

TURBULENCE MODELING ISSUES IN ADS THERMAL AND HYDRAULIC ANALYSES

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ABSTRACT

Accelerator Driven nuclear reactor Systems (ADS) have in several respects a prototypical character of the flow and cooling conditions combined with narrow operating conditions due to the materials engaged. E.g. the high local thermal load in the liquid metal cooled spallation target requires a very careful analysis by experimental and numerical means. Some of the main goals of the numerical analyses of the thermal dynamics of those systems and of required experiments are discussed. The prediction of locally detached and recirculating flows suffers from insufficient turbulence modeling; this has to be compensated by using prototypical model experiments, e.g. with water, to select the adequate models and numerical schemes. Some sensitivities and model uncertainties are discussed; some of them are reduced by so-called layered models like in the SST turbulence model or the DES. The well known problems with the Reynolds analogy in predicting the heat transfer in liquid metals requires prototypic liquid metal experiments to select and adapt the turbulent heat flux models. The uncertainties in liquid metal experiments cannot be neglected; so it is necessary to perform CFD calculations and experiments always hand in hand and to develop improved turbulent heat flux models. One contribution to an improved 3 or 4-equation model is deduced from recent Direct Numerical Simulation data. Of course, the ADS community would need such extended heat flux models, but even realizing standard 3- or 4-equation ASM heat flux models in the commercial CFD codes would allow for an improved heat transfer modeling, especially when buoyancy is involved.

1. INTRODUCTION

Transmutation is considered a promising technology for significantly reducing the amount of highly radioactive waste. One of the designs of a transmutation reactor is the Accelerator Driven System, ADS, in which a spallation target and an accelerator are used to produce the missing neutrons for the weakly sub-critical reactor, called blanket, by a proton beam [1]. The protons are injected into the spallation target through a vacuum beam pipe which is closed at the end by a beam window, Fig. 1.

The issues in designing and analyzing local details in such a liquid metal cooled nuclear reactor are manifold: One needs detailed methods to describe the momentum and heat transfer to get the local maximum temperature e.g. in simple channels like in the piping system or annular channels, including forced, mixed, and buoyant convection. More complicated channel geometries need to be treated in the fuel elements with the axial flow between the fuel pin bundles and with the cross flow through the heat exchanger bundles. The detailed analysis of the locally time-dependent flow through the thermally stratified large pool areas gains increasing interest because of the thermal striping phenomenon which causes thermal fatigue in the structures; similarly it may be expected that the instantaneous pressure fluctuations in the heavy fluid could also lead to some mechanical problems. Similar problems have also to be investigated in T-junctions of the piping system. And the heat transfer by purely buoyant convection within the complete reactor system has to be considered for some decay heat removal situations, or in some reactor concepts even for operating conditions.

Some of these thermal and hydraulic issues are obvious from considering the target. The proton beam will have some MWs which are deposited in a fluid volume of a few liters only. Thus, there are high thermal loads in such liquid metal cooled targets and the type of flow and cooling conditions are quite prototypical. In addition the technological challenges in working with Pb-Bi as spallation fluid needs a

lot of development and testing to allow for the design of a target which can safely and reliably be operated. This requires a careful analysis by experimental and numerical means.

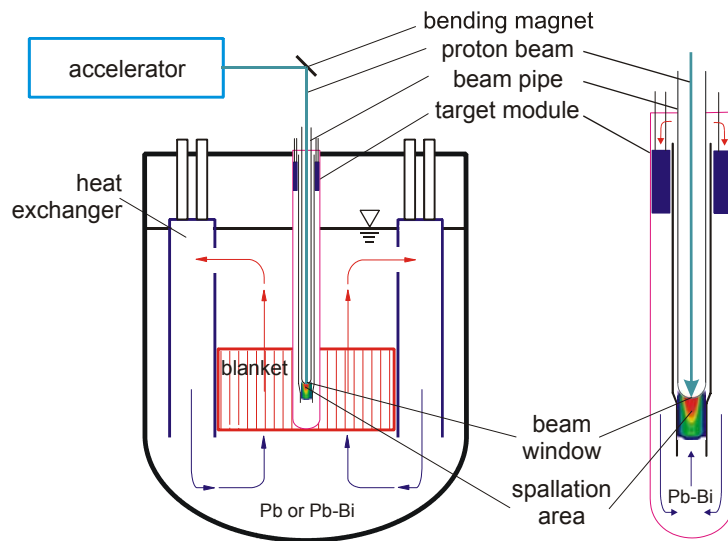


FIG. 1. Flow paths through the components of an ADS.

The steps which are in principle chosen by the international ADS research partners to develop an ADS target are explained in [2]: Loops are developed operating with Pb-Bi for the development of the special liquid metal cooling technology, e.g. [3], and the related measurement techniques, e.g. [4], to investigate the chemical interactions of the materials and develop new materials, e.g. [5], to determine in single effect experiments the most important data for improvement of the required turbulent heat transfer models, e.g. [6], and to analyze in larger loops complete target components or modules to demonstrate and validate the proper design [7,8]. Supplemental water experiments are performed where more information is required on the velocity field [9,10]. In parallel the Computational Fluid Dynamics tools (CFD), which are required for detailed heat transfer analyses [11,12,13,14] are investigated regarding their suitability for adequate predictions [15,16], and model developments are ongoing basing on turbulence data from Direct Numerical Simulations (DNS) e.g. in [17].

All these results are coming together in a project in which a model target, MEGAPIE, is developed and built [18]. It will be operated and irradiated at PSI in Switzerland at the SINQ accelerator, and will also be dismantled and decommissioned at the end. This model target has all prototypical features of a ADS target as shown in Fig. 1, except that the fluid and vacuum side of the target are exchanged, Fig. 2. Finally all the experimental and numerical data are used to investigate the heat transfer in an ADS reactor mainly by system codes and by CFD tools. Due to this key role of CFD in scaling up the results from model investigations to reactor applications and due to the narrow window of operating conditions for the allowed velocities and temperatures, a high accuracy and reliability of the CFD codes is required in nuclear reactor hydraulic and thermal analysis.

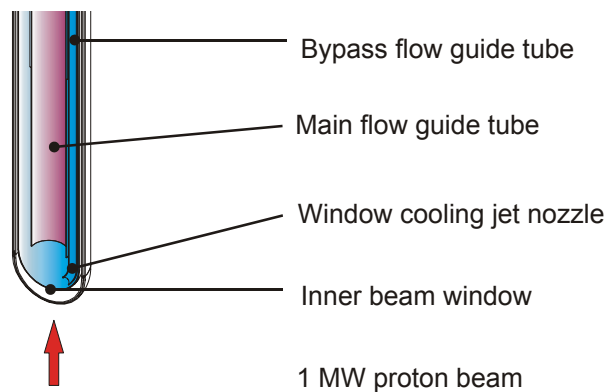


FIG. 2. Window and spallation zone in the MEGAPIE target.

The objectives of this contribution are to extend the discussion of the development procedure of a target in [2] to the modeling issues in the ADS development. The discussed special problems in the current CFD tools are related to the velocity field calculation, like (a) the not sufficiently accurate numerical predictions of a detached flow as it may occur in an ADS target, or (b) the strong deviations in stagnation point flow calculations for the target window for which water experiments are ongoing to select the adequate turbulence models. In a short chapter (c) the status of CFD regarding axial bundle flow predictions is discussed. The problems in calculating the temperature field are related to (d) that the turbulent heat transfer models basing on Reynolds analogy are not sufficiently accurate for liquid metals, which is demonstrated by two benchmark results; (e) this is found to be a serious problem especially for the large scale mixing by the buoyancy influenced flows in large plena. Finally (f) the ongoing model development activities basing on theoretical methods and DNS data are used to gain more accurate turbulent heat transfer models which avoid the Reynolds analogy.

