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COMPUTATIONAL MODELING OF GAS LIQUID INTERFACES USING DIFFERENT MULTIPHASE MODELS.

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Abstract

A time dependent Computational Fluid Dynamics analysis of gas jets impinging onto liquid pools has been conducted. The aim of the study is to obtain a better understanding of highly complex, and industrially relevant flows in jetting system. Three different multiphase models, i.e., The Eulerian model, the volume of fluid model and the mixture model are used to analyze the surface deformations namely dimpling, splashing and penetration. The Standard k-ε model is used to incorporate the Turbulence in the continuous phase. Two-dimensional axisymmetric geometries with different dimensions have been used in the study. Simulations are performed using commercial CFD code Fluent 6.1. PISO (pressure- implicit with splitting of operators) algorithm was employed to compute the pressure velocity coupling. The computed results are compared with experimental and theoretical data reported in the literature. Also the results of the study highlight and compare the discrepancies between the three multiphase models in capturing the flow structure and cavities formed at gas-liquid interfaces.

NOMENCLATURE

C Vertical distance from nozzle exit to undisturbed liquid free surface. [m]
d_c cavity diameter. [m]
h_c cavity depth [m]

h_L Lip height.
H undisturbed liquid height in the receiving pool [m]
D nozzle diameter [m]
D Vessel diameter [m]
U_{inlet} gas jet inlet velocity [m]

1. INTRODUCTION

The metallurgical industry is one that demands a superior level of efficiency for processing operations in order to minimize material and operating costs whilst maximizing productivity. To fulfill such requirements, it is necessary to collect the information directly or indirectly affecting the process system, and subsequently have the opportunity to react in real time to any potentially unproductive anomalies, which may arise. The injection of gas streams into molten metals is used extensively in the process metallurgical industry as a means of refining and agitation e.g. Oxygen steel making, vacuum degassing, argon agitated ladles, top blown copper converting and as a method of contracting gas and liquid phases.

Most of the steel making processes involve gas jetting ;(1) Gas jetting is used in steel making process involving top blowing e.g. LD (Linz-Donawitz) converter. This process is widely used and stands for 60% of the total world steel production. The main principle of the LD process is to reduce, by oxidation and the contents of Mn, C, Si and Fe in the molten metal. In the LD converter, oxygen is jetted onto the liquid iron surface from the top, through lance, at supersonic speed. When blown oxygen strikes the steel melt a cavity is formed on the liquid surface. The chemical reaction takes place both in the cavity and in the foam or slag that is produced in the process. The slag contains bubbles and provides a large surface area for the oxidation. The depth and diameter of the cavity, heat and mass transport at the interface and in the liquid, are important parameters in the process. (2) The interaction of liquid steel and an inclined impinging oxygen jet in an electric arc furnace is of interest both commercially and scientifically. (3)In both the acid Bessemer and Basic Bessemer Processes of steel making Molten pig iron is refined by blowing air through it in an egg shaped vessel,known as a converter.In the interaction area between the gas and liquid, a cavity is formed, where some of the oxidation occurs, The gas travels racially outwards from the impact point thereby dragging the liquid into motion and setting up a recirculation flow with in the bulk as shown in Fig.1

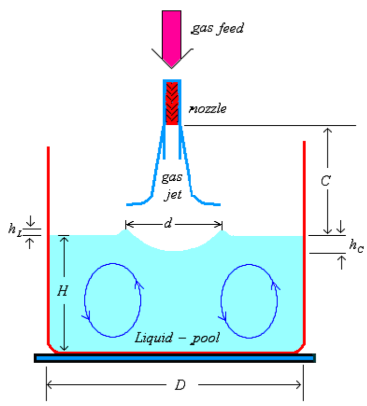

Fig.1 Gas Jet impinging onto liquid pool.

