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REPORT

FOR

PREDICTIVE MODELLING OF BOILER FOULING

DE-AC22-90PC90098

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1.0 SUMMARY

The overall aim of fouling control in boilers is to reduce the power generation cost in coal fired utilities. The improved control can reduce the power generation cost by reducing the down time required to clean the tubes. It can also provide greater flexibility to utilities in terms of choice of coal selection and improved control of pollutants formed.

Fouling in coal fired systems is a highly complex phenomenon governed by the interactions between reactive gas phase, mineral matter evolution and transformation from coal and its transport to the tube surface, and deposit, erosion, and bonding of the mineral matter on the tube surface.

Gas flow field in the vicinity of the tube surface is highly turbulent and complex and governs the transport of mineral matter from the gas surface to the tube surface. The present work focuses on the prediction of gas phase behavior in an attempt to develop a comprehensive model for transport of mineral matter to the tube surface. It assumes a priori knowledge of other sub models.

The geometry in the vicinity of the tubes is complex and turbulent. Simpler or lower level models, e.g 2 equation k-e model, does not provide accurate flow results for reliable prediction of fouling behavior. On the other hand, simulation by the Direct Numerical Simulation method for the typical flow Reynolds numbers is not within the realm of present day computers. Large Eddy Simulation technique is a viable method for providing sufficient accuracy within practical limits. In particular, a spectral element method embodying Large Eddy Simulation technique based on the Re-Normalization Group theory for simulating Sub Grid Scale viscosity was chosen for the present work. This method is embodied in a computer code called NEKTON.

NEKTON solves the unsteady, two or three dimensional, incompressible Navier Stokes equations by a spectral element method. The code was later extended to include the variable density and multiple reactive species effects at low Mach numbers; density is a function of temperature and molecular weight. The code was also extended to compute transport of large particles governed by the inertia. Transport of small particles is computed by treating them as trace species.

Code computations were performed for a number of test conditions typical of flow past a deep tube bank in a boiler. The computed results indicate qualitatively correct behavior. Predictions of deposition rates and deposit shape evolution also show correct qualitative behavior. These simulations provide the first attempts to compute flow field results at realistic flow Reynolds numbers of the order of 10^4 . Detailed code validation studies were not performed. Detailed comparisons with experimental conditions also could not be made as many of phenomenological model parameters, e.g. sticking or erosion probabilities, and their dependence on the experimental conditions were not known. The predictions however demonstrate the capability to predict the fouling behavior from the first principles. Further demonstration of the code capability will require importing the code to a large or massively parallel machine to reduce the computer time. The code validation studies and parametric studies can then be undertaken to provide a deeper understanding of the processes controlling fouling with an aim to develop phenomenological models and engineering correlations

2.0 INTRODUCTION

Fouling results from the deposition or adhesion of the mineral matter on the tube surface. It involves highly complex interactions between the gas phase combustion products, fuel, and mineral matter carried by the fuel, such as coal. Physical and chemical changes occurring in the gas phase and the deposit phase as well as the transport of different species and phases from and to the surface of the deposit govern the time evolution of the deposits.

Combustion of coal with utility grind coal results in ash carrying the majority of mineral matter, with the size distribution of ash evolving from the initial coal particle size distribution [Raask, 1985]. Alkali and chlorides may evolve as gas phase constituents in the combustion zone and condense again on the cooled tube surfaces or in the thermal boundary layer. These processes lead to a very wide range of size and composition distribution [Bryers, 1977; Barrett, 1984].

A number of mechanisms control the transport of particles and mist to the surface of the tubes. For larger sized ash particles with diameters greater than 10 microns, the dominant deposition mechanism is via inertial transport. Sub-micron sized particles or condensable mist, less than 0.1 microns, are transported via particle (Brownian) diffusion. Intermediate sized particles are most likely transported via thermophoretic diffusion mechanism. In many coal combustion systems most of the mineral mass is contained in the large sized particles, hence inertial deposition is the most dominant transport mechanism. However, very minute quantities of condensable gases can have pronounced effect on wettability, and hence sticking behavior of the deposits.

Flow in the deep tube bank of a boiler is extremely complex and unsteady exhibiting large variations between tubes and along the circumference of each tube. Detailed experimental measurements on the heat exchange around tube banks are available in the literature. It is expected that particle deposition rates are closely related to the flow and heat transfer characteristics and a good understanding of the deposit behavior in boiler tubes will require an accurate and detailed understanding of the flow behavior.

Most of the turbulent flow simulations rely on some kind of closure model, for example k- ϵ model. Such simulations neglect the chaotic or unstationary nature of turbulence by modeling the flow as steady state flow. Comparison of model predictions for a simplified geometry, e.g. flow around a single cylinder [Schuh et al, 1989], with experimental measurements indicate the inadequacy of steady state models. Time accurate turbulent simulations are required to avoid uncertainties associated with closure models. Also, because of the non-linearity of the deposition process, it is expected that the time average deposition rate for an unsteady flow will be different from the steady deposition rate for the steady flow.

It is generally recognized that the turbulent flows are adequately described by the time dependent Navier-Stokes equations. Time accurate solutions of Navier-Stokes equations, however, warrants a careful selection of the numerical algorithm to eliminate numerical diffusion and correct choice of grid sizes to simulate the wide range of length and time scales present in the turbulent flow. Direct Numerical Simulations (DNS) are usually reported at low Reynolds numbers [Hunt, 1988]. Typical Reynolds number for the flow around a boiler tube is around 10^4 . With the minimum eddy length scale of the order of Kolmogorov length scale ($Re^{3/4}$), the solution requires $Re^{9/4}$ points and of the order of $Re^{3/4}$ time steps so that the total computational effort is of the order of Re^3 [Oran and Boris, 1993]. Needless to say that it is impossible to solve this problem with 1 billion grid points.

Large Eddy Simulation (LES) technique can bring this problem in the realm of practicality. LES resolves all large energy containing eddies but models the smaller energy dissipating eddies which are up to 10 -100 times Kolmogorov length scale. Thus minimum grid size requirements are reduced by at least a factor of 10 in each direction, i.e. factor of 1000 in three dimensions, while the number of time steps required to reach steady state is also reduced by at least a factor of 10. Key to the success depends on the ability to model the effects of small unresolved length scales on the larger eddies (Sub-Grid Scale modelling). Selection of appropriate numerical algorithm for minimizing the numerical diffusion and perhaps minimizing the number of grid points by selecting non-uniform grids is also equally important. A number of successful cases comparing DNS and LES results at low Reynolds have been reported in the literature [Oran and Boris, 1993].

The numerical algorithm selected for LES methodology was based on the spectral element formulation. The spectral methods involve approximating the flow by using appropriate combinations of Fourier, Chebyshev, Legendre etc. polynomial series. The spectral methods achieve high accuracy and appear excessively complicated compared to lower order finite difference methods. They also lack the flexibility to simulate the complicated tube bundle like geometry. Spectral element methods [Patera, 1984] combine the high order accuracy of the spectral methods with the geometric flexibility of the finite element methods. Spectral element computer code was provided by Prof. Karniadakis & Orszag of Princeton University.

Sub Grid Scale (SGS) turbulence model selected for the computations was based on Re-Normalization Group (RNG) theory [Yakhot and Orszag, 1986]. RNG techniques have been applied only recently to the turbulence flow. They provide a means of systematically eliminating smaller length scales from the Navier-Stokes equations by modifying the governing equations. For SGS model, this implies replacing the molecular viscosity with an effective model viscosity. RNG technique has also been used to derive an effective Prandtl number for the transport of energy or passive scalar quantity as well as an improved k-e model. All the parameters appearing in the equations are determined from the theory; it is not necessary to treat parameters as adjustable constants to be determined by matching experiments and predictions.

A number of test cases were studied to examine the applicability of RNG based LES model to the conditions typical of flow around boiler tube. These included calculating 2-dimensional and 3-dimensional flow past a single circular cylinder, flow past a single cylinder in a channel, flow past a notch in a channel, flow past deep tube bank array of 2 x 2 cylinders with large cylinder separation so that cylinder-cylinder interactions are minimized, flow past a deep tube bank array of 3 x 3 cylinders with small cylinder separation so that cylinder-cylinder interactions are significant. The computations were performed at flow Reynolds numbers typical of boiler tube flow conditions at Reynolds number based on free stream velocity and cylinder diameter of about 4000. These simulations are the first LES simulations carried at such high Reynolds number. Typical results for a 2 x 2 cylinder geometry and a 3 x 3 cylinder geometry are shown in chapter 5.

In order to obtain information on the particle deposition rates, particle tracking algorithms were coupled with LES code. Accurate particle trajectory computation requires use of instantaneous gas phase velocity at each particle position which was obtained from the appropriate interpolation algorithms for velocity computed at the grid node points. Instantaneous deposition rates are calculated from trajectory calculations using instantaneous velocity field, while time averaged deposition rates are obtained from calculating trajectories over a large number of instantaneous velocity field. Trajectory computations provide information only on the particle impaction (arrival) rate. Such information needs to be coupled together with particle sticking, erosion, and deposit deformation information to predict the time evolution of the deposit shape. Typical evolution of the deposit shape were obtained for the limiting case of complete capture (sticking coefficient unity, erosion coefficient zero). Transformation of the particle arrival rate in the deposit thickness also requires information on the deposit density, which can vary significantly between loose and dense

deposits and the deposit sintering, although such information is lacking, the predicted shape provides qualitatively correct shape.

Particle sticking probability depends on the deposit composition, in particular on the wetting and glue like characteristics of the deposits. In order to apply such correlation, it is necessary to solve coupled fluid flow and multi-phase, multi-species transport problem. As an example of the code capability, typical results for the reactive species transport were also obtained.

After an initial stage of deposit formation on the clean cylindrical surface, subsequent deposits are formed on non-circular cylinders. Fluid flow characters, especially vortex shedding behind bluff bodies, and flow acceleration due to additional area blockage due to thick deposits can significantly affect the subsequent deposit formation and erosion rates. RNG based LES code was tested for its ability to calculate the flow past smooth non-circular cylinders. Typical results are discussed in chapter 5. It is to be noted that the gas phase turbulence may induce random or chaotic deposit shape with a roughness on the scale of the deposit non-uniformities. Deposit roughness may in turn induce additional flow turbulence. Non-uniform deposit shapes shown in chapter 5 are most probably due to the inadequate sample size and should not be construed as prediction of chaotic deposit evolution.

Significant progress has been made so far in demonstrating the capability of RNG based LES model in calculating fluid flow, multiple species transport, and particle transport problem for complex geometry typical of boiler tube applications. Such simulations require extremely large computer resources. Detailed validation of the flow predictions, understanding of the significant flow processes, and their interactions with the deposition process will require many more detailed simulations than has been possible in the present contract. Use of faster computers, especially parallel processing machines, will significantly reduce the real time [Karniadakis and Orszag, 1993].

3.0 GAS PHASE BEHAVIOR

Boiler fouling is a result of complex interaction between gas phase, mineral matter, and condensate phase. Initial step in the formation of tube deposits is the transport of the mineral matter to the tube surface through the intervening turbulent gas phase. A thorough understanding of the turbulent gas phase is therefore a pre-requisite to the development of the comprehensive model of boiler fouling. The gas phase turbulent behavior is governed by the incompressible, time dependent Navier Stokes equations. A review of the available methods for solving time dependent Navier Stokes equations for fluid flow was undertaken to examine their appropriateness for solving the flow for realistic flow conditions and geometries typical of flow in the convective pass of a boiler.

The method selected was based on a spectral element algorithm [Patera, 1984]. The method, incorporating RNG techniques [Yakhot and Orszag 1986] to provide sub-grid models, serves as the basic flow analyzer for the effort in this program. As such techniques have not been widely publicized in the literature regarding their algorithmic details and/or physical assumptions embodied in their basic structure, the following is intended to provide a brief overview. The code that incorporates the aforementioned computational algorithm and physical models is given the acronym NEKTON and will be referred to frequently in the following discussion.

3.1 Governing Equations

The computational algorithm solves the unsteady, incompressible, two-dimensional, axisymmetric or three-dimensional Navier Stokes equations with forced or natural convection heat transfer in both stationary or time dependent geometry.

The solution variables are the fluid velocity $\mathbf{u} = (u_x, u_y, u_z)$, the pressure p , the temperature T , and a specified number of independent passive scalar fields f_i ; all of the above field variables are functions of space $\mathbf{x} = (x, y, z)$ and time t . The governing equations used are:

Momentum equation:

$$\rho(\partial_t \bar{\mathbf{u}} + (\bar{\mathbf{u}} \cdot \bar{\nabla}) \bar{\mathbf{u}}) = -\bar{\nabla} p + \bar{\nabla} \cdot [\mu(\bar{\nabla} \bar{\mathbf{u}} + (\bar{\nabla} \bar{\mathbf{u}})^T)] + \rho \beta T \hat{\mathbf{g}} + \rho \bar{\mathbf{f}} \quad (1)$$

Continuity (mass conservation) equation:

$$\bar{\nabla} \cdot \bar{\mathbf{u}} = 0 \quad (2)$$

Energy equation:

$$\rho C_p [\partial_t T + (\bar{\mathbf{u}} \cdot \bar{\nabla}) T] = \bar{\nabla} \cdot (k \bar{\nabla} T) + q_{vol} \quad (3)$$

and a convective-diffusive equation for each passive scalar

$$(\rho C_p)_i [\partial_t \phi_i + (\bar{\mathbf{u}} \cdot \bar{\nabla}) \phi_i] = \bar{\nabla} \cdot (\kappa_i \bar{\nabla} \phi_i) + (q_{vol})_i \quad (4)$$

The above governing equations are subject to boundary conditions and initial conditions described below.

3.1.1 Spatial Discretization

The spatial discretization used in the formulation is based on the spectral element method, a high-order finite element method for partial differential equations. Here the computational domain is represented as a set of (disjoint) macro-elements, with the solution, data and geometry being approximated by high-order polynomial expansions within each macro-element.

This approach offers high order (spectral) accuracy, while maintaining the geometric flexibility of low-order finite-element techniques. In the rest of this section the key features of the spectral element method are discussed with special emphasis on mesh generation.

Domain Decomposition.

For two-dimensional domains, the isoparametric spectral element spatial discretization proceeds by first breaking the two-dimensional domain up into (non-degenerate) quadrangles, which are denoted as "macro-" or "spectral" elements. An example of such a decomposition is shown in Figure 3.1a. Three-dimensional domains are broken up into "bricks" in which the two horizontal parallel faces (top and bottom) are non-degenerate quadrangles, Figure 3.2.

Elemental Mesh:

Within each element, a local continuum mesh is constructed corresponding to a $N \times N$ (xN) tensor product. Gauss-Lobatto-Legendre collocation points are shown in figure 3.1b. The Gauss-Lobatto points are clustered near elemental boundaries, and are chosen because of their accurate approximation, interpolation and quadrature properties. The D_x, D_y, D_z notation used in the following discussion refers to the distance between the collocation points.

Element and Continuity Requirements:

The requirements that are placed on individual spectral elements are:

a) Two-dimensional spectral elements are quadrangles, as shown in Figure 3.3a with the interior angle at each of the four corners q in the range $0 < q < 180$ (strict inequality). This is to ensure unique elemental transformations (non-zero Jacobians). Elements that do not satisfy this condition, and are therefore not permitted, are shown in Fig. 3.3b.

b) Three-dimensional elements are defined by two quadrangles on different (parallel) planes which make up the "top" and "bottom" faces of the element. These quadrangles are subject to the rules of the previous paragraph. The four "side" faces of the spectral element are defined by the four surfaces which connect each of the four respective sides of the two quadrangles. Points on the "side" faces are interpolated linearly from the corresponding points on "top" and "bottom" edges, see Figure 3.2.

c) The number of Gauss-Lobatto collocation points in the two or three directions within each spectral element (see Fig 3.1) must be the same and will be denoted by N . It is remarked that whereas (a) is a fundamental restriction, (c) is an artificial constraint (conforming elements).

Regarding how elements may be placed together, the fundamental rule dictated by the form of the governing equations is that the solution and geometry must be continuous across elemental boundaries. Given the restrictions on individual elements, (a) - (c), this continuity requirement translates into the following rules of connection for assemblies of elements.

- i) No part of the element may lie in the interior of another element. Figure 3.4a
- ii) Two elements may be connected only by spatial coincidence of two neighboring vertices of each element (from which it follows that they share an entire common side or face). Examples of correct and incorrect assembly are given in Figure 3.4b.
- iii) To describe a domain, D , elements must cover the entire domain. That is, the only element sides that are not connected to other element sides (per (ii)) must lie on the domain boundary ∂D .
- (iv) The number of Gauss-Lobatto collocation points, N , in each spatial direction within each element is the same for all elements. This follows from the functional and geometrical conformity (continuity) requirement and the restriction (c). It should be noted that (c) and (iv) are automatically taken care of in the code.

Function Interpolation: Similar to standard finite element techniques, within each element the depend variables (u, p, T) are expanded in terms $(N-1)^{th}$ order tensor-product (polynomial) Lagrangian interpolants through the Gauss-Lobatto-Legendre collocation points. For instance, the temperature is expanded as $T = \sum h_i T_i$ where the h_i are the Lagrangian interpolants (that is polynomials which are unity at the i^{th} Gauss-Lobatto node and zero at all others), and T_i are nodal values of the temperature.

Generation of Discrete Equations: The semi-discrete equations (discrete in space) are generated using weighted residual (variational, Galerkin) techniques, corresponding to inserting the assumed forms for the dependent variables (e.g., $T = \sum h_i T_i$) into the governing equations, and requiring that the resulting residual vanish in some integral, weighted sense. Note that, since the basis functions chosen are Lagrangian interpolants, the numerical variables that are solved (e.g., the T_i) correspond to the values of the function of interest (e.g., the temperature) at the collocation points of the mesh.

Convergence: Convergence to the exact solution is obtained either by increasing the number of macro-elements, K , ("finite element"), in which case the error decreases algebraically like K^{-N} , or by increasing the order of the interpolants, N , in elements of fixed identity ("spectral") in which case the error decreases exponentially for smooth solutions e^{-a^N} . As always, any solution obtained numerically is verified to be converged (mesh-independent) by repeating the calculation on a finer mesh.

3.1.2 Temporal Discretization

Most simulations to be carried out during the course of this effort are time-dependent, that is, the governing equations are solved in the time-dependent evolution form given in (1-4). If a steady state solution exists to the problem, it will be achieved by NEKTON as the time asymptotic result of a transient calculation. The solution is updated to the new time-level using various combinations of multistep and multistage schemes.

