# VALIDATING THE GALERKIN LEAST-SQUARES FINITE ELEMENT METHODS IN PREDICTING MIXING FLOWS IN STIRRED TANK REACTORS

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## INTRODUCTION

A novel approach for computer aided modeling and optimizing mixing process has been developed using Galerkin least-squares finite element technology. Computer aided mixing modeling and analysis involves Lagrangian and Eulerian analysis for relative fluid stretching, and energy dissipation concepts for laminar and turbulent flows. High quality, conservative, accurate, fluid velocity, and continuity solutions are required for determining mixing quality.

The ORCA Computational Fluid Dynamics (CFD) package, based on a finite element formulation, solves the incompressible Reynolds Averaged Navier Stokes (RANS) equations. Although finite element technology has been well used in areas of heat transfer, solid mechanics, and aerodynamics for years, it has only recently been applied to the area of fluid mixing. ORCA, developed using the Galerkin Least-Squares (GLS) finite element technology, provides another formulation for numerically solving the RANS based and LES based fluid mechanics equations.

The ORCA CFD package is validated against two case studies. The first, a free round jet, demonstrates that the CFD code predicts the theoretical velocity decay rate, linear expansion rate, and similarity profile. From proper prediction of fundamental free jet characteristics, confidence can be derived when predicting flows in a stirred tank, as a stirred tank reactor can be considered a series of free jets and wall jets (Bittorf and Kresta, 2001).

## PART I: CFD CODE

The analysis of mixing flows in stirred tank reactors involves the solution of the governing partial differential equations (PDE's), incompressible Reynolds Averaged Navier Stokes (RANS) Equations, for fluid mechanics.

The solution of these PDE's is generally accomplished through the notion of approximate solution methods, a general class under which virtually all numerical solution formulations and algorithms are defined. Approximate solution methods transform the continuous form of the governing differential equations to a discrete form operating on either a collection of points, volumes, or both, to produce a set of nonlinear algebraic equations. Into this class of solutions fall Finite Difference (FD), Finite Volume (FV), and Finite Element (FE) methods. Within each of these classes are many variations.

The Galerkin Least Squares (GLS) formulation, one of the variations of the Finite Element Method, has at its roots the Upwinding Finite Element work of Hughes (1978), Hughes (1979), and Hughes and Brooks (1979); the SUPG methods of Brooks and Hughes (1982), Franka, et. al. (1986), Hughes and Shakib (1988); and GLS formulation, Hughes, et. al. (1989) and Shakib (1989).

Further, the GLS formulation has been proven to possess mathematical characteristics relating to stability and convergence, Johnson and Szepessy (1985) Johnson and Szepessy (1986), Hughes et al. (1989), Franka and Frey (1992), Franka, et. al. (1992), and Franka and Hughes (1993).

This formulation begins with a basic Galerkin – Method of Weighted Residuals discretization, but adds a number of additional stabilization terms to maintain stability while maintaining the continuity on each cell and the entire system. The application of new computational methods requires accuracy to be established before it is considered a predictive tool. Fundamental accuracy within the limitation of the discretization is guaranteed by the formulation. Thus, validation is defined in a new, stronger qualitative and quantitative sense Zalc, et. al. (2001, 2002). In the present work, validation is considered to be achieved when the differences between computational and experimental methods, on a full field basis, are found to be very small and when computational results are achieved without introduction of arbitrary constants or other arbitrary or artificial diffusion terms for maintaining stability and convergence.

The following outlines the salient characteristics and superiority of the GLS formulation, the consideration of validation for stirred tank reactor flows, and results of specific studies to demonstrate validity.