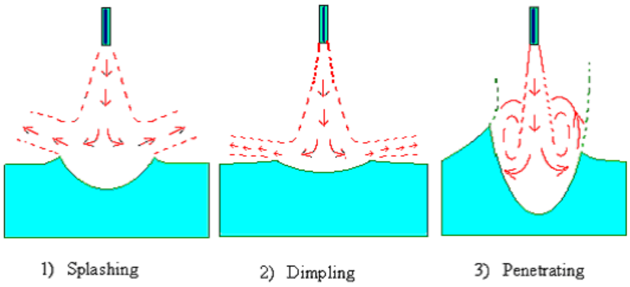

Fig.2 Modes of free surface deformation

The jetting also produces slag, where much of the process chemical reaction takes place. Understanding the effects of a gas jet impinging on a liquid surface would give more insight into the process behavior and improve the efficiency of blowing, since lance position and oxygen flow are usually used as manipulating variables. The important parameters, determining heat and mass transport at the interface and in the liquid, are the interface shape, the width and depth of the cavity and the height of the peripheral lip.

Three different modes of the surface deformation have been identified in the process: dimpling, splashing and penetrating, depending on the properties of the gas jet and the liquid. Splashing and penetration are mostly encountered in industrial situations.

This knowledge has been Valuable in the design and scale-up stages of new process development, to ensure the system will perform as required and to minimize potentially harmful behaviour such as excessive splash or surface wave action. Three different modes of surface deformation are illustrated in Fig. (2).This paper is written in the perspective that how CFD helps to understand the more complex industrial phenomena. In this paper three multiphase model e.g. Volume of fluid, Mixture model and the Eulerian model are used to study the modes of surface deformation by the impinging gas jet. Commercial CFD code Fluent 6.1 has been used to perform simulations. The results are compared with the experimental and theoretical data reported in the literature[4].

2. FREE SURFACE FLOWS

Flows with free surface area difficult class of flows with moving boundaries. The position of the boundary is known only at the initial time; its position later has to found as a part of the solution. The SCL (Space Conservation Law) and the boundary conditions at the free surface make this possible. In most cases the free surface is boundary between air and water (or another liquid or gas). If phase change at the free surface can be neglected the following boundary conditions apply:

1. The free surface is a sharp boundary between the two fluids with no flow through it, i.e

$$[(\upsilon-\upsilon_b).n]_{fs}=0 \quad \text{Or} \quad \dot{m}_{fs}=0 \tag{2.1}$$

Where "$\dot{m}_{fs}$" denotes that mass flux through free surface.

2. The forces acting on the fluid at the free surface are in equilibrium (momentum conservation or the dynamic condition condition at the free surface). This means that the normal forces on either side of the free surface are of equal magnitude, while the forces in the tangential direction are of equal magnitude and direction:

$$(n.T)_l.n = (n.T)_g.n + \sigma K, \tag{2.2}$$

$$(n.T)_l.t = (n.T)_g.t + \tfrac{\partial \sigma}{\partial t}, \tag{2.3}$$

$$(n.T)_l.s = (n.T)_g.s + \tfrac{\partial \sigma}{\partial s}, \tag{2.4}$$

Here σ is the surface tension, n, t and s are the unit vectors in the local orthogonal coordinate system (n, t, s) at the free surface (n is normal to the free surface and directed outwards), the indices 'l' and 'g' denote the liquid and gas, respectively, and K is the curvature of the free surface,

$$K = \tfrac{1}{R_t} + \tfrac{1}{R_s} \tag{2.5}$$

With R_t and R_S being the radii of curvature along coordinates t and s. The surface tension is the force per unit length of a surface element, acting tangential to the free surface. Free turbulent flows are of significant engineering importance. A mixing layer forms at the interface of two regions: one with fast and and other with slow moving fluids. In jet a region of high-speed flow is completely surrounded by stationary fluid. Velocity changes across an initially thin layer are important in all free flows: transition to turbulence occurs after a very short distance in the flow direction from the point. Where the different streams initially meet, the turbulence causes vigorous mixing of adjacent fluid layers and rapid widening of the region (cavity formation) where the velocity changes take place. The flow inside the jet region remains fully turbulent, but the flow in the outer region far away from the jet is seen to be smooth and largely unaffected by the turbulence.

Many methods have been used to find the shape of a free surface. They can be classified into two major groups. These are:

1. Methods that define the free surface as a sharp interface whose motion is followed (interface –tracking methods). Boundary fitted grids are used, and they are adjusted each time the free surface moved. In explicit methods, which must use small time steps, the problem associated with grid movement is often ignored.