2. MODELING ISSUES IN FLOW DISTRIBUTION PREDICTIONS

The calculation of the velocity field with sufficient accuracy should not be an ADS-specific problem, because in forced convection only the Reynolds number enters into the similarity analysis of the hydraulic problem. Nevertheless, one should get acquainted with the behavior of the current codes. This is required, because in the last years there was a change in the basic CFD tools used in the nuclear community: Several years ago mostly research codes were used, like AQUA, FLUTAN and TRIO, which were usually adapted in their physical models to the requirements of the nuclear applications and which were tested intensively in related benchmark comparisons. Meanwhile, mainly commercial codes are applied like CFX, FLUENT or Star-CD; those codes are multi-purpose codes which are not adapted to the special requirements of liquid metal heat transfer.

In order to gain experience with these codes and to find their practical limitations in ADS applications, a European Concerted Action was performed for the Assessment of CFD codes for Heavy Liquid Metals (ASCHLIM), in which benchmark calculations were performed and in which so far as possible the results were compared to experimental data [15] to find conclusions for the required model developments. Here we use published results of our FZK contributions to some benchmarks in ASCHLIM, combined with the results of additional investigations of target relevant flows from [2], to extend our conclusions on the required model developments and qualification on the hydraulic side, and on the thermal side in the next chapter, which are required for a successful detailed ADS analysis.

2.1 Detached flow predictions

The modeling issues on the fluid dynamics side of the ADS target development are due to the fact, that the flow geometry, which is optimized for the window cooling, may cause flow separation. This could be expected in the diffuser-type widening of the cross section around the window, see target sketch in Fig. 1. As it is well known that the standard $k-\varepsilon$ turbulence model, which is the basis of most commercial and research codes, has serious problems in predicting the existence and extensions of detached recirculating flow areas [19], the benchmark WP3 was performed within the ASCHLIM project, in which the isothermal flow around an ADS typical target window had to be predicted and compared to data from the COULI water experiments [10]. In the preparation of this benchmark blind predictions for the experiments were performed by some of the partners. The geometry specifications are given in [15,20] in which we presented also details of our blind predictions.

The calculations were performed with the FLUTAN code [21,22] which was developed at FZK. It is a code to simulate single-phase flows with heat transfer of several fluids with small compressibility in complex geometries using structured rectangular grids with additional discretization features like local grid refinement and body fitted grids. Several turbulence models are available in FLUTAN like models based on transport equations for some turbulence quantities. Two cases, one for a small Reynolds number at the inlet, $Re=2 \times 10^4$, and one for a realistically high one, $Re=9 \times 10^5$, were given. The water temperature is 60 °C. Most calculations were performed with the standard $k-\varepsilon$ turbulence model and

with a first order upwind method of the convective terms in the equations for the momentum and turbulence quantities. The system of equations was solved on a structured rectangular grid.

The results for the high Reynolds number case are presented in terms of the calculated modulus of the velocity vector in the plotting plane normalized by the inlet velocity into the funnel, Fig. 3. FLUTAN simulates very low velocity values with a flow detachment at the inner wall downstream of the beam window. Calculations with second order discretisation methods like QUICK and LECUSSO were likewise performed with the same grid. The length of the recirculation zone increases downstream in going from first to second order schemes. However, a qualitative influence from the discretisation method on the occurrence and on the size of the recirculation zone can only be avoided when adequate iteration parameters are used as the higher order schemes need sharper criteria. All results are fully converged calculations and show a flow detachment at the inner wall.

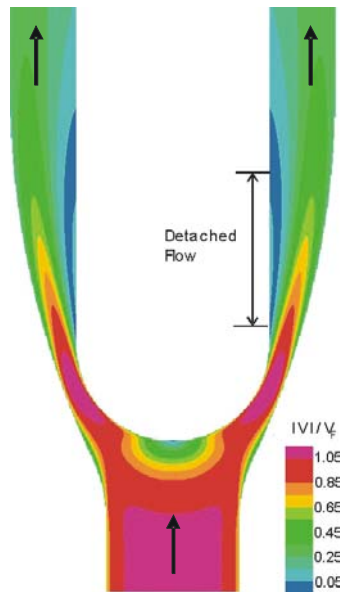


FIG. 3. FLUTAN results for the COULI benchmark: Modulus of the velocity vector normalized by the axial inlet velocity W_{in} , $Re=9 \times 10^5$.

The reliability of this result is doubtful because the standard k- ϵ model uses wall functions to approximate the wall shear stresses, but wall functions are not valid near stagnation points and in the detached flow area. Therefore, turbulence models without wall functions must be used for this case. Calculations for the smaller Reynolds number with a low-Reynolds number k- ϵ model, which contains additional terms in the transport equations for k and ϵ for the near wall area, do not need wall functions, but require fine grids near walls. Such calculations with FLUTAN show velocity fields with a strong reduction of the size of the detached area at the inner wall, but at the same time the area with small velocities increased at the outer wall, so that there may be a tendency to develop also a detached flow at the outer wall. However, this result is not representative for a reliable analysis because the used grid is near the walls too coarse for this kind of turbulence models.

The pre-test results from other codes presented at the first benchmark discussion showed in some cases the detached area not at the inner wall, but at the outer wall. E.g., Star-CD gave with a low-Reynolds number model at the larger Reynolds number the detached area near the outer wall and for the smaller Reynolds number in addition one near the inner wall. Finally, in the experiment a flow separation was found at the outer wall [10]. The pre-test calculations showed that no computer code participating in the COULI benchmark could reliably “predict” the location and the extension of the flow detachment at least with the used models. And even the post-test calculations showed that the physical models have to be carefully selected to gain acceptable results [15]. Therefore, already without heat transport a complex interaction turns out between physical models and code-dependent numerics in the simulation of typical ADS target flows which at the current status of the two-equation

turbulence models always requires accompanying experiments which should provide detailed velocity and turbulence field information for choosing adequate models and for validation.

2.2 Recirculating flow predictions

Extensive recirculation is appearing in the MEGAPIE model target which is developed in an international cooperation and which is now under construction [18]. This model target has all important features of a typical ADS target except the vacuum and spallation sides are exchanged; compare Fig. 1 and Fig. 2. In MEGAPIE the downward flow in the annulus and the upward flow inside the guide tube are combined with a sideward flow across the window to remove the stagnation point from the hottest zone by using a nozzle to produce a jet flow across the beam window. In the conceptual design phase of the MEGAPIE target, several design concepts were proposed for effective cooling of the window and the target itself [13,14]. In the first design configuration there is no bypass injection and the guide tube is cut horizontally. The numerical work by using CFX 4 and CFX 5.5 is focused on this first configuration which also was the topic of the first HYTAS experiment series [9]. The detailed specifications and computational results are summarized in [23].

The flow domain is geometrically axisymmetric. With axisymmetric inlet conditions and boundary conditions, a two-dimensional flow would be expected. Three different kinds of computational configurations are selected, i.e. a 2D axisymmetric one, which is discussed here, a 3D half-scale (180°), and a 3D full-scale (360°) configuration. Five turbulence models are selected to assess their effect on the calculated velocity field, the $k-\epsilon$, RNG $k-\epsilon$, low-Re $k-\epsilon$, $k-\omega$, and the SST model. The SST turbulence model (Shear Stress Transport) is a layered version of the $k-\omega$ model in CFX 5.5.1 [24]. Coupled with the turbulence models, the mesh sizes of the structured grid in the near wall region are adapted adequately. The flow Reynolds number is 10,000, where Re is based on the mean velocity and hydraulic diameter in the annular gap. The thermal properties of water at 20 °C are used.

The axial velocity component W calculated with the standard $k-\epsilon$ model shows downward flow not only in the annular downcomer, but also near the centre of the widow and inside the guide tube near its lower end, Fig. 4. The recirculation zone in the guide tube concentrates the upward flow into a narrow area around the axis of the target. With increasing height z the cross section which is available for the upward flow is increasing so that the maximum of the axial velocity component is decreasing.

