PREDICTIVE MODELLING OF BOILER FOULING

QUARTERLY TECHNICAL PROGRESS REPORT

FOR THE PERIOD
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1.0 PROGRAM OBJECTIVE AND SCOPE OF WORK

The primary objective of this work is the development of a comprehensive numerical model describing the time evolution of fouling under realistic heat exchanger conditions. As fouling is a complex interaction of gas flow, mineral transport and adhesion mechanisms, understanding and subsequently improved controlling of fouling achieved via appropriate manipulation of the various coupled, nonlinear processes in a complex fluid mechanics environment will undoubtedly help reduce the substantial operating costs incurred by the utilities annually, as well as afford greater flexibility in coal selection and reduce the emission of various pollutants. In a more specialized context, the numerical model to be developed as part of this activity will be used as a tool to address the interaction of the various mechanisms controlling deposit development in specific regimes or correlative relationships. These should prove of direct use to the coal burning industry.

The Statement of Work comprises a series of related and logically structured tasks described as follows:

Phase I

Task 1

Perform semi-quantitative evaluations of solution and algorithmic details of Higher Level Simulation (HLS) techniques applicable to flow in and around a tube bundle.

Task 2

Assess (quantitatively) HLS predictions for flow and turbulence characteristics of related, simpler problems.

Task 3

Reformulate the algorithm to predict flow details around a cylinder in an isothermal, but otherwise representative environment.

Task 4

Predict heat transfer characteristics for the problem in Task 3.

Task 5

Generalize the algorithm to predict flow, turbulence and heat transfer details for multi-tube configurations including in-line and staggered arrangements.

Task 6

Provide project management and financial control with the required technical and financial reports and documentation.

Phase II

Task 1

Develop an appropriate multi-phase, multi-species transport algorithm for a "frozen" gas aerothermal field.

Task 2

Develop sub-modules for surface related processes including adherence and removal.

Task 3

Provide project management and financial control with the required technical and financial reports and documentation.

Phase III

Task 1

Extend the algorithm to couple multi-species, multi-phase transport and deposition models with a comprehensive HLS of flow and heat transfer in a tube bundle for a representative case.

Task 2

Perform pertinent parameter variation studies and develop improved engineering correlations to model fouling in practical boiler configurations and operating environments.

Task 3

Provide project management and financial control with the required technical and financial reports and documentation.

2.0 SUMMARY OF PROGRESS TO DATE

Efforts were continued to apply the algorithm for predictions of flow, turbulence and heat transfer details around an isolated cylinder as well as a deep tube bank. 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.

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.

3.0 TECHNICAL PROGRESS

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:

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

$$\underline{\nabla} \cdot \underline{v} = 0 \quad (3.1a)$$

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.,

$$\underline{N}(\underline{v}) = \frac{1}{2} [\underline{v} \cdot \underline{\nabla} \underline{v} + \underline{\nabla} \cdot (\underline{v} \cdot \underline{v})] + \underline{f} + \underline{\nabla} \cdot (\underline{v} - \bar{\nu}) [\underline{\nabla} \underline{v} + \underline{\nabla}^T \underline{v}] \quad (3.1b)$$

where ν 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 Ω . However, before proceeding with the spatial discretization of the equation, details of the time stepping algorithm are briefly reviewed.

3.1 Semi Discrete Formulation

The separation of terms in Equation (3.1a) 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:

$$\frac{\hat{\underline{v}} - \sum_{q=0}^{J-1} \alpha_q \underline{v}^{n-q}}{\Delta t} = \sum_{q=0}^{J-1} \beta_q [-N(\underline{v}^{n-q})] \quad (3.2a)$$

where α_q, β_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:

$$\frac{\hat{\underline{v}} - \underline{v}}{\Delta t} = \underline{\nabla} p^{n+1} / \rho \quad (3.2b)$$

$$\underline{\nabla} \cdot \hat{\underline{v}} = 0 \quad (3.2c)$$

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

$$\frac{\gamma_0 \underline{v}^{n+1} - \hat{\underline{v}}}{\Delta t} = \bar{\underline{v}} \underline{\nabla}^2 \underline{v}^{n+1} \quad (3.2d)$$

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 (3.1) results in a very efficient calculation procedure as it decouples the pressure and velocity equations as in (3.2b) and 3.2c) 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:

$$\underline{\nabla}^2 p^{n+1} = \underline{\nabla} \cdot \left(\frac{\hat{\underline{v}}}{\Delta t} \right) \quad (3.3a)$$

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

$$\frac{\partial p^{n+1}}{\partial n} = \underline{n} \cdot \left[-\sum_{q=0}^{J-1} \beta_q \underline{N}(\underline{v}^{n-q}) - \text{Re}^{-1} \sum \beta_q [\underline{\nabla} \times (\underline{\nabla} \times \underline{v}^{n-q})] \right] \quad (3.3b)$$

where $\underline{n}$ denotes the unit normal to the boundary Γ . Equation (3.3) therefore is a Poisson equation with constant coefficients which can be rewritten in the standard form:

$$\underline{\nabla}^2 \phi = g(x) \quad (3.4)$$

where ϕ is defined as p^{n+1} and $g(x) = \underline{\nabla} \cdot (\hat{\underline{v}}/\Delta t)$. In the following section reference is specifically made to this equation in order to discuss the spatial discretization of equations (3.2) in three dimensions using the spectral element method.