2. Methods, which do not define a sharp boundary (interface tracking methods). The computation is performed on a fixed grid, which extends beyond the surface. The shape of

the free surface is determined by cells, which are partially filled. This is achieved by either following massless particles introduced into liquids phase near the free surface initially (e.g. Marker –and –Cell or MAC scheme, Harlow and Welsh, 1965), by solving a transport equation for the void fraction of the liquid phase (e.g. Volume -of-Fluid or VOF scheme, HIRT and Nichols, 1981).
In VOF-like methods, in addition to the conservation equations for mass and momentum, one has to introduce and solve an equation for the volume fraction, c. One sets e.g. $c = 1$ for CVs (Control Volumes) filled by liquid and $c = 0$ in CVs filled by gas. The change of c is governed by the transport equation.

$$\frac{\partial c}{\partial t} + div(c\upsilon) = 0 \tag{2.6}$$

In incompressible flows this equation is invariant with respect to the interchange of c and 1-c; for this to be assured in the numerical method, mass conservation has to be strictly enforced. The critical issue in this type of methods is the discretization of convective term in equation above. Low order schemes (like first-order upwind) smear the interface and introduce artificial mixing of two fluids; so higher order schemes are preferred. Since c must satisfy the condition. $0 \le c \le 1$ Local grid refinement is important for accurate resolution of the free surface. The refinement criterion is simple: cells with $0 \le c \le 1$, need to be refined. Alternatively one can treat both fluids as a single fluid whose properties vary in space according to the volume fraction of the each phase, i.e.

$$\rho = \rho_1 c + \rho_2 (1-c) \, , \mu = \mu_1 c + \mu_2 (1-c) \tag{2.7}$$

Where subscripts 1 and 2 denote the two fluids (e.g. liquid and gas). In this case one does not treat the interface as a boundary and prescribes no boundary condition.

3.FLUENT-6.1 MODELING

A time dependent two-dimensional axisymmetric model of a gas jet impinging onto a liquid pool has been developed using the computational fluid dynamics package fluent 6.1.The different geometries used in the simulations as summarized in table.1.Since the gas velocities exiting the nozzle are relatively high, it is appropriate to simulate the flow in jetting system using a turbulent flow model. . Standard k-ε model is used to incorporate the Turbulence in the continuous phase. The k-ε model is most widely used and validated turbulence model. It has achieved notable success in calculating a wide variety of thin shear layer and recirculating flows without the need for case-by-case adjustment of model constants. This model performs particularly well in confined flows where the Reynolds shear stresses are most important. This includes a wide range of flows with industrial engineering applications, which explains its popularity.

The Pressure –Implicit with Splitting of Operators (PISO) pressure –velocity-coupling scheme is used in the analysis. PISO is a part of SIMPLE family of algorithms, based on higher degree of the approximate relation between the corrections for pressure and velocity. One of the limitations of the SIMPLEC and SIMPLE algorithms is that new velocities and the corresponding fluxes do not satisfy the momentum balance after the pressure-correction equation is solved. As a result, the calculations must be repeated until the balance is satisfied. To improve the efficiency of this calculation, the PISO algorithm performs additional corrections: neighbor correction and skew ness correction. In this study the PISO algorithm with neighbor correction is used. As it is highly recommended for both steady state and transient calculations on meshes with a degree of distortion.

In this paper Euler-Euler approach has been used. In the Euler –Euler approach, the different phase are treated mathematically as a interpenetrating continua. The concept of basic volume fraction is incorporated, as volume of phase cannot be occupied by the other phase. These volume fractions are assumed to be continuous functions of time and space and their sum is equal to one. In Fluent, three Euler-Euler multiphase models are available: the volume of fluid (VOF) model, the mixture model, and the Eulerian model.

3.1 The VOF Model

The VOF model is designed for two or more immiscible fluids where the position of interface is of interest. In the VOF method the computations are performed on a fixed grid, It is a surface tracking technique, where a single set of momentum equations is shared by the fluids, and the volume fraction of each of the fluids in each computational cell is tracked throughout the domain.The VOF can be successfully applied to free surface flows, filling, sloshing, stratified flows, the motion of large bubbles in a liquid, the motion of liquid after a dam break, the prediction of jet break up, and the steady or transient tracking of any liquid-gas interface.