In all transient simulations, the convective terms in $(\bar{u} \cdot \bar{\nabla})\bar{u}, (\bar{u} \cdot \bar{\nabla})T, (\bar{u} \cdot \bar{\nabla})\phi_i$ (1), (3) and (4) are usually treated explicitly, that is only data from previous time steps are used. The standard time-stepping procedure in NEKTON uses a third-order Adams-Bashforth scheme and the temporal accuracy associated with these terms are therefore $O(Dt^3)$, where Dt is the time step. The reason for the explicit treatment of the convective terms is to avoid the solution of a nonlinear, non-

symmetric system of algebraic equations at each time level. However, due to this explicit treatment, a restriction on the time step, Δt , must be enforced in order to obtain stability.

The stability restriction (Courant condition) can be written in the form:

$$\Delta t < C_{\min_{DF}} \left\{ \frac{\Delta x}{|u_x|}, \frac{\Delta y}{|u_y|}, \frac{\Delta z}{|u_z|} \right\} \quad (5)$$

where C is the Courant number, Δx , Δy , Δz are the x,y,z distances between spatial collocation points (see Figure 3.1b), u_x , u_y , u_z are the x,y,z velocities, respectively and $\min_{DF}$ refers to the minimum over the entire flow field. The formulation will always ensure that the Courant condition (5) is satisfied.

The (prescribed) volumetric forcing functions, f , $-rbgT$, q_{vol} , $(q_{vol})_f$ including the subgrid scale contributions to the resolved scales in Eq. (1), (3) and (4) are also treated using a third order-explicit Adams-Bashforth time stepping procedure. However the stability restriction (5) does not apply to these terms.

The diffusion terms $\nabla \cdot [\mu (\nabla \bar{u}) + (\nabla \bar{u})^T], \nabla k \nabla T, \nabla \cdot k, \nabla \phi_i$

in Eq. (1), (3), and (4) and the pressure incompressibility condition in Eq. (1) - (2) are always treated implicitly using a Q^{th} order backward differentiation multistep scheme. Possible values of Q range from 1 to 3 resulting in a temporal accuracy of $O(\Delta t^Q)$. Due to the implicit treatment, there is no stability restriction associated with these terms, however, a set of linear algebraic equations must be solved at each time level. This can be done efficiently using iterative solvers as described in Section 3.3.

Remark 1: In general, the stability determining convective terms (explicit) and the work-intensive pressure/diffusion terms (implicit) do not coincide in a traditional semi-implicit treatment of the unsteady Navier-Stokes equations. In order to address this issue, a new high-order operator splitting method has been implemented in a variant of the numerical formulation. This method can potentially yield significant speed-up, Section 3.4. Although this scheme can be interpreted as the method of characteristics, it is in fact a particular example of a scheme generated from a more general methodology based on operator integration factor methods.

Remark 2: The algorithm also provides the option of integrating the unsteady Navier-Stokes equations using the classical splitting method (fractional step method). This scheme cannot be applied to stress boundary conditions and the temporal accuracy is $O(\Delta t)$.

3.2 Solution Methods

The selection of the fully discrete set of equations are characterized by use of iterative solvers and tensor-product sum-factorization techniques. For the explicitly treated convective terms, there is no matrix inversion, but only matrix vector product evaluations. This is done efficiently, both in terms of operation count and memory requirement by using sum-factorization techniques on an element-by-element basis.

The implicitly treated diffusion and pressure terms result in a large linear system of equation, which are solved using iterative solution procedures. The basic solver in NEKTON is an elliptic Helmholtz solver, appropriate for inverting the diffusion operator. This solver is based on conjugate gradient iteration, in which the computationally intensive part in each iteration is

dominated by a single matrix vector product evaluation. As for the explicit terms, this evaluation is performed using sum-factorization techniques on an element-by-element basis. It is worth emphasizing that the global or elemental matrixes are never formed explicitly, an essential feature for solving large (three-dimensional) problems. The storage requirements in NEKTON is therefore minimal; it is on the order of the number of collocation points in the mesh.

Remark 3. The classical splitting scheme for solving the steady Navier-Stokes equations only involves one elliptic solve for the pressure and one for each of the velocity components. In contrast, a discretization based on consistent approximation spaces (polynomial degree N for velocity and polynomial degree $N-2$ for the pressure) results in nested elliptic solves for the pressure (Uzawa algorithm). While the latter approach is slow, it is generally more accurate.

Remark 4. NEKTON has the capability of using two different elliptic solvers. The first is based on conjugate gradient iteration, while the second one is based on intra-element multigrid procedure. The multigrid technique is particularly attractive for large problems, as the associated convergence rate is almost resolution independent.

The data structure used in the code also allows NEKTON to run efficiently on modern architectures, in particular on distributed memory parallel machines. The loosely coupled spectral elements can readily take advantage of medium-grained parallelism by distributing the elements on different processors, while each individual (tightly coupled) elemental matrix-vector product evaluation can be vectorized. This is in contrast to direct solution techniques such as Gaussian elimination, which are cross-coupled and less effective at exploiting parallel computer architecture.

The motivation behind spectral element (rather than low-order finite element) methods is that the increased coupling introduced by high-order methods increases the work only algebraically, whereas the increase in accuracy is exponential. These argument only apply for problems with smooth solutions. However, with the exception of boundary-induced singularities, incompressible flow and heat transfer problems will generally satisfy these requirements

3.3 Method Tradeoff

NEKTON uses several different algorithms for solving problems in fluid mechanics. The selection of the algorithm most appropriate for a given problem can greatly affect the speed and accuracy with which that problem can be solved. In this section, a discussion is provided to outline and compare the capabilities, relative speeds, and accuracies associated with each solution algorithm used by NEKTON.

The solution algorithm has two parts, the problem formulation in which the partial differential equations comprising the Navier-Stokes equations are converted into a set of discrete equations, and the solution, a numerical procedure in which the set of discrete equations are solved simultaneously. The formulation uses three variants, the non-stress formulation, the stress formulation, and the classical splitting scheme. These formulations convert the Navier-Stokes equations into a series of discrete elliptic problems, which are solved iteratively using an elliptic solver; in the code this solver is based on conjugate gradient iteration.

The split formulation gives the fastest solution for any given time-dependent flow problem. Its primary limitation is that it incurs splitting errors which are of order $u\Delta t$, where u denotes kinematic viscosity. Splitting errors are significant where the viscosity is high and the time step is large, as in creeping or Stokes flows. For high Reynolds number problems, the viscosity is low and the time step is small due to stability restrictions (Courant condition), so that generally the splitting errors are small. The split formulation is hence suitable for flows in which $Re > 25$.

The non-stress formulation uses consistent approximation spaces for the velocity and pressure, and gives accurate results for the entire range of Reynolds numbers. It can be used for flows ranging from Stokes flows (where $Re=0$) through transition flows. It is slower than the split formulation by a factor of approximately four.

The stress formulation is a variant of the non-stress formulation in which the three (or two) velocity components are solved for simultaneously and all components of the stress tensor are retained. This formulation allows for additional stress-related boundary conditions: imposed stress, zero stress and moving boundaries, which can be defined in terms of local (tangential and normal) coordinate components. This formulation is the most general and rigorous of the three, but also the most CPU-intensive. It is slower than the non-stress algorithm by a factor of approximately two.

As discussed in Section 3.2, NEKTON solves any convection diffusion problem as a transient problem, with the convective terms treated explicitly. For convection dominated flows ($Re \gg 1$) this explicit treatment can give very severe time step restrictions due to the Courant condition (5). For the standard semi-implicit time-stepping strategy, NEKTON uses a default Courant number of $C = 0.25$. However, if the flow problem has prescribed velocity on the whole (fluid) domain boundary, substantial time saving benefits can be realized by increasing the Courant number to about $C = 0.4$.

Bigger savings can be achieved for convection-diffusion problems, however, if the method of characteristics is used, in which the convective terms are decoupled from the pressure and viscous treatment. Hence, the time step for the (expensive) integration of viscous term, together with the imposition of the incompressibility constraint, can be set much larger than the (restrictive) time step for the integration of the explicitly treated convective terms. If the work is dominated by the pressure solver, an increase in the Courant number (measured using the bigger time step) from $C = 0.25$ to $C = 2.0$ can sometimes give a factor 8 in speed up. The limitations using the method of characteristics are typically related to problems with steep (marginally resolved) normal boundary layers, and if the prescribed in flow boundary conditions do not correspond to fully developed flows.

3.4 ReNormalization Group Treatment of Turbulent Flows

Current trends in turbulence modelling employ methods from statistical mechanics, with turbulence regarded as exhibiting both universal and non-universal behavior [Orszag et al 1993, Yakhot et al, 1986]. Universal behavior can conceivably be modelled, with the model having a wide range of application. Non-universal behavior is brought about by large scale inhomogeneities, such as geometry, boundary conditions, imposed unsteadiness, etc. Such inhomogeneities must be resolved by the governing equations and cannot be modelled in any general manner. A statistical mechanics approach addresses the universal behavior, looking for ways to model it, or at least its gross effects, on the non-universal part of the flow. A perturbation series is usually applied to the instantaneous equations, resulting in an infinite series in powers of mean flow gradients. The first term in such a series expansion is the isotropic formula, the second term is linear in the mean velocity gradient, and the third term produces quadratic non-linearity.

The constitutive approach to turbulence modelling suffers even on an intuitive level: turbulence is not a material and does not exhibit the necessary characteristics to be considered a optimum material. Constitutive and statistical mechanic approaches also suffer a common weakness: these theories provide no logical means to terminate the expansion, i.e., the theory cannot indicate when a satisfactory order or number of terms has been achieved. Thus one is left to terminate the series when the desired phenomenon is obtained or the algebra inundates the researcher. More problematic, no proof of convergence can be produced for these series, and arbitrarily obtaining higher order terms invites problems. In common with the more widely used

phenomenologically based models, all the constants arising in such formulations must be established by comparing with data - again the theory fails to provide any clue to the values of the constants.

ReNormalization Group (RNG) techniques, like the previous statistical approaches, have proven to be useful tools in theoretical physics and statistical mechanics to study systems with a very large number of degrees of freedom. Although RNG theory has found its way into fluid mechanics relatively recently, particularly in developing turbulence theory, it has provided a series of interesting theoretical and numerical results. A milestone for RNG theory in fluid mechanics was the establishment of the so-called correspondence principle, stating that in the inertial range, the behavior of the small scale Navier-Stokes turbulence is statistically equivalent to the modelled Navier-Stokes equation with the addition of a random noise term. This principle makes it possible to use all the formalism of the classical RNG theory.

Recently RNG methods have been developed to analyze a variety of turbulent flow problems. For homogeneous turbulent flows, such important quantities as the Kolmogorov constant, Batchelor constant, turbulent Prandtl number, rate of decay to isotropy, skewness factor, etc. have been obtained directly from this theory in good agreement with available data. Efforts in developing RNG methods for sub-grid (large eddy simulation) model constants have also been notably successful.

RNG methods involve systematic approximations to the full Navier-Stokes and energy equations that are obtained by using perturbation theory to eliminate or decimate infinite small bands of small scale modes, iterating the perturbation procedure to eliminate finite bands of modes by constructing recursion relations for the renormalized transfer coefficients, and evaluating the parameters at a fixed point in the lowest order of a dimensional expansion around a certain critical dimension. The decimation procedure, when applied successively to the entire wave number spectrum, leads to the RNG equivalent of full closure of the Reynolds averaged Navier-Stokes and temperature equations. The resulting RNG transport coefficients are differential in character as opposed to ad hoc algebraic coefficients of conventional closure methods. All constant and functions appearing in the RNG closures are fully determined by the RNG analysis. In essence, the RNG method provides an analytical method to eliminate small scales from the Navier-Stokes and passive scalar equations, thus leading to a dynamically consistent description of the large scales. The formal process of successive elimination of small scales together with re-scaling of the resulting equations results in a calculus for the derivation of the transport approximations in turbulent flows.

The renormalization group method has been used to derive a formula for the inverse turbulent Prandtl number, and three different types of models for the eddy viscosity: an algebraic model, a differential k- ϵ , and a subgrid scale turbulence model for large eddy simulations. The governing equations for the flow motion are the Navier Stokes equations:

$$\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial v_i}{\partial x_j} \right) \quad (6)$$

along with the incompressibility constraint

$$\frac{\partial v_i}{\partial x_i} = 0 \quad (7)$$

and the governing equations for the temperature field:

$$\frac{\partial T}{\partial t} + v_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial T}{\partial x_j} \right) \quad (8)$$

Here n is the total viscosity defined as $n = n_0 + n_T$ (the sum of the molecular and turbulent viscosity, respectively) and $\Gamma = \alpha \nu$ where α is the inverse total Prandtl number. It has been shown in the literature that elimination of small scales from the original Navier-Stokes and energy equations written in terms of the molecular properties of a passive scalar leads to the following relation between the inverse total Prandtl number α and the total viscosity n :

$$\left(\frac{\alpha - 1.3929}{\alpha_0 - 1.3929} \right)^{0.6321} \left(\frac{\alpha + 2.3929}{\alpha_0 + 2.3929} \right)^{0.3679} = \frac{\nu_0}{\nu} \quad (9)$$

where α_0 refers to the molecular inverse Prandtl number. It is obvious from Equation (9) that in the limit $n \rightarrow n_0$ one obtains $\alpha = \alpha_0$; however for larger values of n only one root is chosen from (9).

Use of Equation (9) assumes that the distribution of n at every nodal point in the computational domain is available; this distribution can, for example, be based on fittings of experimental data or it can be computed entirely via the renormalization group analysis that provides different types of models as discussed next:

3.4.1 RNG Algebraic Model

This model [Yakhot et al, 1986] is the simplest of all, however it is not very general as it requires the a priori postulation of the characteristic integral length scale, and thus an assumption needs to be made based on physical considerations. The eddy viscosity n is obtained from the following relation:

$$\nu = \nu_0 \left[1 + H \left(\frac{a\varepsilon}{(2\pi)^4 \nu_0^3} \Delta^4 - C \right) \right]^{1/3} \quad (10)$$

where $H(x)$ is the Heaviside function defined by $H(x) = x$ for $x \geq 0$ and $H(x) = 0$ otherwise and D is an integral length scale of turbulence in the inertial range. Constants a and C are assigned values of 0.120 and 100 respectively. The mean dissipation rate ε can be expressed entirely through the resolvable field as:

$$\varepsilon = \frac{\nu}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)^2 \quad (11)$$

The total viscosity is then obtained by solving an algebraic cubic equation at every node of the computational domain at each time step [Sakya et al 1993].

3.4.2 RNG k-ε Model

This is a differential model based on differential recursion relations [Yakhot et al, 1992]. It is free of adjustable parameters, however two additional equations are derived for the turbulent kinetic energy k , and the rate of dissipation ϵ .

$$\frac{Dk}{Dt} = P - \epsilon + \frac{\partial}{\partial x_i} \left(\alpha \nu \frac{\partial k}{\partial x_i} \right) \quad (12)$$

$$\frac{D\epsilon}{Dt} = -\bar{P} - Y + \frac{\partial}{\partial x_i} \left(\alpha \nu \frac{\partial \epsilon}{\partial x_i} \right) \quad (13)$$

The production term P is based on the turbulent viscosity and is defined as:

$$P = \frac{\nu_T}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)^2 \quad (14a)$$

while the terms P , Y are subsequently defined by:

$$P = 0.656 \epsilon^{1/2} Y_e P \quad (14b)$$

$$Y = \epsilon^{3/2} Y_e \quad (14c)$$

The RNG procedure provides the additional two differential equations for Y_e and $k/\epsilon^{1/2}$ which can be integrated as follows:

$$Y_e \nu_o^{1/2} = \alpha_y - \gamma_y \int_1^{v/\nu_o} \frac{dt}{(t^3 - 1 + C)^{1/2}} \quad (15a)$$

$$\frac{k}{\epsilon^{1/2}} = \alpha_k + \gamma_k \int_1^{v/\nu_o} \int \frac{tdt}{(t^3 - 1 + C)^{1/2}} \quad (15b)$$

Here the coefficients (α_y, γ_y) and (α_k, γ_k) are known constants derived from the asymptotic behavior of the model. The total viscosity ν is implicitly defined from equations (15) at each node of the computational domain. In the high Reynolds number region where $\nu \gg \nu_o$, one obtains:

$$\nu = 0.0845 \frac{k^2}{\epsilon} \quad (16)$$

This high Reynolds number approximation is similar to that commonly used in algebraic models. Thus, the algebraic models contain terms like e^2/k , which diverge when $k \rightarrow 0$ (i.e. near wall regions or separation zones) creating immense computational difficulties. The differential relations obtained via RNG techniques, however do not contain such singular behavior and thus have great potential for success with separating flows. The differential relations provide definitive interpolation formulae to connect low and high Reynolds number regions of the flow.

3.4.3 RNG Sub-Grid Scale Model

In large eddy simulations (LES), the velocity field v_i is decomposed into large scale v_i and sub-grid component v_i . It is the modelling of terms involving these latter components that is crucial for accurate computations as previous attempts using various sub-grid models have indicated. The RNG sub-grid model is derived by elimination of modes from the interval L_0 - L , where

$L = g(e/n_0^3)^{1/4}$ ($g=0.20$ is a dissipation cut-off limit) and the wave vector

$L_0 = Le^{-1}$ can be expressed through the computational mesh size D . The general RNG derived viscosity given by:

$$\nu_r = \nu_0 \left(1 + \frac{a\varepsilon}{\nu_0^3 \Lambda^4} (e^{4r} - 1) \right)^{1/3} \quad (17)$$

can then be expressed in terms of a length scale D , which in LES represents the width of a suitably chosen Gaussian filter. Thus, Equation (17) reduces to an identical equation as in (10) where D is expressed through an integral in terms of the size of the computational domain.

3.5 Potential Practices to Reduce Computational Resources

Even though optimum values of the relevant computational and algorithmic variables can be obtained only after a careful analysis of a large number of cases and are invariably problem specific, certain conclusions regarding potential practices to reduce computational resources associated with a solution are readily apparent and can be outlined as follows:

Most solutions employ a default description of the initial field to correspond to a zero field excluding the boundary conditions specified. To economize on this wasteful practice, restarts are generally made from a coarse mesh to a finer mesh, where the macro-elemental mesh is the same, but the order of the basis functions (NORDER) is higher in the finer mesh. In this strategy, an initial start-up coarse mesh will typically have NORDER=5. The solution produced with this mesh is then utilized as initial conditions for a final simulation with a higher NORDER. The NORDER to be employed in these accurate solutions varies between 7 and 9. This strategy can also be used effectively to obtain improved convergence for problems with high Reynolds numbers. The steady solution of a low Reynolds number problem in which low resolution is used can be used as initial conditions for the solution of a high Reynolds number problem with higher resolution. In this way, part of the expensive and slow transient associated with high Reynolds number flows can be avoided.