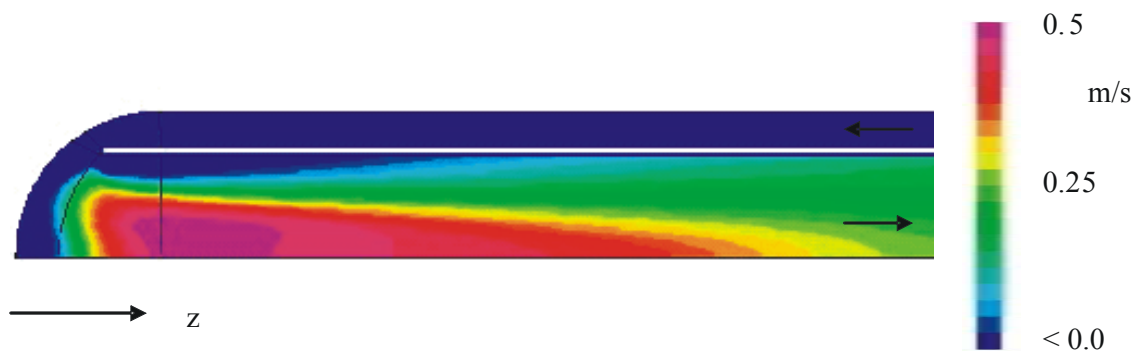


FIG. 4. Axial velocity W in half of a MEGAPIE target without bypass jet, standard $k-\epsilon$ model, $Re=10^4$. Blue areas indicate zero velocities or downward flow (to the left).

The maximum axial velocity values which are predicted by the five different turbulence models differ by about 10%, Fig. 5. However, there exist significant qualitative differences in the flow fields near the window centre and in the region downstream around $z=0.4$ to 0.8 m. Near the window the SST turbulence model doesn't predict any recirculation while the other turbulence models do. In the region downstream of the lower guide tube end, large differences in the flow fields exist. The steeper decrease of the axial velocity, which is at the upper end of the recirculation zone at the inside of the guide tube, is at different axial positions. This shows that the different turbulence models predict very different axial extensions of the recirculation area. In the target this recirculation would be exactly on

the height of the spallation zone; therefore, these differences could have strong consequences on the calculated temperature distributions.

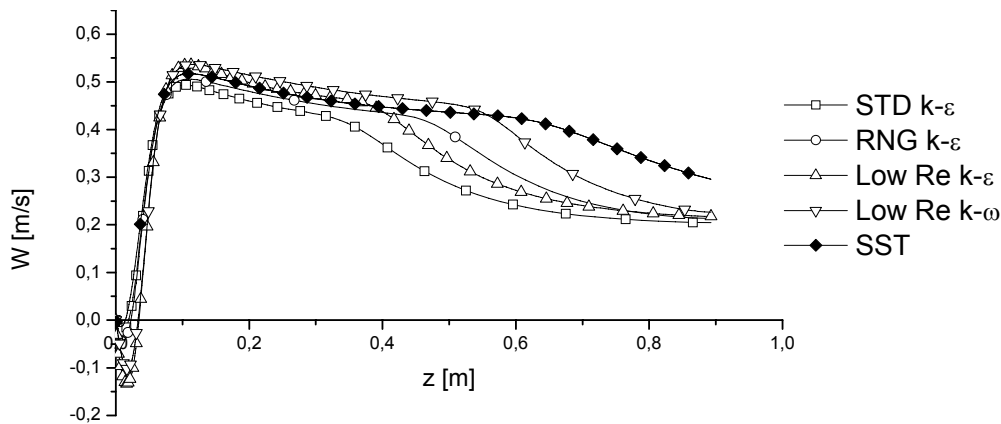


FIG. 5. Axial velocity W along the vertical axis of the jet-less target calculated with different turbulence models, $Re=10^4$.

Thus, detailed experimental data for the velocity field and some turbulence data in the prototypic geometry with jet are strongly required for the selection of an adequate turbulence model and its validation, especially in certain regions, i.e. near the window and between $z=0.4$ and 0.8 m. Other parameters, like the chosen mesh or the size of the computational domain, have compared to this sensitivity only a weak influence on the predicted results. In [25] it is shown that the type of the advection scheme has a strong influence on the temperature field; as the advection scheme is influencing the temperature by means of the velocity field, the selection of an adequate scheme should be performed on the basis of velocity data from such detailed water experiments. Performing the HYTAS experiments was found to be rather challenging. Therefore, there are currently no direct comparisons to the experimental data possible.

2.3 Other issues in flow field predictions

There exist no universal turbulence models which could be used for any type of turbulent flows at any Reynolds number. Therefore, our CFD codes provide a list of different models from which the user has to select the suitable one. One important difference occurs in the different modeling approaches in the near-wall area. Standard models use wall functions to calculate the wall shear stresses in the mean flow direction. With these models it is not required to use very fine grids near the wall to resolve the viscous sublayer; just the opposite is required: the grids must be coarse enough so that logarithmic wall functions can be applied. So, these models are the preferred ones for high Reynolds number flows, but they are not valid e.g. for detached and recirculating flows, because we don't have adequate wall functions for such flows. For detached flows one prefers the so-called low-Reynolds number models which need to resolve the viscous sublayer, but which then need special near-wall adaptations in the transport equations of the turbulence models. Those adaptations are expected to be more universal than the wall functions. So, such models are the preferred ones for flows at lower Reynolds numbers, or on powerful computer systems also for computations for somewhat larger Reynolds numbers. Of course, in practice there is a large sensitivity found in switching between these models and the adequate grids, which always requires verifying the calculated data on experimental data. So, what is needed is to achieve less sensitivity against this selection of the models. Or, as it is realized now in CFX 5, to develop intelligent methods which use a kind of blending between the different types of models so that this sensitivity can strongly be reduced because the resulting turbulence modeling, called SST [24], can be applied for a wide Reynolds number range.

The statistical turbulence models basing on the time-averaged Navier-Stokes equations, called Reynolds-Averaged Navier-Stokes models (RANS), are not the adequate tool when the consequences of the high energy containing low frequent turbulence has to be investigated, e.g. the consequences of

thermal stripping or of the pressure fluctuations in fluid-structure interaction. For such investigations Large Eddy Simulation (LES) is increasingly used which simulates directly the large scales of turbulence and models by sub-grid scale models (SGS) only the small scales which cannot be resolved by the grid [26]. The results of such LES are in principal less sensitive against modeling assumptions; nevertheless, there exist also no universal SGS models and no universal wall modeling. Thus, we find in these promising field similar challenging problems regarding the universality of the models, regarding their applicability to near wall flows at all Reynolds numbers, and regarding the wall treatment. An attractive compromise, which was recently developed to avoid part of these problems especially for flows around air foils, is the Detached Eddy Simulation (DES), which combines low-Reynolds number RANS modeling near the walls and Large Eddy Simulation apart from walls [27]. This DES may also be a powerful method to investigate low-frequent time-dependent phenomena in an ADS. The method is realized in the actual CFX 5 version. What hinders usually the wider application of LES or DES is that one needs finer grids and more time steps to get sufficient data, and that in channels with an inlet and an outlet it is hard to specify meaningful time-dependent turbulence at least at the inlet. So, more efficient methods are required to provide suitable inlet data.

All these issues in modeling and calculating velocity fields are not ADS specific. Some of them are known since decades and could not be solved by the turbulence modeling community despite tremendous research. So, it is not expected that the ADS community could seriously contribute to new solutions. Thus, if one has to treat one of these problematic cases one has always carefully to select the adequate modeling by checking the results of the chosen method by means of experimental results for the underlying flow regime or by means of experimental data directly for this prototypical flow. Of course one should consider using the recent combinations of methods like the SST and the DES which are especially intended to reduce or even to avoid some of the general problems. Finally, these or similar combined models which should have a wide range of applicability should be made available in all typically applied CFD codes.