### BACKGROUND AND MOTIVATION

The fundamental equations of fluid mechanics for incompressible flow, generally referred to as the Navier-Stokes equations, may be written as the following:

$$u_{i,i} = 0$$

$$\rho u_{i,t} + \rho u_j u_{i,j} = -p_{,i} + \tau_{ij,j} + \rho b_i \quad (1)$$

$$\rho C_p T_{P,t} + \rho u_i C_p T_{P,i} = \tau_{ij} u_{i,j} - q_{i,i} + q_{src}$$

Turbulence is modeled using the one equation Spalart-Allmaras closure model solving the transport equation for $\tilde{n}$ Spalart and Allmaras, (1992):

$$\tilde{n}_{,t} + u_i \tilde{n}_{,i} = c_{b1} \tilde{S} \tilde{n} + \left( \frac{n + \tilde{n}}{s} \tilde{n}_{,i} \right)_{,i} + \frac{c_{b2}}{s} (\tilde{n}_{,i} \tilde{n}_{,i}) - c_{w1} f_w \left( \frac{\tilde{n}}{d} \right)^2 \quad (2)$$

This turbulence closure model has been evaluated relative to several others Bardina, et. al., (1997) and was found to be among the leading methods for overall performance.

Although within the domain of the approximate solution methods the overwhelming majority are very similar, differences exist in areas such as differencing stencils, volume constructs, and variations in stabilization methods, up to and including the Total Variation Diminishing (TVD) constructs for introducing artificial diffusion/viscosity for nonlinear equation convergence,Tannehill, et al(1997).

Finite Difference/Volume methods operate directly on a discrete form of the differential equations, or the differential equations applied to discretized control volumes of linear approximation, respectively. As such, the basic formulations are relatively easy to construct and appear similar to the original equations. However, difficulties arise in maintaining stability and applying general classes of boundary conditions, etc. While each of the popular formulation classes has its own utility, engineers skilled in the formulations are generally required to achieve viable solutions.

The GLS Finite Element formulation, when coupled with an effective code implementation, represents a solution structure that is stable, robust, and efficient. Hughes and Shakib (1988).

The present issue concerns the lack of a wide body of validation work in the subject matter of mixing class flows, upon which confidence in the accuracy and subsequent predictive characteristics are based.

## GENERAL FINITE ELEMENT CONSIDERATIONS

The general finite element formulation seeks to define a system of equations that minimizes the error of approximating functions with respect to a minimizing principle. Depending on the nature and consistency of the overall formulation, issues of stability and numerical formulation difficulties have varying effects.

## MIXED VARIATIONAL METHODS/PENALTY METHODS

While there is no direct variational statement for the governing equations of fluid mechanics, a functional statement can be minimized in the context of variational calculus methods and mixed variational methods operating on variables, in conjunction with various augmenting techniques, such as penalty methodsHughes (1987). This has the effect of scaling undesired responses with a large penalty, which pushes the solution in the desired direction.

## *GENERAL GALERKIN – WEIGHTED RESIDUALS*

The general Galerkin method works directly on the discretized form of the governing equations which seeks to minimize the error of the product of the approximating trial functions with the weighting functions on the residual. The error of the product is minimized globally by solving the resultant set of nonlinear algebraic equations minimizing the error of the approximation. This approach suffers stability difficulties similar to the above formulations, for the case of nonlinear fluid mechanics Huges et al. (1989).

Weighted residual methods are a standard approximate mathematical construct for solving general PDE's, and hence, are not intractable for understanding basic formulation details. The weighted residual formulation for the continuity and momentum equations may be stated as: find the solution $\{\boldsymbol{u},p\} \in \boldsymbol{S}^h$ such that for all $\{\boldsymbol{w},q\} \in \boldsymbol{n}^h$ the following equation is satisfied Huges et al. (1989)

$$\begin{aligned}
&\int_\Omega (w_i(\boldsymbol{r}u_{i,t} + \boldsymbol{r}u_j u_{i,j} - \boldsymbol{r}b_i) - w_{i,i}p + w_{i,j}\boldsymbol{t}_{ij})d\Omega \\
&- \int_\Omega q_{,i}u_i d\Omega \\
&+ \sum_e \int_{\Omega_e} (\boldsymbol{r}w_{i,t} + \boldsymbol{r}u_j w_{i,j} + q_{,i})\boldsymbol{t}_m(\boldsymbol{r}u_{i,t} + \boldsymbol{r}u_k u_{i,k} + p_{,i} - \boldsymbol{t}_{ik,k} - \boldsymbol{r}b_i)d\Omega_e \\
&+ \sum_e \int_{\Omega_e} w_{i,i}\boldsymbol{t}_c u_{j,j} d\Omega_e \\
&= \int_\Gamma - w_i(pn_i + \boldsymbol{t}_{ij}n_j) - q(u_i n_i P)d\Gamma
\end{aligned} \quad (3)$$

