PARALLEL NUMERICAL SIMULATION OF CONJUGATE HEAT TRANSFER IN THE TARGET SYSTEM OF AN ADS BY DOMAIN DECOMPOSITION METHOD

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Abstract. Accelerator Driven Sub-critical nuclear reactor System (ADS) are envisaged to enhance neutronics of reactors as well as safety physics. The spallation target module or target system is the most innovative and key component for an ADS. In the target module, a high energy proton beam from the accelerator irradiates a heavy metal target like Lead Bismuth Eutectic (LBE) to produce spallation neutrons, which initiate the fission reaction in the sub-critical core. The removal of the spallation heat by the same LBE is a challenging thermal-hydraulic issue. Also the presence of any recirculation or stagnation zones of LBE in the flow path may lead to local hot spots either in the window or in the flowing liquid metal which is detrimental to the performance of the target. The beam window, a physical barrier separating the liquid metal (LBE) from the proton beam, is a critical component as it is subject to high heat fluxes as well as thermal and mechanical stresses. In addition to heat deposited in the bulk of LBE in the spallation region, large amount of heat also gets deposited on the window. To incorporate the physical situation in a more realistic way, a conjugate heat transfer problem (solving the conduction equation of the beam window in conjunction with the energy equation) is accomplished. As the conjugate heat transfer problem is found to be computationally very demanding, the energy equation module is parallelized following the paradigm of domain decomposition method using MPI (Message passing Interface) library. In this study, the equations governing the axisymmetric flow and thermal energy are solved numerically using a Streamline Upwind Petrov-Galerkin (SUPG) Finite Element (FE) method. The turbulent kinetic energy and its dissipation rate are modeled using k-ε model with standard wall function approach. The interface temperature as a result of conjugate heat transfer and Nusselt number distribution at the interface with a reasonable speedup is computed and quantified.

Key words. ADS, Thermal Hydraulics, Conjugate heat transfer, Streamline Upwind Petrov-Galerkin technique, Parallel Computing

1. Introduction

In the near future, ADS will play a significant role in nuclear power generation due to their ability to enhance both the neutronics of reactors as well as safety physics (Rubbia et al. [13]). The target system is the critical part of an ADS which is shown in Figure 1 (i). In the target system, a high energy proton beam from the accelerator irradiates a heavy metal target to produce spallation neutrons which initiates fission reaction in the sub-critical core. The protons are induced on the target through vacuum pipe closed by a window at the end. Therefore, the beam window is exposed to a huge amount of thermal and mechanical load and suffers from radiation damage due to spallation neutrons. Lead-Bismuth Eutectic (LBE) is preferred as the target material due to its high production rate of neutrons, effective heat removal rate and a very small amount of radiation damage properties. In addition, it can be used as a reactor coolant simultaneously. Thus the spallation target module is the most innovative component of ADS which constitutes the physical interface between the accelerator and the sub-critical core.
Even though it is relatively easy to take away the total spallation heat by the LBE, what is crucial is that this has to be achieved without target temperature exceeding the stipulated temperature in any region of the flow. There should not be any recirculation or stagnation zones leading to the hot spots, inadequate window cooling, generation of vapors etc. This necessitates detailed flow analysis in the spallation region, flow region near the entrance of the annular zone along with the temperature distribution on the window. Investigations concerning the development of target system of an ADS have been summarized by Maiorino et al. [9]. A review of the recent literature reveals that there have been few investigations focussing on the design of the target system of an ADS. Dury et al. [6] have analyzed the spallation zone near the beam window of the European Spallation source liquid-metal target facility numerically using CFX-4. They considered liquid mercury as the spallation target. Cho et al. [4] have computed the heat transfer and flow characteristics in a simplified version of the target system model called HYPER using ANSYS and CFX packages. Recently, window based target modules, such as, XADS (Batta et al. [1]), with nozzle shaped flow guides have been proposed. In the ADS model considered in this study, the downcomer part of the ADS is separated from the riser part by using a flow guide. The flow takes a 180° turn around the tip of flow guide. In order to simulate the target system an in-house SUPG-FE code based on the projection scheme of Chorin [5] has been developed and validated. The two equation k-ε model with standard wall function approach is used for analyzing turbulent flows. Further, we account for the high energetic proton beam impingement on the window surface by introducing isothermal condition on the window. Simulations have been carried out to analyze the flow and heat transfer characteristics in the target system of an ADS for a wide range of Reynolds numbers. The optimization of the target modules are also carried out based on the suitable design of flow guide which separates the hot rising flow from the cold one. In the region where the flow takes a 180° turn different shapes of flow guide are introduced. Initially a straight flow guide with cylindrical bottom container is simulated (Prakash et al. [11]). Finally a funnel shape flow guide with spherical bottom container is designed in order to accelerate the liquid metal and thereby enhance the cooling of the window (Prakash et al. [11]).