2.4 Development needs for bundle flow predictions

The fuel element analysis is an important application field; therefore, some specific requirements for calculating the axial flow through fuel bundles should be discussed shortly. There are already applications of CFD to study heat transfer in bundles [28] or even to optimize mixing vanes at the spacers of reactor fuel elements [29]. By using different variants of the k - ϵ model and a full second order closure model it was found that the k - ϵ models give more or less insufficient accuracy for the bundle flow, that some of them give good secondary currents (which are the induced flows in the plane perpendicular to the axial mean flow), and that the second order model gives better results. It is concluded, that the used models are inadequate to capture the anisotropy and that other models should be investigated or new models should be developed. To analyze this conclusion we shortly discuss what is known from historical experiments in bundle flows and from former numerical analyses.

Basic experiments with detailed flow, heat transfer, and turbulence measurements in bundles were performed at FZK between the eighties and the mid nineties, see e.g. in [30]. These experiments, in which e.g. the gas flow through a large 4-rod arrangement in a rectangular channel was investigated, are still the basis for code benchmarks. The main results which are of interest if one decides to use CFD are that the flow is strongly anisotropic, especially in the near wall zones, that the expected secondary currents are near the measurement accuracy and can therefore hardly be detected. In addition systematic periodic oscillations were found in the spanwise velocity components and in the pressure in densely packed bundles which cause intensive mixing between subchannels [31].

First experiences with numerical analyses of axial bundle flows were basing on two-dimensional mixing lengths approaches. So, e.g. in [32,33] it is found that such flows need at least the use of anisotropic eddy diffusivities to reproduce bundle flows adequately; especially the azimuthal turbulent diffusion of momentum and heat near walls needs special care. In [34] it is found that bundle flows need the modeling of the secondary currents to get the correct azimuthal variation of shear stresses and heat fluxes. In [35] it is shown by means of LES that eddy diffusivities are a transportable quantity and

that they are considerably influenced by secondary currents so that only transport equation models will have a chance to record adequately flows with secondary currents. If densely packed bundles have to be considered, the highly intermittent periodic oscillations coming from the transport of coherent structures in the narrow gaps between fuel pins can well be treated by LES [36].

So, one has to expect that successful CFD applications can nowadays only be performed if the user of the CFD code is aware of the problematic physical background so that he can select the adequate models. From our nowadays knowledge we have to conclude that anisotropic turbulence modeling is required whereas the secondary currents are smaller than expected; they are usually automatically reproduced in a three-dimensional CFD. This means, it is known that there is no chance to record axial bundle flows with any isotropic eddy diffusivity and eddy conductivity model, i.e. all isotropic or standard k- ϵ models will fail. One has to use at least good Algebraic Stress Models (ASM) or sophisticated second order models. And for the strong inter-subchannel mixing in densely packed bundles one has to use either LES or DES. Whether the existing models are really sufficient, or whether further development of them is needed, cannot be deduced from the available investigations.

3. MODELING ISSUES IN TEMPERATURE DISTRIBUTION PREDICTIONS

3.1 Reynolds analogy and liquid metal heat transfer

To realize the challenges which we face when doing heat transfer predictions for liquid metal flows with RANS methods one should consider what are the methods which we use in our CFD tools on the momentum transfer side and on the heat transfer side. The conservation equations for mass, momentum, and thermal energy do not form a closed set of equations if the statistical or Reynolds approach is used to describe turbulence. In fact, unknown correlations between velocity fluctuations u_i and u_j called turbulent shear stresses $\overline{u_i u_j}$ and between velocity fluctuations and temperature fluctuations θ called turbulent heat fluxes $\overline{u_i \theta}$ exist in these equations. These terms which represent the turbulent transport of momentum and heat have to be modeled.

A widely used class of turbulence models is based on the eddy viscosity / eddy heat diffusivity concept [37]. The eddy viscosity ν_t and eddy heat diffusivity Γ_t are respectively introduced by a mean gradient approach in terms representing the turbulent transport of momentum and heat. There was already tremendous research in how to model the eddy viscosity for the turbulent momentum transport. It is usually approximated by using any variant of the k- ϵ model. The much more complicated and nevertheless less investigated eddy heat diffusivity is approximated mostly much less sophisticated; it is assumed to be also isotropic and to be linked to the eddy viscosity by a fixed turbulent Prandtl number $Pr_t = \nu_t / \Gamma_t$. This implies that the turbulent transport of heat is assumed to be strictly analogous to the turbulent momentum transport. These assumptions are the basis of the Reynolds analogy. This analogy works well for a wide class of flows but not for liquid metal flows. Due to the strongly different values of the relatively small molecular viscosity ν and the relatively large thermal diffusivity Γ , the statistical features of the turbulent velocity and temperature fields are not similar, like it is indicated by the different thicknesses of the molecular wall layers or the differing positions of the fluctuation maxima of the velocities and temperatures. This means, the Reynolds analogy should not be applied because it has no basis for fluids with small molecular Prandtl numbers $Pr = \nu / \Gamma$. At least for these fluids the turbulent Prandtl number is no longer a fixed value, but it depends on a number of parameters like Pr , Re , and wall distance, see e.g. in [38,39]. As the turbulent Prandtl number at all Pr below one is found to increase strongly near walls, and as the near-wall area is at a heated wall the most important area in heat flux modeling, any concept of using a spatially constant value of Pr_t will lead to insufficient results; nevertheless, this is the status quo of our current CFD tools in modeling liquid metal heat transfer.

In contrast to this modeling, formulations should be used which approximate the turbulent eddy conductivity Γ_t in liquid metals independent of ν_t , like in the first order 4-equation model [40]. Such 4-equation models based not only on k- and ϵ -equations, but in addition on transport equations for the

temperature variance $\overline{\theta^2}$ and its dissipation or destruction ε_θ , allow also for different time scales in the turbulent velocity and temperature fields.

For buoyant flows one gets strong anisotropy in the turbulence field due to the orientation of the buoyancy force. In such flows even a second-order description of the turbulent transport of heat should be applied, which means the use of independent transport equations for the three components of the turbulent heat flux vector. Such models are not constrained by any of the above mentioned problems. Therefore, in order to simulate turbulent flows in liquid metals with buoyancy influences it is reasonable to use a second-order model at least for the turbulent transport of heat. The Turbulence Model for Buoyant Flows (TMBF) [21,41] which is developed and implemented in the CFD Code FLUTAN [22] belongs to this class of models. It is suitable for the simulation of the turbulent transport of heat in liquid metals because it uses a second order model for the turbulent heat transport with special model extensions. The model extensions are widely basing on DNS data, e.g. by [42,43].

Similar turbulent heat flux models are missing in the commercial CFD tools which use at least some transport equations for statistical features of the thermal field. So, one has to live with the uncertainties of the Reynolds analogy, has to investigate from application to application which formulation for the turbulent Prandtl number is the more suited one, and has to verify carefully the finally computed results by comparisons to directly related liquid metal heat transfer experiments.

3.2 Heated annulus heat transfer predictions using Reynolds analogy

Here the limits of our current CFD capabilities are investigated by applying the Reynolds analogy to an experiment in our KALLA laboratory [44]. We use an annulus with a heated inner rod cooled by flowing liquid Pb-Bi. More detailed specifications and experimental as well as numerical results are given in [6,45].

The rod with an outer diameter of $d=8.2$ mm is installed concentrically in a pipe with $D=60$ mm inner diameter in the THESYS loop of the KALLA laboratory. The rod has a total length of 2,500 mm, the heated length is 228 mm. The rod can be traversed axially in z -direction by 240 mm to measure with the radially traversable Pitot probe and thermocouple at different axial positions relative to the begin of the heated length, Fig. 6. The helical Inconel heater inside the rod is DC current heated. In this experiment a maximum surface heat flux of $q''=34$ W/cm² was used. The inlet temperature is $T_{in}=300$ °C. This corresponds to a molecular Prandtl number of the fluid of $Pr=0.022$. The mean Reynolds number in the pipe zone basing on mean velocity and hydraulic diameter is $Re=10^5$.