3.2 The Mixture Model

Mixture model uses a single fluid approach like the volume of fluid model. Mixture model solves the following equations:

1. Continuity equation for the mixture.
2. Momentum equation for the mixture.
3. Energy equation for the mixture.
4. The volume fraction equation for the secondary phase.
5. Algebraic expressions for the relative velocities.

The mixture model can also be used without the relative velocities for the dispersed phases to model homogeneous multiphase flow.

3.3 The Euler Model

It is the most complex of the multiphase models in the Fluent. It solves a set of n momentum and continuity equations for each phase.

4. GEOMETRY

Four different axisymmetric models are used to investigate the flow field due to gas jet impinging onto liquid pool. The dimensions of the models are shown in table.1.

Geometry	d (mm)	D (mm)	C (mm)	H (mm)	U_{inlet}
1	6	290	154	111	56.2
2	11	300	220	1500	100
3	11	200	220	1000	100
4	11	100	220	500	100

Table.1 Dimensions of the models used in simulations.

5.GRID GENERATION

For 2D axisymmetric simulations structured grids are modeled using Gridgen.15.04 software**.**Grid Independence studies were done using grids of different sizes. Each grid consists of two blocks. The region with air is named as Block.1.While the liquid phase is representing the Block.2 see Fig. (). Here we are only discussing the grid independence study of geometry.1The various computational grids used in the study are given in table.2. for geometry.1.

Grid Number	Grid size, Block.1	Grid size, Block.2
1	100 x 150	120 x 150
2	80 x 100	100 x 120
3	70 x 90	90 x 110

Table.2 Different grids used for grid independence study of geometry.1

The changes in the cavity depth and cavity diameter are used to decide upon a final grid. Based on these studies it was decided that grid number 1 in the above table (100 x 150 block.1 & 120 x 150 block.2) was adequate and refinement beyond this was not necessary. Because the results of this grid are consistent with those presented in[4]. The selected grids for different geometries used in this paper are shown in Fig.3, 4, 5.

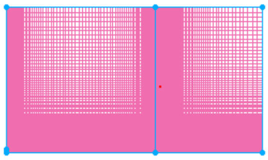

Fig3. A 2D axisymmetric structured grid for Geometry 1.

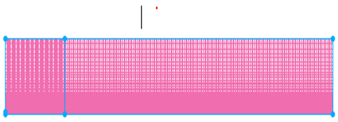

Fig.4 A 2D axisymmetric structured grid for Geometry 2.

Fig.5 A 2D axisymmetric structured grid for Geometry 3.

Fig.6 A 2D axisymmetric structured grid for Geometry 4.

6. BOUNDARY CONDITIONS

The boundary conditions used to describe the flow field with in the computational domain are shown in Fig.7.Five types of boundry conditions are used to describe the flow field with in the computational domain.

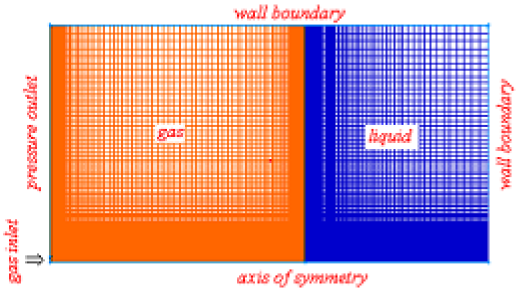

Fig.7 Boundary Conditions used for the analysis of gas jet impinging onto liquid pool

7. RESULTS AND DISCUSSIONS

A time dependent study of gas jet impinging onto liquid pool has been done in this paper using different multiphase models detailed above. Simulations are carried out for air-water systems at ambient temperature and pressure. The gas jet at the nozzle exit depends upon the nozzle design such as nozzle shape and length to diameter to ratio. In this study, a uniform nozzle velocity profile is considered. Initially fast moving gas jet loses momentum to speed up the stationary fluid. Owing to entrainment of the surrounding fluid the velocity gradients decrease in magnitude in the flow direction. This causes the decrease of the mean speed of the jet at its centerline as shown in fig.8

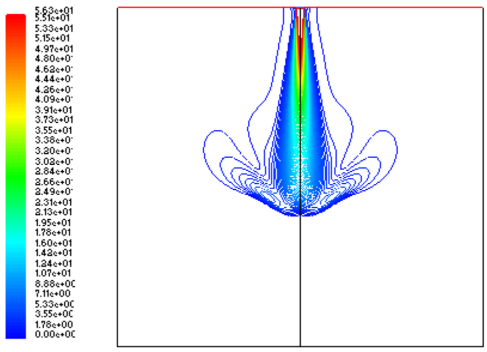

Fig.8 Contours of gas jet centerline velocity (Geometry.1)

Analysis has been done using VOF model for geometry.1 that how the surface of the liquid pool deforms with time, when gas jet strikes with it. The deformed shape of the gas-liquid interface becomes stable with in 2 seconds as shown in Fig.9a, b, c, d.

