CHALLENGES IN SIMULATION AND MODELING OF HEAT TRANSFER IN LOW-PRANDTL NUMBER FLUIDS

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Abstract

Nuclear heat transfer applications with low-Prandtl number fluids are often in the transition range between conduction and convection dominated regimes. Most flows in reactors involve also anisotropic turbulent fluxes and strong buoyancy influences. The relevance and complexity of the required heat flux modelling is discussed depending on engineering issues. The needed acceptable models range from turbulent Prandtl number concepts, over algebraic flux models, to full second order models in RANS as well as in LES, all with special liquid metal extensions. Recommendations are deduced for the promising HYBRID models. The listed remaining challenges show the need for further development of models and instrumentation.

1. Introduction

Thermal hydraulics of low-Prandtl number fluids is of wide interest in technical processes or applications, not only in fission reactor engineering. Simulation and modelling of heat transfer in such fluids is of essential economical interest to better understand and optimise e.g. steel production by continuous casting of metals [1] or crystal growth in semi-conductor production [2]. Thermal hydraulics is further of some interest in the feasibility studies of liquid metal targets; e.g., as a first step there is the stability of a free surface jet investigated for application in the high flux synchrotron radiation source at GSI Darmstadt [3]. Similarly the target system for the International Fusion Materials Irradiation Facility IFMIF is investigated [4], or the targets for many different blanket designs for breeding Tritium in fusion reactors [5].

Most research and engineering work on thermal-hydraulics of liquid metal flows was and is in the field of fission reactor cooling. A number of liquid metal (LM) cooled test reactors and Fast Breeder Reactors (FBRs or LMFBRs) were investigated in projects, or even built and operated [6]. The world-wide need for more energy was leading to new projects like the European Sodium Fast Reactor ESFR [7], the Indian Prototype Fast Breeder Reactor PFBR [8], or the Heavy Liquid metal (HLM) applying European Lead faSt Reactor ELSY [9] and the Russian lead cooled BREST-OD-300 [10]. The strong motivation to reduce extremely long living radioactive waste brought the transmutation concept up with HLM cooled fast reactors. Examples are the European eXperimental Accelerator Driven System XT-ADS with a spallation target with steel window and the Belgian windowless MYRRHA ADS with a free surface target [11].

The possibilities for detailed measurement of local flow parameters in LM cooled reactor components are challenging [12]. From a fundamental research point of view the measuring capabilities are quite limited to get data for more detailed physical modelling. Therefore, numerical simulation and modelling of basic and prototypic flow configurations is more important with low-Prandtl number (*Pr*) flows than usual for analysis of the relevant physical phenomena and model development; here $Pr=\nu/a$, where ν = diffusivity for momentum, a = diffusivity for heat. The typical goals of numerical investigations are related to analyses for the design of experiments, to parameterisation to reduce the experimental effort, to extend and complete experimental data, and to select and adapt correlations for use in system codes. Numeric tools are also used to up-scale and transfer the experimental data from model experiments to reactor conditions, and to optimise details of reactor components.