The formulation uses for problems involving convection, a solution technique which is inherently unsteady. Steady solutions, if they exist, are calculated by running an unsteady problem for sufficient time for it to reach steady state. The two problems for which a steady solution technique can be used directly are conduction heat transfer and Stokes flow. The implications of

the unsteady solution technique are important in the calculation of the CPU time that is required for the solution of a given problem; the total run time will thus be the CPU time per time step, summed over all time steps.

The CPU time naturally depends on the number of elements, the order of the elements and the number of time steps. Both the elemental solution and the number of time steps required for a given problem invariably increase with increasing Re. The Reynolds number is a primary consideration in CPU time estimates.

The number of time steps required in an unsteady algorithm depends strongly on the Reynolds (or Peclet) number where the time step is constrained by the Courant criterion. This constraint has the effect of limiting the distance that a particle of fluid can move in a single time step to on the order of a local mesh spacing. For a computational domain of characteristic length L , the number of steps required to convect the fluid throughout the domain will be $2L/Dx$ based on a convective time scale of L/u , where u is a characteristic velocity. The time to steady state, if it exists may also include a diffusive time scale, which will depend on the existence, location and thickness of boundary layers. At worst case, the diffusive time scale would be of order (Re) times the convective time scale. The arrival of steady state is usually verified by checking the temporal behavior of the flow using prespecified history points.

3.6 Details of RNG Methodology

The specific details of the spectral element methodology incorporating the ReNormalization Group (RNG) large eddy descriptor are given below for a better appreciation of the pertinent computational issues.

The renormalized equation of motion (incorporating the full stress tensor) for $\underline{v}$ is cast in the following form:

$$\frac{\partial \underline{v}}{\partial t} = \frac{\nabla p}{\rho} + \bar{\nu} \nabla^2 \underline{v} + \underline{N}(\underline{v})$$

$$\underline{\nabla} \cdot \underline{v} = 0 \quad (18a)$$

where the last term in the first equation includes all nonlinear and forcing terms (due to RNG formulation) as well as the viscous terms, i.e.,

$$\underline{N}(\underline{v}) = \frac{1}{2} [\underline{v} \cdot \underline{\nabla} \underline{v} + \underline{\nabla} \cdot (\underline{v} \cdot \underline{v})] + \underline{f} + \underline{\nabla} \cdot (\underline{v} - \bar{\nu}) [\underline{\nabla} \underline{v} + \underline{\nabla}^T \underline{v}] \quad (18b)$$

where n denotes the total RNG viscosity, while $\bar{\nu}$ is an artificial (constant in space) viscosity introduced for stability reasons. $\underline{f}$ denotes the renormalized force due to RNG of the original Navier-Stokes equations. The convective terms are written in a skew-symmetric form for aliasing control purposes. Numerical solution of the above system of equations is obtained in a three dimensional computational domain W . However, before proceeding with the spatial discretization of the equation, details of the time stepping algorithm are briefly reviewed.

Semi Discrete Formulation

The separation of terms in Equation (18a) leads naturally to a splitting scheme of mixed explicit/implicit type. In particular, a specific high-order splitting algorithm based on mixed stiffly

stable scheme is used. Considering first, the nonlinear terms $\underline{N}$, the following time stepping form results:

$$\frac{\hat{\underline{v}} - \sum_{q=0}^{J-1} \alpha_q \underline{v}^{n-q}}{\Delta t} = \sum_{q=0}^{J-1} \beta_q [-\underline{N}(\underline{v}^{n-q})] \quad (19a)$$

where a_q, b_q are implicit/explicit weight-coefficients for the stiffly stable scheme of order J (especially 3). The next substep incorporates the pressure equation and enforces the incompressibility constraint as follows:

$$\frac{\hat{\underline{v}} - \underline{\hat{v}}}{\Delta t} = \underline{\nabla} p^{n+1} / \rho \quad (19b)$$

$$\underline{\nabla} \cdot \underline{\hat{v}} = 0 \quad (19c)$$

Finally, the last substep includes the viscous corrections and the imposition of the boundary conditions, i.e.,

$$\frac{\gamma_0 \underline{v}^{n+1} - \underline{\hat{v}}}{\Delta t} = \bar{\nu} \underline{\nabla}^2 \underline{v}^{n+1} \quad (19d)$$

where γ_0 is a weight -coefficient of the backwards differentiation scheme employed by Karniadakis, et al.

The above treatment of the system of equations (18) results in a very efficient calculation procedure as it decouples the pressure and velocity equations as in (19b) and (19c) respectively. As regards the time accuracy of this splitting scheme, a key element in this approach is the specific treatment of the pressure equation, which can be recast in the form:

$$\underline{\nabla}^2 p^{n+1} = \underline{\nabla} \cdot \left(\frac{\hat{\underline{v}}}{\Delta t} \right) \quad (20a)$$

along with the consistent high-order pressure boundary condition (Karniadakis, et al):

$$\frac{\partial p^{n+1}}{\partial n} = \underline{n} \cdot \left[-\sum_{q=0}^{J-1} \beta_q \underline{N}(\underline{v}^{n-q}) - \text{Re}^{-1} \sum_{q=0}^{J-1} \beta_q [\underline{\nabla} \times (\underline{\nabla} \times \underline{v}^{n-q})] \right] \quad (20b)$$

where $\underline{n}$ denotes the unit normal to the boundary G . Equation (20) therefore is a Poisson equation with constant coefficients which can be rewritten in the standard form:

$$\underline{\nabla}^2 \phi = g(x) \quad (21)$$

where f is defined as p^{n+1} and $g(x) = \underline{\nabla} \cdot (\underline{v}/Dt)$. In the following section reference is specifically made to this equation in order to discuss the spatial discretization of equations (19) in three dimensions using the spectral element method.

Spatial Discretization

The spatial discretization of (19) is obtained using the spectral element methodology. In the standard spectral element discretization, the computational domain W is broken up into general brick elements (hexahedra) in three dimensions, which are mapped isoparametrically to canonical tubes. The accuracy of interpolating the geometry therefore is of the same order as the accuracy of interpolating the field unknowns. Geometry, unknowns and data are then expressed as tensorial products in terms of Legendre-Lagrangian interpolants. The final system of equations to be solved is obtained via a Galerkin variational statement. In particular, a typical computational domain W is covered with K spectral elements of resolution N_1, N_2, N_3 (ranges from 5 to 16) in respective directions.

To illustrate the spectral element methodology in more detail, consideration is given to the model equation (21) which represents the elliptic contributions of the governing equations. If H_0^1 is defined as the standard Sobolev space which contains functions that satisfy homogeneous boundary conditions, and test functions are introduced in the manner $y \in H_0^1$, the resulting equivalent variational statement of (21) can be expressed as:

$$\int_{\Omega} \frac{\partial \chi}{\partial x_j} \frac{\partial \phi}{\partial x_j} ds = - \int_{\Omega} \chi g ds \quad (22)$$

The conforming spectral element discretization corresponds to the numerical quadrature of the variational form (22) restricted to the space $X_h \in H_0^1$. The discrete space X_h is defined in terms of the spectral element discretization parameters (K, N_1, N_2, N_3) where K is the number of spectral elements, and N_1-1, N_2-1, N_3-1 are the degrees of piecewise high order (Legendre) polynomials in the three directions respectively that fill the space X_h . By selecting appropriate Gauss-Lobatto points x_{pql}^k and corresponding weights $r_{pql} = r_p r_q r_l$, equation (22) can be replaced by:

$$\sum_{k=1}^K \sum_{p=0}^{N_1} \sum_{q=0}^{N_2} \sum_{l=0}^{N_3} \rho_{pql} J_{pql}^k \left[\frac{\partial \chi}{\partial x_j} \frac{\partial \phi}{\partial x_j} \right]_{\xi_{pql}^k} = \sum_{k=1}^K \sum_{p=0}^{N_1} \sum_{q=0}^{N_2} \sum_{l=0}^{N_3} \rho_{pql} J_{pql}^k [\chi g]_{\xi_{pql}^k} \quad (23)$$

Here J_{pql}^k is the Jacobian of the transformation from global to local coordinates (x, y, z) to (r, s, t) for the three dimensional element k . The Jacobian is easily calculated from the partial derivatives of the geometry transformation at the nodal point (pql) via collocation as follows:

$$J = z_t (x_r y_s - x_s y_r) + z_s (x_t y_r - x_r y_t) + z_r (x_s y_t - x_t y_s) \quad (24a)$$

The partial derivatives are calculated from standard Lagrangian interpolations as for example:

$$(X_r)_{pql} = D_{pm} X_{mq1} \quad (24b)$$

where X_{mq1} is the x global coordinate of node (pql) ; here the derivative operator is defined $D_{ij} = dh_j/dz(x_i)$, and h_j is the Lagrangian interpolant.

The next step in implementing (23) is the selection of a basis that reflects the structure of the piecewise smooth space X_h . A choice is made to employ an interpolant basis with components defined in terms of Legendre-Lagrangian interpolants $h_i(r_j)=d_{ij}$. Here r_j represents the local coordinate and d_{ij} is the Kronecker-delta symbol. It was shown previously that such a spectral element implementation converges spectrally fast to the exact solution for a fixed number of elements K and $N_{1,2,3} \in \mathbb{N}$, for smooth data and solution even in non-linear geometries. Having selected the basis, the procedure then resumes by writing the local to the element spectral element approximations for the test functions, data and geometry and obtains the system matrix; details are presented elsewhere.

The natural choice of solution algorithm for Eq. (23) is an iterative procedure; in this case the large matrices (i.e., $P^{k_{ijmnpq}}$) need not be stored, but instead computed during the time stepping by matrix-vector products (i.e., $P^{k_{ijmnpq}} f_{mnq}$). Two different iterative techniques have been implemented in the literature in this context; conjugate gradient techniques and multigrid methods. A difference of the formulation adopted here as compared to similar schemes employed in the literature is that the high-order splitting scheme used here results in separate, elliptic equations for the pressure and velocity that can be solved very efficiently and robustly by using those iterative techniques without the need of case dependent preconditioners and other convergence acceleration techniques.

3.6.1 RNG Prandtl Number Derivation

The specific details of the spectral element methodology incorporating the ReNormalization Group (RNG) large eddy descriptor are given below with a view to derive a formula for the inverse turbulent Prandtl number in addition to the previously mentioned subgrid scale turbulence model. The governing equations for the flow are the Navier-Stokes equations:

$$\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial v_i}{\partial x_j} \right) \quad (26)$$

along with the incompressibility constraint:

$$\frac{\partial v_i}{\partial x_i} = 0 \quad (27)$$

and the governing equation for the temperature field:

$$\frac{\partial T}{\partial t} + v_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j} \left(k \frac{\partial T}{\partial x_j} \right) \quad (28)$$

In the above equations ν is defined as the total viscosity, i.e., $\nu = \nu_0 + \nu_T$ (the sum of the molecular and turbulent viscosity respectively, and $k = \frac{\nu_0}{\alpha}$ where α is the inverse total Prandtl number. It has been shown by Yakhot and Orzag that elimination of small scales from the original Navier-Stokes and energy equations written in terms of the molecular properties of a passive scalar leads to the following relation between the inverse total Prandtl number α and the total viscosity ν .

$$\left| \frac{\alpha - 1.3929}{\alpha_0 - 1.3929} \right|^{0.6321} \left| \frac{\alpha + 2.3929}{\alpha_0 + 2.3929} \right|^{0.3679} = \frac{\nu_0}{\nu} \quad (29)$$

where a_0 refers to the molecular inverse Prandtl number. It is obvious from equation (29) that in the limit $n \rightarrow \infty$, $a = a_0$; however, for large values of n only one root should be chosen from (29). Searching parametrically for possible zeros of (29) for various values of $n \geq 10$ ($a_0 = \nu_0 = 1$) a unique root exists, however for smaller values there can be two roots provided by (29) from which only the smaller is physically acceptable.

Use of equation (29) assumes that one has the distribution of n at every nodal point of the computational domain; this distribution can, for example, be based on fittings of experimental data or it can be computed entirely via the ReNormalization Group analysis as is done in this effort. This is discussed next for the sake of completeness.

In large eddy simulations (LES) the velocity field v_i is decomposed into large scale v_i and subgrid components v_i . It is the modelling of these latter components that is crucial for accurate computations as previous attempts using various subgrid models have indicated. The RNG subgrid model is derived by elimination of modes from the interval

$$\Lambda_0 \Lambda, \text{ where } \Lambda = \gamma \left(\frac{\varepsilon}{\nu_0^3} \right)^{1/4} (\gamma = 0.20)$$

is a dissipation cut-off limit and the wave vector. $L_0 = L e^{-T}$ can be expressed through the computational mesh size D . The general RNG derived viscosity given by:

$$\nu_r = \nu_0 \left(1 + \frac{a\varepsilon}{\nu_0^3 \Lambda^4} \right) (e^{4r} - 1)^{1/3} \quad (30)$$

can then be expressed in terms of a length scale D , which in LES represents the width of a suitably chosen Gaussian filter.

3.6.2 Details of the RNG Subgrid Viscosity Model

Subgrid scale viscosity model was developed and applied for prediction of flow, turbulence and heat transfer details around an isolated cylinder as well as a deep tube bank, using an ReNormalization Group (RNG) large eddy simulator. Specifically, the following expression for the RNG subgrid viscosity is employed after Yakhot and Orszag:

$$\nu^{(q)} = \left[1 + H \left(\gamma_{rng} \gamma_{iso} \frac{\bar{\varepsilon}^{(q)} \Lambda^{-4}}{\nu_0^3} - C \right) \right]^{1/3} \quad (31)$$

where

$$\gamma_{rng} = \frac{3}{8} (1.594) A_d, A_d = \frac{d^2 - d}{2(d^2 + 2d)} \quad d = 3 \quad (32)$$

$$\gamma_{iso} = \frac{3w^2}{(u^2 + v^2 + w^2)} \quad (33)$$

$$\bar{\epsilon}^{(q)} = v^{(q)} |S_{ij}^{(q)}|^2$$

$$I = \Lambda^{-4} = \pi^{-1} \int_{\Lambda_1}^{\infty} \int_{\Lambda_2}^{\infty} \int_{\Lambda_3}^{\infty} \frac{dq_1 dq_2 dq_3}{(q_1^2 + q_2^2 + q_3^2)^{7/2}} \quad (35)$$

where $(L_i = (p/D_i) \ i = 1,2,3$

In equation (33) g_{iso} depends on the local resolvable velocities, which reflects the anisotropy of the small-scale structure of the complete flow. Additionally, function $H(x)=x$ when $x \geq 0$ and 0 otherwise, representing the fact that scale elimination only occurs when there are scales to be removed. In the expression for subgrid viscosity, the "average" inverse grid scale L also follows directly from the RNG calculus. In principle, the scale elimination procedure leading to the RNG subgrid model may be performed with confidence only for scales much smaller than that corresponding to the energy containing scales of turbulence. If all length scales up to $l \gg \max(D_i)$ are eliminated, where D_i is the filter length scale related to the computational mesh size, then the geometrical structure of the mesh is anticipated not to be important and a simple procedure that replaces L by $p/$ suffices. In this case, use of a commonly employed expression, i.e.,

$$D = (D_x D_y D_z)^{1/3} \quad (36)$$

(a practice that was also adopted during the course of this study) also produces reasonable predictions. However, only the scales up to $2D_i$ are removed; then it is logical to account more properly for the grid anisotropy. A suitable procedure to numerically evaluate(35) to obtain an appropriate integral scale for a grid of general asymmetry, was devised during the course of this work. Specifically, the integral was evaluated in the following manner:

$$I = I_s + I_N - (I_{13} + I_{21} + I_{32}) \quad (37)$$

where:

$$I_s = \int_L^{\infty} \int_0^{\pi/2} \int_0^{\pi/2} \frac{r^2 \sin \theta dr d\theta d\phi}{(r^2)^{7/2}} = \frac{\pi}{8L^4} \quad (38)$$

(using spherical coordinates, L is chosen arbitrarily)

$$I_N = \int \int \int_{ABCD} \frac{dk dp dq}{k^2 + p^2 + q^2} \quad (39)$$

(evaluated numerically using trapezoidal rule)

$$I_{13} = \int_0^{\Lambda_2} \int_{\varphi_3}^{\pi/2} \int_L \frac{dq_2 r dr d\theta}{(r^2 + q_2^2)^{7/2}} = \frac{2\pi/2 - \varphi_3}{5 L^4} \Im(\alpha_2)$$

$$\text{where } \varphi_3 = \sin^{-1} \frac{\Lambda_3}{L}$$

$$\alpha_2 = \tan^{-1} \frac{\Lambda_2}{L}$$

(40)

$$I_{32} = \int_0^{\Lambda_1} \int_{\varphi_2}^{\pi/2} \int_L \frac{dq_1 r dr d\theta}{(r^2 + q_1^2)^{7/2}} = \frac{2\pi/2 - \varphi_2}{5 L^4} \Im(\alpha_1)$$

$$\text{where } \varphi_2 = \sin^{-1} \frac{\Lambda_2}{L}$$

$$\alpha_1 = \tan^{-1} \frac{\Lambda_1}{L}$$

(41)

$$I_{21} = \int_0^{\Lambda_3} \int_{\varphi_1}^{\pi/2} \int_L \frac{dq_3 r dr d\theta}{(r^2 + q_3^2)^{7/2}} = \frac{2\pi/2 - \varphi_1}{5 L^4} \Im(\alpha_3)$$

$$\text{where } \varphi_1 = \sin^{-1} \frac{\Lambda_1}{L}$$

$$\alpha_3 = \tan^{-1} \frac{\Lambda_3}{L}$$

(42)

$$\Im(\alpha) = \sin(\alpha) - \frac{1}{3} \sin^3(\alpha)$$

(approximately using cylindrical coordinates).

4.0 MINERAL MATTER TRANSPORT MECHANISM

Boiler fouling is a result of complex interactions between gas phase, mineral matter, and the condensate phase. After developing a comprehensive model for describing the gas phase behavior, in the frame work of RNG- Spectral Element Simulation, it is necessary to develop modules for incorporating the mineral matter and condensable species transport behavior in their comprehensive model. A brief survey of the literature revealed the following possible mechanisms for transporting different ash constituents from the host gas to boiler tubes as deserving prominence in building the overall comprehensive model.[see Rosner, 1986, Rosner et al, 1992, Baxter et al, 1993].

i) Flame-volatilized species, chiefly sulfates, are deposited on cooled boiler tubes via the mechanism of classical vapor diffusion. This mechanism is more efficient than the particulate ash deposition, and as a result there is usually an enrichment of condensable salts, chiefly sulfates, in boiler deposits.

ii) Particle diffusion (Brownian motion) may account for deposition of some fine particles below 0.1 mm in diameter in comparison with the mechanism of vapor diffusion and particle depositions, however, the amount of material transported to the tubes via this route is probably small.

iii) Eddy diffusion thermophoretic and electrophoretic deposition mechanisms are likely to have a marked influence in transporting 0.1 to 5 mm particles from the host gas to cooled boiler tubes.

iv) Inertial impaction is the dominant mechanism in transporting particles above 5 mm in diameter to water and steam tubes in pulverized coal fired boiler, where the typical flue gas velocity is between 10 to 25 m/s. Particles above 10 mm usually have kinetic energies in excess of what can be dissipated at impact (in the absence of molten sulfate or viscous slag deposit), resulting in their entrainment in the host gas.