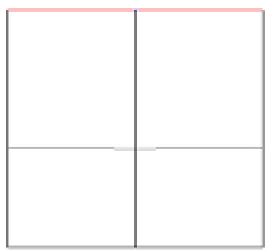

Fig. a Shape of free surface, t=0.6 sec

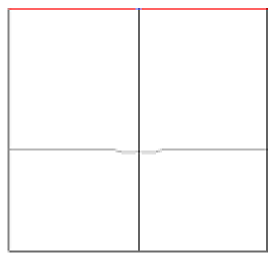

Fig. b Shape of free surface, t=0.8 sec

Fig. c Shape of free surface, t=1.2 sec   Fig. d Shape of free surface, t=1.8sec

Fig.9 Fluent cavity shape results

Adhesive forces among the molecules of the liquid are strong enough to keep the molecules of the liquid tight together. The water surface due to surface tension behaves as a stretched piece of rubber. When gas jet having a considerable amount of kinetic energy collides with the surface molecules of the liquid. The kinetic energy of the gas molecules is lost which is gained by the liquid molecules. The liquid surface is depressed in the down ward direction making a cavity on the surface of the liquid as shown in Fig.9.The problem of cavity formation is long standing and has been addressed by many researchers since the 1960's i.e. Banks and Chandrasekhara (1963), Turkdogan (1966), Wakelin (1966) etc. Due to difficulties of estimating the form of cavity, the researchers have concentrated on a few key parameters such as depth and diameter of the cavity. Many suggessions on the cavity profile, such as paraboloid, ellipsoid or Gaussian form have been made in the past. The parabolic shape of the cavity have been been observed in our analysis of gas jet impinging onto liquid pool using VOF, mixture and the Euler model as in.Fig.10, 11,12&13.

Close scrutiny of the qualitative results of geometry.1 suggests that the flow field inside the jet region is fully turbulent, but the flow in the outer region far away from the jet is smooth and unaffected by the turbulence.Fig.10 shows the cavity profile predicted by the different multiphase models with a gas jet velocity of 56.2 m/s and nozzle to liquid pool diameter ratio of 0.02068 for geometry.1.It is seen that at this gas jet velocity and d/D ratio, the liquid is only slightly depressed which explains the dimpling mode of surface deformation. The cavity profile predicted by the different multiphase models has almost the same parabolic shape. Also the predicted cavity diameter and the cavity depth has a good agreement with the data given in[4]. It can be inferred that when d/D ratio is in the order of 0.02068 and the gas jet velocity is not very high, the flow field predicted by VOF, Mixture and Euler model is almost same.

Fig.11 shows the cavity profile predicted by VOF, Mixture and the Euler model respectively. The depression depth, cavity width and lip height can be analyzed in this figure. It is seen that the cavity predicted by the VOF and the Mixture model has almost the same shape. But the Euler model predicts a deeper cavity. The gas jet velocity is high in this case i.e. 100m/s. Due to the increased gas jet velocity, the deeper cavity is predicted by the multiphase models used in this paper. Also the cavity diameter has increased in this case due to increased gas jet velocity and greater d/D ratio.

The cavity dimensions predicted by the VOF, mixture and Euler model for geometry .3 with nozzle to pool diameter ratio of 0.055 are shown in fig.12.The shape of the cavity formed by the VOF model is similar to one reported in the literature[4]. Although its dimensions deviate from the data given in the literature. A splashing mode is clearly seen for the mixture model analysis in fig.10b.While the results of Euler model show the penetration mode for this case. Fig.13 shows the qualitative results for geometry .4 using the different multiphase models.e.g VOF, Mixture and Euler model. It is shown in the Fig.11 that the cavity width predicted by the different multiphase models used in this analysis has a 100% agreement with the one given in the literature [4]. It can be inferred that when gas velocity is high and d/D ratio is increased to 0.11, the VOF, mixture and Euler model predict the same flow filed.