Figure 1. (i) Schematic diagram of the target module of an ADS (ii) Domain of Interest with boundary conditions.
These cases are computed in order to trace the temperature distribution on the beam window and in LBE which is useful for its mechanical design. In our earlier studies the thickness of the beam window is not considered. In situations where the thickness of the solid wall is considerable or the thermal conductivities of fluid and solid are comparable, the conjugate heat transfer analysis is necessary and more appropriate to assess the model. The beam window of ADS considered here is of considerable thickness (say 3 mm). Hence, conjugate heat transfer study is performed by solving simultaneously the solid heat conduction equation and energy equation. The domain decomposition parallelization method using MPI library is implemented and a reasonable speedup is achieved.

2. Governing Equations and Boundary Conditions

2.1. Governing equations. The flow is considered to be viscous, incompressible and turbulent. The Reynolds analogy is applied to calculate the turbulent heat transfer. The geometry of interest is axisymmetric. The computational domain shown in Figure 1 (ii) is discretized using small quadrilateral elements. All variables including the velocity components, pressure, temperature, kinetic energy and dissipation rate are located at element nodes. The dimensionless equations governing the axisymmetric mean flow [11, 12] are as follows:

Continuity Equation

\[ \frac{1}{x^5} \frac{\partial}{\partial x} (x^5 u) + \frac{\partial v}{\partial y} = 0 \]  

Momentum Equations

\[ \frac{\partial u_j}{\partial \tau} + u_j \frac{\partial u_j}{\partial x_i} = - \frac{\partial p}{\partial x_i} + \frac{1}{Re x^5} \left\{ \frac{\partial}{\partial x} \left[ x^5 \nu_{eff} \left( \frac{\partial u_i}{\partial x} + \frac{\partial u_j}{\partial x_j} \right) \right] - \frac{2 \beta \nu_{eff} u_j}{x_i} \right\} \]

where \( p \) is the pressure, \( (u_j) \) are the radial and axial mean velocity components respectively and \( (x_i) \) the radial and axial coordinates, respectively. The effective turbulent viscosity, \( \nu_{eff} = (1 + \nu_{t,n}) \) is calculated using the \( (k - \epsilon) \) model of turbulence (Launder and Spalding [8]) as:

\[ \nu_{eff} = 1 + c_p Re \frac{k^2}{\epsilon_n} \]

Transfer of the dimensionless turbulent kinetic energy \( k_n \), its dissipation rate \( \epsilon_n \) and the temperature distribution \( \theta \) are modeled as follows:

\( k \)-Equation

\[ \frac{\partial k_n}{\partial \tau} + u \frac{\partial k_n}{\partial x} + v \frac{\partial k_n}{\partial y} = \frac{1}{x^5 Re} \left[ \frac{\partial}{\partial x} \left( x^5 \frac{\nu_{t,n}}{\sigma_k} \frac{\partial k_n}{\partial x} \right) + \frac{\partial}{\partial y} \left( x^5 \frac{\nu_{t,n}}{\sigma_k} \frac{\partial k_n}{\partial y} \right) \right] + G_n - \epsilon_n \]