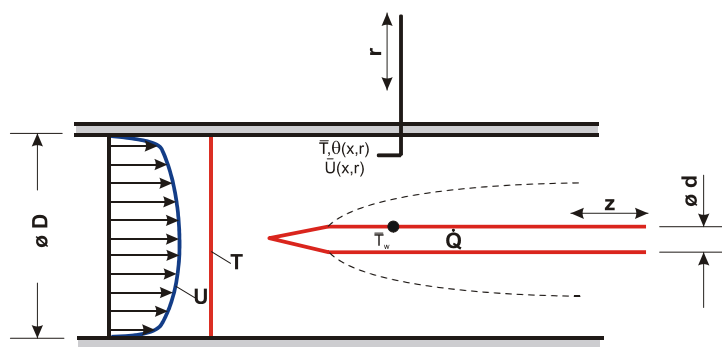


FIG. 6. Heated rod experiment in the KALLA loop.

The calculations have been performed using CFX 4.4. 2D and 3D structured grids were applied. Special attention has been paid to keep the first grid point from the wall in the range of $30 \leq y^+ \leq 50$ because this is on one hand side required to work with wall functions in the velocity field; on the other hand side this is still in the conductive wall layer, so that it can be avoided to apply the thermal wall function formulation which is in this code version inadequate for liquid metals. The standard $k-\varepsilon$ model has been used and the turbulent Prandtl number has been set to $Pr_t=0.9$. A first order hybrid

scheme has been selected for the advection terms. In order to examine the effect of buoyancy 3D calculations were performed including the full developing length of the flow as in the experiment. The thermal insulation has been taken into account using a constant temperature at the outer boundary.

The results of the first experiment series were the basis of ASCHLIM benchmark WP 4 [15]. The comparison of these results with the computational results leads to considerable discrepancies in the temperature field near the heated wall [45]. So, a systematic investigation was performed to learn about the most sensitive uncertainties in the modeling. By changing the effective thermal conductivity in the insulation in the calculation it could be excluded that support structures going through the insulation could have a considerable influence. By changing the turbulence level at the inlet into the computational box its influence could be excluded because with altered data the measured velocity profile could not be reproduced. Serious problems with an inadequate turbulent Prandtl number could be excluded because in increasing this value the deviations even increased. The near wall resolution was adequate because a further refinement had no effect on the results. And switching over to a low-Reynolds number turbulence model and adapting the grid in the required manner lead to the same temperature profiles. With the full 3D calculation it could finally be excluded that buoyancy influences the results at this Reynolds number. Thus, after intensive discussions of possibly missing phenomena in the calculations and of possible uncertainties on the test section side it was expected that the fixation of the rod was not sufficient to avoid that an eccentricity of the rod in the pipe may have been built due to the swimming up of the light rod in the heavy fluid in the horizontal channel. So the construction of the test section was changed and additional spacers were introduced.

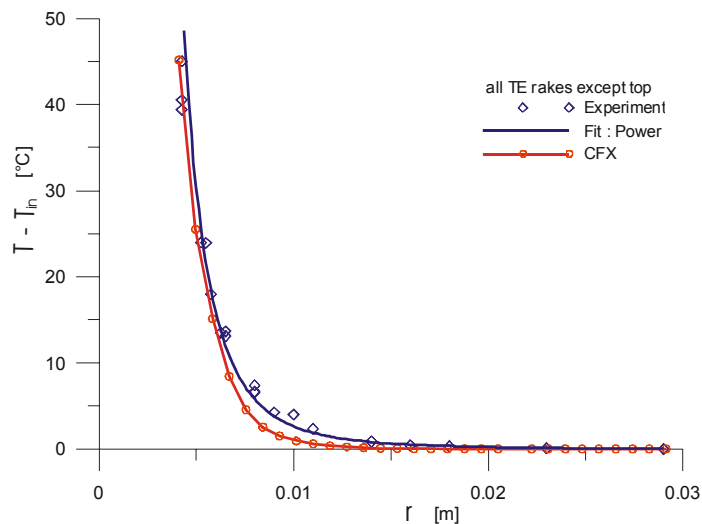


FIG. 7. Measured and calculated radial temperature profiles at half heated length of the heated rod experiment, $Re=10^5$, $q''=34 \text{ W/cm}^2$.

The new experiment series shows much better radial temperature profiles if one takes the data from the thermocouple array below or beneath the rod [6]; the data from above the rod indicate that the temperature field is still not fully axisymmetric. The originally calculated numerical results are now in much better agreement with the new experimental data, Fig. 7. Nevertheless, the agreement is not perfect: The computed fluid-wall interface temperature is for all axial positions larger than the measured one, e.g. at half of the heated length by about 10%. The deviation would increase if more realistic turbulent Prandtl numbers with values above one would have been used; but this would not help to bring the calculated profile around $r=0.01 \text{ m}$ nearer to the measured one.

This benchmark indicates that heat transfer investigations for Pb-Bi have considerable uncertainties on both sides, on the numerical as well as on the experimental side, even if simple channel configurations are used. The measured temperature profiles cannot be reproduced by using a constant turbulent Prandtl number; at least a radially varying value should be used to achieve a better agreement. To adapt higher order turbulent heat flux models requires additional experimental data for velocity-temperature cross correlations which can currently hardly be provided. On the other hand it gets

obvious that not only CFD needs assistance, here by experiments, for quality assurance, but also vice versa the quality of experiments profits considerably from parallel CFD analyses.

3.3 Heated jet heat transfer predictions using a second order turbulent heat flux model

A number of experiments in literature provide data for time mean temperature fields in turbulent liquid metal flows, but reliable turbulence data of the temperature field in liquid metal flows are rare. Such data are required to investigate the performance of more sophisticated turbulent heat flux models basing on transport equations. One data set, which was already once used in an IAHR benchmark [46] is the one of the TEFLU experiments. There, the turbulent mixing of momentum and heat was investigated in the co-flow of a multi-jet arrangement using liquid sodium, $Pr=0.006$ [47], Fig. 8. Some of the TEFLU data were chosen also in ASCHLIM in work package WP 2 to investigate the performance of some codes and their models [15].

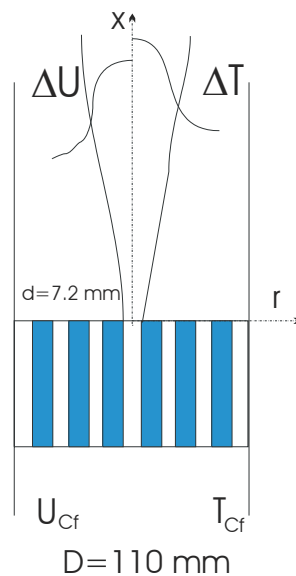


FIG. 8. TEFLU geometry with a heated sodium jet in the co-flow from a multi-bore jet block.

Here we show results which we got by using the latest version of the TMBF model [21]. This is a combination of a low-Reynolds number $k-\epsilon$ model and a second order turbulent heat flux model consisting of the transport equations for the three heat fluxes, for the temperature variance $\overline{\theta^2}$, and for its dissipation ϵ_θ . The calculated turbulent stresses and heat fluxes are not related through a fixed turbulent Prandtl number Pr_t . Thus the TMBF represents a compromise between the classical $k-\epsilon-Pr_t$ model and a full Reynolds stress model. In addition, the TMBF contains a number of special model extensions for liquid metal heat transfer which were deduced by theoretical means and by using our DNS data for liquid metal buoyant convection, see e.g. [48].

The extended modeling is verified at small Prandtl numbers without and with buoyancy contributions by means of some TEFLU experiments. Using a free jet experiment in a highly turbulent multi-jet surrounding to analyze the performance of turbulence models has the advantage that the results are mainly governed by the turbulence models and do not suffer from any inadequate wall modeling. Three different buoyancy regimes were considered in the benchmark; they were classified as forced jet, buoyant jet, and plume. The FLUTAN calculations applied not only the TMBF but also the standard $k-\epsilon-Pr_t$ model in order to investigate the advantage of the TMBF compared to the $k-\epsilon-Pr_t$ model. The specifications of the calculations and a detailed discussion of the results are given in [21].