Compared to common fluids with *Pr* around one, LM cooled systems need quite improved, extended, or different physical modelling. In low-*Pr* number heat transfer, even in simple channels it is problematic to apply the Reynolds analogy to calculate local turbulent heat fluxes. In validating a correlation for the turbulent Prandtl number it was found by a valuable consistency test that most of the at that time available data were not suited to deduce an improved model and to validate it [13]. This situation is only slowly becoming better. The much more complicated anisotropic flow in tight lattice fuel bundles leads to moving regular coherent structures which cause intensive mixing and may also lead to serious structure vibrations. The phenomena are now understood as well as the type of modelling which is required to numerically simulate the more or less regular pulsations [14], [15]. In contrast to this, the thermal hydraulics modelling in LM cooled reactor cores still needs development and research [16]. When buoyancy dominated flows are engaged in the reactor core and in the plenum, the understanding of the mechanisms and the physical modelling need improvement in water cooled reactor systems [17], as well as in LM cooled systems where experiments and numerics are used up to now in combination [18]. Unfortunately, much of the early LM work was done for sodium, so that additional thermal hydraulics work has to be done by involving experiments, further model development and numerical analysis because the *Pr* numbers of the fluids and their chemistry are quite different [19], [11]. The target of an ADS is a new component with new cooling conditions. Therefore, special assessment of the available tools is needed by involving realistic model experiments [20] and in-pile experiments [21]. The demand in accuracy of the analysis and in the degree of recorded details is ever increasing in experiments and in modelling. Thus, even for the new sodium systems, like the French ASTRID, additional work will be necessary for many of the thermal hydraulic issues [22]. Fortunately, many of the LM issues in fission reactors are common with those in fusion reactors [23]. Nevertheless, the possibilities of numerical analysis of thermal hydraulics in low-*Pr* flows by CFD methods are also limited. An assessment of the widely used turbulence modelling leads to quite some required model improvements and corresponding model proposals [24].

In this paper a discussion of the status and needs of methodological issues in low-Prandtl number thermal hydraulics is given and of some challenges which need very specific knowledge. The work is limited to single-phase flows and concentrates on theoretical or numerical methods. The evaluation is partially from a personal and European point of view from academia. Nevertheless, most of the discussed problems are of general interest. Many of them are known and more or less tolerated in daily engineering CFD-applications, but the ever growing increase in recorded details and in accuracy requests makes improvements and further development of the current physical modelling necessary. The discussion starts from some specific statistical features of turbulent temperature fields in low-Prandtl number flows which are relevant for heat flux modelling or adequate selection and application of models. Following some of the challenges in CFD applications to LM cooling, peculiarities are elaborated of Reynolds Averaged Navier-Stokes (RANS) heat flux modelling by Reynolds analogy and by transport equation based heat flux models. As nuclear engineering is one of the large fields in which Large Eddy Simulation (LES) is of growing importance, the heat flux modelling in LES by subgrid scale (SGS) turbulent Prandtl numbers and by extended SGS heat flux models are also discussed, and the HYBRID methods combining RANS and LES. For most of these five topics it is shortly mentioned which modelling is currently available in codes; this is complemented by remarks regarding the current practically applied methods and regarding the in academia available better methods; finally some remaining challenges are mentioned to each topic which need improved modelling in the near future.

2. Thermal hydraulic peculiarities of turbulent LM flows

To get a better access to some of the specific problems which occur in heat flux modelling for low-*Pr* fluids, some of the peculiarities of the temperature fields and of their turbulent fluctuations are summarised. In forced convection the value of *Pr* does only influence the temperature field and the heat flux modelling, whereas in buoyancy influenced flows *Pr* does also influence the velocity field and the shear modelling. Here the focus shall be on the temperature field and on the heat flux modelling.

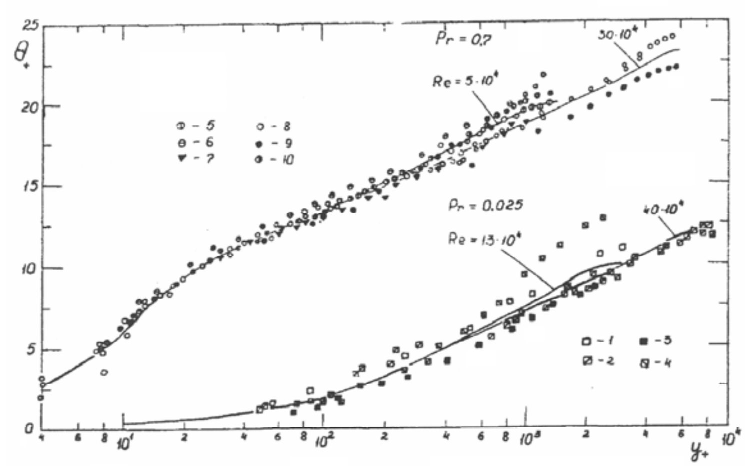

Figure 1 Universal temperature profiles T^+=Θ^+=$f(y^+)$ for two *Pr* values [25]. y^+=wall distance in wall units.