In the vicinity of cooled tubes, alkali sulfates, formed prior to entry in the boiler by conversion of primarily alkali hydroxides and chlorides, may condense on ash, fume and fly ash or alternatively through self-nucleation owing to the large supersaturation in the boundary layer. Thus, a comprehensive nucleation model may be required to predict the size distribution and composition of aerosols formed from condensation of ash vapor/alkali sulfates. Such a model should be formulated to incorporate significant mechanisms of homogeneous/heterogeneous nucleation, agglomeration and adsorption as dictated by kinetic processes. Coupling of nucleation/agglomeration with the deposition mechanisms outlined in (i) to (iv) should duly account for a combination of simultaneous deposition processes and hence enable to accurately predict fouling phenomena for this practically important operating range.

4.1 Ash Particle Transport

Typical range of particle sizes for normal boiler operating experience comprises particles >0.1 mm and 40 mm; hence a judiciously formulated model incorporating a non-linear combination of transport processes including inertial impaction, turbulent eddy diffusion and possible thermophoresis is strictly warranted.

On the question of the particle equation of motion, the analysis presented by Maxcy and Riley regarding the equation of motion of a small rigid sphere in a non-uniform flow, i.e.,

$$\begin{aligned}
\frac{d\bar{v}}{dt} = & \frac{2(\rho-1)}{2\rho+1} \bar{g} + \frac{2}{2\rho+1} \left(\frac{D\bar{u}}{Dt} + \frac{1}{2} \frac{d\bar{u}}{dt} + \frac{r^2}{20} \frac{d\nabla^2 \bar{u}}{dt} \right) \\
& - \frac{9/(r^2 \text{Re})}{2\rho+1} \left(\bar{v} - \bar{u} - \frac{r^2}{6} \nabla^2 \bar{u} \right) \\
& - \frac{9/(r\sqrt{\pi \text{Re}})}{2\rho+1} \\
& \times \int_0^t \frac{(d/d\tau) [\bar{v} - \bar{u} - (r^2/6) \nabla^2 \bar{u}]}{(t-\tau)^{1/2}} d\tau
\end{aligned} \tag{4.1}$$

needs to be appropriately simplified for incorporation in the RNG-Spectral Element code. In the above v is the velocity of the sphere, u is the velocity of the undisturbed fluid evaluated at the center of the sphere, t is the time, r is the radius of the sphere, ρ is the ratio of the density of the sphere to the density of fluid, d/dt denotes a time derivative following the sphere, and D/Dt denotes a time derivative using the undisturbed fluid velocity as the convective velocity. The variables in Equation (4.1) have been made dimensionless in terms of a characteristic length D_c and velocity u_0 of the undisturbed flow and $\text{Re} = u_0 D_c / \nu$ where ν is the kinematic viscosity of the fluid.

In the above equation, if it is assumed that the density of the particle is sufficiently great compared to the density of gas, virtual mass effects are unimportant. Furthermore, for a sufficiently small particle, the Bassett history terms and the buoyancy terms should be small compared to the Stokes drag term. The same reasoning would suggest that the Saffman lift term (which does not appear explicitly in the above equation of motion) should be small compared to the Stokes drag term, and this is generally the case, except in the viscous sublayer where the combination of a large normal component of velocity and a large normal gradient of the streamwise component of the velocity can make the lift term significant for particles in certain size ranges.

The Saffman lift force takes the form:

$$f_s = 6.46 \mu r^2 \left[\left(\frac{1}{\nu} \right) \left| \frac{du_x}{dy} \right| \right]^{1/2} (v_x - u_x) \tag{4.2}$$

In equation (4.2) f_s is the lift force acting on a rigid spherical particle in a uni-directional time dependent shear flow that points in the x direction and is a function of y . The sign of the right hand side of (4.2) is valid provided that (du_x/dy) is positive.

When divided by the particle mass and expressed in a dimensionless form, the Saffman lift force contributes an additional term to the right hand side of Equation (4.1) of the form:

$$f_s / m_p = - \left(\frac{0.343}{\rho r \text{Re}} \right) \left| \frac{du_x}{dy} \right|^{1/2} (v_x - u_x) \quad (4.3)$$

As is shown above, while the large/intermediate size region of the spectrum can be conveniently treated using a Lagrangian formulation with due regard to eddy diffusion, sub/micron particle deposition rates are strongly influenced by thermophoretic effects and typical particle deposition rates are enhanced by many orders of magnitude over the inertial deposition rates. Furthermore, particle diffusion can no longer be neglected; thus the merits of an approach that treats them in a Eulerian framework needs to be evaluated. Generally, the mass loading of submicron particles as well as the vapor phase constituents is negligibly small, allowing the possibility of employing an approach that treats them as trace species, semi-independent of the main bulk motion. The extent to which the behavior of the two distinct trace species is coupled to each other is presently unclear. There are indications that condensation of vapor phase constituents forms a "glue-like" material which then determines the sticking and erosion probability of impacting particles. Assuming that such interactions can be modelled or experimentally determined, it should, in principle, be feasible to incorporate in a comprehensive model the combined influence of micron, submicron and aerosol or vapor phase constituents for multi-species deposition. When formulating such a model, for turbulent flow problems where embedded laminar sublayers cannot be resolved adequately owing to excessive computational requirements, means have to be provided to couple the relevant "wall transfer and deposit" processes to bulk flow computations. Here, a first order treatment might be conveniently employed that utilizes turbulent boundary layer correlations for particle deposition rates in a fashion analogous to the use of turbulent wall boundary conditions for the treatment of wall shear stress calculations.

4.2 Condensable Species & Particle Transport

The following discussion develops criteria to assess the significance of simultaneous presence of both condensable vapors and aerosol particles on mass transfer (deposition) rates.

It has been proposed in the literature that the simultaneous presence of aerosol particles and condensable vapors in a saturated boundary layer may affect deposition rates to subcooled surfaces because of vapor-particle interactions. Scavenging of condensable vapors by aerosol particles may lead to increased particles size (and mass) and decreased vapor mass fraction, thus altering both vapor and particle deposition rates. Particles, if sufficiently concentrated may also coagulate. Analysis presented below to assess the significance of such phenomena assumes particles are already present in the mainstream and are not created inside the boundary layer via homogeneous nucleation.

The boundary layer mass conservation equations for the condensable vapor and aerosol particles (dilute) in two dimensions (for clarity) can be expressed as: (assuming sufficiently small particles, incapable of inertially impacting on surfaces):

$$\rho u \frac{\partial w_i}{\partial x} + \rho v \frac{\partial w_i}{\partial y} = \rho D_i \frac{\partial^2 w_i}{\partial y^2} - \dot{r}''' \quad (4.4)$$

(condensable species i)

$$\rho u \frac{\partial w_p}{\partial x} + \rho(v + v_T) \frac{\partial w_p}{\partial y} = \rho w_p \frac{\partial v_T}{\partial y} + \dot{r}''' \quad (4.5)$$

where v_T is the aerosol particle thermophoretic velocity given by:

$$v_T = \alpha_{T,p} D_p \frac{\partial \ln T}{\partial y} \equiv -\alpha_{T,p} D_p \frac{\Delta T}{T_w} \frac{1}{\delta_h} \quad (4.6)$$

and r''' denotes the mass of vapor locally scavenged by the aerosol particles per unit time and volume. If one approximates the shapes of the aerosol particles by spheres, neglects the relative velocity of condensable vapors with respect to aerosol particles, and takes the largest possible mass transfer driving force, the $(r''')_{\max}$ can be expressed in terms of the diffusion flux of condensable vapors onto the surfaces of aerosol particles, i.e.,

$$\begin{aligned} (r''')_{\max} &= \left(2 \frac{D_i}{d_p} \rho w_{i,\infty} \right) \pi d_p^2 \left(\frac{\rho w_{p,\infty}}{\frac{\pi}{6} d_p^3 \rho_p} \right) \\ &= 12 \frac{D_i}{d_p^2 \rho_p} \rho w_{i,\infty} \rho w_{p,\infty} \end{aligned} \quad (4.7)$$

where the mass transfer Nusselt number is taken to be 2, corresponding to mass transfer to/from spheres in a quiescent medium. Note that the analysis below will provide a conservative estimate of the significance of the above mentioned effects because use is made of the largest possible reaction (condensation) rate, $r'''_{\max}$. In reality, the actual reaction rate r''' will be smaller because (a) the local mass fractions of both condensable vapors w_i and aerosol particles w_p inside the boundary layer will be smaller than their corresponding mainstream values $w_{i,\infty}$ and $w_{p,\infty}$ and (b) the driving force for condensation onto the aerosol particle is determined by the difference between the condensable vapor local mass fraction, w_i in the boundary layer and the mass fraction locally prevailing on the aerosol particle surface at the gas/condensate interface (assumed to be much smaller than w_i here).

Now considering the effects of the presence of condensable vapors on particle deposition rates, it is seen that the thermophoretic velocity v_T of aerosol particles depends on the thermophoretic diffusivity $\alpha_{T,p} D_p$ as shown in Eq. (4.6). However, because the thermophoretic diffusion fraction $\alpha_{T,p}$ is inversely proportional to the Brownian diffusion coefficient, D_p , the thermophoretic velocity is actually independent of D_p (and hence d_p). Therefore, it is known a priori that vapors condensing on aerosol particle surfaces will not affect their thermophoretic velocity. However, the deposition rate of aerosol particles will still be affected because the depositing particles will be larger (heavier). A proper way to measure the significance of this effect is to consider the maximum fraction change in the aerosol particle diameter due to vapor condensation. The rate of change of mass of an aerosol particle Dm/Dt , is given by:

$$\frac{\Delta m}{\Delta t} = \rho_p \left(\frac{\pi \Delta(d_p^3)}{6} \right) = \rho_p \frac{\pi d_p^2}{2} \frac{\Delta d_p}{\Delta t} \quad (4.8)$$

But Dm/Dt is also given by the mass deposition rate of saturated vapors condensing on the aerosol particle surface, i.e.,

$$\frac{\Delta m}{\Delta t} = (\pi d_p^2)(\dot{m}_i) = \pi d_p^2 \left(2 \frac{D_i}{d_p} \rho \omega_{i,\infty} \right) \quad (4.9)$$

Hence,

$$\Delta d = 4 \frac{D_i}{d_p} \frac{\rho \omega_{i,\infty}}{\rho_p} \Delta t \quad (4.10)$$

In (4.10) Δt is the residence time of the aerosol particles traveling with a thermophoretic speed $|v_T|$ inside the thermal boundary layer of thickness δ_h and can be estimated from:

$$\Delta t \approx \frac{\delta_h}{v_T} = \frac{\delta_h}{\alpha_{T,p} D_p \frac{\Delta T}{T_w} \frac{1}{\delta_h}} = \frac{\delta_h^2}{\alpha (\alpha_{T,p} Le_p) \Delta T} \frac{T_w}{\Delta T} \quad (4.11)$$

where α is the thermal diffusivity of the mixture and Le denotes the particle Lewis number. Combining, Equations (4.10) and (4.11), the fraction change in the aerosol particle diameter is given by:

$$\frac{\Delta d_p}{d_p} = 4 \frac{Le_i}{(\alpha_{T,p} Le_p) \Delta T} \frac{T_w}{\rho_p} \frac{\rho \omega_{i,\infty}}{\Delta T} \left(\frac{\delta_h}{d_p} \right)^2 \quad (4.12)$$

The parameters in Equation (4.12) can be readily estimated for the prevailing operating conditions to assess the significance of vapor scavenging by particles.

A further effect relates to the influence of the presence of aerosol particles on vapor deposition rates. In this context, a measure of the importance of the presence of ash particles acting as a sink for vapor molecules can be obtained by comparing the relative magnitude of the reaction ($\dot{r}'''$) term in Equation (4.7) to the diffusion term. An effective Damkohler number defined as:

$$Da \equiv \frac{\text{characteristic vapor diffusion time across mass transfer boundary layer}}{\text{characteristic reaction (condensation) time}}$$

is such a quantity. The characteristic vapor diffusion time is given by:

$$t_i = \frac{\delta_{m,i}^2}{D_i} \quad (4.13)$$

and the characteristic reaction (condensation) time is given by:

$$t_r = \frac{\rho \omega_{i,\infty}}{\dot{r}_{\max}'''} = \frac{1}{12} \frac{d_p^2 \rho_p}{D_i \rho \omega_{p,\infty}} \quad (4.14)$$

Thus,

$$Da = \frac{t_i}{t_r} = 12 \frac{\rho \omega_{p,\infty}}{\rho_p} \left(\frac{\delta_{m,i}}{d_p} \right)^2 \quad (4.15)$$

The quantities in Equation (4.15) can be estimated for prevailing operating conditions.

Finally, considering the effect of particle coagulation on aerosol particle deposition rates, it is assumed that the residence time of the aerosol particle inside the thermal boundary layer is determined by thermophoretic velocity as the aerosol particle transport is demonstrated by thermophoresis. A comparison of the characteristic particle residence time inside the thermal boundary layer with the characteristic coagulation time is a measure of the significance of particle coagulation. If one assumes a nearly monodisperse system with Brownian coagulation, then the ratio of two characteristic time is given by:

$$\frac{t_{\text{thermophoresis}}}{t_{\text{coagulation}}} = \frac{\delta_h}{\frac{v_T}{\left(\frac{\beta \rho \omega_{p,\infty}}{\frac{\pi}{6} d_p^3 \rho_p} \right)^{-1}}} \quad (4.16)$$

$$= \frac{6}{\pi} \left(\frac{\beta}{d_p \alpha} \right) \left(\frac{1}{\alpha_{T,p} Le_p} \right) \left(\frac{T_w}{\Delta T} \right) \left(\frac{\rho \omega_{p,\infty}}{\rho_p} \right) \left(\frac{\delta_h}{d_p} \right)^2$$

where b is the binary coagulation rate constant given by:

$$\beta = \frac{8}{3} \frac{kT}{\mu}$$

Again, the relevant quantities can be readily obtained from operating conditions.

It is tentatively concluded from the above analysis that $(d/d_p)^2$ is the single most critical factor to consider in deciding when to neglect vapor-particle interactions for thermophoretically dominated systems.

4.3 Particle Impact Mechanism

The efforts were continued to supplement the comprehensive flowfield description obtained from the RNG-Spectral Element Simulations by incorporating, in a general framework, appropriate modules to model particle and condensable species transport to the surface. Specifically, attention was focused on describing particle-surface interaction and related phenomena and the nature of surface topography in influencing deposition patterned for the tube banks.

Regarding the former topic, experimental measurement of the restitution coefficient is difficult, but the information is necessary for solving the equations governing the trajectories of

particles rebounding from surfaces and subsequently striking the surface again. The data are generally provided as least square fits to polynomial functions of the form:

$$\frac{V_2}{V_1} = a + b\beta_1 + c\beta_1^2 + \dots \quad (4.17)$$

$$\frac{\beta_2}{\beta_1} = a' + b'\beta_1 + c'\beta_1^2 + \dots$$

where V_1 and β_1 are the particle incidence speed and angle and V_2 and β_2 the corresponding rebound values, β_1 and β_2 measured relative to the target to the surface at the input location, in the V_1 - V_2 plane. The numerical values of the coefficients a , b , c , etc. in Eq. (4.17) depend on the material properties of the specific particle surface pair. Similar data for the rotation velocities of particles rebounding from surfaces apparently are unavailable.

Representative conditions regarding particle impact and rebound from target surface involve large spatial and temporal conditions in the vicinity of the target. However, such conditions are fairly difficult to control and measure, because they require the use of nonintrusive techniques, especially close to the impacted surface.

The restitution characteristics of particles rebounding from surfaces require a statistical description. For fixed incidence values β_1 and V_1 , the rebound values β_2 and V_2 have statistical distributions resulting from (a) variations in particle shape, size and rotational velocity at the time of impact; (b) variations in the topography and properties of the surface; (c) uncontrollable phenomena, such as particle and/or surface fragmentation, particle-particle collisions, changes in properties of materials owing to sudden highly localized temperature increases; and (d) variations in near-surface fluid flow conditions which significantly affect particle trajectories if the momentum equilibration number is less than 1.

Studies of typical histograms showing statistical distribution of the velocity distribution ratio for the case of relatively hard particles striking a ductile surface reveal that shapes of the distributions for V_2/V_1 and β_2/β_1 as well as the mean values of these ratios vary strongly with β_1 . Nevertheless all attempts to date to use restitution coefficient information at boundaries for predicting particle trajectories have been limited to the use of the mean values of the distributions, with the information contained in the shape of the distribution being ignored. This practice raises serious questions about the validity of predictions of particle trajectories when particles are subjected to sequential impacts.

The distributions of V_2/V_1 and β_2/β_1 , as well as their variations with the incidence angle β_1 are highly dependent on the physical properties of the impacting particle/impacted material surface pair. The highly specific dependence of the restitution coefficient of the materials evolved and the unknown influence of transverse Magnus and Saffman forces make deriving general theoretical relations or postulating generally applicable empirical correlations for these from experimental measurements very difficult.

On the question of surface topography, as it influences substantially deposition patterns for tube banks, the role of surface roughness in mechanisms for explaining deposition cannot be ignored. Except for the isolated interesting turbulent flow studies reported in the literature, little attention however, has been paid to the synergistic effects between deposition-induced surface evolving topographies and the associated fluid motion. One particular study reported in the literature centers on large scale changes in topography of bends. However, the local influence of

surface roughness on fluid and particle motions was not investigated. This topic is discussed briefly next.

The wall region of a developed turbulent flow is characterized by a large spectrum of scales of motion and vigorous unsteady dynamics. However, the average velocity component, U_f , of fluid moving parallel to the surface can be expressed as:

$$\frac{U_f}{U_\tau} = \frac{1}{\chi} \ln\left(\frac{yU_\tau}{\nu}\right) + f\left(\frac{hU_\tau}{\nu}\right) \quad (4.18)$$

where U_τ is the wall friction velocity defined at $U_\tau = (\tau_w/\rho)^{1/2}$, y is the normal distance from the surface, h is the "equivalent" roughness height and c is the Von Karman constant. The wall region to which Eq. (4.18) applies is bounded by $40\nu/U_\tau < y < 0.2d$ where d is the boundary layer thickness. For values of $hU_\tau/\nu > 5$ roughness has the effect of reducing the mean fluid velocity relative to that which would develop along a smooth wall and for $hU_\tau/\nu > 70$ this effect becomes pronounced. Appropriate forms for the fraction $f(hU_\tau/\nu)$ in Equation (4.18) are provided in the literature.