When we start decreasing the diameter of the liquid pool and increase the gas jet velocity. The cavity diameter and the cavity depth also start increasing.

The Quantitative results are shown in Fig.14 &15.The graph in Fig.14 shows the comparison of the cavity diameter predicted by different multiphase models with the CFD and theoretical data given in literature [4]. The graph clearly shows that for d/D ratio of 0.02068,for geometry .1, the results of all the models show a good agreement with data given in [4], the error is 21.31% for VOF model, 27.8% for mixture model and 27.8% for the Euler model. Also the cavity diameter results of different models are in good agreement with the CFD literature and theoretical data for geometry.1. The nozzle to liquid pool diameter ratio (d/D) is increased to 0.03666,while the gas jet velocity is taken as 100m/s for geometry.2.It is shown in the graph that under these conditions the cavity diameter calculated by the mixture and the VOF model has a good agreement with the theoretical and CFD literature data[4]. But the the Euler model results for d/D ratio of 0.03666 deviate from the results of other multiphase models used in this study and the data given in the literature, the error is 24.65%. The results of the VOF and mixture model show a close approximation with the CFD literature and theoretical data for d/D ratio of 0.055 for geometry.3.But the cavity diameter calculated by the Euler model shows a greater deviation, with %age error of 34.45. When the d/D ratio is increased to 0.11 with a gas jet velocity of 100m/s the results of all the multiphase models used in this paper show a 100% agreement with the data[4].

The graph in Fig.15 shows the comparison of cavity depth predicted by different multiphase models with the data given in literature[4].The graph shows that for d/D ratio of 0.02068 the cavity depth predicted by all the multiphase models is almost the same. For geometry .2,the results of VOF and mixture model show a good agreement with the literature data. But the cavity depth calculated by Euler model shows a deviation of 32.81% for geometry.2.When d/D ratio is further increased, the results of all the models show deviation from each other and the data[4] as shown in graph, Fig.15.For geometry.4,the cavity depth calculated by all the multiphase models has a good agreement with each other, but deviate from the one in [4].It is clear from the above discussion that VOF,Mixture and Euler model results are same for the dimpling mode. But when we increase the gas jet velocity, and also the d/D ratio the flow becomes complex due to splashing and penetration mode. Due to this reason deviation is observed in the results of the different multiphase models used in this study. But if the d/D ratio is increased to a certain value in such a way that the liquid pool behaves like a capillary tube, the results of all the models show a good agreement with other. However the results of VOF model show a overall good match with the data [4]. The mixture and Euler model can be used for flows with low gas jet velocity and lower d/D ratio. The results of different multiphase models used in this paper are summarized in Table.3&4.

When the gas jet velocity is increased to 100m/s, the Euler model results deviate form the CFD literature and Theoretical data.

In short VOF model results have a overall good agreement with CFD Literature and Theoretical data [4].

Geometry	Multiphase model results for cavity Diameter			CFD [4]	Theoretical [4]
	VOF	Mixture	Euler		
1	74	78	78	61	56
2	146	150	182	146	123
3	140	120	160	119	122
4	100	100	100	100	100

Table.3. Comparison of Different multiphase model results of cavity Diameter with literature data [4]

Geometry	Multiphase model results for cavity Depth. (mm)			CFD [4]	Theoretical [4]
	VOF	Mixture	Euler		
1	10	11	13.2	12	14
2	68	68	85	64	66
3	48	30	72	64	66
4	56	57	64	27	159

Table.4 Comparison of Different multiphase model results of cavity depth with literature data [4]

8.CONCLUSION

The interest of applying Computational Fluid Dynamics in industrial multiphase processes has increased during the last few years. In this study we investigated the gas jet impinging onto liquid pool using different multiphase models. The emphasis was given to highlight and compare the discrepancies between the three multiphase models in capturing the flow structure and cavities formed at gas-liquid interfaces. At low velocities of gas jet and low d/D ratio, VOF, Mixture and Euler model predict the same flow field. But when we increase the gas jet velocity and also increase the d/D ratio, the results of VOF and mixture model show close results with literature data [4]. While the results of Euler model deviate to a greater value. But it is interesting to note that when d/D ratio is increased to certain value, the results of three multiphase models detailed above show a 100% agreement with data[4] .At this value of d/D ratio the liquid pool diameter is so small that it acts like a capillary tube. Also there is jet velocity over which splashing will occur and below which a smooth cavity is formed. The analysis shows that the VOF model is suitable for such type of free surface flows.