Liquid metals have a large thermal conductivity or diffusivity. In fluids with *Pr* around one the statistical features of the turbulent velocity and temperature fields are similar: The diffusive and conductive wall layers have about the same thickness and their fluctuation fields behave similar so far as heated or cooled walls are considered. With decreasing *Pr* the conductive sublayer in the time-mean temperature field becomes thicker so that the conductive heat flux is near walls increasing in importance, Figure 1. Thus, there is no similarity between time-averaged velocity and temperature profiles at low *Pr*. As a consequence of the large thermal diffusivity, the turbulent thermal diffusivity ε_h is only becoming larger than the molecular thermal diffusivity *a* when e.g. for *Pr*=0.025 the Reynolds number *Re* is beyond 60,000, or for *Pr*=0.007 when *Re* is beyond 214,000, where $Re=u_b/(D_h*\nu)$ and u_b=bulk velocity, Figure 2. This means, many of the nuclear applications are in the transition range between conduction dominated and convection dominated turbulent heat transport, i.e. the effect of the turbulent heat flux models extends from minor to large importance.

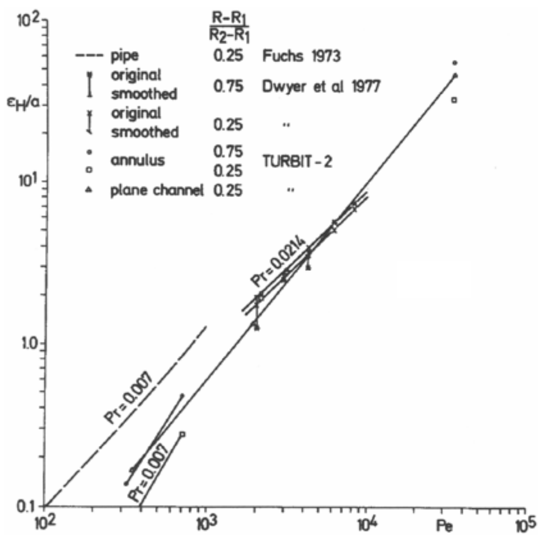

Figure 2 Relative importance of thermal turbulent diffusivity ε_h/a over Peclet number [26]. *Pe=Re*Pr*.

The radial turbulent heat flux in a RANS turbulence model is expressed as the time mean $\overline{u_3' T'}$. So it is governed by the radial velocity fluctuation u_3' and the temperature fluctuation *T'*. In channel flows, the behaviour of u_3' is well known [27]; in wall units its size and radial distribution are widely independent on *Re*, except for values near the critical Reynolds number. In contrast, the temperature fluctuations show a much more complicated behaviour, Figure 3. In both figures data belonging to the same Prandtl or Schmidt (*Sc*) number are connected by lines; single dots belong to differing *Pr* or *Sc* values. Plotted are Direct Numerical Simulation (DNS) data from [28], [29], [30] and LES data from [31] for maxima of the rms values of the temperature fluctuations $T'^{+}_{max}=\sqrt{\overline{T'^2}}/T*$, where $T^*=q_w/(\rho\ c_p\ u_\tau)$, q_w=wall heat flux, ρ=density, c_p=specific heat at constant pressure, u_τ=shear velocity. These show, like the experimental data summarised in [26], that T'^{+}_{max} increases with Pe_τ. For *Pr*=0.71 and larger the data are roughly independent on Re_τ, this means they depend only on *Pr*, whereas the results for low *Pr* strongly depend also on Re_τ. It may be expected that at large Re_τ the LM data should also become independent on Reynolds number. A similarly complex behaviour is also found in the wall distance y^{+}_{max} of the position of the fluctuation maximum. Again, the data for *Pr*=0.71 and larger are roughly independent on Re_τ, this means they depend only on *Pr*, whereas the results for low *Pr* strongly depend on *Pr* and Re_τ. By analysing where the y^{+}_{max} values are found in the universal temperature profiles given in Figure 1 one notes that at *Pr*=0.71 the maximum of *T'* is found about 10 to 15% below the begin of the logarithmic range, and that at *Pr*=0.025 it is at about the same position but moves with increasing Re_τ into the logarithmic range. These complicated differences at low *Pr* between the normalised velocity and temperature fluctuations and their differences in the spatial distribution point to the fact that there will be no simple way to use any analogy between turbulent fluxes in the velocity and temperature field to approximate the turbulent heat fluxes at least at medium and large *Re*.