For a pipe flow at room temperature with $Re_D = 10^5$, the magnitude of the friction velocity is $U_\tau = 0(10 \text{ ms}^{-1})$. Thus, roughness elements of height $h > 100 \text{ mm}$ or $h > 10 \text{ mm}$ in water significantly reduce the mean speed of fluid near a surface (relative to a smooth surface) at this value of Re_D . Photographic evidence suggests that typical values of h for surfaces roughened by particle impacts range from 1 to 1000 mm. Because of viscous damping in the sublayer region of the flow, fluids with high kinematic viscosity, ν are less sensitive than fluids with low ν to the presence of protrusions on a surface. However, in both cases roughness retards the mean component of fluid motion and hence particle motion parallel to the surface.

The ultimate consequences for deposition owing to surface roughness are hard to generalize, because particle incidence speeds and angles that determine the amount and spatial distribution of surface deposition depend markedly on momentum equilibration number, I , and local flow turbulence. Nevertheless, relative to a smooth pipe, we can reasonably expect that in an initially rough pipe, particles with $I > 1$ approaching the pipe wall at shallow incidence angles on average will be deviated less from their damaging trajectories by the component of fluid motion parallel to the wall.

Even from such a crude picture, based on mean flow interpretation of a region of flow characterized by intense velocity fluctuations distributed randomly in time and over space, one concludes that roughness elements can alter both the magnitude and topography of surface deposit by affecting the flow. Thus, such influences have to be accounted for when planning experiments and interpreting observations or when attempting to calculate particle trajectories near a surface.

4.4 Method for Solving Reacting Species

As this study incorporates in a general framework, appropriate modules to model condensable species transport to the surface along with particles, the need for a suitable solver for the reaction component of the species equations with regard to issues of stability, stiffness, economy, etc. becomes obvious.

It is generally agreed in the literature that the major problem associated with the simultaneous integration of large sets of chemical kinetic rate equations is that of stiffness. Although stiffness does not have a simple definition, it is characterized by widely varying time constants. For example, in hydrogen-air combustion, the induction time is of the order of

microseconds whereas the nitric oxide formation time is of the order of milliseconds. These widely different time constants present classical methods (such as the popular explicit Runge-Kutta method) with the following difficulty: to ensure stability of the numerical solution, these methods are restricted to using very short time steps that are determined by the smallest time constant. However, the time for all chemical species to reach near-equilibrium values is determined by the longest time constant. As a result, classical methods require excessive amounts of computer time to solve stiff systems of ordinary differential equations (ODE's).

Several approaches for the solution of stiff ODE's have been proposed. Of all these techniques, the general purpose codes EPISODE and LSODE are regarded as the best available "packaged" codes for the solution of stiff systems of ODE's. However, although these codes may be the best available for solving an arbitrary systems ODE's, it may be possible to construct superior methods for solving a particular system of ODE's governing the behavior of a specific problem. In this view, an exponentially fitted method, CREK1D, deserves a special mention and is described briefly next.

CREK1D is a computer algorithm designed for transient chemical kinetics problems and combustion kinetics problems in particular. It is based on the exponentially fitted trapezoidal method described adequately in the literature. It consists of a predictor-corrector algorithm and includes automatic step size selections. Given a prescribed error tolerance, it selects either a Newton-Jacobi or a Newton iteration for convergence. It compares favorably with LSODE for lower accuracy requirements and costs somewhat more when higher accuracy is required.

The decision whether to solve the implicit equations using a Newton-Raphson iteration or Jacobi-Newton iteration (which does not require evaluation of the Jacobian matrix) is automated. The trade-offs involve accuracy, convergence rate and total computation time. A Newton-Raphson iteration converges quadratically, but the Jacobian and its inverse must be evaluated frequently to ensure this convergence.

In CREK1D, Jacobi-Newton iteration is used during the early part of the integration of chemical equations involving the chemical induction time and early heat release stages. During this time, when small step sizes are required for stability, this iteration minimizes the work involved. During the late heat release stages and the equilibration region, the Newton-Raphson iteration is preferred, since it has better convergence properties and large step sizes must be used. A test is performed to identify each regime based on the differences between the forward reverse reactions.

Efforts were continued to supplement the flow field description obtained from the RNG Spectral Element Simulations by incorporating, in a general framework, appropriate modules to model particle and condensable species transport to the surface. Specifically, attention was focused on incorporating a stiff chemical kinetics solver in the Spectral Element algorithm to model species related transport. This is described next:

The reaction step of the species transport equations describing hetro/homogeneous chemical reactions can be expressed as follows upon operator splitting:

$$\dot{y}_i = \frac{dy_i}{dt} = f_i(y_k) \quad i, k = 1, NS$$

$$y_i(t = 0) = y_i(0) = \text{given} \quad (4.19)$$

$$y_{NS+1} = T \quad ; \quad N = NS + 1$$

where NS denotes the number of species and T is the temperature. In vector notation equation (4.23) becomes:

$$\underline{\dot{y}} \frac{dy}{dt} = f(\underline{y})$$

$$\underline{y}(t=0) = \underline{y}(0) \text{ given} \quad (4.20)$$

where the underscore is used to denote a vector quantity. A matrix is denoted by a boldface letter.

The initial-value problem is to determine values for y_i ($i=1,N$) at the end of a prescribed time interval, given f_i ($i=1,N$) and the initial values $y_i(0)$ ($i=1,N$).

The method adopted in the present effort attempts to distinguish the physical and computation characteristics of induction, heat release and equilibration regimes. The code that embodies the formulation, CREK1D, consists of two algorithms developed for the two distinctly different regimes of the reaction. These regimes are (a) induction and early heat release, when the relevant equations are dominated by positive time constants, and (b) late heat release and equilibration, when the equations are more stable. Both algorithms are based on an exponentially fitted trapezoidal rule, but they use different iterative methods for convergence.

In CREK1D, the temperature is not treated as an additional independent variable so the number of equations in (4.24) is equal to NS. The temperature is calculated from the algebraic energy conservation equation. In the following discussion the variables y_i ($i=1,NS$) therefore refer only to the species mole numbers.

The species rate expression f_i (right side of Equation (20) can be expanded in a first-order-truncated Taylor series about the current approximate solution, $[t_{n-1}, y_{n-1} (=y_{i,n-1}, i=1,NS), T_{n-1}]$ as follows:

$$f_i = f_{i,n-1} + \left(\frac{df_i}{dy_i} \right)_{y_{n-1}} (y_i - y_{i,n-1}) \quad (4.21)$$

where df_i/dy_i is the total derivative of f_i with respect to y_i and is given by the chain rule as:

$$\begin{aligned} \frac{df_i}{dy_i} &= \sum_{k=1}^{NS} \frac{\partial f_i}{\partial y_k} \frac{dy_k}{dy_i} \frac{dt}{dt} + \frac{\partial f_i}{\partial T} \frac{dT}{dy_i} \frac{dt}{dt} \\ &= \frac{1}{f_i} \left(\sum_{k=1}^{NS} \frac{\partial f_i}{\partial y_k} f_k + \frac{\partial f_i}{\partial T} \frac{dT}{dt} \right) \end{aligned}$$

To avoid confusion with the partial derivative of f_i with respect to y_i , ($\partial f_i / \partial y_i$), a special notation is employed :

$$Z_i \equiv \frac{df_i}{dy_i}$$

With this new notation, Equation (4.21) becomes:

$$f_i = f_{i,n-1} + Z_{i,n-1}(y_i - y_{i,n-1}) \quad (4.22)$$

or

$$\frac{dy_i}{dt} = f_{i,n-1} + Z_{i,n-1}(y_i - y_{i,n-1})$$

which can be integrated to give:

$$y_{i,n} = y_{i,n-1} + h_n f_{i,n-1} \left[\frac{\exp(h_n Z_{i,n-1}) - 1}{h_n Z_{i,n-1}} \right] \quad (4.23)$$

Consider now, an approximate solution to Equation (4.20) based on a variation of the second order trapezoidal rule, the tunable trapezoid,

$$y_{i,n} = y_{i,n-1} + h_n [U_{i,n} f_{i,n} + (1 - U_{i,n}) f_{i,n-1}] \quad (4.24)$$

The substitution of Equation (4.23) into Equation (4.24) gives:

$$U_{i,n} = \frac{1}{h_n Z_{i,n-1}} + \frac{1}{1 - \exp(h_n Z_{i,n-1})} \quad (4.25)$$

In order to maintain A-stability of Equation (4.24) (i.e., $y_{i,n}$ remains bounded as h_n is increased indefinitely), U_i must be restricted to the interval (0.5, 1.0). For values of $Z_i > 0$ Equation (4.25) gives $U_i < 0.5$. CREK1D resolves this problem by setting $Z_i = 0$ whenever it is greater than zero. This gives $U_i = 0.5$, so that Equation (6) defaults to the second-order-accurate trapezoidal rule. However, for $Z_i \leq 0$ Equations (4.24) and (4.25) together are equivalent to the locally exact or exponential solution, which has an equivalent polynomial accuracy of order six to eight. Thus, Equations (4.24) and (4.25) with the constraint (0.5 < U_i < 1.0), constitute an exponentially fitted trapezoidal rule, a method which is A-stable and has a polynomial order of accuracy at least two and as great as six to eight.

At each integration step, Equation (4.24) must be solved for $y_{i,n}$. This is accomplished by Newton-Raphson iteration in regime b and Jacobi-Newton iteration in regime a.

A Newton-Raphson function $F_{i,n}^{(m)}$ ($i=1, NS$) for the species mole numbers is defined from Equation (4.24) by:

$$F_{i,n}^{(m)} = \frac{y_{i,n}^{(m)} - y_{i,n-1}}{h_n U_{i,n}} - \left(\frac{1 - U_{i,n}}{U_{i,n}} \right) f_{i,n-1} - f_{i,n}^{(m)} \quad (4.26)$$

For temperature the functional $F_{T,n}^{(m)}$ is defined from the enthalpy conservation equation as :

$$F_{T,n}^{(m)} = \sum_{k=1}^{NS} y_{k,n}^{(m)} \tilde{h}_k[T_n^{(m)}] - H_o(T_o) \quad (4.27)$$

where m is the iteration number, $T_n^{(m)}$ is the m th approximation to the exact value $T(t_n)$, $h_k[T_n^{(m)}]$ is the molal specific enthalpy of species k at temperature $T_n^{(m)}$ and $H_o(T_o)$ is the initial mixture mass-specific enthalpy at the initial temperature T_o .

Newton-Raphson corrector equations with log variable corrections (for self-scaling of the widely varying mole numbers) are given by:

$$\sum_{k=1}^{NS} \frac{\partial F_{i,n}^{(m)}}{\partial \log y_{k,n}^{(m)}} \Delta \log y_{k,n}^{(m)} + \frac{\partial F_{i,n}^{(m)}}{\partial \log T_n^{(m)}} \Delta \log T_n^{(m)} = -F_{i,n}^{(m)}$$

$$\sum_{k=1}^{NS} \frac{\partial F_{T,n}^{(m)}}{\partial \log y_{k,n}^{(m)}} \Delta \log y_{k,n}^{(m)} + \frac{\partial F_{T,n}^{(m)}}{\partial \log T_n^{(m)}} \Delta \log T_n^{(m)} = -F_{T,n}^{(m)} \quad (4.28)$$

To start the iteration process, the predicted values $y_{i,n}^{(o)}$ and $T_n^{(o)}$ are obtained quite simply by setting them equal to the values at the previous time step,

$$y_{i,n}^{(o)} = y_{i,n-1} \quad i=1, NS$$

$$T_n^{(o)} = T_{n-1}$$

The Jacobi-Newton iteration technique can be derived from the Newton-Raphson iteration procedure by neglecting the off-diagonal elements of the Jacobian matrix $\partial f_i / \partial y_k$. With this simplification, Equations (10) reduce to:

$$\frac{\partial F_{i,n}^{(m)}}{\partial \log y_{i,n}^{(m)}} \Delta \log y_{i,n}^{(m)} = -F_{i,n}^{(m)} \quad (4.29)$$

$$\frac{\partial F_{T,n}^{(m)}}{\partial \log T_n^{(m)}} \Delta \log T_n^{(m)} = -F_{T,n}^{(m)} \quad (4.30)$$

The iteration procedure is further simplified as follows: the expression for $\partial F_{i,n}^{(m)} / \partial \log y_{i,n}^{(m)}$, derived from Equation (4.26) is given by:

$$\frac{\partial F_{i,n}^{(m)}}{\partial \log y_{i,n}^{(m)}} = \frac{y_{i,n}^{(m)}}{h_n U_{i,n}} - y_{i,n}^{(m)} \frac{\partial f_{i,n}^{(m)}}{\partial y_{i,n}^{(m)}}$$

In deriving an expression for $\partial f_{i,n}^{(m)} / \partial y_{i,n}^{(m)}$, the partial derivatives with respect to the inverse mean molar mass n_m are assumed to be negligible in comparison with the other terms. This results in the following approximation for $\partial f_{i,n}^{(m)} / \partial y_{i,n}^{(m)}$.

$$\frac{\partial f_{i,n}^{(m)}}{\partial y_{i,n}^{(m)}} = -[\rho y_{i,n}^{(m)}]^{-1} \sum_{j=1}^J (\dot{\gamma}_{ij} - \ddot{\gamma}_{ij}) (\dot{\gamma}_{ij} R_j - \ddot{\gamma}_{ij} R_{-j})$$

For Jacobi-Newton iteration, this expression is further approximated by:

$$\frac{\partial f_{i,n}^{(m)}}{\partial y_{i,n}^{(m)}} = -[\rho y_{i,n}^{(m)}]^{-1} \sum_{j=1}^J (\dot{\gamma}_{ij} R_j + \ddot{\gamma}_{ij} R_{-j})$$

which can be simplified to yield

$$\frac{\partial f_{i,n}^{(m)}}{\partial y_{i,n}^{(m)}} = -\frac{D_{i,n}^{(m)}}{y_{i,n}^{(m)}}$$

where $D_{i,n}^{(m)}$ is the destruction rate of species i. Using the above form, Equation (4.29) can be solved explicitly for the iterative corrections:

$$\Delta \log y_{i,n}^{(m)} = \frac{F_{i,n}^{(m)}}{y_{i,n}^{(m)} / h_n U_{i,n} + D_{i,n}^{(m)}}$$

From Equation (4.27) the following expression can be derived:

$$\frac{\partial F_{T,n}^{(m)}}{\partial \log T_n^{(m)}} = T_n^{(m)} \sum y_{k,n}^{(m)} C_{p,k} [T_n^{(m)}]$$

where $C_{p,k} [T_n^{(m)}]$ is the constant pressure mole-specific heat of species k at temperature $T_n^{(m)}$. Substituting the preceding equation into Equation (4.30) gives:

$$\Delta \log T_n^{(m)} = \frac{-F_{T,n}^{(m)}}{T_n^{(m)} \sum_{k=1}^{NS} y_{k,n}^{(m)} C_{p,k} [T_n^{(m)}]}$$

To start the iteration process, the predicted values $y_{i,n}^{(0)}$ are obtained from Equation (4.23).

$$y_{i,n}^{(0)} = y_{i,n-1} + h_n f_{i,n-1} \left[\frac{\exp(h_n Z_{i,n-1}) - 1}{h_n Z_{i,n-1}} \right]$$

The predicted temperature $T_n^{(0)}$ is obtained by a single Newton-Raphson iteration:

$$T_n^{(0)} = T_{n-1} + \frac{H_o(T_o) - \sum_{k=1}^{NS} y_{k,n}^{(0)} \tilde{h}_k [T_{n-1}]}{\sum y_{k,n}^{(0)} C_{p,k} [T_{n-1}]}$$

For both Newton-Raphson (NR) and Jacobi-Newton (JN) iteration schemes, the current values $y_{i,n}^{(m+1)}$ and $T_n^{(m+1)}$ are updated by the approximate equations

$$\begin{aligned} y_{i,n}^{(m+1)} &= y_{i,n}^{(m)} [1 + \Delta \log y_{i,n}^{(m)}] \\ T_n^{(m+1)} &= T_n^{(m)} [1 + \Delta \log T_n^{(m)}] \end{aligned} \quad (4.31)$$

The test for convergence of the iterates $y_{i,n}^{(m+1)}$ is based on the value $\Delta \log y_{i,n}^{(m)}$ and is given by:

$$\sqrt{\frac{\sum_{i=1}^{NS} [\Delta \log y_{i,n}^{(m)}]^2}{NS}} \leq EPS \quad (4.32)$$

This test is used only with variables whose magnitudes are greater than 10^{-20} . If convergence is not obtained after ITMAX iterations, the step length is reduced and the step retired. If convergence is achieved in M iterations ($M \leq \text{ITMAX}$), the step is accepted as successful and the solution is updated.

$$y_{i,n} = y_{i,n}^{(m)} \quad i = 1, NS$$

$$T_n = T_n^{(m)}$$

CREK1D automatically selects the iteration scheme (JN or NR) to be used for solving Equation (6). During induction and heat release, when small step lengths are required for solution stability, the JN iteration is used to minimize computational work. During late heat release and equilibration, when the equations are more stable and larger step lengths can be used, NR iteration is preferred since it has a much larger radius of convergence than JN iteration. The regime identification test exploits the fact that during equilibration many reactions achieve a condition in which the forward and reverse rates are large, but have vanishingly small differences. The actual test employed at the beginning of each time step is:

$$|f_i| \leq 10^{-3} (Q_i + D_i) \quad (4.33)$$

Where Q_i and D_i are the production and destruction terms, respectively, for species i . If any of the species satisfies Eq. (4.33), regime b is obtained and the NR iteration is used for the step. If none of the species satisfies Eq. (4.33), regime a is obtained and the JN iteration is used for the step.

