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APPLICABILITY OF THREE-DIMENSIONAL CFD SIMULATION OF THE SPALLATION NEUTRON SOURCE MERCURY TARGET

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ABSTRACT

Computational fluid dynamics (CFD) is being used to predict the thermal-hydraulic performance of the liquid mercury target for the Spallation Neutron Source (SNS). Features in the liquid mercury flow through the target present problems to the credibility of the simulated results because the turbulence models and wall functions have not been validated for these flow conditions. Discussion is presented in this paper of the plan for establishing the relevance of the CFD simulations to the SNS target. Some of the tasks proposed as a part of this plan have been completed, some (such as the three experimental loops) are currently underway, and some have yet to be performed.

The SNS is a high-power accelerator-based pulsed spallation source being designed by a multi laboratory team led by Oak Ridge National Laboratory (ORNL) to achieve high fluxes of neutrons for scientific experiments. In addition to thermal shock and materials compatibility, the thermal-hydraulic performance of the target is an important issue in prolonging the life of the target.

The mercury flows through a stainless steel target vessel at a rate of 23 L/s. Temperatures calculated in the steel and mercury are subsequently used in predicting thermal stresses. The target is subjected to the radiative (internal) heat generation that results from the proton collisions with the mercury nuclei. The liquid mercury simultaneously serves as the neutronic target medium, transports away the heat generated within itself, and cools the metallic target structure.

The target design includes a complete U-turn flow redirection which leads to flow separation, high streamline curvature, and strongly adverse pressure gradients. These aspects of the flow present uncertainty in the application of turbulence models and wall functions typically used in CFD. To build confidence in the analyses, three experiments are currently underway which will provide validation data for various aspects of the CFD model.

INTRODUCTION

The Spallation Neutron Source (SNS) is a high-power accelerator-based pulsed spallation source being designed by a multi-laboratory team led by Oak Ridge National Laboratory (ORNL) to achieve high fluxes of neutrons for scientific experiments (Siman-Tov et al., 1997). The SNS will utilize a 2-MW proton beam (60% of which will be deposited as heat in the target) with a beam cross-section of 7 × 20 cm. The proton beam consists of 0.5 μs pulses that are repeated at 60 Hz. The target, which has dimensions of 65 × 40 × 10 cm (about 20 L), consists of liquid mercury flowing through a stainless steel target vessel (Fig. 1). The distribution of the power deposited within the mercury and stainless steel has been calculated using Monte Carlo methods and a Green's function extrapolation technique. The nominal peak current density is 0.25 amp/m^2, and the peak heat deposition is 800 W/m^3.

The liquid mercury serves both as the neutronic target medium and as the working fluid that removes the heat generated within itself and cools the metallic target structure. If the mercury cooling is insufficient, the stainless steel will overheat and lose strength, or will possibly fracture due to thermal stresses induced by high thermal gradients. The proton beam is parallel to the primary direction of flow. The beam first passes through the stainless steel

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window on the front of the target which is provided with supplemental exterior cooling by a wide, shallow window coolant channel that wraps around the target window lengthwise. Figure 2 (with one-half of the target structure removed) shows that the window coolant channel constricts and then expands to provide maximum cooling at the beam centerline. The transverse extent of the window coolant channel is limited to the width necessary to contain the proton beam path. The window coolant flows along the bottom of the target, cools the window, and then returns along the top before merging with the main mercury flow in the return channel.

For the past three years, computational fluid dynamics (CFD) has been used to assist in the R&D and the design of the SNS target by predicting pressures, velocities, turbulence quantities, temperatures and thermal gradients in the liquid mercury and stainless steel target structure. These numerical simulations have been both two- and three-dimensional (2D and 3D).