Here, $w_i$ and q are the weighting function counterparts corresponding to the trial functions $u_i$ and p respectively; further, $\boldsymbol{S}^h$ and $\boldsymbol{n}^h$ are the interpolation function space for the trial and weighting functions respectively. The standard Galerkin formulation is represented by the first two integral terms and the last integral term on the right hand side of the equal sign. An in-depth discussion of the GLS technology is found in Hughes, (1987).

## GLS EXTENSIONS, STABILIZATION, RESIDUALS, CONVERGENCE

The GLS extensions to the basic Galerkin Weighted Residuals formulation is defined in a consistent fashion with respect to the specific physics and in a symmetric matrix form. These are seen as the third and fourth terms of (3) corresponding to the momentum and continuity equation respectively.

The ***tau*** matrix metric is defined to appropriately operate on each class of physics and determine the appropriate governing scaling to be applied. The net effect is that each class of physics involved in the computation is introduced with its own set of stabilization terms, as a function of the residual, to aid in the nonlinear convergence Huges and Shakib (1986), Shakib (1989) Hughes and Mallet (1986a)

The GLS terms are structured so that a stabilization influence is introduced into the nonlinear system, which is consistent with each individual set of physics involved in the problem. The result is that as each of the physics converges, the stabilization is removed in a consistent fashion. This structure of the GLS terms permits rigorous mathematical proofs for stability and convergence. This formulation has the characteristic that if the exact solution was substituted into the formulation, all stabilization reduces to zero and the original governing equations are exactly satisfied. This is not the case for the general class of approximate solution formulations. Huges and Shakib (1988), Shakib (1989), Johnson and Szepessy (1985) Johnson and Szepessy (1986), Hughes et al. (1989), Franka and Frey (1992), Franka, et. al. (1992), and Franka and Hughes (1993)

Another characteristic in the formulation that promotes consistency is the definition of pressure in terms of an equal order interpolation with respect to the other variables. This builds a necessary consistency between the continuity equation and the momentum equation. Further, in this case, pressure is introduced in a fashion that precludes effects such as element locking and artificial spurious modes emanating from the element formulations Huges (1987)

**IMPLEMENTATION CONSIDERATIONS**

Fundamental mathematical fidelity to the governing PDE's is an absolutely necessary condition for a high performance, robust, accurate computational package, but it is not sufficient for stability and convergence. The complete structure of code implementation is also a necessary condition. When taken together with the proper formulation, fundamental mathematical fidelity to the governing PDE's and the complete structure of code implementation produce the results of high performance, accuracy, and robustness. The convergence of the above concepts is exemplified in the base of the ORCA CFD package that uses Acusim Software's numerical solver.

**CONSERVATION OPERATORS**

Within the implementation of Acusim's finite element solvers ACUSOLVE, each of the physics is formulated separately, because of the GLS structure. In addition to the basic formulation, conservation operators have been derived and implemented, requiring that conservation is strictly observed for the solution variables. Hence, conservation is not an accident of the formulation, but rather is strictly guaranteed by solution in the implementation Shakib (1989)

**DISCONTINUITY CAPTURING OPERATOR**

It is not always possible to have sufficient discretization everywhere that is necessary, particularly in transient flows where conditions are changing throughout the field. The discontinuity operator seeks to handle under-resolved flow structures, relative to such effects as boundary layers, and flow around sharp corners. This operator is derived in a consistent fashion relative to the GLS formulation, such that stability and convergence are strictly maintained.Hughes et al. (1989), Hughes and Shakib (1988), Shakib (1989), Hughes and Mallet (1986b).

**FULLY COUPLED LINEAR EQUATION SOLVER**

Nonlinear solution performance is enhanced within the formulation, relative to the structure of the left hand side system matrix, producing high quality tangent matrices for the Newton class nonlinear equation solver. Additionally, the total nonlinear performance is enhanced by introducing creative iterative linear algebraic methods that solve the system of velocities and pressures, as well as temperature if necessary, in a fully coupled manner.