For this method much computation time can be involved in calculating Z_i because it requires the evaluation of the Jacobian matrix. To avoid evaluating this matrix, $Z_{i,n-1}$ is estimated as follows: if Eq. (4.32) is applied to the entire time step h_n

$$f_{i,n} = f_{i,n-1} + Z_{i,n-1} (y_{i,n} - y_{i,n-1})$$

which when substituted into Equation (4.33) gives:

$$f_{i,n} = f_{i,n-1} \exp(h_n Z_{i,n-1})$$

or,

$$Z_{i,n-1} = \frac{1}{h_n} \log \left(\frac{f_{i,n}}{f_{i,n-1}} \right)$$

However, $f_{i,n}$ is not known at the start of the step, so approximations have to be developed for $Z_{i,n-1}$. For the NR iteration, $Z_{i,n-1}$ is approximated by:

$$Z_{i,n-1} = \frac{1}{h_n} \log \left(\frac{f_{i,n-1}}{f_{i,n-2}} \right) \text{ for } 0 < \frac{f_{i,n-1}}{f_{i,n-2}} < 1$$

$$= 0 \text{ otherwise}$$

For the JN iteration, $Z_{i,n-1}$ is approximated by:

$$Z_{i,n-1} = \frac{1}{h_n} \frac{f_{i,n-1} - f_{i,n-2}}{f_{i,n-1}} \text{ for } f_{i,n-1} f_{i,n-2} > 0$$

$$\text{and } f_{i,n-1} \neq 0$$

$$= 0 \text{ otherwise}$$

CREK1D also includes an algorithm for filtering the initial conditions that may be ill-posed. These ill-posed conditions may arise, for example, in multi-dimensional modelling because of the averaging of mole numbers over adjacent grid modes. CREK1D therefore "filters" the initial conditions to provide physically meaningful initial mole numbers and net species production rates. On the first call to CREK1D it uses a predictor-corrector algorithm over one time step of length h_1 which is determined by:

$$h_1 = \frac{1}{\max L_i} \quad L_i = D_i / y_i$$

The predictor-corrector algorithm uses the following equation as the predictor:

$$y_{i,1}^{(0)} = y_i^{(0)} + h_1 f_i^{(0)} \left\{ \frac{1 - \exp[-h_1 L_i(0)]}{h_1 L_i(0)} \right\}$$

An implicit Euler corrector is then iterated to convergence:

$$y_{i,1}^{m+1} = y_i^{(0)} + h_1 f_{i,1}^{(m+1)}$$

In these equations $y_i^{(0)}$ are the initial values and the subscript 1 is used to indicate that this is first step. Using approximations $Q_{i,1}^{(m+1)} = Q_{i,1}^{(m)}$ and $L_{i,1}^{(m+1)} = L_{i,1}^{(m)}$, it can be

shown that the preceding corrector equation can be rewritten to provide the following expression for the log variable corrections $\Delta \log y_{i,1}^{(m)}$:

$$\Delta \log y_{i,1}^{(m)} = \frac{y_i^{(0)} - y_{i,1}^{(m)} + h_1 f_{i,1}^{(m)}}{y_{i,1}^{(m)} + h_1 D_{i,1}^{(m)}} \quad (4.34)$$

Equation (4.34) is iterated until convergence, which is ascertained by the criterion given by Equation (4.32). If convergence is not obtained after 10 iterations, the step length is halved and the step retried. If convergence is obtained after M iterations ($M \leq 10$) the step is accepted as successful, the solution for the mole numbers is updated:

$$y_{i,1} = y_{i,1}^{(m)} \quad i = 1, NS$$

and the temperature T_1 is obtained by a single Newton-Raphson iteration:

$$T_1 = T_o + \frac{H_o(T_o) - \sum_{k=1}^{NS} y_{k,1} \tilde{h}_k(T_o)}{\sum_{k=1}^{NS} y_{k,1} C_{p,k}(T_o)}$$

Specifically, the stiff chemical kinetics solver incorporated in the Spectral Element algorithm was exercised to solve the following reacting flow problem for a "massively fouled" heat exchange surface:

In the above, M denotes a typical third body. Resulting predictions will be reported in due course. However sample output from the kinetics solver used in a "batch" mode is provided in the attached appendix for a critical evaluation of the predictive capability of the formulation.

4.5 Particle Adhesion Mechanism

A brief survey of the adhesion mechanisms for the depositing ash particles was carried out and is reported next.

The ash particles deposited on boiler tubes are centrally held in place by surface forces, i.e., van der Waals and electrostatic attraction forces. [Zimon, 1982, Dahneke, 1975]. van der Waals forces become important when molecules or solid surfaces are brought close together without a chemical interaction taking place. For a hemispherical particle of radius r held at a distance of nearest approach h from a plane the resultant force F is given by:

$$F' = \frac{2B\pi r}{3h^3} \quad (4.35)$$

where A is the Hamaker constant [Hamaker, 1937].

Equation (4.35) applies over short distances up to $150\text{\AA}$ ($1.5 \cdot 10^{-8}\text{m}$) and for longer distances the "retarded" van der Waals forces decay rapidly. An equation based on the dielectric properties of solids for the retarded van der Waals forces F' between a sphere of radius r at the distance h from a flat surface is:

$$F' = \frac{2B\pi r}{3h^3} \quad (4.36)$$

where B is the appropriate constant for the given material.

The changeover from the unretarded to retarded van der Waals forces occurs at a distance of about $150\text{\AA}$ and the corresponding value of the Hamaker constant A in Equation (4.35) is found to be 10^{-19} Newton and that of the Lifshitz constant B in Equation (4.36) is 8.9×10^{-29} Nm. These values have been used to compute the ratio of van der Waals forces to the gravitational force on small ash particles approaching a flat surface.

The gravitational force F_g on any ash particle of radius r and the density ρ is given by:

$$F_g = \frac{4}{3}\pi r^3 \rho g \quad (4.37)$$

where g is the gravitational acceleration constant, 9.81 ms^{-2} . Thus, the ratio of F_r of the short distance van der Waals forces F to the gravitational F_g on a particle is:

$$\frac{F}{F_g} = F_r = \frac{A}{8\pi\rho g r^2 h^2} = \frac{1.62 \times 10^{-25}}{r^2 h^2} \quad (4.38)$$

where the value of r for ash particles is taken to be 2500 kgm^{-3} and when $h < 150\text{\AA}$. The corresponding ratio F_r' of the retarded van der Waals forces F' to be gravitational forces is given by:

$$\frac{F'}{F_g} = F_r' = \frac{B}{2\rho g r^2 h^3} = \frac{2.04 \times 10^{-34}}{r^2 h^3} \quad (4.39)$$

where $h > 150\text{\AA}$.

A comparison of van der Waals and gravitational forces on small ash particles approaching a collecting surface indicates that sub-micron sized particles are readily held on a surface by van der Waals forces. The capture of small particles of ash on boiler tubes is further enhanced by surface irregularities of oxidized metal. Also, it has been suggested that electrostatic attraction forces enhance the transport and retention of sub-micron sized particles on steel probes inserted in the flue gas of coal fired boilers. A layer of electrically precipitated deposit of ash can have a cohesive strength between 5 and 40 times higher than that formed by sedimentation because, particles in an electric field have permanent dipole characteristics which lead to these being oriented to form a cohesive layer of ash. It appears, therefore, that the combined effects of van der Waals and electrostatic forces of attraction, and surface irregularities are sufficient to hold the sub-micron diameter particles on the surface of boiler tubes for the subsequent liquid phase adhesion, and chemical and mechanical bond formation.

Concerning the nature of adhesion by surface tension forces, it is generally agreed that the formation of strong adhesive bonds of enamel coatings and glass/metal seals on heating requires the presence of a liquid phase. The role of the liquid film is to provide the initial adhesion of solid particles as a result of surface tension. The work of adhesion W_a is given by:

$$W_a = \pi + \gamma(1 + \cos\theta) \quad (4.40)$$

where γ is the surface tension of the liquid and θ is the contact angle at the solid/liquid interface. With perfect wetting, i.e., when θ equals zero, W_a has the highest value:

$$W_a = \pi + 2\gamma \quad (4.41)$$

The work of cohesion of a liquid W_c is given by:

$$W_c = 2\gamma \quad (4.42)$$

With wetting liquids, therefore, W_a can be higher than W_c and failure will take place within the liquid layer, whereas with non-wetting liquids rupture occurs at the solid/liquid interface.

Alkali-metal sulfates frequently constitute a liquid phase in ash deposits, and the molten sulfates readily wet and spread on the surface of boiler tubes. In a reducing atmosphere and when in contact with carbon, sulfates are reduced to sulfides which wet and spread on any surface. The coefficient of surface tension of sulfates is fairly high, 0.20 Nm^{-1} for Na_2SO_4 and 0.14 Nm^{-1} for K_2SO_2 near their respective melting point temperatures. Thus the work of cohesion of molten sulphate layer in a boiler deposit is between 0.3 and 0.4 Nm^{-1} and the work of adhesion is higher because of a low contact angle at the sulphate/tube surface interface. The surface tension of coal ash slag has been measured and a typical value is 0.3 Nm^{-1} . It is about twice that of the sulphates and thus the work of adhesion and the cohesive bond strength are those corresponding to the slag/solid interface.

Only a small amount of liquid, about a hundred molecule thick layer, is sufficient for the adhesion contact of sub-micron diameter particles. In the case of a volatile liquid, the equilibrium thickness of the film, and thus adhesion, varies with partial pressure of the vapor in the surrounding atmosphere. When evaporation from a liquid film occurs as a result of increased temperature, the adhesion first rises to a maximum value due to the meniscus effect but it breaks down as the film thickness is reduced to molecular dimensions. However, before the breakdown of the surface tension, chemical and mechanical bonds may develop between the deposited ash and boiler tube surface.

5.0 RESULTS & DISCUSSIONS

A three-dimensional spectral element code was installed on the in-house STARDENT computer. As this code was intended for exclusive use as the base flow code to model finite length effects in a practical boiler, it does incorporate state-of-the-art ReNormalization Group techniques to provide sub-grid scale effects. The code was subsequently set up to predict a number of related flow problems. Specifically, these refer to non-isothermal flow around a backward facing step, laminar flow in a periodic (streamwise and spanwise) three-dimensional channel and impulsively started flow around, a wedge attached to one of the plates of a two dimensional channel.

As the spectral element code incorporates a variety of computational options and physical sub-models, a substantial effort was devoted to get a reasonable feel for the influence of some of the relevant solution variable, e.g., order of the basis functions, nature of the time stepping algorithm, iterative solution details, imposition of the incompressibility constraint, variations on the Courant number, etc.

Efforts were then continued to reformulate the algorithm for application to flow and turbulence evolution around an isolated cylinder. Practical issues related to computational and algorithmic characteristics including number of points, domain sizes, convergence and accuracy degradation due to disparate discretization practices across various zones were studied.

Subsequently, an energy balance formulation was used to predict surface heat transfer details as a prelude toward developing meaningful deposition modules. Temperature was treated as a "passive" scalar regarding the turbulence dynamics, although local mean flow is expected to be directly influenced by the details of the heat transfer process.

Predictions for the cases that have been simulated appear qualitatively reasonable. For turbulent cases, due consideration was also given to the resolution requirements of the various eddy scales involved, treatment of the near-wall region, implementation of non-homogeneous boundary and initial conditions, solution and algorithmic details including cost versus accuracy, etc. Such an effort has helped clearly delineate critical accuracy bounds for the fluid mechanics description, as well as establishing comparable criteria for the remaining module development effort. It has also provided for a greater insight into the physical and mathematical nature of the dominant transport mechanism, thereby enabling the development of a rational comparison basis to guide the rest of the effort.

5.1 Flow Past Circular Tubes & Tube Banks

A number of predictions were performed to simulate the representative configuration and conditions of utility boilers along with pertinent test problems. These include:

a) V-groove laminar flow that either simulates the flow in the vicinity the boiler hose or flow around a hypothetical deposit layer. Figs. 5.1.

b) A single cylinder in an inflow/outflow configuration where the remaining directions are treated periodically. Reynolds number studied is 20,000 and the computations have been carried out to an integrated time unit of 26.08. Figures 5.2 depict various variable evolutions in the field for select viewing angles. These predictions do include the RNG description to simulate subgrid effects.

c) Flow around a single cylinder in a duct where the horizontal boundaries are treated periodically for a Reynolds number of 4000. Integrated time is 5.46 and Figures 5.3 display

turbulent flow field evolution including heat transfer, where subgrid effects are provided via the previously discussed RNG model.

d) 3-D multi-cylinder flow (four cylinders arranged in tandem configuration) including heat transfer; these predictions refer to a turbulent case of $Re=4000$. The choice of length to diameter ratio (L/D) was made to eliminate various cylinder to cylinder flow interactions. Figures 5.4.

e) The same as above, but focusing on the effect of the L/D ratio on the flow structure where cylinder to cylinder flow interactions do occur. These refer to a 3×3 matrix of in-line geometry, Figures 5.5. These predictions were carried out for a turbulent case of Reynolds number 4000 including heat transfer as modelled by RNG.

From the preliminary cases, as well as those reported extensively in the literature, the following qualitative picture emerges regarding cross flow features over tubes within a bundle.[Chambrel et al, 1991].

The flow over tubes is controlled by the pressure gradient, the fluid viscosity and the Reynolds number, Re . The flow upstream of a single tube usually has a relatively low turbulence intensity and a uniform velocity profile. Flow over tubes within a bundle involves significant blockage of the flow passage; the pressure gradient at the tube surfaces is affected by the degree of flow constriction. Nonisotropic turbulence into discrete eddies prevails within the bundles where the mean flow has a nonuniform velocity profile. For this reason, the flow structure near the tube surfaces differs from that of a single tube; consequently, the location of the boundary layer separation shifts and affects the flow in the wake.

The velocity distribution over the cross-section of tube bundles varies depending on the net cross-section area within the bundle. The characteristic velocity in the study of flow over tubes is that outside of the tube's boundary layer, i.e., velocity related to the average velocity in the smallest cross-section of the bundle.

The adjoining tubes in each transverse section of the staggered and in-line bundle constrain the flow and affect the pressure gradient dp/dx . This changes the velocity distribution outside the boundary layer and the nature of the vortical flow over the trailing part of the tube within a bundle as compared with the case of a single tube in unbounded flow. The location of the boundary layer separation on a tube within a bundle is shifted downstream. This shift is affected by the relative transverse pitch of the bundle, since then the pitch is reduced, the favorable pressure gradient over the leading part of the tube increases. Thus the laminar boundary layer over the leading part of the tube becomes more stable than that of a single tube, and the separation is shifted downstream. In bundles with large relative transverse pitch, the boundary layer separation at critical Re occurs at the same value of the azimuthal angle ϕ , for a single tube. In a tightly packed bundle, the separation location is influenced by the availability of space for eddy formation.

At low Re , the mainstream within the bundle is laminar with regions of circulating macroscale eddies whose effect on the boundary layer over the front part of the tube is attenuated by viscous forces and by the favorable pressure gradient. The boundary layer is laminar, whereas the trailing part of the tube lies in a region of circulating flow. The flow pattern over a tube bundle which occurs at $Re < 10^3$ can be regarded as predominantly laminar.

As Re increases, the flow pattern within the bundle changes significantly. the flow in the space between the tubes becomes turbulent. This change in the flow pattern within bundles depends on their configuration and relative pitches. At a relatively small transverse pitch, intensive fluctuations are generated at the exit from an upstream row. However, when the flow

enters the next row, these eddies are damped out more rapidly than in the case of large transverse pitches due to the favorable pressure gradient.

In bundles with large longitudinal pitches, transition from laminar to turbulent flow in the space between tubes occurs gradually with rising Re . First, large vortices appear in the flow and then as the velocity increases, the additional energy of the flow causes small eddies to develop. In bundles with small longitudinal pitches this occurs over a narrower range of Re ; small eddies are generated at $Re \approx 10^3$. In this case, the flow in the space between the tube becomes turbulent very rapidly.

When this happens, the tube is exposed to a complex turbulent flow. Although the front part of the tube is situated in this flow, the boundary layer that develops over it is laminar, since the favorable pressure gradient around the leading part accelerates the flow outside the boundary layer. A convex velocity profile forms over the tube's leading part and the boundary layer thickness remains small, changing little with increasing distance from the stagnation point. Accordingly, a new flow pattern appears which can be regarded as mixed, since over the leading part of the tube, a laminar boundary layer prevails that is influenced by the free stream turbulence, whereas the trailing part is exposed to an intensive turbulent flow.

A change in the flow mode effects the distribution of location velocities and pressures over the tube perimeters; it also influences the location of vortex shedding from the surface and other features of the flow. This changes the flow forces acting on the tubes, the drag on them and their flow induced vibrations.

A tube bundle is actually a turbulizing grid and the turbulence within it is governed by the relative pitches. Tubes deep within the bundle are situated in a highly turbulent flow whose characteristics depend on the given bundle configuration. For this reason, the free stream turbulence is not capable of changing the flow pattern over tubes deep within the bundle. It is thus reasonable to expect that a developed flow pattern within the bundle sets on earlier in a highly turbulent flow than in a low turbulence free stream.

The flow structure behind a cylinder undergoes a drastic alteration as it passes from a quasi-laminar instability to one in which there are two distinctly different scales of instability. The variations in base pressure, vortex strength and formation length with Reynolds number are substantial as revealed in a number of previous investigations. These traditional parameters are generally interpreted in the literature within the context of unstable shear layer from the cylinder.

In the event that the separating shear layer supports a purely convective instability, one may view the initial fluctuation level (near separation) to be a direct function of the upstream-induced velocity/pressure fields. In general, in a Biot-Savart induction, the largest initial fluctuation levels would be associated with the smallest values of the vortex formation length. The importance of accounting for upstream influence was also emphasized by Michalke in his assessment of jet instabilities. It is generally agreed in the literature that compatibility exists between the most simplified disturbance in the shear layer from the cylinder and the downstream vorticity dynamics.

However, there is another type of upstream influence that may potentially exert a strong, if not the controlling influence: upstream wave motion due to the existence of an absolute instability in the near wake. It is emphasized that the fluctuation levels of instability near separation are, over certain ranges of Reynolds number, very large. Indeed this fluctuation level takes on values much higher than those typically achieved in purely hydrodynamic oscillations of jets and mixing layer where no acoustic resonance or fluid-elastic effects come into play. The issue remains as to the relative predominance of upstream influence through: Biot-Savart induction; and upstream influence from the region of absolute instability.

In a rigorous sense, one must account for the nonlinear character of the disturbance. Nonlinearity is evident in the relatively high fluctuation levels at separation. Furthermore, the non-parallelism of the mean shear layer, arises from the Reynolds stresses which are in turn a higher-order product of the velocity perturbation, requiring accommodation of nonlinearity. An additional complication arises from the simultaneous existence of large scale shedding frequency f_v , and the smaller convective instability frequency f_{BG} due to the separating shear layer. In the spirit of the unstable wave growth in fully turbulent flows one may view the growth of the wave at f_v in the presence of f_{BG} instability (which may be three-dimensional) as a degenerate case of organized wave growth in a turbulent flow. In fact, as noted by Wygnanski and Petersen, the small scale motions do not exert substantial influence on the macroscale dynamics of the flow. In essence one views the growth of the smaller scale instabilities at f_{BG} , as well as that at f_v , as contributing to the thickening of the mean shear layer. This thickened shear layer, however, then serves as the base mean flow for a quasi-linear description of the disturbance development at f_v again following the principles of organized wave growth in turbulent flow.