The CFD simulations have all utilized numerical turbulence models, usually assuming an eddy viscosity related to turbulent kinetic energy that is solved for the computational domain. Although turbulence models are commonly applied (often with good success) to engineering problems such as the forced convective cooling of the SNS target, certain aspects of the SNS target flow differ significantly from the empirical conditions that were used to develop these models. The inlet flows to the target separate from the wall as they turn around the flow baffle and thus generate highly turbulent, large recirculation zones in the return channel. Also, near the window, there is a stagnation point with associated adverse pressure gradient that occurs due to the symmetric target design. These complications of high streamline curvature, flow separation and adverse pressure gradients raise concern over the applicability of the turbulence model.

In most of the simulations, a steady-state condition has been assumed with the proton pulse energy averaged over time. However, it is expected that the flow will be significantly perturbed (for at least some small amount of time) by the sudden impact of each proton pulse which will create ~30 MPa pressure waves in the mercury due to thermal expansion of the liquid. The impact of these severe pressure waves on the target structure is being assessed separately using both experimental and analytical methods (Riemer et al., 1999 and Taleyarkhan et al., 1999).

Three experiments, funded by the SNS project and are presently underway, will be used to reduce uncertainty in the current predictions for target thermal performance. Using the measured quantities from these three experiments (none of which include all of the physics that define the normal operating state of the target), confidence in the SNS CFD model to accurately predict normal operating temperatures and temperature gradients can be increased.

DESCRIPTION OF THE MODEL

The general-purpose CFD code CFX4.2,[1] which uses a finite-volume, pressure-correction method, is being used to predict the temperature and velocity distribution in the liquid mercury target.

In addition to the mercury flow regions, the model includes solid conducting regions that represent the stainless steel target walls and internal baffle. Beam heat deposition is included for both the mercury and stainless steel, with a total target heat loading of 1.2 MW, corresponding to the 2-MW proton beam. The heat generation distribution provided to the model is based on an efficient Green's function technique that is used to extrapolate more complex Monte Carlo radiation transport simulation results.

The baseline CFD model for the SNS target uses a renormalization-group isotropic, two-equation turbulence model in combination with the standard law-of-the-wall boundary condition (wall function) for imposing wall heat flux in the energy equation and shear stress in the momentum equations. The boundary conditions include no-slip at the walls, specified inlet velocity at the inlets to the window coolant flow region and main flow region, and specified pressure on the outlet boundaries. The density is normally assumed to be constant, but the viscosity and thermal conductivity are allowed to vary with temperature. The temperature variation of the viscosity was included primarily for its impact on results in the near-wall region (outside the boundary layer, the eddy viscosity dominates).

The discretization used for the full target design includes up to 3 million computational cells which leads to long simulation times of up to 2–4 weeks of CPU time on the 500 MHz Dec ALPHA Personal Workstation to become well converged. A hybrid differencing scheme (first-order accurate) and the algebraic multigrid (AMG) linear solver were used to produce results where the cumulative mass conservation error was less than 1%.

KEY RESULTS

Although a comprehensive experimental program is underway to demonstrate the thermal-hydraulic feasibility of the SNS target to perform for a several-week lifetime, there will be no prototypical target experiments with mercury heated at the 2 MW beam power level. The intent is to use these separate effects experiments to validate the applicability of the CFD model and then to rely on the CFD results for quantifying the margins to the thermal limits.

The purpose of the CFD is to predict (in order of anticipated importance) the *temperatures, temperature gradients, flow patterns, flow stability, pressures, and pressure drops,*

[1] CFX is developed by AEA Technology whose U. S. offices are located in Bethel Park, PA.

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associated with the flow of liquid mercury through the main target body and piping pieces that connect the target to the hot and cold leg headers.

The temperatures are important because if they get too high, the stainless steel strength could be significantly reduced. The temperature gradients produce thermal stresses in the stainless steel target structure. These thermal stresses are included in a comprehensive finite-element structural model for the target. An R&D effort is underway to determine the strength of the stainless steel target material subjected to radiation and in contact with liquid mercury.

The overall flow pattern is important for general knowledge of the facility. It may be important in certain accident scenarios or in future modifications to the target, such as the implantation of monitoring devices or experiments.