In addition to the above considerations, ORCA's solver has implemented both high performance linear algebra solvers and highly scalable domain decomposition parallel architecture that minimizes interdomain communications.

## PART II: CFD VALIDATION

A major contribution of this work is to establish a more rigorous basis for comparison of experimental and computational results. Experimental results embody many variations from a variety of sources. Although this is often termed experimental error, a more precise term would be experimental variation. Further, resolution of experimental results in a temporal, phase, and/or spatial resolution may be required for more direct comparison between the experimental and computational results. The CFD code that embodies all of the characteristics as described above carries substantial detail and accuracy, in both the spatial and temporal domains. Therefore, the best comparison is direct, on a time, space, phase, and physics basis.

The computational methods outlined herein are both sufficiently fast and accurate, relative to the level of discretization, to allow the direct comparisons with actual experimental information that generally produce the best results. That is to say, the better the agreement between the physical boundary conditions from the experiment and the computational model, the better the agreement is between the methods. This becomes a driving principle; hence, arbitrary constants are not introduced to drive results to converge to known solutions.

Another principle of consideration is that results should be validated relative to full field results. A limited scope of comparison may indicate some level of agreement and lead to a particular conclusion regarding flow physics, but also has the potential to mislead, if results are completely off in another location. Therefore, in this study it was important to use a full three dimensional model to insure the widest possible field of comparison. The formulation and implementation of the GLS model is derived to be accurate, within the limits of discretization and model approximation. Consequently, full field comparisons with experimental data demonstrate the strength of this method.

Validation is completed for test cases relevant to stirred tank reactors and the resultant jet flows. Since validation of basic flow is essential in prediction of more complex flows, the first case examined concentrates on base free jet principles. A free round jet similar to that found as an injector for stirred tank reactor is modeled and similarity, velocity decay, and expansion rate of the jet are modeled.

From proper prediction of fundamental free jet characteristics, confidence can be derived when predicting flows in a stirred tank because a stirred tank reactor can be considered a series of free jets and wall jets (Bittorf and Kresta, 2001, & Kresta et al. 2001). The second case examines the three dimensional wall jet along the baffle of the tank induced by an axial flow impeller (Bittorf and Kresta, 2001). The 3-D wall jet created in the stirred tank reactor acts ideally; the velocity decays inversely to the distance traveled; and the jet expands linearly as shown experimentally by Bittorf and Kresta (2001).

## FREE JET

The round free jet solution has been well characterized by many authors, and Rajaratnam (1976) reviews the basic theory. Decay and expansion rate can be analytically derived from RANS equations. This basic jet flow, which can be related in inlets to tanks, reactors, heat exchangers, septic tanks, water treatment basins, and many more applications, is one of the most important flows in the process industry. Without proper validation of this base flow, the CFD engineer can not expect to attain accurate results to more complex problems.

Figure 1 illustrates the free jet examined. Like any jet, it expands as the jet travels and the velocity decays. The velocity decay and expansion, as derived from the RANS equations is:

$$\frac{V}{V_{Nozzle}} \propto \left(\frac{z}{D_{Nozzle}}\right)^{-1} \qquad \frac{b_{1/2}}{D_{Nozzle}} \propto \left(\frac{z}{D_{nozzle}}\right) \qquad (4)$$

Here, $V_m$ is the local maximum velocity at any distance from the nozzle and $b_{1/2}$ corresponds to the half width of the jet when velocity is equal to $0.5V_m$.