3.2 Spatial Discretization

The spatial discretization of (3.2) is obtained using the spectral element methodology. In the standard spectral element discretization, the computational domain Ω 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 Ω 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 (3.4) 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 $\psi \in H_0^1$, the resulting equivalent variational statement of (3.4) can be expressed as:

$$\int_{\Omega} \frac{\partial \chi}{\partial x_j} \frac{\partial \phi}{\partial x_j} ds = - \int_{\Omega} \chi g ds \quad (3.5)$$

The conforming spectral element discretization corresponds to the numerical quadrature of the variational form (3.5) 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 ξ_{pql}^k and corresponding weights $\rho_{pql} = \rho_p \rho_q \rho_l$, equation (3.5) can be replaced by:

$$\sum_{k=1}^K \sum_{p=0}^{N_1} \sum_{q=0}^{N_2} \sum_{\ell=0}^{N_3} \rho_{pql} J_{pql}^k \left[\frac{\partial \chi}{\partial x_j} \frac{\partial \phi}{\partial x_j} \right]_{\xi_{pql}^k} = \quad (3.6)$$

$$\sum_{k=1}^K \sum_{p=0}^{N_1} \sum_{q=0}^{N_2} \sum_{\ell=0}^{N_3} \rho_{pql} J_{pql}^k [\chi g]_{\xi_{pql}^k}$$

Here J_{pql}^k is the Jacobian of the transformation from global to local coordinates $(x, y, z) \Rightarrow (r, s, t)$ 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:

$$J = z_t (x_r y_s - x_s y_r) + z_s (x_t y_r - x_r y_t) + z_r (x_s y_t - x_t y_s) \quad (3.7a)$$

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

$$(X_r)_{pql} = D_{pm} X_{mq} \quad (3.7b)$$

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

The next step in implementing (3.6) 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 $h_i(r_j) = \delta_{ij}$. Here r_j represents the local coordinate and δ_{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 $N_{1,2,3} \rightarrow \infty$, 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 equation (3.6) 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., $P^k_{ijpmnq} \phi_{mnq}$). 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 very efficiently and robustly solved using those iterative techniques without the need of case dependent preconditioners and other convergence acceleration techniques.

Using the above formulation along with the RNG descriptor previously discussed, studies were continued to simulate various single and multi-cylinder configurations as well as other relevant test problems.

3.3 Sample Predictions

In addition to the previously reported cases, more refined predictions were carried out to simulate the representative configuration and conditions of utility boilers along with pertinent test problems. These include:

a) 3-D multi-cylinder flow (four cylinders arranged in tandem configuration) including heat transfer; these predictions primarily refer to laminar conditions $Re=400$ however, the numerical formulation is currently being extended to cover 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 1 to 3.

b) The same as above, but focussing on the effect of the L/D ratio on the flow structure where cylinder to cylinder flow interactions do occur. These refer to a 3x3 matrix of in-line geometry, Figures 4 to 8. These predictions were carried out primarily for laminar Reynolds number of 400.

c) A single cylinder in an inflow/outflow configuration where the remaining directions are treated periodically. Reynolds number studied is 4000 and the computations have been carried out to an integrated time of unit 6.0. Figures 9 to 18 depict various variable evolutions in the field for select viewing angles. These predictions do include the RNG description to simulate subgrid effects.

These predictions, as well as others studied appear qualitatively reasonable and are currently being studied in detail to assess the predictive nature of the formulation including issues of computational resources.

4.0 CONCLUSION AND PLANS FOR FUTURE WORK

4.1 Conclusions to Date

Good technical progress has been made. As accurate large eddy simulations in the past have concentrated on resolving the turbulence details of semi-idealized geometrically simple flow problems, applications involving configurations and physical complexity comparable to those in typical tube banks are naturally rare. The effort in this reporting period has shown spectral element algorithm incorporating RNG techniques can be conveniently used to provide detailed flow and heat transfer information for a truly complex transport field. Furthermore, the RNG technique as reported in the literature, seems to give a faithful description of the turbulence in the wall region including approximately correct Reynolds number independent value of the spacing between the streaks for turbulent channel flow. However, results presented so far for case (c) are only preliminary and can only provide a qualitative assessment of the resolution capabilities of the RNG subgrid model in describing inhomogeneous turbulence and, in particular separated flows. Work still underway addresses the issue of mesh dependence and compares in detail results of large eddy simulations with direct simulations for the same flow.

4.2 Plans for Next Reporting Period

Efforts direct towards algorithm development and applications involving flow, turbulence evolution and heat transfer characteristics around an isolated cylinder and a tube bank will be continued.

cylht61 Uvel $Re=400$

Figure 1

cylht61 T Re=400

Figure 2

cylht61 vec $Re=400$

Figure 3

In-line Uvel $Re=400$

Figure 4

In-line W Re = 400

Figure 5

In-line $P \cdot Re = 400$

Figure 6

In-line T Re = 400

Figure 7

Figure 8

c3d12 Uvel $Re=4000$ $t=6.0$

Figure 9

c3d12 Vvel Re=4000 t=6.0

Figure 10

c3d12 Wvel $Re=4000$ $t=6.0$

Figure 11

c3d12 vel $Re=4000$ $t=6.0$

Figure 12

c3d12 pres Re=4000 t=0

1.0

0.8

Figure 13

c3d12 Uyplt Re=4000 t=6.0

Figure 14

c3d12 Wyplt Re=4000 t=6.0

Figure 15

c3d12 Pyplt Re=4000 t=6.0

Figure 16

c3d12 Wxplt Re=4000 t=6.0

Figure 17

c3d12 vec $Re=4000$ $t=6.0$

Figure 18

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