Flow stability is a concern since it relates to dynamic loading of the target and possible asymmetry in target loads and temperatures. The flow through the target has two separate inlets that resemble impinging jets at the front center of the target. Within the single return channel for the flow, some degree of asymmetry is expected.

The local pressure is important in considering the possibility of cavitation, and overall pressure drop dictates required pumping power.

Computed results for the target bulk flow show two large recirculation zones downstream of the flow baffles around which the liquid mercury makes the U-turn (Fig. 3). These large zones are of different sizes and together obstruct about one-half of the cross-sectional area in the central rectangular return channel. Two smaller stagnation zones are also predicted in the corners of the target volumes. Temperatures and temperature gradients are highest in two regions: (1) near the front of the target on the centerline where a stagnation point occurs and the heat generation is the highest, and (2) behind the flow baffles in the recirculation zones where the fluid residence time is long and velocities are low.

IMPORTANT FLOW FEATURES

It is important to consider how appropriate the sub-models used in the CFD code are for use in predicting the thermal hydraulic performance of the SNS liquid mercury target.

Most of the heat is generated in the bulk mercury flowing through the target and is quickly transported out of the main target body. However, there are two problem areas in the bulk flow region that involve heat transfer between the mercury and the stainless steel target vessel: (1) the recirculation zone located behind the flow baffles in the return channel, and (2) the front window zone located at the front of the target near the centerline. The use of the sub-models to predict flows in these regions must be carefully considered to assess the accuracy of the CFD results.

Recirculation Zone

The inlet flow streams separate from the flow baffles as they make the U-turn, leaving two large zones of recirculating flow in the path of the beam. Although the turbulence intensity is very high in these zones (the model predictions indicate eddy viscosities as high as 30,000 times the molecular viscosity), the residence time of the mercury is also higher thus allowing more time for the temperature to elevate.

Higher mercury temperatures present a problem primarily to the extent that they lead to higher steel temperatures in the surrounding target vessel. In Fig. 4, a cross-section through the baffle is shown that illustrates the target structure that surrounds the recirculation zone. The target structure is cooled both above and below by the window coolant passages. The baffle is cooled on the back side by the inlet flow. Despite the forced cooling of the structure on these top, bottom and back surfaces, it is possible that the temperatures and/or temperature gradients developed in the stainless steel will exceed acceptable values based on material strength considerations.

The flow pattern in this region of separated multidimensional flow is quite different from the flow conditions for which the law-of-the-wall formulation was developed. However, it has been shown (Heyerichs and Pollard, 1996) that the wall function approach leads to under prediction of the wall heat transfer in the recirculation zone behind a backward facing step, which is similar to the flow pattern behind the baffle.

Due to the additional mesh refinement required to resolve the viscous sublayer, the use of low-Reynolds number turbulence models which do not use wall functions is not considered feasible at this stage of the analysis. Instead of having to rely upon the CFD result obtained with the wall function, three other options are available to address this problem:

(1) Use a conservative assumption that forces a large amount of heat through the wall. For instance, if half of the heat deposited in the recirculation zone were forced to pass through the flow baffle, a bounding estimate for the peak temperature and thermal gradient could be made (apart from any CFD).

(2) Gather experimental data that will validate the CFD, either by measuring near wall profiles, or by measuring local wall heat flux in the recirculation zone. The WTHL and TTF facilities could be used to acquire these measurements.

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(3) Design around the problem to alleviate the recirculation zone. Some design modifications that could be made include putting holes (or slots) in the baffle or top/bottom walls that would break up the recirculation zone, placing a curved flow vane at the leading edge of the baffle to smooth the flow, or putting some extra flow resistance towards the center of the return channel that might force more flow near the wall.

Front Window Zone

The highest heat loads are on the target centerline at the front, near the window where the proton beam impinges onto the target. The beam first passes through the outer window wall. The outer boundary of this wall is exposed to a 1 atmosphere helium environment with possible radiation to or from the surrounding water shroud. The outer boundary is assumed to be adiabatic, so the peak temperatures in the outer window wall will be located on the outside surface and all of its heat must be removed by the window coolant.