When a simulation was completed to ensure compliance, the results matched the theory indicated in Equation 4. The computational set-up is shown in Table 1

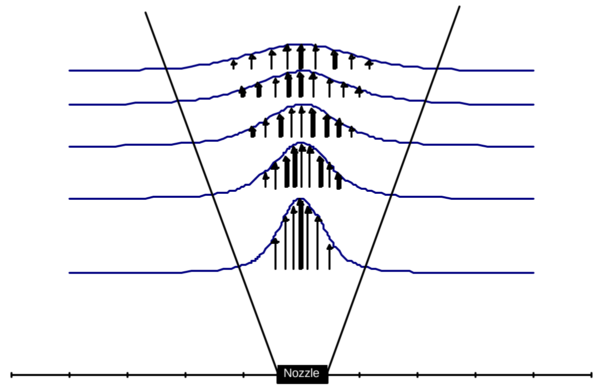


**Figure 1:** Jet expansion and progression of a round free jet in a stagnant fluid

Table 1: Properties Used in CFD Simulation of Free Jet

| ***Dimensions and fluid properties*** | ***CFD properties*** |
|---|---|
| Nozzle<br>Diameter, $D_{Nozzle}$=0.005m<br>Fluid Depth=0.5m<br>Fluid Viscosity, $\nu=1\times10^{-6}$ m$^2$/s<br>Nozzle velocity=1 m/s<br>Reynolds Number=5000 | Software:ORCA, distributed by Dantec Dynamics<br>1.3 million unstructured tetrahedral mesh<br>Solved Linux Cluster of FOUR -900 MHz processors, 512 MB RAM<br>Convergence tolerance $1\times10^{-3}$<br>Solution time = 3 hours |

## SIMILARITY SOLUTION OF THE JET

The first property examined is the jet similarity profile of a jet with velocities that are made dimensionless as shown above. A similarity profile will occur as seen in Figure 2. This matches the ideal similarity profile from Goertler (1942):

$$\frac{V}{V_m} = 1 - \tanh^2\left(c\frac{b_{1/2}}{r}\right) \quad (5)$$

Goertler's similarity compares well with the CFD. The slight deviation from the ideal near the bottom of the profile is expected since experimental comparisons to Goertler’s profile indicate the same phenomena (Rajaratnam, 1976). The predicted expansion rate $b_{1/2}$ is linear, which is congruent with the theory from Equation 4.

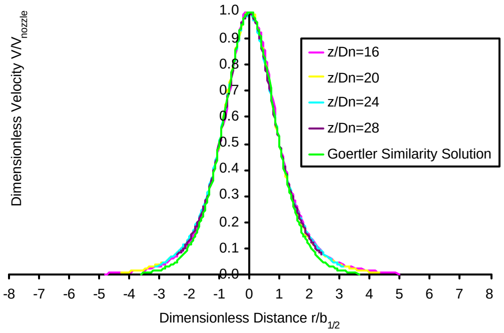


**Figure 2**: Similarity profile of a round free jet as predicted by the CFD program compared to the Goertler's (1946) Similarity solution.

## VELOCITY DECAY

Figure 3 shows the center line velocity decay of the round free jet. The ideal decay of the jet is proportional to the distance traveled. Velocity decay predicted by the CFD matches extremely well with theory, indicating that the GLS finite element numerics are not over-diffusive and provide good prediction for velocity decay.

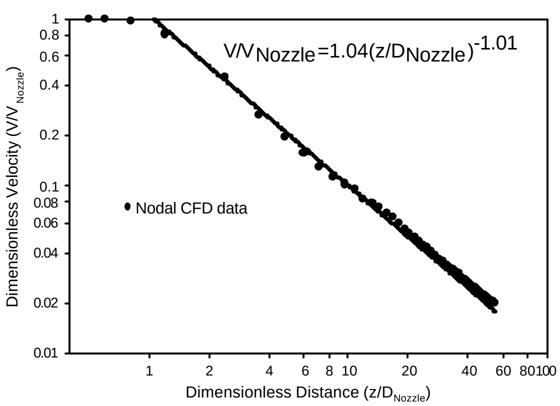


**Figure 3:** Shows the velocity decay of the circular free jet notice that it closely matches the theoretical decay in Equation 4.

## STIRRED TANK

The next case study examines the three dimensional wall jets that are created in a stirred tank reactor. After completing the base study on free jet decay, the next test for the CFD is to insure predictability of the three dimensional wall jet created in a stirred tank. This case involves much more complicated geometry as the flow structure in a stirred tank is considered chaotic, with many different turbulent structures influencing the flow.