The radial temperature profiles predicted by the $k-\epsilon-Pr_t$ model for the forced jet case are flatter than the measured ones, Fig. 9. The reason is the over-estimation of the radial heat transport from the axis to the outer flow. The mean temperature field is better predicted by the TMBF. This model calculates a smaller turbulent heat flux in the radial direction than the one calculated by the $k-\epsilon-Pr_t$ model.

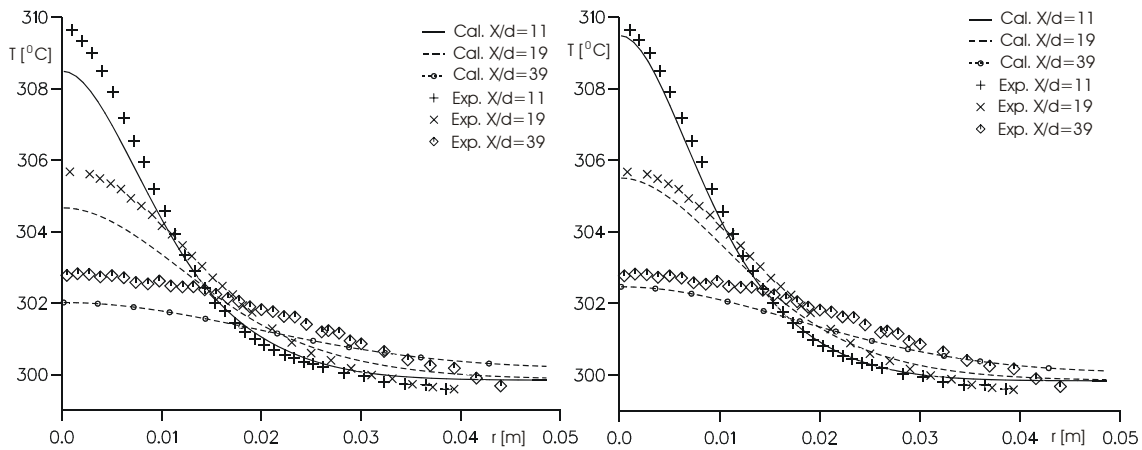


FIG. 9. Forced jet, radial temperature profiles at three different axial positions x/d , measurements and calculations with the $k-\varepsilon-Pr_t$ model (left) and TMBF model (right).

In considering the velocity and temperature profiles for the buoyant jet and for the plume it was found that the results of both models, of the $k-\varepsilon-Pr_t$ model and of the TMBF, agreed quite well with the experimental data. This astonishing result is caused by the fact that the local Reynolds numbers in these cases were too small so that the corresponding temperature fields were mainly governed by heat conduction and were only weakly influenced by turbulent convection. As many technical applications of liquid metal heat transfer are in the transition range between having mainly conduction dominated temperature fields and convection dominated ones, these cases were analyzed in more detail. Indeed, the results of the TMBF for the plume case indicate the need for further improvements in the TMBF model: Whereas the predicted temperature variances for the forced and buoyant jet agree with the experimental data, the results for the plume deviate considerably. So, the focus of further research was on the closure terms in the equations for the temperature variances and its dissipation; see chapter 4.

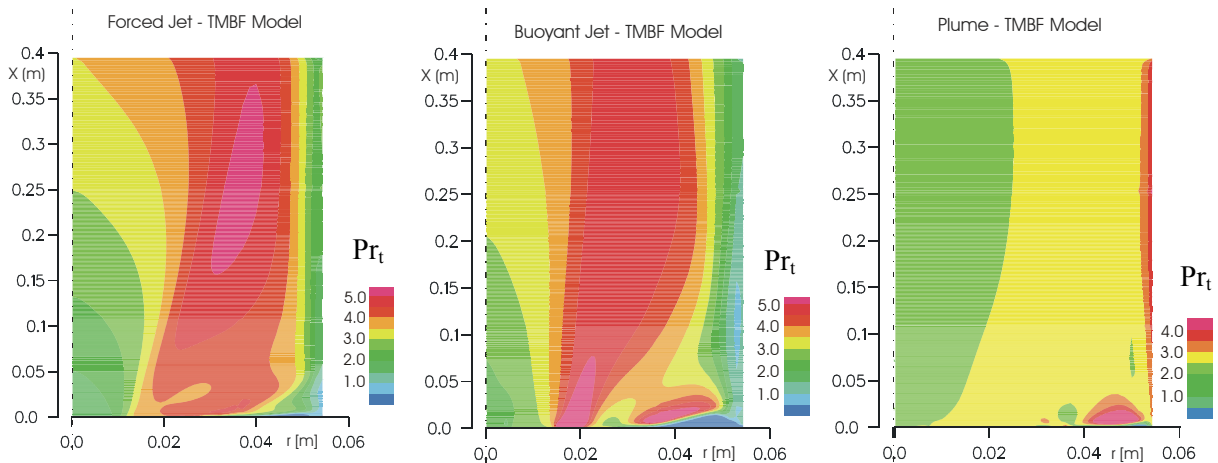


FIG. 10. Turbulent Prandtl number Pr_t calculated by the TMBF model for the forced jet (left), buoyant jet (middle), and plume (right). x -axis in the vertical direction along the centre line starting at begin of computational domain ($6d$ behind jet block), r radial co-ordinate starting at jet axis.

The TMBF uses the full transport equations for the turbulent heat fluxes; thus, it is possible to analyze from its numerical results the turbulent Prandtl number which would be required to produce the same temperatures with the Reynolds analogy. The fields of the such calculated Pr_t reaches values beyond 5, Fig. 10. Thus the values are locally much higher than the value of $Pr_t=0.9$ which is usually applied in calculations with the $k-\varepsilon-Pr_t$ model. Moreover, it is not constant. It depends not only on the fluid, but also on the flow regime and on the position. Indeed it was found that the $k-\varepsilon-Pr_t$ model can only give good results by adjusting the value of Pr_t to reduce the turbulent heat flux perpendicular to the flow direction [41]. This is consistent with the findings of other partners in the ASCHLIM project that only

those results were roughly acceptable which are based on physical models applying at least non-constant turbulent Prandtl numbers. The TMBF results were evaluated to be the most promising ones.

3.4 Issues in buoyant flow predictions

Flows, which are influenced or exclusively driven by buoyancy forces, like in large reactor pools, have some peculiarities compared to forced flows. One is the fact that in such flows there is not only a coupling from the velocity field into the temperature field equation by means of the convective term, but also the coupling back from the temperature field by means of the buoyancy force into the momentum equation. As a consequence the velocity field is influenced by the Prandtl number and thus detailed experiments to study the turbulence in buoyant flows need model fluids with about the same Prandtl number as the operating fluid for which the investigation is performed. Thus, one is faced with the serious problem of finding sensors to measure e.g. the local turbulence in the velocity field in liquid metals. As there aren't sufficient possibilities available, DNS is the standard tool to provide the data which are required for model development, see chapter 4.

The other important peculiarity is that the turbulence in buoyant flows is not only anisotropic due to the presence of the walls, but also in the complete channel due to the presence of the directional buoyancy force. It is well known, see. e.g. [49], that such flows can only be calculated with sufficient accuracy by means of models which use additional transport equations for quantities of the thermal field, like for the temperature variance $\overline{\theta^2}$ and in some cases also for its dissipation or destruction ε_θ . Such 3- or 4-equation models could also be extended to treat the influence not only of augmenting buoyancy but also of damping buoyancy in case of stable stratification.

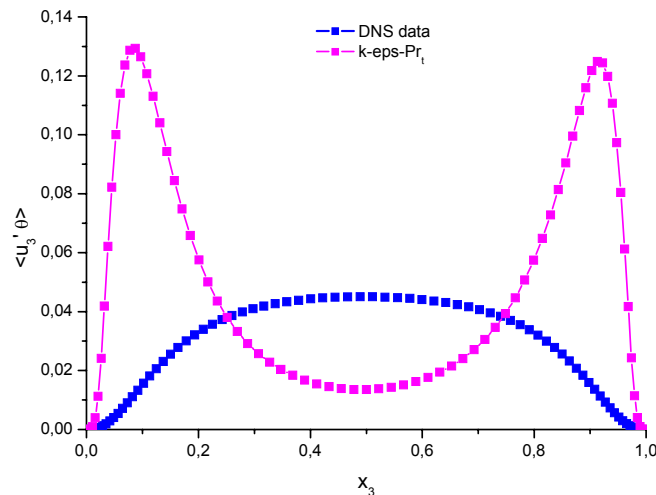


FIG. 11. DNS data for the vertical profile of the turbulent heat flux $\overline{u_3 \theta}$ in Rayleigh-Bénard convection and for the prediction by a $k-\varepsilon-Pr_t$ model, $Ra=10^5$, $Pr=0.025$.