The beam then passes through the mercury window coolant which is flowing in an annulus and into the inner window wall before reaching the mercury bulk flow. The window coolant keeps the structure cool in this region of high volumetric heat deposition, and since the geometry is a narrow annulus (with moderate curvature) the CFD (RANS turbulence models with wall functions) is expected to do very well at predicting temperatures and heat fluxes on the surfaces in contact with this flow.

The inner wall is more complicated. Heat is removed on one side by the window coolant flow, but the other side contacts the bulk flow in a region where a stagnation point will occur.

Because of the strongly adverse pressure gradient and high stream line curvature, the law-of-the-wall assumption is again questionable. However, Heyerichs and Pollard (1996) have shown that for a jet impinging on a wall, using the law-of-the-wall assumption leads to under-predicting the heat transfer by 30% in the stagnation region of their test case. Using this information, a bounding case can be defined that will not be overly conservative.

It is likely that the peak volumetric heat deposition is located in the bulk flow, therefore the possibility exists that the bulk mercury temperature may be higher than the inner window wall temperature, and the bulk mercury may actually heat the wall from the inside. If this is the case, a bounding assumption can be used where the wall heat transfer is enhanced based on the findings of Heyerichs and Pollard (1996).

However, if it is determined that this is not the case and that the heat flows from the stainless steel into the bulk mercury, then a conservative assumption can be made that no heat crosses this boundary and the inner wall temperature will be over predicted.

In any event, wall heat transfer measurements could be conducted in the TTF facility to gain confidence in the CFD.

VERIFICATION OF THE MODEL

Verification is assessing how well the governing equations (which reflect the modeling assumptions) are being solved. Numerical errors and machine-dependent problems can lead to incorrect solutions to the Reynolds-averaged Navier Stokes conservation law system.

As described by Roache, 1998, the sensitivity of the CFD solution to the specified numerical grid is the most convenient measure of how well the governing equations are being solved. A method based on Richardson extrapolation using two solutions based on two different grids is proposed by Roache. It is this method that is being used to assess the SNS CFD baseline solution. Multiple levels of grid refinement will be used to quantify the uncertainty in the solution of the equations for the SNS target model.

Verification will be partially accomplished through a benchmarking procedure. In cooperation with the Japan Atomic Energy Research Institute (JAERI), which is planning its own accelerator using a liquid mercury target, four benchmark problems have been proposed using two different analytical tools.

The purpose of the benchmarking effort is to verify that the most appropriate CFD modeling assumptions are being made in the analyses as well as to verify that the numerical solutions to the RANS conservation law system obtained by each CFD code are consistent. Four test problems were selected because they are relevant to the turbulent forced convection with separated flow and high streamline curvature that is characteristic of the liquid mercury flows in spallation targets.

The first benchmark problem is straight tube flow, with heat transfer to an isothermal wall. The SNS solution to this problem and comparison to data is presented in this paper in the next section. Comparisons will be made with the JAERI solution to the same problem. The second problem will involve a duct with ribs attached on the sides to enhance turbulence. The third and fourth problems will be two-dimensional solutions of flow through the respective target designs (SNS and JAERI).

VALIDATION OF THE MODEL

Validation of the model should answer the question of whether adequate physical models are being used to render the computed results relevant to the problem of interest. For the SNS target flow, the wall heat transfer and shear stress boundary conditions are

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important to the key results of this forced convection problem; however, with the internal heat generation and complex flow field, turbulent mixing in the region away from the wall is also very important.

The turbulent mixing predicted by the model rests upon the turbulence model. In this case all of the available models are Reynolds-Averaged Navier Stokes (RANS) models, most of which utilize the eddy viscosity hypothesis and the Reynolds analogy for diffusion of heat. An important assumption in applying these models is the turbulent Prandtl number (Pr_t). Since liquid mercury has such a low molecular Prandtl number, Pr_t is somewhat higher than unity (White, 1974).