The theoretical decay and expansion rate of a three dimensional wall jet is the same as Equation 4; however, the assumptions and the derivation to attain the equation are different. A full derivation and a list of the assumptions can be found in Bittorf and Kresta, 2001

Figure 4 shows the stirred tank and the locations of the three dimensional wall jets. The experimental work completed on this system by Bittorf and Kresta (2001) will be compared to the CFD results attained from ORCA. The experimental and computational configuration is shown in Table 2.

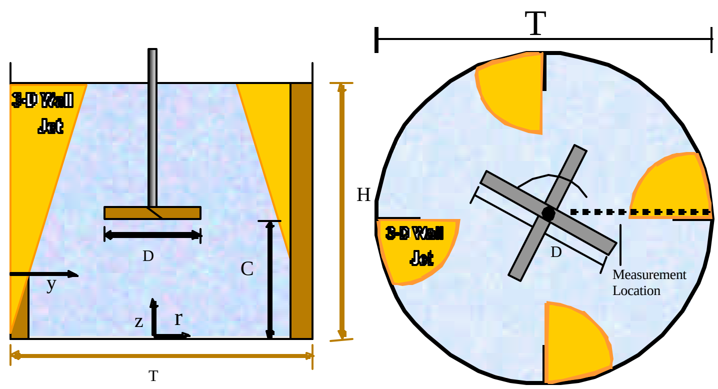


**Figure 4:** Tank Configuration for the PBT impeller indicating: the locations of the three dimensional jets; the measurement location experimental data from Bittorf(2001)

**Table 2**: Properties Used in CFD Simulation for Axial Impeller Stirred Tank

| ***Experimental Set-Up*** | ***Computational Set Up*** |
|---|---|
| Impeller - 45° Pitched Bladed Turbine<br>Impeller Diameter, D=80mm=T/3<br>Impeller Clearance, C=80mm or C/D=1<br>Tank Diameter, T=240 mm<br>Liquid Height, H=240mm<br>Liquid used is water<br>Viscosity, $\nu=1\times10^{-6}$ m$^2$/s | ORCA CFD Software<br>2.0 million unstructured tetrahedral mesh<br>Solved Linux Cluster of THREE -900 MHz processors, 512 MB RAM<br>Convergence tolerance $1\times10^{-3}$<br>Solution time = 3.5 hours |

Figure 5 indicates the progression of the local maximum velocity for the three dimensional wall jet created in a stirred tank. Notice the four distinct regions that develop for the wall jet which correspond to the findings of Bittorf and Kresta, 2001. The first three regions (potential core, characteristic decay, and radial decay) correspond to the three regions of a stirred tank discussed by Swamy, (1974). The characteristic decay region is system depended and the radial decay region is system independent, with the velocity decay proportional to the distance traveled ($V_m \propto z^{-1}$). As well, Figure 5 shows the velocity decay rates for the characteristic and radial decay regions. The CFD data in the radial decay region compares well with the theoretical velocity decay from Equation 4.

Figure 6 compares experimental data from Bittorf and Kresta (2001). The CFD compares well to experimental data providing similar shape although the experimental data decays faster near the end region. The jet quantities are predicted with suitable accuracy and predictability.

**CONCLUSION**

The GLS finite element solver found within ORCA has been experimentally shown to accurately predict theoretical jet decay for a free round jet and a three dimensional wall jet found in a stirred tank. This provides excellent indication that the numerical methods are not diffusive and hence provide reliable predictability for simple and complex jet flows.

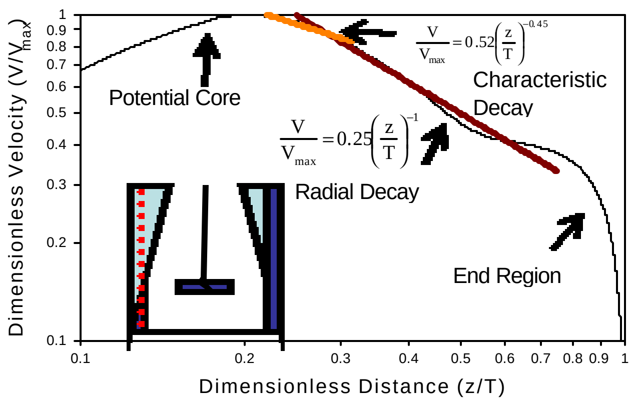


**Figure 5:** CFD results indicating the decay of the local maximum velocity as the jet progresses from the bottom of the tank to the top. The first three regions are characteristic of any 3-D wall jet; while the end regions is only a characteristic of stirred tank systems. The CFD matches the theoretical radial decay rate exponent for much of the data.

