17.786 | 0.149 | 2.085 | 0.000 | 0.321 | 0.563 | 0.936 |

**Figure (4-6) The format of Drop-Size.DAT file**

### 4.6.2   Mass Flow Rate distribution

By selecting Mass Flow option, the file "Spray.DAT" will be opened which has the general format as shown in Figure (4-7). This file shows the mass flow rate distribution of the spray in a 360 angle which can be a good indication how efficient the nozzle design is.

The first line is heading with 4 columns and the rest of the data are divided in these 4 columns.

- The first and second columns indicate the starting and ending angles of the segments.

- The third column shows the mass flow rate passing that specific segment in kg/s.

- The forth column shows the percentage of the total mass flow rate passing through the specific segment.

Please note due to the numerical errors, the total mass flow rate calculated for the whole domain may be slightly different with the total mass flowrate indicated by user.

| ANGLE1 | ANGLE2 | Mass Dist.[kg/s] | % Mass Flow |
|--------|--------|------------------|-------------|
| 0.00 | 10.00 | 0.635E-03 | 3.051 |
| 10.00 | 20.00 | 0.580E-03 | 2.787 |
| 20.00 | 30.00 | 0.361E-03 | 1.737 |
| 30.00 | 40.00 | 0.689E-03 | 3.314 |
| 40.00 | 50.00 | 0.748E-03 | 3.594 |
| 50.00 | 60.00 | 0.328E-03 | 1.579 |
| 60.00 | 70.00 | 0.657E-03 | 3.160 |
| 70.00 | 80.00 | 0.658E-03 | 3.162 |
| 80.00 | 90.00 | 0.611E-03 | 2.935 |
| 90.00 | 100.00 | 0.276E-03 | 1.327 |
| 100.00 | 110.00 | 0.414E-03 | 1.992 |
| 110.00 | 120.00 | 0.264E-03 | 1.269 |
| 120.00 | 130.00 | 0.598E-03 | 2.877 |
| 130.00 | 140.00 | 0.684E-03 | 3.286 |
| 140.00 | 150.00 | 0.307E-03 | 1.475 |
| 150.00 | 160.00 | 0.569E-03 | 2.737 |
| 160.00 | 170.00 | 0.571E-03 | 2.747 |
| 170.00 | 180.00 | 0.590E-03 | 2.836 |
| 180.00 | 190.00 | 0.247E-03 | 1.185 |
| 190.00 | 200.00 | 0.412E-03 | 1.982 |
| 200.00 | 210.00 | 0.305E-03 | 1.467 |
| 210.00 | 220.00 | 0.505E-03 | 2.430 |
| 220.00 | 230.00 | 0.613E-03 | 2.947 |
| 230.00 | 240.00 | 0.687E-03 | 3.301 |
| 240.00 | 250.00 | 0.708E-03 | 3.402 |
| 250.00 | 260.00 | 0.719E-03 | 3.455 |
| 260.00 | 270.00 | 0.373E-03 | 1.792 |
| 270.00 | 280.00 | 0.524E-03 | 2.519 |
| 280.00 | 290.00 | 0.639E-03 | 3.072 |
| 290.00 | 300.00 | 0.485E-03 | 2.333 |
| 300.00 | 310.00 | 0.769E-03 | 3.696 |
| 310.00 | 320.00 | 0.909E-03 | 4.371 |
| 320.00 | 330.00 | 0.527E-03 | 2.534 |
| 330.00 | 340.00 | 0.669E-03 | 3.217 |
| 340.00 | 350.00 | 0.984E-03 | 4.733 |
| 350.00 | 360.00 | 0.513E-03 | 2.465 |

**Figure (4-7) Mass flow rate distribution**

## 5. APPENDIX: DROPLET DISTRIBUTION FUNCTION

The droplet distribution function according to Li and Tankin[8] can be described as follows:

$$\frac{dN}{dD} = \frac{\pi}{2}\frac{\rho_l \dot{n}}{\dot{m}_l} D^2 \exp\left(-\frac{\pi}{6}\frac{\rho_l \dot{n}}{\dot{m}_l} D^3\right) \tag{1}$$

Where $\rho_l$ is the density of the liquid, $\dot{n}$ is the total number of droplets produced per unit time, and $\dot{m}_l$ is the liquid mass flow rate. This distribution has been obtained based on a Nukiyama-Tanasawa Distribution model, using the concept of Maximum Entropy Formalism.

From the definition of volume (or mass) mean droplet, $D_{30}$, one has:

$$D_{30} = \sqrt[3]{\frac{\sum_{i=1}^{N} D_i^3}{N}} \tag{2}$$

(Note that based on the linear instability analysis, the average droplet size that is calculated is the mass mean diameter of droplets). The above equation can be re-written as:

$$D_{30}^3 = \lim n \to \infty \left(\frac{\int_0^n D^3 \, dN}{\int_0^n dN}\right) \tag{3}$$

Eq. (1) can be substituted in Eq. (3) to give:

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[8] Li X., and Tankin R.S., *Combust. Sci. Technol*, 1987, 56, p65.

$$D_{30}^3 = \frac{\int\limits_0^\infty \frac{\pi}{2} \frac{\rho_l \dot{n}}{\dot{m}_l} D^5 \exp\left(-\frac{\pi}{6} \frac{\rho_l \dot{n}}{\dot{m}_l} D^3\right) dD}{\int\limits_0^\infty \frac{\pi}{2} \frac{\rho_l \dot{n}}{\dot{m}_l} D^2 \exp\left(-\frac{\pi}{6} \frac{\rho_l \dot{n}}{\dot{m}_l} D^3\right) dD} \tag{4}$$