Tube Flow

The near wall region predictions depend upon the applicability of the law-of-the-wall logarithmic profile assumption. It is known that for regions where adverse pressure gradients, curved walls and separated flows exist the applicability of the wall law is questionable. However, the capability of the computational tool to predict forced convection liquid metal heat transfer even for simple geometries must be confirmed as a baseline. For this reason, the simple geometry case of flow in a tube is examined.

Experimental data and theoretical correlations are available (Lubarsky and Kaufman, 1995) for turbulent, forced-convection heat transfer for liquid metal flowing in a tube. A CFX4 model was assembled for a circular pipe with a diameter of 0.01 m and a length of 0.50 m. The computed Nusselt numbers were compared with the experimental and theoretical results. Figure 5 shows the comparison over a range of Peclet numbers. The computed results match the Lyon-Martinelli theoretical correlation (Lyon, 1949) to within 10% when Pr_t is assumed to be 1.0. When the recommended Pr_t given by White (1974) is applied to the tube flow, the Nusselt numbers settle nicely into the scatter of measured data.

MTHL

The Mercury Thermal Hydraulic Loop (MTHL) will provide heat transfer characteristics of the liquid mercury/stainless steel system in a geometry representative of the window coolant channel. Straight channel measurements are currently being taken for both cooled and heated test sections. Also, a curved test section will be used to quantify the effects of curvature on the mercury heat transfer.

Temperature measurements on the outside wall of the test section will provide the information necessary to calculate wall heat flux from the steel to the mercury and then correlate these data with channel Reynolds number. For validation, simulations will be performed with CFX for the same geometry using various turbulent Prandtl numbers and turbulence models.

WTHL

The Water Thermal Hydraulic Loop (WTHL) is a full-scale water loop for testing of the target module only. This loop is being used for flow visualization and laser-Doppler velocimetry (LDV), providing details of velocity and turbulence quantities.

The transparent plastic test section has the same geometry as the SNS target with the window coolant channel removed. The following measurements are being obtained for the expressed purpose of code validation: overall flow visualization using dye and bubble injection, pressure distribution, velocity distribution, and Reynold's stress distribution (related to turbulent kinetic energy).

TTF

The Target Test Facility (TTF) is a full-scale mockup of the entire SNS mercury loop which will not be heated, but will provide a venue to directly measure mercury target velocities and possibly turbulence quantities at nominal conditions. The main target flow and window coolant flows will both be represented, but they will be separated for convenience in taking measurements. An ultrasonic velocity profilometer will be used to obtain the velocity profiles. Also, by measuring the flow in each of the inlet lines, the flow stability of the target can be characterized.

CONCLUSIONS

CFD has been used extensively to investigate the thermal-hydraulic performance of the SNS liquid mercury target design. Two flow features, important to the key results, have been identified for which the application of the RANS turbulence model and wall law assumption are suspect. Results indicate very large regions of highly turbulent recirculation downstream of the flow-baffle separator plate and a stagnation region near the front of the target where heat loads are very high. These flow patterns present a challenge to the reliability of the results because they differ from the conditions under which the empirical turbulence models and wall functions were developed.

Verification of the model is being performed using grid sensitivity studies and Richardson extrapolation. Also an independent calculation performed in Japan using another CFD code will be used to verify the 2D results.

The SNS project is using the following activities to quantify the uncertainty in CFD predictions and to build confidence in the ability to predict the margins to the thermal limits: (1) comparison with published data, (2) validation experiments that are currently underway at the Oak Ridge National Laboratory, and (3) design changes to alleviate potential problems.