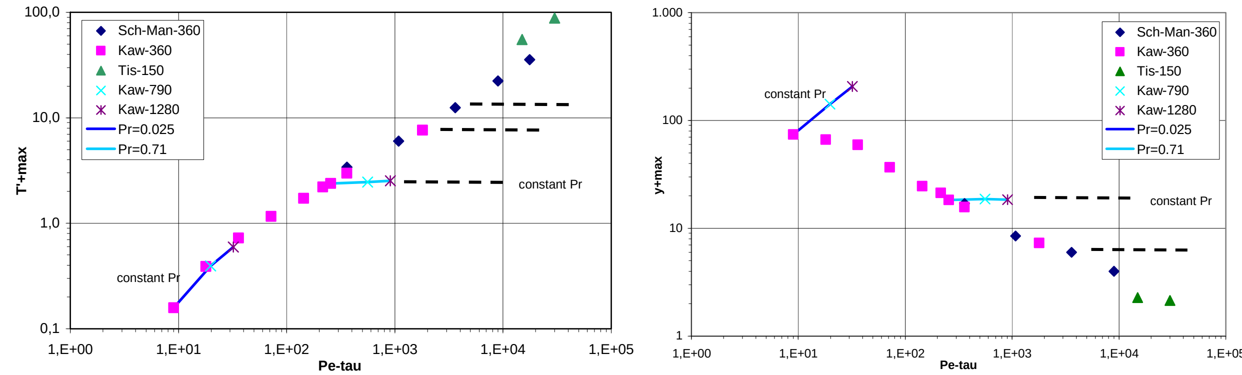

Figure 3 Influence of *Pr, Re_τ* and *Pe_τ* on the maximum of the rms value of the radial temperature fluctuation profile T'^{+}_{max} and on its position y^{+}_{max}. $Pe_\tau = Re_\tau * Pr$, $Re_\tau = u_\tau / (D*\nu)$, and $y^{+}_{max} = y/D*Re_\tau$. Curve identifiers indicate author names and Re_τ. Data connected by lines belong to a fixed *Pr* but varying Re_τ, whereas unconnected data with same identifiers belong to a fixed Re_τ but varying *Pr*. DNS data from [28], [29], [30], LES data from [31].

The differences in the spatial scales of the two fluctuation fields may be analysed from the distributions of the energy spectra, Figure 4. The velocity fluctuations distribute over a wide range of wavenumbers *k*. The wavenumber is a reciprocal length scale. Most energy is found at large scales; at smallest scales the energy is dissipated. Scaled in wall units, the energy distributes with increasing *Re* to ever higher wave numbers. The temperature spectrum for *Pr* around one has the same distribution and dependence on *Re*. With decreasing *Pr*, the increasing thermal diffusivity reduces the amplitude of the temperature fluctuations, compare T'^{+}_{max} in Figure 3, and damps strongly the temperature fluctuations at small scales. There are indications that the temperature spectra for low *Pr* flows extend somewhat to larger scales, i.e. to lower wavenumbers [32]. A third parameter in this figure is the wall distance *y*. As the magnitude of velocity and temperature fluctuations is varying with wall distance, all these spectra depend also on *y*. These distributions give LES for low *Pr* fluids a special chance because it will be easy to record widely or even completely all temperature fluctuations; this means there are chances to get rid of any SGS heat flux models for LES applications at very low *Pr* values.