The above discussion addresses the nature of the instability leading to the classical Karman vortex street. As noted in a number of studies in the literature, small scale Bloor-Gerard vortices can exist in the separation shear layer at sufficiently high Reynolds numbers. Particularly remarkable is the fact that there is no evidence of successive coalescence of the Bloor-Gerard vortices at f_{BG} . In the corresponding free jet or mixing layer, one observes successive pairing of the neighboring vortices to produce large-scale structures in the downstream regions of the flow. Inspired by flow visualization studies, one viewpoint regarding the small scale vortices envisages them as a frill upon large scale vortices. In fact, one may make the interesting observation that as Reynolds number increases, the initial fluctuation level near the upstream separation increases as well.

Another feature of the unstable shear layer that distinguishes it from its classical counterpart is the dominance of fluctuation kinetic-energy at the large scale vortex formation frequency f_v over that at the smaller-scale frequency f_{BG} . This dominance persists from separation onwards. In accordance with the lack of subharmonics of f_{BG} , there is not successive energy transfer from smaller to larger scales as the shear layer evolves in the streamwise direction. It is suggested that this dominance of energy at f_v is due to pronounced upstream influence from Biot-Savart induction, existence of an absolute instability, or a combination of both.

Regarding wake interference and vortex shedding for multiple bluff body (cylinder) configurations, the following qualitative/quantitative picture emerges from the predictions carried out in this effort.

Wake interference between cylinders is extremely complex involving various aspects of flow conditions, number of cylinders and spacing and arrangements. The wide variety of changes of the interference fluid forces reflect the complex nature of the corresponding flow patterns. Basic interference patterns however, have been clarified via the predictions carried out in this effort as well as studies reported in the literature.

The most striking feature in the wake interference of cylinders arranged side-by-side is that the flow passing through the gap is biased to one side or the other in an unstable or stable manner when the gap is smaller than a critical size. This leads to a bistable biased flow or multiple stable flow patterns for a single transverse spacing ratio. Cylinders on the biased side show high drag and lift and regular vortex shedding, while those on the unbiased side show the opposite. The difference in the wake interference of various cylinders arrayed side by side appears in the direction of the lift force.

When a body is submerged in the wake of other bodies, the aerodynamic force on the downstream body is strongly influenced by the wake interference for a wide range of spacings, even over 50 diameters. However, forces on upstream bodies attain almost constant values except for a limited range of small spacings $L/D < 3.5$ where reattachment of the shear layers separated from the front body is so complicated, that the flow around two in-line cylinders can be classified into six distinct flow patterns as a function of certain critical spacing dimensions. Then a new critical spacing is proposed to be added as the boundary, where a new vortex street begins to be independently shed behind the downstream cylinder. Aerodynamic forces at transcritical Reynolds numbers can also be inferred to have critical spacings like the ones at subcritical Reynolds numbers from wind tunnel tests using roughened cylinders.

When two cylinders are neither in side-by-side nor tandem arrangement, then they are staggered. Since in the configuration of two staggered cylinders the gap flow is always biased to the side of the upstream cylinder, the upstream cylinder has a much smaller wake and a higher frequency of vortex shedding than the downstream one. All possible arrangements of two circular cylinders are classified into five distinct categories depending on the size of the lift force or whether the drag is greater or less than that of a single cylinder. Drag and lift forces on the downstream cylinder shows two prominent aspects. First, there are two separate curves representing the maximum lift force with the direction pointing towards the axis of the upstream cylinder wake. One lies well inside the upstream wake for L/D up to 3, and the other is near the wake boundary for $L/D > 2.7$. The second feature is that minimum drag force occurs at the same transverse spacing where an inner maximum lift force is found. Finally, there exists a discontinuity in the lift force for some staggered arrangements due to the bistable flow patterns in the gap.

For a single cylinder, the prevailing flow field depends strongly on the Reynolds number. For $6 \leq Re \leq 40$ a steady state exists, with a pair of symmetric separation bubbles on the leeward side. At higher Reynolds numbers the flow field is inherently unsteady and is characterized by cyclic vortex shedding. Still at higher Reynolds numbers (critical Re range) the laminar boundary layer over the cylinder separates with the formation of the so called separation bubble, followed by reattachment at $Re \approx 100$ in the form of a turbulent boundary layer. The pressure on the cylinder surface in the region of the separation bubble remains constant. Here the flow becomes turbulent. In the course of this transition, the boundary layer acquires additional kinetic energy from the free stream, and the separation point moves abruptly to $Re \approx 140$. When this type of separation occurs, the wake region downstream of the cylinder narrows and the pressure distribution around the cylinder approaches that of a potential flow over a large portion. At critical Re , when the location of the boundary layer separation is abruptly shifted downstream, a departure from the regular pattern of vortex shedding from the surface occurs. Experimental evidence in the literature indicates that the eddy shedding frequency in supercritical flow over bodies at $Re \geq 3.5 \times 10^6$ is highly regular.

Concentrating on the laminar, asymmetric region of the flow map, it is generally agreed that at a Reynolds number higher than 40, any perturbation excites an unsteady flow, and eventually a periodic vortex shedding is established generating the well-known Von Karman vortex shedding street. In the present effort, the laminar vortex shedding over a cylinder was simulated at select Reynolds numbers. Examination of these cases, as well as evaluation of related predictions reported in the literature (e.g. $Re=200$) reveals that following a relatively short transient flow, the onset of periodic flow dominated by a single frequency is observed [Song et al, 1990]. The amplitude of oscillations and the Strouhal number of the vortex shedding increase with the Reynolds number. Examining instantaneous streamlines for five equally spaced instances along one vortex shedding cycle, the following qualitative picture emerges. Time is normalized by the period and $t=0$ corresponds to the instant when the lift coefficient is maximum. The lift coefficient is minimum and the drag coefficient is maximum at $t=0.5$, while at $t=0.25$ and $t=0.75$ the lift coefficient vanishes and the drag coefficient is minimum.

The flow fields at the beginning of the cycle ($t=0$) and the end of the cycle ($t=1$) are eventually identical indicating the periodic nature of the flow. Moreover, the flow field at $t=0.5$ is a mirror image of the flow field at $t=0$. A similar relationship is found between the flow fields at $t=0.25$ and $t=0.75$, when the instantaneous lift coefficient vanishes. A large separation bubble is created at the upper side of the cylinder at $t=0$. The bubble induces a low pressure field, which causes a large positive lift coefficient as well as maximum drag. The bubble ultimately separates from the body and is washed downstream ($t=0.25$). The lift coefficient is decreased to zero and the drag coefficient is minimum at that time. At $t=0.5$, a large separation bubble is created at the lower side, reversing the direction of the lift coefficient. The bubble is washed downstream and creates the lower vortex of the Von Karman vortex street. The centers of the shed vortices are characterized by a low pressure region.

Regarding the heat transfer details of deep tube bank, the following qualitative picture emerges from a study cases predicted as well as those reported extensively in the literature.

In the range of Reynolds numbers of interest in this study (i.e. $2 \cdot 10^3 \leq Re \leq 2 \cdot 10^5$), high intensity in the space between tubes in a bank causes a transition from laminar flow in the boundary layer to a turbulent flow. The transition point coincides with large values of the circumferential angle f , resulting in reduced dimensions of the recirculation zone behind the tube.

With the appearance of turbulence in the boundary layer, the distribution and character of the local heat transfer coefficient changes substantially. Considering the flow around the frontal region of a tube in the first and inner rows of a staggered bank, the flow accelerates and after crossing the minimum cross-sectional area it decelerates. The location of the minimum cross-sectional area depends on the pitches and could be at $f=90^\circ$ or at another angle. For in-line banks it is always located at $f=90^\circ$. The acceleration of flow effectively decreases the thickness of the boundary layer, increasing heat transfer; however, transverse velocity fluctuations which enhance turbulent heat transfer are reduced. Vortices generated in intertubular spacing and in the boundary layer spread under the influence of a negative pressure gradient. The local heat transfer, as a result, decreases. The decrease in velocity in intertubular spacing leads to an increase in boundary layer thickness and to the separation of the boundary layer. In the region of positive pressure gradient, velocity and temperature fluctuations increase, particularly the transverse component of velocity, which promotes local heat transfer.

As is evident from experimental studies reported in the literature, for flow through the first rows of banks, turbulence caused by the first and second rows plays a principal role, and the difference in heat transfer of the third and fourth rows lies within the bounds of measurement errors. In the inner rows of in-line and staggered banks, the character of heat transfer is different, particularly in the frontal side of tubes.

It is important to note the specific features of heat transfer in inner rows of in-line and staggered banks at different Reynolds numbers. In the region $f=90^\circ-110^\circ$, heat transfer increases as a result of the flow transition from laminar to turbulent and $f=150^\circ$, the increase is due to separation of the turbulent boundary layer.

Local heat transfer, h/h in an inner row of in-line banks varies slightly. The maximum value of h/h occurs at the point of collision of flow and tube, after which h/h decreases. In the region of boundary layer transition from laminar to turbulent ($f=100^\circ-115^\circ$) and separation of the turbulent boundary layer h/h increases. The relation between the maximum and minimum values of h/h in in-line banks amounts to 2.5 which indicates strong non-uniformity of thermal loading of the tube in this range of Reynolds numbers.

It is also worth noting that, for a non-gradient flow of the laminar boundary layer, turbulence of the external flow does not give rise to an increase of the local heat transfer coefficient. But for gradient flow, even slight turbulence (1-2%) of the external flow leads to an increase of local heat transfer by 40-60%.

5.2 Flow Past Non-Circular Tubes

Efforts were continued to perform predictions for a mildly fouled tube with the surface geometry provided a priori. The calculated flow field at about one convective time step is shown in Figures 5.6.1-5.6.4. The computed pressure profiles at mid-span are shown in Figure 5.6.1 and the corresponding velocity vectors are shown superimposed in Figure 5.6.2. Low pressure regions indicate the vortex shedding phenomenon. Pressure contours behind the cylinder are shown in Figure 5.6.3 exhibiting three dimensional effects in the spanwise directions. Three dimensional effects are more clearly exhibited by the spanwise velocity contours shown in Figure 5.6.4.

5.3 Particulate Deposition Rates

Work was also continued on calculating particle deposition rates. Code improvements were made to reduce the computational effort for calculation of stochastic particle trajectories. As a test case, the frozen gas flowfield for the flow past a single cylinder in a channel was selected. Initial conditions for the injection of particle trajectories were selected stochastically from a uniform distribution at the channel entrance. The initial particle velocities were assigned values equal to the local gas velocity. Results for 5000 particle trajectory computations are shown in Figure 5.7.1 where each square represents a particle impacting the wall surface. Based on correlation of Rosner for sticking coefficient, particles were either allowed to stick or rebound from the surface. Coordinates of sticking particles are shown in Figure 5.7.2. Particles impacting the cylinder surface were analyzed for their radial distribution. The fraction of particles hitting a 10 degree interval are shown in Figure 5.7.3. The distribution is not symmetric about the stagnation point (90 degrees) and peaks on the cylinder side away from the wall.

Development of engineering correlations for the deposition rates will require sampling of gas phase flows at many time intervals and computations of about hundred thousands trajectories to obtain statistically meaningful results.

Computations were performed to calculate the instantaneous particle deposition rates for the flow past a deep tube bank. About 5000 stochastic particle trajectories were computed by distributing particles uniformly at the inlet cross section. Stokes numbers corresponding to the average particle diameter is 0.3, with Stokes number varying between 0.13 and 0.52 for the minimum and maximum particle diameters. Flow Reynolds number based on channel height is 25000. The computed particle impaction points are shown in Figure 5.8.1. Approximately 40% of incoming particles experience an impact with the one of nine cylinders. Correlations of Rosner [Rosner et al, 1992] were used to decide if an impacting event would lead to particle adhesion or sticking to the tube surface. Locations of particle sticking to the tube surface are shown in Figure 5.8.2. Approximately 5.4% of incoming particles stick to the tube surface, resulting in an average sticking probability of 0.13. Local instantaneous sticking probability depends on the conditions of the deposit surface, properties of the incoming particles, and the local gas phase species concentrations and temperature. Currently we have used simplified sticking probability distribution with an arbitrary value of parameter V_{crit} to test the code behavior. More accurate correlations can be easily incorporated later once the relevant information is available from Yale group. The distribution of impaction and sticking probability on individual cylinders is shown in Figures 5.8.3 and 5.8.4, respectively. The instantaneous probability exhibits large fluctuations with angle and cylinder-to-cylinder variations so that definitive conclusions about cylinder-to-cylinder variations

are not possible yet. The averaged results for all cylinders are shown in Figure 5.8.5. Both impaction and sticking probabilities tend to peak in the upper left hand quadrant.

The flow field calculated from the Large Eddy Simulation (LES) method was used to obtain improved estimates (increased sample size) for the particle impaction rates. Poly-disperse size distribution corresponding to the realistic ash particle size distribution was used. The results are reported for three different conditions of (1) flow past a single cylinder in a channel (Fig. 5.9), (2) flow past a deep tube bank of 3 x 3 in-line cylinders (Fig. 5.10.1-5.10.4), and (3) flow past a deep tube bank of 2 x 2 in-line cylinders at large separation (Fig. 5.11.1-5.11.3). Flow Reynolds number based on the cylinder diameter was approximately 4000 for all three cases. For typical boiler tube conditions of tube diameter = 0.05 m, cross stream velocity of 10 m/s, the flow Reynolds number may lie between 8,000 - 10,000. Particle trajectories are, however, governed by the particle Stokes number. Particle diameters were therefore scaled to match Stokes number between the simulations and actual boiler conditions. Since no reliable correlation were available for the particle sticking coefficients, we have carried the simulations by neglecting particle rebound (sticking coefficient =1) and obtained upper bound on the particle deposition rates. The frame work for accommodating non-unity sticking coefficients is in place.

5.4 Time Averaged Results

Work was also performed to calculate the time averaged flow field. As an initial step, the computations were performed to calculate the unsteady state flow field at many times intervals for the case of flow past a single cylinder in a channel. The computed flow field was stored after every 20 iteration time steps. The ensemble of stored results provides many snap shots of the flow history, which can be analyzed for their statistical properties. As an example, the calculated axial velocity at 4 different field points is shown in Figure 5.12.1 as a function of dimensionless time. These results correspond to 2000 integration steps, or 100 sampling events stored at 20 step intervals. Storing results at 20 step intervals provides some degree of filtering of high frequency components. In order to average the results over large turbulent eddies, or coherent structures of the order of axial flow dimension, it is necessary to sample results for approximately $t^* = 10$, where t^* is dimensionless time. Computations are continuing to gather more samples. The samples collected so far were analyzed for their statistical properties. The average flow properties, $\bar{u}$, $\bar{v}$, $\bar{w}$ and $\bar{p}$, are shown in Figures 5.12.2-5.12.5, while higher moments, $\langle k \rangle$, $\langle u'v' \rangle$, and $\langle u'v' \rangle$ are shown in Figures 5.12.6-5.12.8. The computed results exhibit some spatial fluctuations due to the inadequate smoothing from 100 samples.

Work was continued to calculate the unsteady state flow field at many times intervals for the case of flow past a single cylinder in a channel. The computed flow field was stored after every 20 iteration time steps. The ensemble of stored results provides many snap shots of the flow history, which can be analyzed for their statistical properties. In order to average the results over large turbulent eddies, or coherent structures of the order of axial flow dimension, it is necessary to sample results for approximately $t^* = 10$, where t^* is dimensionless time. The samples collected so far were analyzed for their statistical properties. The average flow properties, $\langle u \rangle$, $\langle v \rangle$, $\langle w \rangle$, and $\langle p \rangle$ are shown in Figures 5.13.1-5.13.4. The computed results exhibit some spatial fluctuations due to the inadequate smoothing from 200 samples. Further averaging of the data can be obtained by averaging over the spanwise direction. Computed averages $\langle\langle u \rangle\rangle$, $\langle\langle v \rangle\rangle$, $\langle\langle w \rangle\rangle$, $\langle\langle p \rangle\rangle$, $\langle\langle k \rangle\rangle$, $\langle\langle u'v' \rangle\rangle$, and $\langle\langle u'p' \rangle\rangle$ are shown in Figures 5.13.5-5.13.11. Averaging in the spanwise direction increases the sample size by an order of magnitude. Even these results show spatial fluctuations. These results point to the difficulties associated with obtaining time averaged results when using higher order simulation methods such as Large Eddy Simulation.

Computed results for the case of flow past a single cylinder in a channel were analyzed for the vortex shedding frequency. Computed contours of axial velocity at the mid-span are shown in Fig. 5.14.1-5.14.6 at time interval of $t^*=0.5$. The shape of downstream vortex appears to repeat after $t^*=2.5$, so that time period $t.U_0/D$, where U_0 = free-stream velocity and D = cylinder diameter, is 4.16 or Strouhal number is 0.24. Estimated Strouhal number is based on the computation of a single cycle. This number is close to the value of 0.2 for vortex shedding from an isolated cylinder which is nearly constant for $Re > 300$. This agreement is one of the many steps required in the code validation process.

5.5 Evolution of Deposit Shape

A simplified frame work for calculating the growth and shape of deposits from the calculated impaction rates was also established. The calculated deposit shapes for all three cases are shown (Fig. 5.15.1-5.15.3). Using this frame work, one can begin to compare the predicted shapes with the experimentally observed shapes.

For the sake of comparison with other theories, we have also established the frame work for calculating deposit shapes based on the potential flow theory for an isolated cylinder in cross flow. This work extends the results reported by Larry Baxter at Sandia Lab. Detailed correlation for the angular distributions of the deposit shapes are provided (Fig. 5.16.1-5.16.9). A comparison of LES and potential flow theory results will enhance the understanding of the deposition process.

The flow field and deposition rates were also calculated for a single thickly-fouled non-circular cylinder in the cross flow. The shape of the fouled cylinder was specified a priori; it could have been calculated from the deposition rate for a clean circular cylinder as reported in the previous section. The three dimensional flow field was calculated by applying in-flow and out-flow boundary conditions in the main flow direction and periodic boundary conditions in the other two directions. Flow Reynolds number based on the free stream velocity and the projected cylinder diameter was set equal to 10^4 . The computations were based on relatively coarse grid with 30 elements, each element containing $5*5*7$ nodes. The calculated results are shown in Fig. 5.17.1-5.17.7. These results exhibit three dimensional effects and vortex shedding phenomena.