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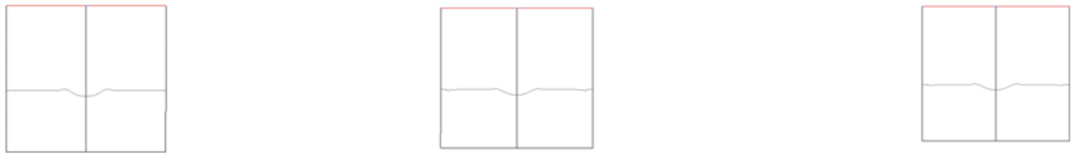
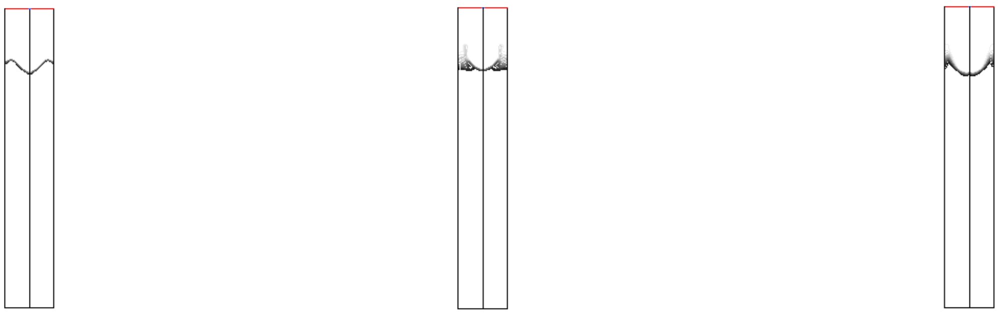


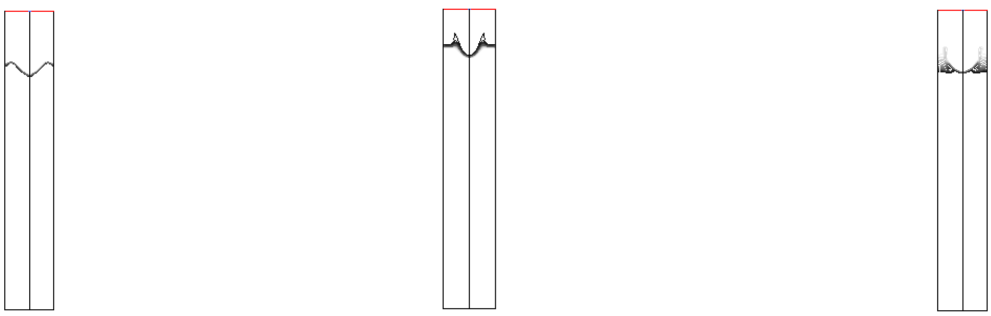
VOF model   Mixture model   Euler Model

Fig.10 Gas-liquid interface profile for geoemtry.1 using VOF, Mixture and Euler model