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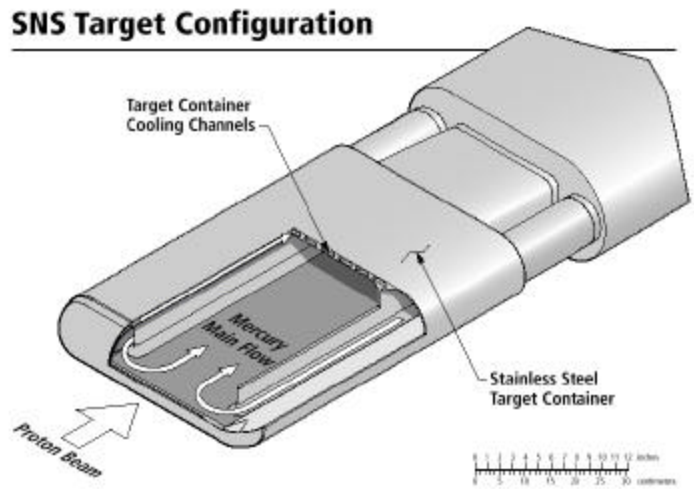

Fig. 1. Design schematic showing the SNS stainless steel target enclosure to be used for liquid mercury containment.

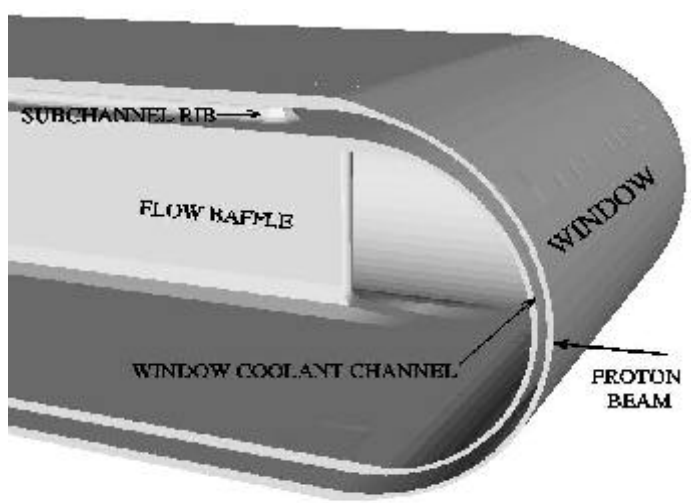

Fig. 2. Stainless steel target structure model geometry.

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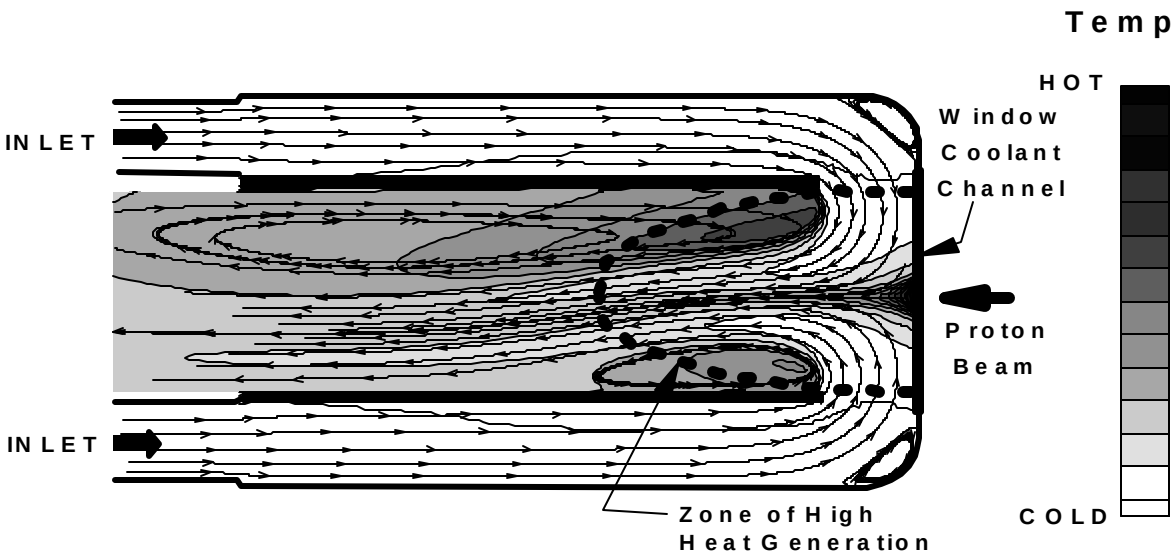

Fig. 3. Typical CFD results showing recirculation zones and hot spots.