\( \epsilon \)-Equation

\[ \frac{\partial \epsilon_n}{\partial \tau} + u \frac{\partial \epsilon_n}{\partial x} + v \frac{\partial \epsilon_n}{\partial y} = \frac{1}{x^5 Re} \left[ \frac{\partial}{\partial x} \left( x^5 \frac{\nu_{t,n}}{\sigma_\epsilon} \frac{\partial \epsilon_n}{\partial x} \right) + \frac{\partial}{\partial y} \left( x^5 \frac{\nu_{t,n}}{\sigma_\epsilon} \frac{\partial \epsilon_n}{\partial y} \right) \right] + \frac{\epsilon_n}{k_n} (C_1 \epsilon_n - C_2 \epsilon_n) \]
Energy Equation

\[
\frac{\partial \theta}{\partial \tau} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} = \frac{1}{x^3 \text{Re Pr}} \left[ \frac{\partial}{\partial x} \left( x^\beta (1 + \alpha_{t,n}) \frac{\partial \theta}{\partial x} \right) + \frac{\partial}{\partial y} \left( x^\beta (1 + \alpha_{t,n}) \frac{\partial \theta}{\partial y} \right) + S_\theta \right]
\]

where \(S_\theta\) is the heat generation source term and \(G_n\) is the turbulence production term. The index \(\beta\) is unity for the axisymmetric cases. The equations describing two-dimensional planar flows can be obtained from equations (1−5) by setting \(\beta = 0\).

Finally, \(\nu_{t,n}\) and \(\alpha_{t,n}\) can be written as

\[
\nu_{t,n} = C_\mu \text{Re} \frac{k_n^2}{\epsilon_n}, \quad \alpha_{t,n} = C_{\mu \text{Re}} \frac{Pr k_n^2}{\sigma_t \epsilon_n}
\]

where the model coefficients are:

\[C_\mu = 0.09, \quad \sigma_k = 1.0, \quad \sigma_c = 1.3, \quad \sigma_t = 0.9, \quad C_{1\epsilon} = 1.44\] and \(C_{2\epsilon} = 1.92\).

The dimensionless variables may be defined as:

\[
u = \frac{u^*}{V_0}; \quad v = \frac{v^*}{V_0}; \quad x = \frac{x^* D}{V_0}; \quad y = \frac{y^*}{D}; \quad \rho = \frac{\rho - \rho_{\text{atm}}}{\rho V_0^2}; \quad \tau = \frac{t^*}{\frac{D}{V_0^2}}; \quad \theta = \frac{T - T_\infty}{\Delta T_{\text{ref}}}; \quad k^* = \frac{k^*}{V_0^2}; \quad \epsilon = \frac{\epsilon^*}{\frac{D}{V_0}}
\]

where, dependent variables with exponent * are dimensional variables and \(\Delta T_{\text{ref}} = T_w\) (wall temperature) − \(T_\infty\) (ambient temperature).

The pertinent non-dimensional parameters are:

Reynolds Number, \(\text{Re} = \frac{V_0 D}{\nu}\) and Prandtl Number, \(\text{Pr} = \frac{\nu}{\alpha}\)

where \(D\) is the hydraulic diameter, \(\nu\) is the kinematic viscosity, \(\alpha\) is the thermal diffusivity and \(V_0\) is the mean inlet velocity.

For conjugate heat transfer, the solid heat conduction equation to be solved is given as follows:

Heat Conduction equation in the solid

\[
\frac{1}{x^3} \frac{\partial}{\partial x} \left( x^\beta \frac{\partial \theta_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial \theta_s}{\partial y} \right) + S_{\theta_s} = 0
\]

where \(\theta_s\) is the non-dimensional solid temperature, and \(S_{\theta_s}\) is the non-dimensional rate of volumetric heat generation in the solid.

\[
S_{\theta_s} = \left( \frac{q''_{\text{max}} D^2}{k_s \Delta T_{\text{ref}}} \right)
\]

where, \(q''_{\text{max}} = \) maximum rate of heat generation (\(W m^{-3}\)), \(k_s = \) thermal conductivity of solid.