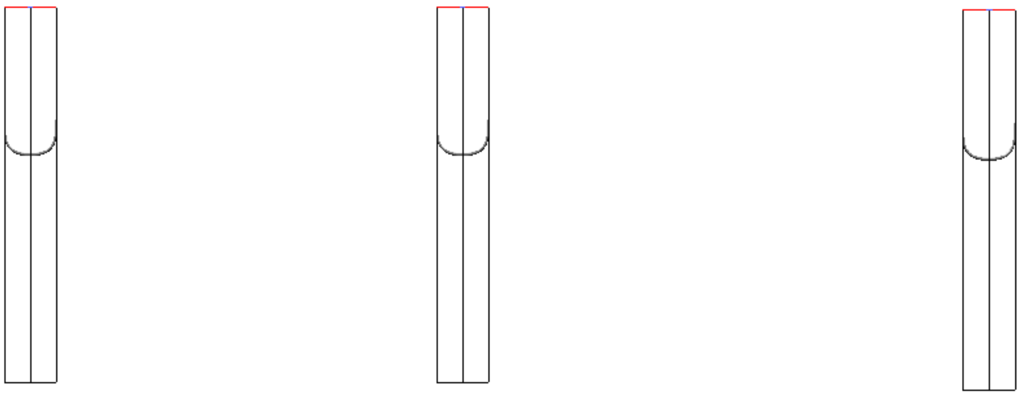
VOF model   Mixture model   Euler Model

Fig.11 Gas-liquid interface profile for geoemtry.2 using VOF, Mixture and Euler model



VOF model   Mixture model.   Euler Model

Fig.12 Gas-liquid interface profile for geometry. 3 using VOF Mixture and Euler model



VOF model Mixture model. Euler Model

Fig.13 Gas-liquid interface profile for geoemtry.4 using VOF Mixture and Euler model

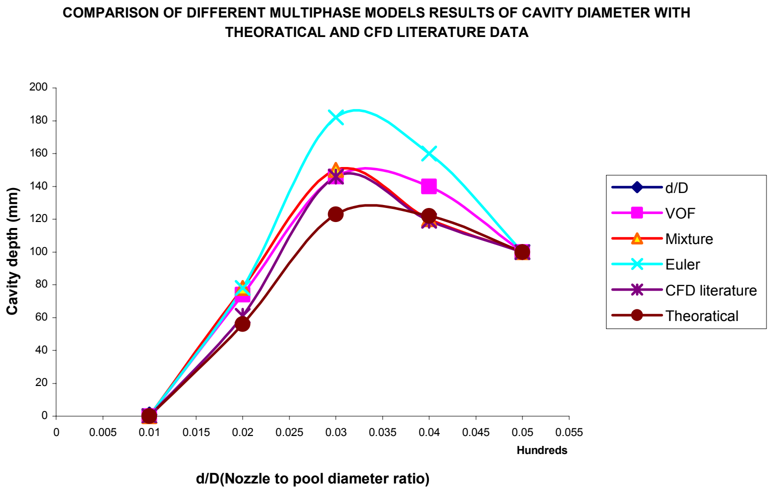


Fig.14 Comparison of cavity diameter results of different multiphase models with data given in the literature.

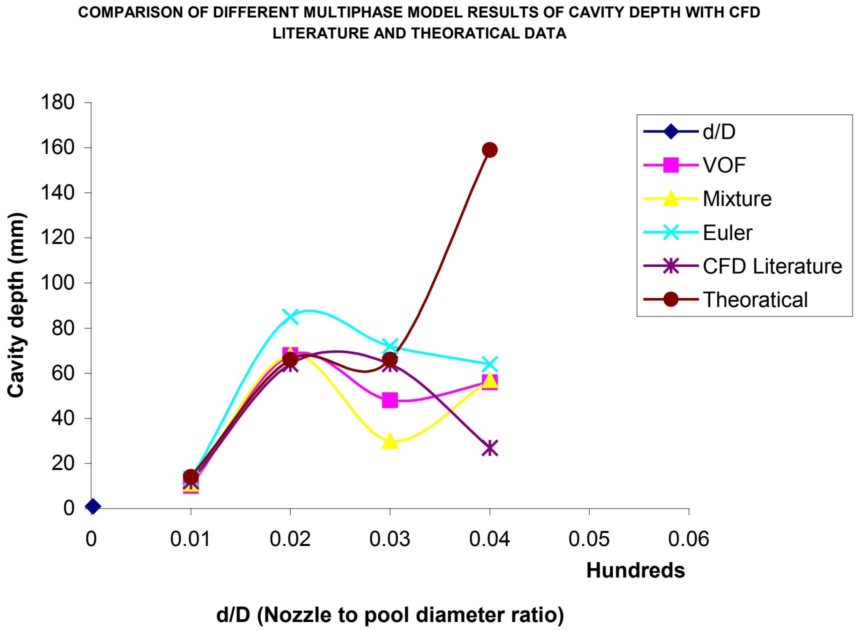


Fig.15 Comparison of cavity depth results of different multiphase models with data given in the literature.