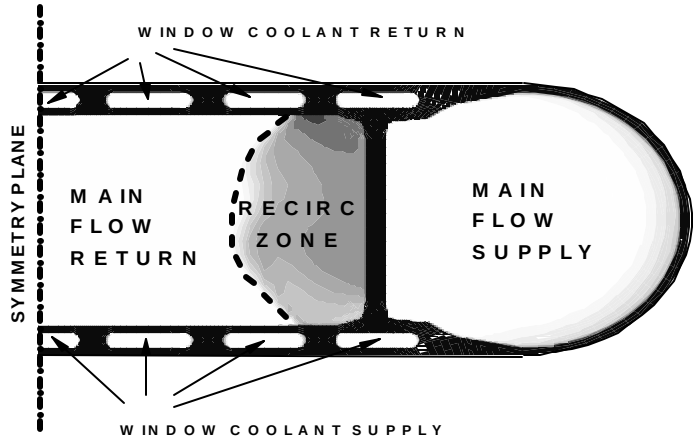

Fig. 4. Cross-section through target structure showing window coolant channels, flow baffle, and recirculation zone.

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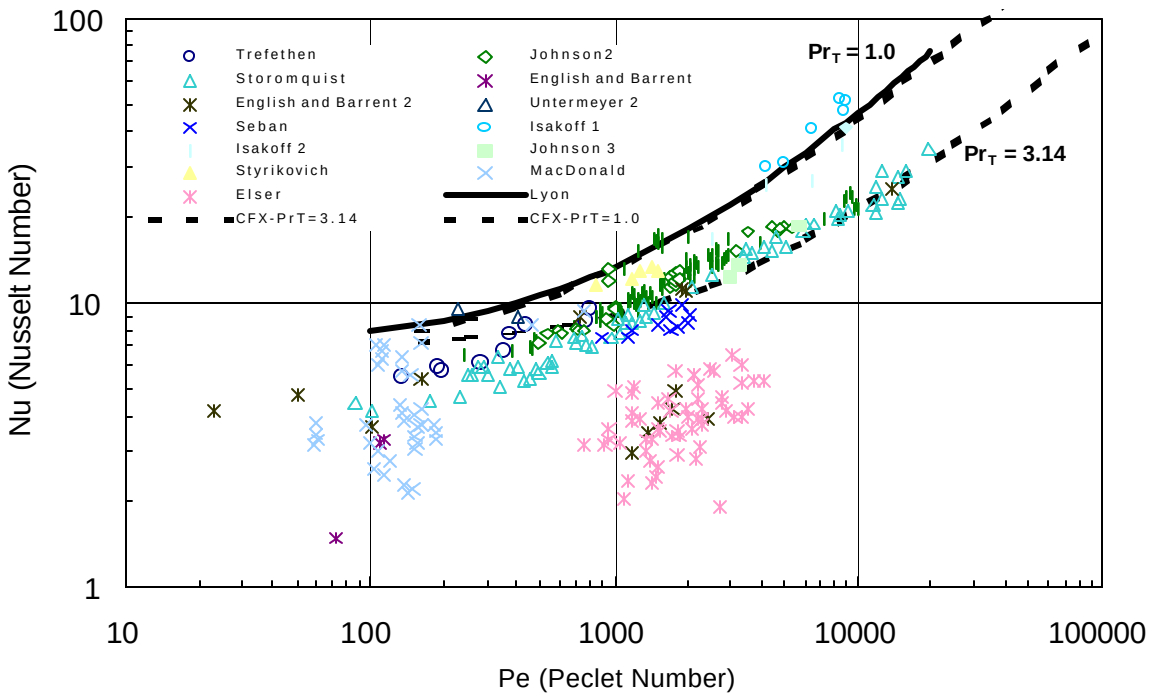

Fig. 5. Comparison of CFX4 forced convection predictions with published data for liquid metals. Data has been digitized from plot published in Kreith (1973).

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