2.2. Boundary Conditions. The detailed analysis of molten LBE flow in the laminar and turbulent regimes are considered. The boundary conditions of interest are:

- Inlet Section: \(u = 0, v = v(x); \quad \theta = 0; k_n = 1.5 \ I^2; \)
  \[
  \epsilon_n(x) = \frac{(k_n^2 C_8^2)}{\chi} \quad \text{for} \quad \frac{x}{(\lambda/\chi)}
  = \frac{(k_n^2 C_8^2)}{\lambda x_p} \quad \text{for} \quad \frac{x}{(\lambda/\chi)} \]
  where \(I\) is the turbulent intensity, \(\chi = 0.42\), which is known as the Von
Karman constant, $\lambda$ is a constant prescribing the ramp distribution of the mixing length in boundary layers and is equal to 0.09, $E = 9.743$ and $p$ refers to the first grid point adjacent to the wall.

- Symmetry Boundary $u = 0, \frac{\partial f}{\partial n} = 0; f = (v, \theta, k_n, \epsilon_n)$
- Outlet Section $\frac{\partial f}{\partial n} = 0; f = (u, v, \theta, k_n, \epsilon_n)$
- Along the beam window:
  \[ \theta = 1.0 \text{ (Isothermal condition) or } \theta = \frac{(S_m - S_i)^2}{S_m^2} \text{ (Variable temperature)} \]
  Where, $S$ - Streamwise distance along the window, $S_i$ = Local non-dimensional arc length from the leading edge of the window and $S_m$ = Non-dimensional total arc length of the beam window.
- For other walls: $\frac{\partial \theta}{\partial n} = 0$ (thermally insulated)

where $n$ represents the normal direction to the surface. For turbulent flows, the standard $k - \epsilon$ turbulence model has been used (Biswas and Eswaran [2]). The standard $k - \epsilon$ relies on the high Reynolds number assumption, is not valid very near the wall where the viscous effects are predominant. Instead of using equations (3) and (4) near the wall, $k_n, \epsilon_n$ at point $p$ are computed from

$$k_{n,p} = \frac{v_{\tau,n}^2}{C_1^2 \mu} ; \epsilon_{n,p} = \frac{v_{\tau,n}^3}{\chi x_p}$$

where $v_{\tau,n}$ is the friction velocity is given as $v_{\tau,n} = C_1^{1/4} k_{n,p}^{1/2}$. The boundary conditions for beam window for computing conjugate heat transfer are imposed as follows:

a. Adiabatic wall: $\frac{\partial \theta_s}{\partial n} = 0$;

b. Temperature specified:

\[ \theta_s = 1.0 \text{ (Isothermal condition) or } \theta_s = \frac{(S_m - S_i)^2}{S_m^2} \text{ (Variable temperature)} \]

c. Fluid-Solid interface

\[ \frac{\partial \theta}{\partial n} = \frac{k_s}{k_f} \frac{\partial \theta_s}{\partial n} \text{ (For Energy equation of the fluid)} \]

$k_s, k_f$ - Thermal conductivities of solid and fluid

\[ \theta_s = \theta \text{ (For heat conduction of the solid equation at the interface)} \]

\[ \theta_s, \theta - \text{Dimensionless temperature of solid and fluid domain} \]

3. Grid Generation, Solution Technique and Code Validation

The computational grid of the target system is generated using an algebraic method, smoothed and clustered by the elliptic partial grid generation technique using Poisson’s equations. A SUPG finite element method (Brooks and Hughes, [3]) has been used to discretize and solve the governing conservation equations. The pressure-velocity iterations follow the method due to Harlow and Welch [7]. The entire procedure has been documented in Maji and Biswas [10] and in the recent work of Prakash et al. [11, 12]. As mentioned earlier, the proton beam impinges
the window and a large amount of heat is deposited on it. To incorporate the physical situation in a realistic way a conjugate heat transfer problem is accomplished using the following numerical procedure. The computations are performed in the target module with a funnel shaped flow guide and spherical bottom. The solution procedure for conjugate heat transfer is as follows:

An interfacial heat flux distribution is guessed on the interface of the solid and fluid domain. Initially, the interface wall condition is taken as adiabatic. This yields highest wall temperature at some point in the solid domain. The heat conduction equation is solved to get the temperature distribution in the solid domain. This is used as an input to the solution of energy equation for the fluid. The energy equation for the fluid domain is solved with the boundary conditions provided in the previous step. This yields a non-zero heat flux distribution at the interface to be used as the input for the heat conduction equation. The heat conduction equation is solved in the solid domain and the heat flux is calculated at the interface. Thus the heat flux distribution calculated in the previous steps is compared and the procedure is repeated if the distributions do not satisfy the preset criteria till the convergence is achieved.

3.1. Parallelization of energy equation solver by domain decomposition method. The conjugate heat transfer problem takes enormous time (approximately 432000 seconds CPU time) for one complete set of calculations. As the computation is found to be very demanding, the energy equation module is parallelized following the paradigm of domain decomposition method using MPI (Message Passing Interface) Library. Under this method the domain under consideration has been discretized into overlapping domains. The overlap is limited to single layer of elements on either sides of the sub-domains. This one layer overlap at either of the boundaries of the subdomains facilitate the full assembly of the neighbourhood contribution at the boundary nodes of the subdomain. This avoids communications within a time step. The overlapping layers of elements referred as ghost elements and the corresponding overlapping nodes are called as ghost nodes. The ghost nodal variable values are updated at the end of every time step following an even-odd processor number communication strategy. The even odd communication strategy (see Figure 2) may be described as follows:

Initially all the even processors send the data corresponding to the side $S_3$ of its sub-domain. The odd processors corresponding to the side $S_1$ receive the data and pass it on the ghost layers. Then the odd processors send the data corresponding to the side $S_1$ of its sub-domain. The even processors corresponding to the side $S_3$ receive the data and pass it on the ghost layers. The communication continues with the side $S_1$ of the even processors sending the data and the side $S_3$ of the odd processors receiving the data for ghost layer update. Finally, the side $S_1$ of the even processors receives the data and the side $S_3$ of the odd processors sends the data. In order to validate our in-house SUPG-FE code, it was tested on many benchmark problems which has been presented in prakash et al [11, 12]. A grid sensitivity analysis study was performed and in the present study a grid consisting of $(51 \times 307)$ nodes was chosen for all computations.

4. Results and Discussions

Figure 3 (i) show streamlines pattern for the flow field obtained with $Re = 500$, 700 and 1000. At $Re = 500$, a primary vortex is observed near the inlet section along the guide due to sudden expansion of the flow domain. In addition, there
are recirculation regions near the 180° turn and also near the exit along both the beam window and the flow guide. Secondary recirculation zones are observed in the stagnation region at the bottom of the downcomer section of the target system along the axis of symmetry and along the solid wall prior to the first change of curvature in the geometry of the target system. At $Re = 700$ and $1000$, although the primary vortex bulges, the reattachment length decreases owing to the increasing velocity field. The pressure developed at the inner edge of the bend of the separating wall will decrease with increasing Reynolds number, which will influence the reattachment length. Also, with increasing velocity, while the secondary recirculation zone in the stagnation region becomes prominent, the secondary recirculation zone, along the solid wall, becomes shorter and drifts upstream. Figure 3 (ii) depicts the streamlines for three higher Reynolds numbers (turbulent regime): (a) $Re = 141340$ (b) $Re = 282000$ and (c) $Re = 565380$. Streamline plots show that there is a flow separation and reattachment near the convex bend along the flow guide downstream to the stagnation zone and the size of the separated eddy increases with the increase in Reynolds number. Near the beam window, the fluid experiences convex flow followed by concave flow, whereas the opposite occurs for flow along the guide near the exit plane. It has been observed for flows with curvature that the quantity, $u'v'$ first increases and then decreases in magnitude on the beam window, whereas the opposite occurs on the flow guide near the exit plane. Therefore, in the case of turbulent flows, the enhanced transverse momentum transport occurs towards the curved section of the beam window and the separation is delayed; in fact, it is prevented owing to the presence of fluid particles with higher kinetic energy. Separated flows are observed in the convex zone of the flow guide. Clearly, three Reynolds numbers give good qualitative consistency and the vortex formation appears to be well reproduced. Figure 4 (i) show the temperature contours of the fluid and solid domain with variable temperature window boundary which is computed sequentially and parallely. It is observed that the sequential and parallel results match exactly. The speed up of the computation is shown in Figure 4 (ii). The speed up is defined as the ratio of sequential computation to parallel computation. A reasonable speed up of is achieved for this case due to the reason that only the energy equation module is parallelized whereas the solid conduction.
(b) STREAMLINES FOR \( Re = 500 \), (b) \( Re = 700 \) AND (c) \( Re = 1000 \) (ii) STREAMLINES FOR (a) \( Re = 1.4 \times 10^5 \), (b) \( Re = 2.8 \times 10^5 \) AND (c) \( Re = 5.6 \times 10^5 \)