Using the definition of Gamma Function, i.e.:

$$\Gamma(x) = \int\limits_0^\infty t^{x-1} \exp(-t) dt \tag{5}$$

One can find that Eq. (4) can be re-written as:

$$D_{30}^3 = \frac{\left(\frac{6}{\pi} \frac{\dot{m}_l}{\rho_l \dot{n}}\right) \Gamma(2)}{\Gamma(1)} \tag{6}$$

From Eq. (6), the term $\left(\frac{\pi}{6} \frac{\rho_l \dot{n}}{\dot{m}_l}\right)$ can be calculated as:

$$\frac{\pi}{6} \frac{\rho_l \dot{n}}{\dot{m}_l} = \frac{1}{D_{30}^3} \frac{\Gamma(2)}{\Gamma(1)} \tag{7}$$

And Eq.(1) or the distribution function can be written in terms of the mass mean diameter. i.e.:

$$\frac{dN}{dD} = \frac{3}{D_{30}^3} \frac{\Gamma(2)}{\Gamma(1)} D^2 \exp\left(-\frac{\Gamma(2)}{D_{30}^3 \Gamma(1)} D^3\right) \tag{8}$$

Considering that $\Gamma(2) = \Gamma(1) = 1$, Eq.(8) can be simplified to:

$$\frac{d\,N}{d\,D} = \frac{3}{D_{30}^3} D^2 \exp\left(-\frac{D^3}{D_{30}^3}\right) \tag{9}$$

This means by only knowing the mass mean diameter of droplets in any section (angle) of the splash plate, one can determine the droplet distribution function for that section. A sample of such distribution is shown in Figure A.1.
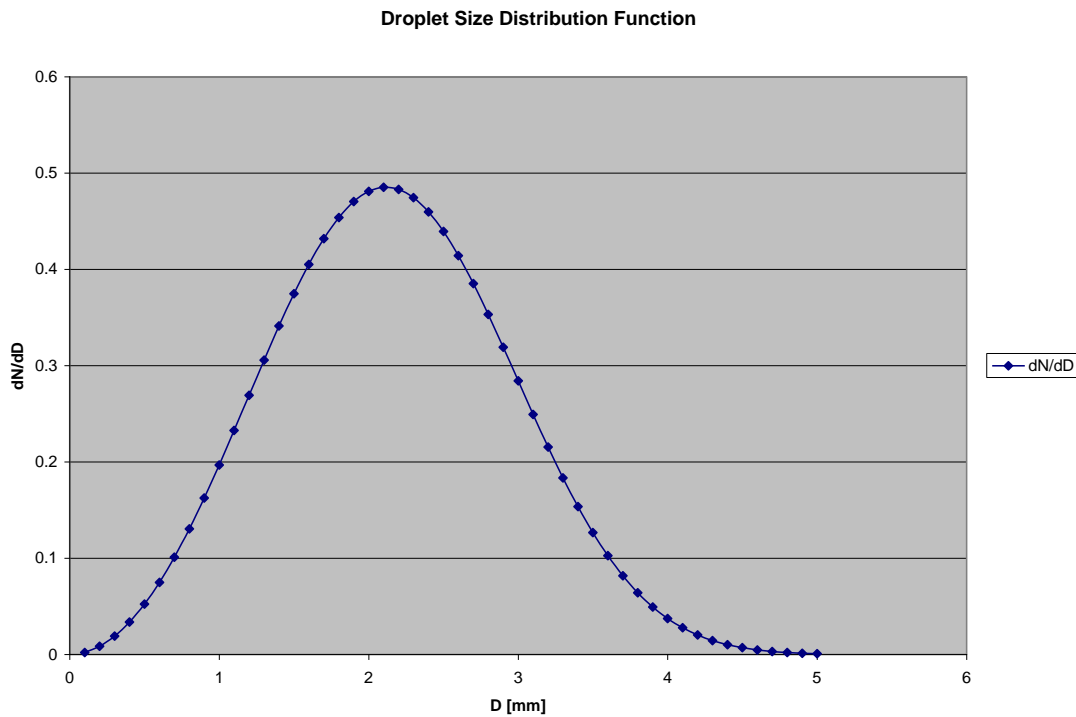


**Figure A.1. Droplet Size Distribution based on Li and Tankin Model, using mean diameter of $D_{30}$ = 2.422 mm.**

An interesting result that can be concluded from Li-Tankin model is the relation between Sauter Mean Diameter and mass mean diameter. According to definition, the Sauter Mean Diameter (SMD) or $D_{32}$, is:

$$SMD = \frac{\int\limits_{0}^{\infty} D^3 \, dN}{\int\limits_{0}^{\infty} D^2 \, dN} \qquad\qquad (10)$$

By substituting Eq.(1) in Eq.(10) and using the definition of gamma Function, one can find that:

$$SMD = \left(\frac{6\dot{m}_l}{\pi \rho_l \dot{n}}\right)^{1/3} \frac{\Gamma(2)}{\Gamma(\frac{5}{3})} \qquad\qquad (11)$$

By combining Eq.(6) and Eq.(11), one can see that:

$$SMD = D_{30} \Big/ \Gamma(5/3) = \frac{D_{30}}{0.9027} \qquad\qquad (12)$$

Of course the above equation is only valid when it is assumed that the distribution function has the form of Li-Tankin function.