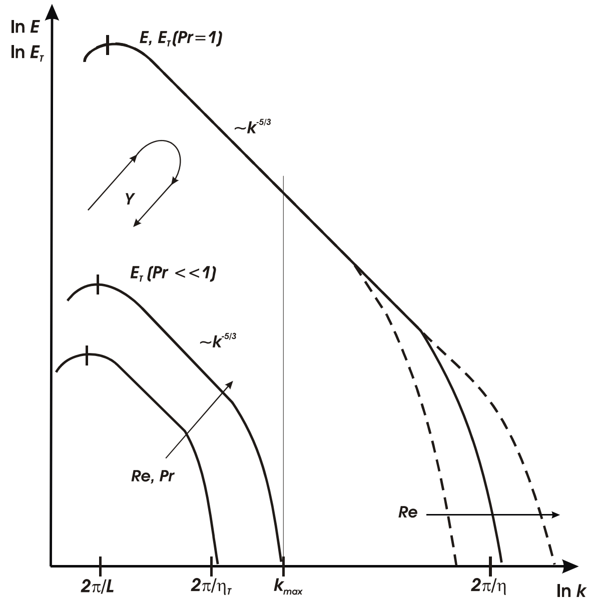

Figure 4 Sketch of three-dimensional energy spectra *E(k)* for velocity fluctuations and $E_T(k)$ for temperature fluctuations at $Pr \leq 1$.

LM, especially HLM, often allow for transport of large amounts of thermal energy with rather moderate velocities. As a consequence, strong distortions of the velocity fields and its turbulence could be expected in such heated or cooled channels due to buoyancy forces. The analyses in [33] of PbBi experiments in an concentric annulus with heated inner rod show that the data could be correlated by the buoyancy parameter $C^{*}=Ra^{0.333}/(Re^{0.8}\ Pr^{0.4})$, where *Ra* is the Rayleigh number calculated using the axial temperature gradient, Figure 5. An increase of Nusselt number *Nu* is found by augmented convection at low *Re*, but also a reduction of *Nu* by some relaminarisation at quite high *Re*. This means, that not only gaining separate effect data for turbulence model development may be quite challenging, but also the selection of adequate models for CFD applications to non-adiabatic liquid metal flows.

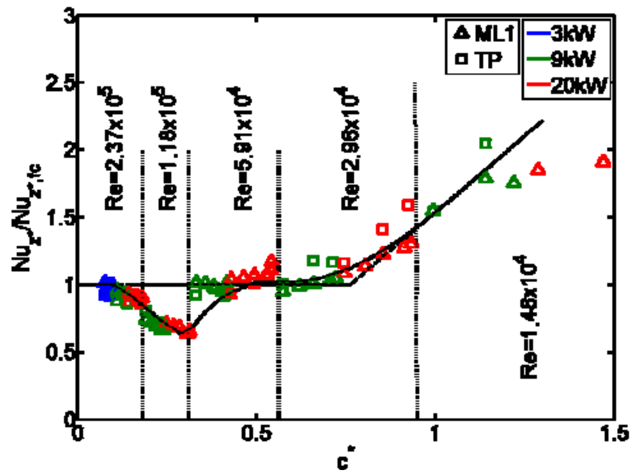

Figure 5 Influence of the buoyancy parameter *c on the Nusselt number in the KALLA heated rod experiments [33].**