equation is computed sequentially. The conjugate heat transfer analysis is thus

\[
\begin{array}{cccccccccccc}
0.929286 & 0.858571 & 0.787857 & 0.717143 & 0.646429 & 0.575714 & 0.505000 & 0.434286 & 0.363571 & 0.292857 & 0.222143 & 0.151429 & 0.080714 & 0.010000
\end{array}
\]

(i) TEMPERATURE CONTOURS WITH VARIABLE TEMPERATURE WINDOW BOUNDARY (ENLARGED VIEW OF THE WINDOW SECTION) FOR \( Re = 1000 \) (A) SEQUENTIAL COMPUTATION (B) PARALLEL COMPUTATION

(ii) SPEED UP OF THE PARALLELIZATION

carried out for different thickness of the beam window with variable temperature and also for different Reynolds numbers on parallel computers with 16 nodes. Here we presented the case of beam window with 3mm thickness.

Figures 5 (i) and 5 (ii) show the temperature distribution on the solid and fluid domains for the low Reynolds numbers and the high Reynolds numbers respectively. The window thickness in this study is 3 mm. It is seen that the thermal boundary layer manifested along the beam window gets decreased with the increase in the Reynolds number. The interface temperature along the beam window (thickness 3 mm) for different Reynolds numbers in the laminar regime is shown in Figure 6
There is a marginal difference in the interface temperature as the convection effect on the window surface is not pronounced. The Nusselt number distribution is shown in Figure 6 (ii). The peak value of the Nusselt number lies immediate downstream of the stagnation zone and the Nusselt number increases with increasing Reynolds number. The interface temperature for the turbulent flow is shown in Figure 7 (i). There is a considerable difference in temperature along the window curvature but at the stagnation zone, and near the exit plane, the temperature distribution remains unchanged. The window temperature decreases with increasing Reynolds number. Nusselt number distribution plot [see Figure 7 (ii)] shows that for the turbulent flows, the convection effects come into play along the window curvature entailing higher heat transfer.

5. Conclusion

A computational study using SUPG-Finite Element Method has been accomplished to determine the laminar and turbulent flow characteristics and heat transfer in the spallation region of ADS geometry. In the laminar case of the ADS geometry, vortices are generated at the concave curvature of the outer wall. It has also been observed that another vortex is generated at the convex surface of the inner wall (window) downstream of the bend for the higher Reynolds numbers. The
size of the vortices grow with the increase in the Reynolds number. The computation is extended for the turbulent flows where the vortex is observed only on the concave downstream of the outer wall. Finally, the conjugate heat transfer analysis on the beam window and the flow domain is accomplished by parallelizing the energy equation solver using domain decomposition method. The analysis is carried out for different thicknesses of the beam window and different Reynolds numbers. The Nusselt number and temperature distribution at the interface is found; the maxima are located along the stagnation zone. These temperature distribution value in the beam window is used to determine the thermal stresses which is useful for its mechanical design.

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References


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