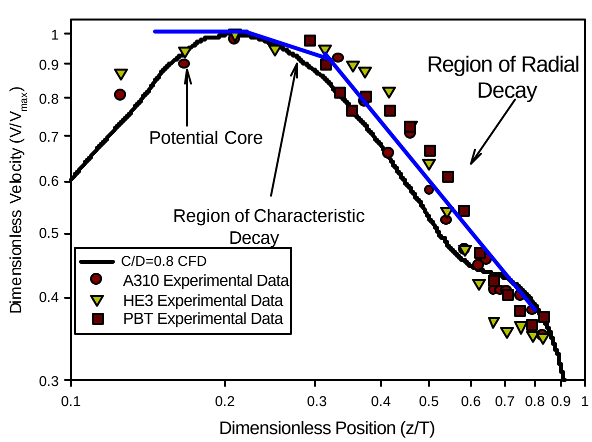


**Figure 6**: Comparison Between the CFD results and Experimental Data from Bittorf and Kresta (2001)

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## Nomenclature

| | |
|---|---|
| $b_i$ | body force vector $\{b_1,b_2,b_3\}^T$ (kg m/s$^2$ ) |
| $b_{1/2}$ | half width of the jet (m/s) |
| c | constant |
| $C_p$ | Constant Pressure Heat Capacity (J/kg K) |
| $D_{Nozzle}$ | Nozzle Diameter (m) |
| $n_i$ | outward normal to boundary (m) |
| p | pressure (Pa) |
| Pr | Prandtl Number, $\rho\mu c_p/\kappa$ |
| $Pr_t$ | Turbulent Prandtl Number, $\rho\mu_t C_p/\kappa_t$ |
| $q_i$ | heat flux vector $=\{q_1,q_2,q_3\}^T = -(\kappa+\kappa_t)\, T_{,i}$ (J s$^{-1}$ m$^{-1}$) |
| $q_{src}$ | volumetric heat generation (J s$^{-1}$ m$^{-3}$) |
| q | weighting function corresponding to pressure interpolation |
| r | radial coordinate (m) |
| $S_{ij}$ | strain rate tensor = $½(u_{i,j}+u_{j,i})$ (1/s) |
| $T_p$ | temperature (K) |
| T | tank diameter (m) |
| $u_i$ | velocity vector $\{u_1,u_2,u_3\}^T$ (m/s) |
| V | axial velocity (m/s) |
| $V_{Nozzle}$ | nozzle velocity (m/s) |
| $V_{max}$ | core velocity in the wall jet (m/s) |
| $V_m$ | local maximum velocity (m/s) |
| $w_i$ | weighting function corresponding to velocity interpolation |
| z | axial position (m) |
| $\Gamma$ | boundary for computational domain (m$^2$) |
| $\Omega$ | computational domain (m$^3$) |
| $\Omega_e$ | domain for discretized element e (m$^3$) |
| $\kappa$ | thermal conductivity (J/s m K) |
| $\kappa_t$ | turbulent thermal conductivity = $C_p\mu_t/Pr_t$ (J/[s m K]) |
| $\mu$ | molecular viscosity (kg/[m s]) |
| $\mu_t$ | turbulent eddy viscosity= (kg/[m s]) |
| $\nu$ | kinimatic viscosity (m/s$^2$) |
| $\rho$ | constant density (kg/m$^{3)}$ |
| $\tau_m$ ,$\tau_c$ | least squares metrics for momentum, continuity |
| $\tau_{ij}$ | stress tensor = $2(\mu+\mu_t)\, S_{ij}$ (kg/m$^2$) |