3. RANS-based CFD

RANS turbulence models form still the basis of the CFD working horses in nuclear engineering. They are used for detailed analyses of experiments and reactor components, for optimization, and for determination of correlations for system codes. Before concentrating on the *Pr* dependent turbulent heat flux modelling, it should be first mentioned that there are a lot of uncertainties in turbulence modelling of the velocity fields. In forced flows these can be independently reduced to a minimum by selecting the best suited momentum transfer model, e.g. by following the Best Practice Guidelines [34]. In channel flows, e.g., especially in bundle flows, since decades the turbulent momentum transfer is known to be highly anisotropic; therefore, anisotropic turbulence models are needed to reproduce the local variations of mean flow data and secondary currents [24]. To reproduce in principle the moving vortices in tight lattice fuel bundles one has to apply at least Unsteady RANS (URANS). Nevertheless, it is also found that LES is doing a better job regarding wavelengths and amplitudes of the moving vortex patterns which are important for inter-subchannel mixing, [35], [36]. Only after having validated the modelling of the momentum field, like e.g. in [37], the heat flux modelling may be parameterised, optimised, and validated.

In strongly buoyancy influenced flows, when the temperature is no longer a passive scalar, the temperature needs to be calculated with utmost accuracy because it forms a strong or total part of the source term for the velocity field. Also buoyant flows are in principle highly anisotropic independent whether these are in channels or in large pools. So, there are similar modelling requirements. Most models existing in the large commercial codes are somehow extended to buoyant flows, but not to its full extend. E.g., there are buoyancy influences hidden in closure terms like in the turbulent diffusion of the kinetic energy *k* which seem to depend on flow type [38], [39], but for which DNS-based improvements could be developed [40] which make the diffusion model obviously independent on flow type. In such flows, selection of adequate turbulent heat flux modelling requires special know how. Sometimes an independent model selection should be avoided because shear stress and heat flux models were developed and validated together. Thus, in flows with active scalars any validation has to be performed with special care, especially in the low-*Pr* range.

3.1 Reynolds analogy and Pr_t

The main issue in this chapter shall be the heat flux modelling in channels with more or less steady wall parallel flow and strong heating, in which the knowledge of accurate temperatures is indispensable. Such heat transfer is the most common problem in turbulent convective heat transfer. It occurs e.g. in subchannels of subassemblies with wider lattice, to some extend also in inter-wrapper flows, and in test rigs with heating or cooling.

Among the currently available RANS heat flux modelling methods the most common one is basing on gradient assumptions for the unknown turbulent heat flux term:

$$\overline{u_i' T'} = -\varepsilon_h^{il} \frac{\partial \overline{T}}{\partial x_l} \tag{1}$$

The introduced unknowns, the eddy conductivities (or eddy diffusivities for heat) ε_h^{il}, should be a tensor. Nonetheless, in most models the anisotropic eddy conductivity tensor ε_h^{il} is replaced by an isotropic scalar ε_h, which means, each heat flux component is governed by the same still unknown eddy conductivity. None of the large commercial codes has up to now a well validated separate model for ε_h. Instead the Reynolds analogy is applied. This means similarity is assumed in the turbulent transport features of momentum and heat, and thus the isotropic eddy conductivity introduced in (1) is assumed to be proportional to the eddy diffusivity for momentum ε_m. The proportionality factor is the inverse of the turbulent Prandtl number Pr_t :

$$\overline{u_i' T'} = -\varepsilon_h^{il} \frac{\partial \overline{T}}{\partial x_l} \approx -\varepsilon_h \frac{\partial \overline{T}}{\partial x_i} = -\frac{\varepsilon_m}{\mathrm{Pr}_t} \frac{\partial \overline{T}}{\partial x_i} \quad \text{with} \quad \mathrm{Pr}_t = \frac{\varepsilon_m}{\varepsilon_h} \tag{2}$$