In using recent DNS data for Rayleigh-Bénard convection in a liquid metal with $Pr=0.025$ at a Rayleigh number of 10^5 we analyzed the turbulent heat flux which would be predicted by a standard $k-\varepsilon$ model using a constant turbulent Prandtl number of 0.9 [50], Fig. 11. The DNS data for the upward directed heat flux shows thick conductive wall layers, whereas the profile which would be predicted by the Reynolds analogy has a much thinner conductive wall layer and large peaks near the walls. Any other spatially constant turbulent Prandtl number would also give such disastrous predictions, so that this concept is not applicable even for this simple buoyant heat transfer problem. A similar problematic experience was e.g. gained with practical applications of the $k-\varepsilon-Pr_t$ model for the calculation of the cooling conditions in core melts, where it was decided to use DNS or LES instead [51]. So, indeed more extended models are required which base at least on 3 or 4 transport equations for turbulence quantities and which should be combined with ASM extensions to record the anisotropy of all turbulent fluxes. One example for such a new ASM heat flux model with 4 equations which is suited for liquid metal convection is discussed in [17]; part of its important extensions for liquid metals is

discussed in chapter 4. Unfortunately, such ASM or second order models which are suited for liquid metal heat transfer are up to now not available in commercial codes.

3.5 Other issues in temperature field predictions

As with the turbulence modeling for the velocity field, we also find that there exist no turbulent heat transfer models which are universal. Especially the additional parameter of the molecular Prandtl number of the fluid leads to large uncertainties for applications to liquid metal heat transfer. Most of the models do not have special adaptations as they are required to include the stronger influences of the molecular conduction in the equations for the temperature variances or the turbulent heat fluxes.

The influence of the molecular Prandtl number occurs also in the wall conditions. The ‘universal’ wall functions for the temperature profile in forced flows depend also on the Prandtl number, and so do also the thicknesses of the conductive wall layers. In liquid metals the conductive wall layer is much thicker than the viscous wall layer. E.g. at moderate Reynolds numbers it may be necessary for usual grids to use wall functions in the velocity field, but it may be possible to resolve with the same grid the conductive wall layer in a liquid metal. It is this fact, which needs separate modeling of both wall layers. Unfortunately this is not correctly treated in most commercial CFD codes, and not all have suitable thermal wall functions for a wide Prandtl number range, so that in some CFD codes, like Star-CD, always coding is necessary to adapt the numerical treatment and the physical models to the ADS typical conditions. This problem is a further argument to use, where ever possible, low-Reynolds number modeling to avoid any problematic wall functions.

A peculiarity occurs e.g. in the stagnation flow at the target window, see Fig. 3. There we have a flow type similar to a wall impinging jet. For this flow type it is known that the turbulent heat transfer from or to the wall strongly depends on the turbulence model for the velocity field. Some k- ϵ models and even second order models are found to over-predict strongly the local turbulence level. As a consequence a too large heat transfer is predicted [52], so that a series of model extensions are required [53]. Again, this is a field of ongoing research in the turbulence modeling community which is not ADS specific. The CFD code developers follow the development and try to provide models which could also be used with limited success for this flow type. So, one has always carefully to check which one of the available more sophisticated models is really the better compromise.

In applying LES for time-dependent problems, like for the thermal striping phenomenon, the influence of the molecular Prandtl number needs also special consideration [26]. SGS heat flux models also depend on the molecular Prandtl number, but the turbulent Prandtl numbers for RANS models and SGS models are not the same. In considering the energy spectra for velocity and temperature fluctuations one can deduce that for fluids with Pr around one, Pr_t for the subgrid scales is around 0.45. For liquid metals Pr_t values can also be deduced from the spectra. Considering that the temperature spectra have vanishing energy at high frequencies with increasing thermal diffusivity or decreasing Pr leads to the result that even on coarse grids nearly all thermal fluctuations are resolved so that with finer grids no SGS heat flux models are required [54] and Pr_t for the subgrid scales approaches infinity. The arguments regarding the calculation of the wall heat fluxes are the same as for the RANS applications; one should avoid thermal wall functions, what is usually possible in ADS applications.

A further problem which is often underestimated is the verification of the complete setup of the numerical model consisting of the geometry specification, numerical grid, specification of the physical features of the involved fluids and structures and their interaction, and the physical model selection. With available computers one cannot reproduce completely the reality. So, simplifications are always introduced and some phenomena are neglected basing on engineering judgment. This holds also for the selection of the adequate models. The problem gets obvious if one considers e.g. buoyant flows: There one has to select which of the structures do thermally interact with the flow field, so that they have to be recorded, and which of the smaller support structures or instrumentation rods may be of second order relevant and can be neglected. In one example we had to learn that even for common fluids like water the engineering judgment could lead to wrong conclusions on what can be simplified and what has to be recorded in the numerical model because we did not expect that some thin support

bolts and cooling pipes going through a large pool had to be recorded in the CFD model to get qualitatively and quantitatively sufficient results [55]. The verification of the assumptions which are done by the code user is the main reason that we will always need prototypical experiments in which a similar combination of the physical phenomena is occurring as in the final technical application. This experiment should be reproduced first by the code user to verify his engineering judgment before going to the prediction of the technically relevant flow and heat transfer problem. Unfortunately the selection of the adequate turbulence models needs some local and very detailed turbulence data of the velocity and temperature field and some cross correlations, so that the instrumentation of such prototypic experiments is also a challenge.

4. ISSUES IN TURBULENT HEAT FLUX MODEL DEVELOPMENT

The results discussed above show that turbulent heat flux models which base on transport equations are superior to the Reynolds analogy using simple turbulent Prandtl number formulations. The challenge in developing the more sophisticated models is that the measurement capabilities are very limited to provide the required detailed local data, especially cross correlations between velocities, pressure, and temperature fluctuations in liquid metal flows. Direct Numerical Simulation of turbulence is the common tool to provide the required data at least for small turbulence Reynolds numbers. Examples for liquid metal forced flows are the data by [40,56], and for liquid metal buoyant flows those from [43].

Our analysis of the closure terms in the transport equations for the temperature variance and its dissipation is aiming to use DNS data for Rayleigh-Bénard convection in several low-Prandtl number fluids. The required DNS data were not yet fully available because liquid metal simulations need extremely fine grids to resolve the small scales in the velocity field and to record a large computational domain because flow structures with long wavelengths exist in this flow type. The available DNS for liquid metal convection by [43,57] did not reach sufficiently high Rayleigh numbers to be in a fully developed turbulent regime in the thermal field. Thus a new simulation was performed for a higher Rayleigh number. Starting from earlier simulations [57] we ran one with the TURBIT code [43] for turbulent convection in mercury or lead-bismuth, $Pr=0.025$, at $Ra=100,000$. Ra is defined by the channel height D and the temperature difference between both horizontal walls ΔT_w . The underlying grid consists of $400 \times 400 \times 75$ mesh cells and uses a periodic computational box of $8 \times 8 \times 1$ normalized by the channel height. The analyses of the simulation show that this Rayleigh number and even somewhat higher ones can be achieved with current computer systems and that the convection at this Rayleigh number gets now closer to the required fully turbulent regime. The data are used to analyze improvements of the TMBF or of the 3- and 4-equation models for ADS applications.