In view of the physical time constraints, these results were repeated by using two dimensional geometry. The computed results are shown in Fig. 5.18.1. Two-dimensional results are less chaotic and exhibit greater symmetry. Some typical particle trajectories are shown in Fig. 5.18.2, while location of particle impaction points is shown in Fig. 5.18.3. These computations were repeated by using 150,000 particles. In order to reduce the computer time, trajectories for particles with initial Stokes number less than 0.1 were not computed as the particle impaction efficiency at $St = 0.1$ is expected to be nearly zero. Computed angular distribution of the impaction points is shown in Fig. 5.18.4 and 5.18.5 for 10 degree and 20 degree collection bins. It is interesting to note that the computed impaction efficiency (based on mass impacted /mass injected) of 13% is very close to the anticipated efficiency of 14.5% based on the correlation for an isolated circular cylinder in a cross flow. Although it is too early to generalize, the results indicate an interesting possibility that impaction rates may be insensitive to the shape of deposit. The increase in the deposition rate observed experimentally for fouled boiler tubes over clean boiler tubes must therefore be attributed to the increased sticking probability.

Due to the lack of appropriate models for predicting sticking coefficient, which depends not only on the inflow conditions of gas and particles but also on the physico-chemical nature of the deposit, we have assumed unity sticking coefficient in the above computations. Typical code computations involving the transport of a passive scalar species can be performed easily. The computed species concentration contours are shown in Fig. 5.19 for the case of flow past a single cylinder in a channel. The species concentration is normalized with respect to the flux at the boundary. Coupled computation of multiple species transport including condensable, non-condensable, and reactive species can be performed by modifying species boundary conditions. Test results involving reactive species have been performed. Thus most of the modules for predicting deposit shape evolution are in place. Phenomenological models for sticking coefficients (and/or erosion coefficients) are required to perform more realistic calculations.

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Figure 3.1a Example of domain decomposition into quadrilateral spectral elements

Figure 3.1b Legendre mesh local to a spectral element

Figure 3.1 Schematic of Domain Decomposition into Quadrilateral Spectral Elements & Legendre Mesh of Spectral Elements

Figure 3.2 Example of Domain Decomposition into Three-Dimensional Hexahedral Spectral Elements

Figure 3.3a Illustration of an admissible element

Figure 3.3b Illustration of inadmissible elements

Figure 3.3 Schematic of Admissible and Inadmissible Spectral Elements

Correct placement

Incorrect placement

Figure 3.4a Illustration of incorrect relative placement of spectral elements

Correct assembly

violates (ii)

Incorrect assembly

Figure 3.4b Illustration of incorrect assembly of spectral elements

Figure 3.4 Schematic of Correct and Incorrect Placement of Spectral Elements

notch vel field

Figure 5.1.1 Computed Velocity Vectors for Flow Past a Notch

notch Pressure

Figure 5.1.2 Computed Pressure Contours at the Mid-Span for the Flow Past a Notch

notch U-vel

Figure 5.1.3 Computed Axial Velocity Contours for the Flow Past a Notch

c3d11 vc Re=20000 t=26.08

Figure 5.2.1 Computed Velocity Vectors for the Flow Past an Isolated Single Cylinder. Flow Reynolds Number 20,000 Dimensionless Time $t = 26.08$

c3d11 U Re=20000 t=26.08

Figure 5.2.2 Computed Axial Velocity Contours

c3d11 V Re=20000 t=26.08

Figure 5.2.3 Computed Radial Velocity Contours

c3d11 W Re=20000 t=26.08

Figure 5.2.4 Computed Spanwise Velocity Contours

c3d11 P Re=20000 t=26.08

Figure 5.2.5 Computed Pressure Contours

c3d11 T Re=20000 t=26.08

Figure 5.2.6 Computed Temperature (Passive Scalar) Contours

c3d11 Py Re=20000 t=26.08

Figure 5.2.7 Computed Pressure Contours in X-Z Plane

c3d11 Wx Re=20000 t=26.08

Figure 5.2.8 Computed W Velocity Contours in Y-Z Plane

c3d11 Wy Re=20000 t=26.08

Figure 5.2.9 Computed W Velocity Contours in X-Z Plane

c3d11 Uy Re=20000 t=26.08

Figure 5.2.10 Computed Axial Velocity Contours in X-Z Plane

cylchv Re=4000 t=5.46

Figure 5.3.1 Computed Velocity Vectors for the Flow Past a Single Cylinder in a Channel. Flow Reynolds Number 4000, Dimensionless Time = 5.46. Flow Is From Left to Right. Top and Bottom Walls are Rigid Walls. Periodic Boundary Conditions are Applied in Z-Direction.

cylchU Re=4000 t=5.46

Figure 5.3.2 Computed Axial Velocity Contours in X-Y Plane

cylchW Re=4000 t=5.46

Figure 5.3.3 Computed W Velocity Contours in X-Y Plane

cylchP Re=4000 t=5.46

Figure 5.3.4 Computed Pressure Contours in X-Y Plane

cylchT Re=4000 t=5.46

Figure 5.3.5 Computed Temperature Contours in X-Y Plane.
(t Treated as Dimensionless Passive Scalar Quantity)

visc cylch $Re=4000$ $t=5.46$

Figure 5.3.6 Computed Turbulent Viscosity in X-Y Plane

cond cylch $Re=4000$ $t=5.46$

Figure 5.3.7 Computed Turbulent Conductivity in X-Y Plane

stry cylch $Re=4000$ $t=5.46$

Figure 5.3.8 Computed Stry in X-Y Plane

visy cylch Re=4000 t=5.46

Figure 5.3.9 Computed Turbulent Viscosity in X-Z Plane

cyl61 vec Re=4000 t=5.232

Figure 5.4.1 Computed Velocity Vectors for the Flow Past a 2x2 Array of Tubes at Large Distance of Separation. Flow Reynolds Number 4000, Dimensionless Time = 5.23. Three Dimensional Vector Plot

cyl61 vec Re=4000 t=5.232

Figure 5.4.2 Computed Velocity Vectors in X-Y Plane

cyl61 Wx Re=4000 t=5.232

Figure 5.4.3 Computed W Velocity Contours in Y-Z Plane

cyl61 W Re=4000 t=5.232

Figure 5.4.4 Computed W Velocity Vectors in X-Y Plane

cyl61 U Re=4000 t=5.232

Figure 5.4.5 Computed U Velocity Contours in X-Y Plane

cyl61 P Re=4000 t=5.232

Figure 5.4.6 Computed Pressure Contours in X-Y Plane

cyl61 T Re=4000 t=5.232

Figure 5.4.7 Computed Temperature (Passive Scalar)
Contours in X-Y Plane

cyl61 Tx Re=4000 t=5.232

Figure 5.4.8 Computed Temperature Contours in Y-Z Plane

cyl61 Uy Re=4000 t=5.232

Figure 5.4.9 Computed Axial Velocity Contours in X-Z Plane

In-line vec. $Re=4000$ $t=4.0$

Figure 5.5.1 Computed Velocity Contours for Flow Past a 3x3 Array of Cylinders. Flow Reynolds Number 4000, Dimensionless Time 4.0

In-line P Re=4000 t=20.

Figure 5.5.2 Computed Pressure Contours in X-Y Plane. Flow Reynolds Number 4000, Dimensionless Time 20.0

In-line U $Re=4000$ $t=20$.

Figure 5.5.3 Computed Axial Velocity Contours in X-Y Plane

In-line Uy Re=4000 t=20.0

Figure 5.5.4 Computed Axial Velocity Contours in X-Z Plane

In-line V_x $Re=4000$ $t=20$.

Figure 5.5.5 Computed Radial Velocity Contours in Y-Z Plane

In-line W $Re=4000$ $t=20$.

Figure 5.5.6 Computed W Velocity Contours in X-Y Plane

In-line W_x $Re=4000$ $t=20$

Figure 5.5.7 Computed W Velocity Contours in Y - Z Plane

In-line T $Re=4000$ $t=20$.

Figure 5.5.8 Computed Temperature Contours in X-Y Plane

In-line Ty $Re=4000$ $t=20$.

Figure 5.5.9 Computed Temperature Contours in X-Z Plane

Figure 5.6.1 Computed Pressure Contours at the Mid Span for Flow Past a Mildly Fouled Cylinder. The Shape of the Cylinder is Specified a Priori.

Figure 5.6.2 Computed Velocity Vectors Superimposed on the Pressure Contours

Figure 5.6.3 Computed Pressure Contours in Y-Z Plane Behind the Cylinder

Figure 5.6.4 Computed Contours of Spanwise Velocity W in X-Y Plane

Figure 5.7.1 Location of Particle Impaction Points for the Flow Past a Single Cylinder in a Channel

Figure 5.7.2 Location of Particle Adhesion Points for the Flow Past a Single Cylinder in a Channel

Particle Impaction Probability
(Cylinder in a Channel)

081093.g1

Figure 5.7.3 Instantaneous Angular Distribution of Particle Impaction.
Angle 90 Corresponds to Stagnation Point, While 0 Corresponds to Top of Cylinder

Figure 5.8.1 Location of Impaction Points for Flow Past a 3 X 3 Array of in-Line Cylinders

Figure 5.8.2 Instantaneous Location of Adhesion Points for Flow Past a 3 X 3 Array of in-Line Cylinders

Particle Impaction Probability

Figure 5.8.3 Angular Distribution of Impaction Probability for a 3 x 3 Array of in-Line Cylinders. Angle 0 Corresponds to the top of Cylinder, While 90 Corresponds to the Stagnation Point.

Particle Sticking Probability

091393.g2

Figure 5.8.4 Angular Distribution of Sticking Probability for a 3 x 3 Array of in-Line Cylinders. Angle 0 Corresponds to the Top of Cylinder, While 90 Corresponds to the Stagnation Point

Particle Impaction & Sticking Probability

Figure 5.8.5 Angular Distribution of Averaged Impaction and Sticking Probability. Average Is Done by Assigning Equal Weight to All Cylinders.

Angular Distribution of Deposition Rate Single Cylinder in a Channel

111193.g1

Figure 5.9 Computed Angular Distribution of Deposition Rate for the Flow Past a Single Cylinder in a Channel. Angle 0 Corresponds to the Stagnation Point, While 90 Corresponds to the Top of Cylinder.

Angular Distribution of Particle Impaction 3 x 3 In-line Cylinders, First Row

Figure 5.10.1 Computed Angular Distribution of the Deposition Rate for the First Row of 3 x 3 In-Line Cylinders

Angular Distribution of Particle Impaction
3 x 3 In-line Cylinders, second row

l10893.g4

Figure 5.10.2 Computed Angular Distribution of the Deposition Rate for the Second Row of 3x3 in-Line Cylinders

Angular Distribution of Particle Impaction 3 x 3 In-line Cylinders, Third Row

110893.g5

Figure 5.10.3 Computed Angular Distribution of the Deposition Rate for the Third Row of 3x3 in-line Cylinders

Figure 5.10.4 Computed Average Angular Distribution of the Impaction Rates for the Flow Past a 3x3 Array of In-Line Cylinders

Angular Distribution of Deposition Rate
2 x 2 In-line Cylinders, First Row

Figure 5.11.1 Computed Angular Distribution of the Impaction Rates for the First Row of an Array of 2 x 2 Cylinders

Angular Distribution of Deposition Rate
2 x 2 In-line Cylinders, Second Row

111193.g6

Figure 5.11.2 Computed Angular Distribution of the Impaction Rates for the Second Row of an Array of 2 x 2 Cylinders

Angular Distribution of Deposition Rate
2 x 2 In-line Cylinders

111193.g3

Figure 5.11.3 Computed Average Angular Distribution of the Impaction Rates for Flow Past an Array of 2 x 2 Cylinders

Axial Velocity History at Selected Points (Cylinder in a Channel)

091393.g4

Figure 5.12.1 Computed History of Axial Velocity at a Few Selected Points for the Flow Past a Single Cylinder in a Channel. Flow Reynolds Number 20,000 Based On Channel Width.

cyl1ch U-avg

Figure 5.12.2 Computed Average Axial Velocity Contours at the Mid Span. Average is Based on 100 Samples Obtained at the Interval of 20 Time Steps Each.

cyl1ch V-avg

Figure 5.12.3 Computed Average Radial Velocity at the Mid Span.

cyl1ch W-avg

Figure 5.12.4 Computed Average Spanwise Velocity W at the Mid Span

cyl1ch p-avg

Figure 5.12.5 Computed Average Pressure Contours

cyl1ch k-avg

Figure 5.12.6 Computed Average Turbulence Kinetic Energy Contours

cyl1ch $\langle u'v' \rangle$

Figure 5.12.7 Computed Average Velocity Correlation Contours

cyl1ch $\langle u'p' \rangle$

Figure 5.12.8 Computed Average Pressure-Velocity Correlation Contours

cyllch <u>

Figure 5.13.1 Computed Average Axial Velocity Contours at the Mid Span. Average is Based on 200 Samples Obtained at the Interval of 20 Time Steps Each. Flow Reynolds Number = 20,000 Based on Channel Width, Reynolds Number = 4000 Based On Cylinder Diameter.

cy1lch $\langle v \rangle$

Figure 5.13.2 Computed Average Radial Velocity at the Mid Span

cy1lch <w>

Figure 5.13.3 Computed Average Spanwise Velocity W at the Mid Span

cy1lch $\langle p \rangle$

Figure 5.13.4 Computed Average Pressure Contours

cyl1ch $\langle \langle u \rangle \rangle$

Figure 5.13.5 Computed Average Axial Velocity Contours. Results Based on Average in Time and Spanwise Direction. No. of Samples = 200*10.

cyl1ch $\langle \langle v \rangle \rangle$

Figure 5.13.6 Computed Average Radial Velocity Contours

Figure 5.13.7 Computed Average Spanwise Velocity W Contours

cyl1ch <<p>>

Figure 5.13.8 Computed Average Pressure Contours

cyl1ch $\langle \langle k \rangle \rangle$

Figure 5.13.9 Computed Average Turbulence Energy Contours

cyl1ch $\langle \langle u'v' \rangle \rangle$

Figure 5.13.10 Computed Average Velocity Correlation Contours

cyl1ch $\langle \langle u'p' \rangle \rangle$

Figure 5.13.11 Computed Average Pressure-Velocity Correlation Contours

Figure 5.14.1 Computed Instantaneous Axial Velocity Contours at the Mid Span for the Flow Past a Single Cylinder in a Channel. Flow Reynolds Number Based On Upstream Velocity and Cylinder Diameter = 4000. Dimensionless Time $t^* = 0.0$

Figure 5.14.2 Instantaneous Axial Velocity at $t^* = 0.5$

Figure 5.14.3 Instantaneous Axial Velocity at $t^* = 1.0$

Figure 5.14.4 Instantaneous Axial Velocity at $t^* = 1.5$

Figure 5.14.5 Instantaneous Axial Velocity at $t^* = 2.0$

Figure 5.14.6 Instantaneous Axial Velocity at $t^* = 2.5$

111193.g2

Figure 5.15.1 Predicted Time Evolution of Deposit Shape for the Flow Past a Single Cylinder in a Channel. Prediction Based on Constant Deposit Density of 2000 and Unity Sticking Coefficient.

Predicted Time Evolution of Deposit 2 x 2 In-line Cylinders

111193.g4

Figure 5.15.2 Predicted Time Evolution of Deposit Shape for an Array of 2x2 in-Line Cylinders. Computed Value Is Average for 4 Cylinders.

Predicted Time Evolution of Deposit 3 x 3 In-line Cylinders

Calculated Deposit Efficiency Correlation for Flow Past an Isolated Cylinder

111293.g1

Figure 5.16.1 Particle Capture Efficiency as a Function of Initial Diameter Based On the Correlation of Israel & Rosner. Solid Curve Represents the Capture Efficiency for the Assumed Ash Size Distribution. Overall Capture Efficiency 16%.

Calculated Deposit Efficiency Correlation For Flow Past an Isolated Cylinder

Figure 5.16.2 Particle Capture Efficiency as a Function of Particle Stokes Number

Impaction Efficiency vs Stokes Number

111593.g6

Figure 5.16.3 Computed Capture Efficiency Versus Stokes Number. Present Calculations Based On the Potential Flow Solution for the Flow Past an Isolated Circular Cylinder.

Angular Distribution of Particle Impaction

111293.g4

Figure 5.16.4 Computed Impact Angle Versus Impact Parameter for Different Initial Stokes Numbers. For Impact Parameter Greater Than the Critical Value, Particle Does Not Impact the Cylinder. Cumulative Weight Fraction Varies Linearly with the Impact Parameter.

Stokes number Dependence of Critical Angle

111593.g5

Figure 5.16.5 Correlation of Critical Impact Angle with Initial Stokes Number. Critical Impact Angle Corresponds to Impact Angle at the Maximum Impact Parameter.

111593.g2

Figure 5.16.6 Results of Figure 5.16.4 are Re-Plotted By Normalizing angle With Critical angle. Curves With Different Stokes Number Merge into a Single Curve.

Normalized Angular Distribution

111593.g1

Figure 5.16.7 Same as Figure 5.16.6 With Axis Interchanged.

111593.g3

Figure 5.16.8 Impact Probability Versus Normalized Angle Impact Probability is Obtained by Differentiating Cumulative Weight Fraction Curve

Angular Distribution of Impaction Rate

111693.g1

Figure 5.16.9 Computed Angular Distribution of Impaction Rate Based on the Potential Flow Solution for an Isolated Single Cylinder and Assumed Ash Size Distribution

$Re = 10,000 \quad U$

Figure 5.17.1 Computed Axial Velocity Contours at the Mid-Span for the Flow Past a Thickly Fouled Non-Circular Cylinder. $Re = 10,000$.

$Re=10,000$ U_x

Figure 5.17.2 Computed Axial Velocity Contours in Y-Z Plane

$Re=10,000$ V

Figure 5.17.3 Computed Transverse Velocity Contours at the Mid-Span

$Re = 10,000$ W

Figure 5.17.4 Computed Spanwise Velocity Contours

$Re=10,000$ P

Figure 5.17.5 Computed Pressure Contours

$Re=10,000$ P_x

Figure 5.17.6 Computed Pressure Contours in Y-Z Plane

$Re=10,000$ vec

Figure 5.17.7 Computed Velocity Vectors at the Mid Span

$$Re = 10,000 \quad U$$

Figure 5.18.1 Computed Velocity Vectors Superimposed on Pressure Contours for Two-Dimensional Flow Past a Thickly Fouled Non-Circular Cylinder

Figure 5.18.2 Typical Particle Trajectories for Two-Dimensional Flow Past a Non-Circular Cylinder

Figure 5.18.3 Computed Location of Impaction Points

Angular Distribution of Deposition Rate Single Non-circular Cylinder in Crossflow

120993.g1

Figure 5.18.4 Angular Distribution of Impaction Rates for Flow Past a Non-Circular Cylinder. Results Based On Sampling in 10 Degree Bins.

Angular Distribution of Deposition Rate Single Non-circular Cylinder in Crossflow

120993.g2

Figure 5.18.5 Same as Figure 5.18.4 but Sampling Based on 20 Degree Bins

cyl re=4000, ps

Figure 5.19.1 Computed Contours for a Passive Scalar Species for the Flow Past a Circular Cylinder in a Channel