The statistical analyses of the DNS data show that several of the closure terms in the temperature variance and destruction of temperature variance equations should be the focus of improvements because the existing models lead to insufficient agreement with the data. In earlier work [48,58] we concentrated on the destruction (or dissipation) of the temperature variance ε_θ . It was found that the standard set of empirical coefficients for this transport equation is not sufficient for getting good agreement with the experimental field of the temperature variances at small Prandtl numbers.

The recent analyses of the DNS data concentrate on the other important closure term in these equations, here especially on the modeling of the turbulent diffusion term $\partial/\partial x_i \overline{u_i \theta^2}$ in the transport equation for the temperature variance [50]. The standard modeling applies the scalar or isotropic Gradient Diffusion Hypothesis (GDH) for the triple correlation:

$$\overline{u_i \theta^2} = -C_{s\theta} \frac{k^2}{\varepsilon} \frac{\partial \overline{\theta^2}}{\partial x_i} \quad (1)$$

This is usually the approach when a k - ε model is used. The results are made dimensionless by using the following scaling measures: D is the length scale, $u_0=(g\beta\Delta T_w D)^{1/2}$ is the velocity scale using g for

the gravity acceleration and β for the volumetric expansion coefficient, and ΔT_w is the temperature scale. In case of using algebraic or second order shear stress modeling, the anisotropic or tensorial form of the gradient diffusion hypothesis may be applied:

$$\overline{u_i \theta^2} = -C_{D\theta} \frac{k}{\varepsilon} \overline{u_i u_j} \frac{\partial \theta^2}{\partial x_j} \quad (2)$$

None of these approaches contains any explicit dependence on the molecular Prandtl number. Consequently, analyzing these equations with the DNS data shows that none of the existing models gives sufficient agreement with the directly analyzed diffusion term, Fig. 12. In contrast to these results we found sufficient agreement of both models for fluids with Prandtl numbers around one.

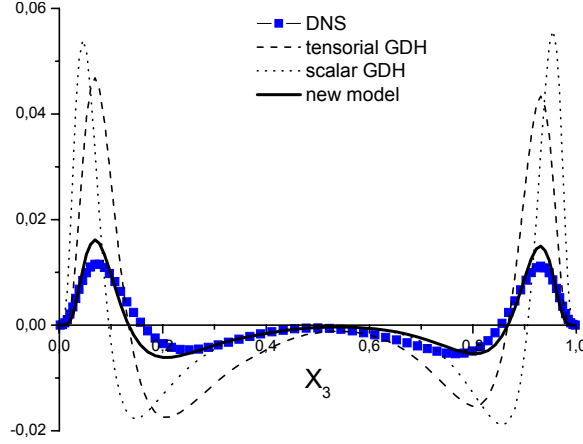


FIG. 12. Vertical profile of the turbulent diffusion in the temperature variance equation, Rayleigh-Bénard convection, $Ra=10^5$, $Pr=0.025$.

Using the two-point correlation technique a new model was developed for the triple correlation appearing in the diffusion term [50]. The model results in a Helmholtz equation and it explicitly depends on the molecular Prandtl number:

$$\overline{u_i \theta^2} = -C_\theta \left[\frac{2}{Re_0 Pr^{1/2}} \sqrt{\frac{k}{\varepsilon} \frac{\theta^2}{\varepsilon_\theta}} \Delta_x \overline{u_i \theta^2} + \frac{k}{\varepsilon} \overline{u_i u_j} \frac{\partial \theta^2}{\partial x_j} \right] \quad (3)$$

This model, in which Re_0 is basing on the scaling data given above, reproduces the DNS data for the turbulent diffusion not only at the Prandtl number of 0.025 quite well, Fig. 12, but also at Prandtl numbers around one. The model coefficient C_θ has been found to be independent on the Prandtl number. A Similar model has also been developed for the ε_θ equation with also convincing results. Thus, this new model is an important extension of the standard modeling used in the temperature variance equation. Combined with the former developments for the corresponding destruction terms one should get more reliable CFD results over a wide range of Prandtl numbers. What should come in the future is to test these models, which were developed for buoyant flows, also for forced flows, e.g. by using the DNS data by [56]. Then, they can be implemented in one of the basic CFD tools used in the ADS community and can be validated in practical applications.

5. CONCLUSIONS

Detailed numerical investigations of an ADS and its components require highly accurate tools on both sides, on the fluid dynamics side, as well as on the thermal dynamics side. The modeling issues on the fluid dynamics side are due to the fact, that the target geometry, which is optimized for cooling the window, may cause flow separation. This occurs especially in the MEGAPIE model target in which the downward flow in the annulus and the upward flow inside the guide tube is combined with a

sideward flow across the window to remove the stagnation point from the hottest zone. Numerical parameterization indicates that the resulting recirculation cannot be accurately described by common CFD tools without the aid of detailed prototypical model experiments, e.g. in water, in which the velocity fields are measured so that the adequate turbulence model can be chosen. Examples are the COULI experiments at CEA for an ADS target and the HYTAS experiments at FZK for the MEGAPIE target. The corresponding recalculations with commercial and research codes show that even more detailed and more accurate measurements in water models are required to achieve an adequate numerical modeling. Other issues which need improved modeling are the sensitivities which are sometimes found in switching from high Reynolds number coarse grid calculations with wall functions to low Reynolds number fine grid calculations without wall functions. An adequate layered modeling as in the SST turbulence model, or the DES in case of time-dependent simulations e.g. for fluid-structure interactions, seems to be a feasible compromise for the future to overcome many of the current limitations and should therefore be made available in suitable forms in most commercial codes. Simple, accurate, and manageable anisotropic models are still missing, but these are absolutely necessary e.g. to investigate the axial flow in fuel bundles.

The modeling issues on the heat transfer side are due to the fact, that we don't have adequate turbulent heat flux models for liquid metal flows in the commercial codes; all use at least the Reynolds analogy which means, similarity is assumed between the statistical features of the velocity and temperature fields. This does not hold for liquid metals. The more sophisticated models are usually not adapted to liquid metal flows. Thus, the capabilities of the available commercial CFD codes are beyond acceptable limits, and the sometimes physically better suited research codes are going out of operation. Therefore, also single effect experiments with detailed instrumentation are required with more realistic fluids. Calculations applying the Reynolds analogy for an experiment in the KALLA laboratory using an annulus with a heated inner rod cooled by liquid Pb-Bi indicate that such investigations have considerable uncertainties on both sides, on the numerical as well as on the experimental side. A turbulent Prandtl number concept which applies a spatially constant value for Pr_t will have no chance to reproduce adequately the recent, more accurate, experimental data. Some results of the sophisticated second order heat flux model TMBF were discussed, which is already in a number of terms extended for liquid metal heat transfer. The considered flow is the TEFLU benchmark, which is the spreading of a heated jet in a highly turbulent multi-jet environment in liquid sodium. Compared to all other benchmark contributions the TMBF results were found promising, but the model is still not adequate for the total investigated parameter range. Therefore, Data from improved basic research-type experiments and from our Direct Numerical Turbulence Simulations are used to develop more suited turbulent heat flux models. Such extended anisotropic models which at least are basing on the temperature variance equation (3- or 4-equation models) are absolutely required if one has to include buoyancy phenomena as they occur at strongly heated surfaces or in large pools of an ADS. Therefore, such models should be realized in the CFD codes. The strong influence of the turbulence models on the predicted heat transfer in an impinging jet needs still further model developments.

Finally, due to all these methodological problems and numerical and experimental uncertainties, as well as due to the simplifications which are always introduced by engineering judgment in building the numerical representation of the ADS or its components there will be always realistic experiments required which contain the typical physical phenomena and interactions. An example for target experiments are those going on in our KALLA laboratory combining the real target geometry with considerable heat input and the original cooling fluid. They use extensive instrumentation to allow for a detailed interpretation so that the selection is assisted of the adequate more sophisticated physical models in the CFD tools. Performing the numerical interpretation in parallel to the experimental activities ensures that the CFD team profits optimally from the experimental data and vice versa that the experimental team profits also from the complementing and often clarifying CFD field data.

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