So the problem is shifted to the unknown proportionality factor $1/\mathrm{Pr}_t$. This variable is defined by the turbulent shear stress and the gradient of the velocity field, and by the turbulent heat flux and the gradient of the temperature field. At least from the discussion of Figure 1 and Figure 3 it is known that these variables are non-similar in LM flows. Therefore, Pr_t will not be constant, but it will depend on many parameters. Accordingly, many correlations are known, see e.g. the overviews in [41], [42], [43]. Churchill [43] used for his proposal a similar approach like it is used in the consistency test for the experimental data in [13]. The approach by Cebeci [41] is attractive because it can be easily extended to local applications in concentric and eccentric annuli and in subchannel flows by using the local wall shear stress $\hat{\tau}_w$, to symmetric or asymmetric heating or cooling by applying different profile lengths $\hat{y}$ in the Nikuradse parabola for the mixing length l_m of the momentum field and $\hat{y}_T$ in the mixing length l_h of the thermal field, and to varying wall roughnesses h^+ ; for more details see [24].

$$\mathrm{Pr}_t = \frac{\varepsilon_m}{\varepsilon_h} \approx \frac{l_m}{l_h} = \frac{\kappa\, \ell_{Nik}(y/\hat{y}) \left\{1-\exp\left(-y^+ \hat{\tau}_w^{1/2} / A_w\left(h^+\right)\right)\right\}}{\kappa_h\, \ell_{Nik}(y/\hat{y}_T) \left\{1-\exp\left(-y_T^{\,+} \hat{\tau}_w^{1/2}\, \mathrm{Pr}^{1/2} / B_w(\mathrm{Pr})\right)\right\}} \tag{3}$$

The Karman constants are those from the universal velocity profiles, respectively temperature profiles, $\kappa = 0.4$ and κ_h = 0.43 to 0.47. For smooth walls, one gets $A_w(h^+=0)=26$. The coefficient $B_w(Pr)$ is according to [44]. Unfortunately, it turns out that this Pr_t correlation has incorrect near-wall behaviour because the calculated Pr_t data for different molecular Prandtl numbers do not converge near the wall to a single value [45]. This convergence is not so strong as expected; this is found in the later DNS results of [28], [29] which were according to [32] gained on sufficiently large computational domains, Figure 6. The proportionality factor $1/Pr_t$ in the approximated turbulent heat flux has a complex dependence on Re_τ, *Pr* and wall distance. At low *Pr* it is increasing with Reynolds number, it is increasing with Prandtl number, and it varies strongly with wall distance.

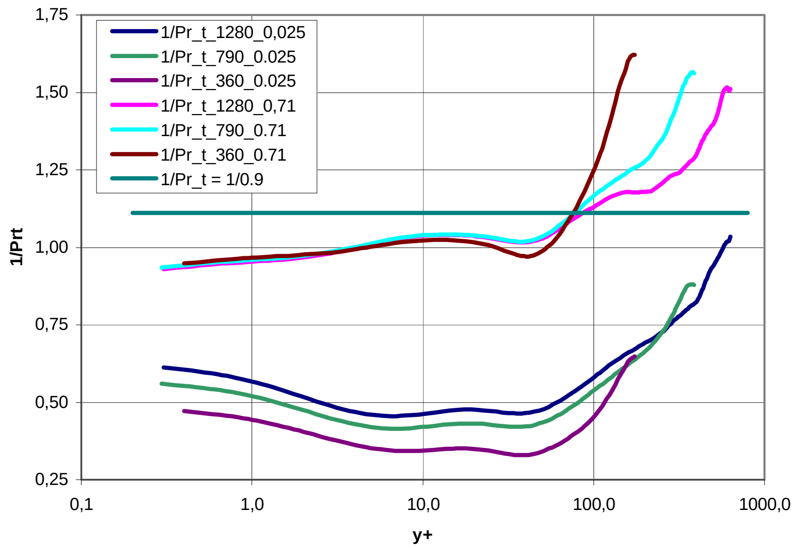

Figure 6 Radial profiles of the inverse of the turbulent Prandtl number Pr_t for Re_τ=360, 790, 1280 and for *Pr*=0.025 and 0.71. DNS data from database of [28], [29].

The relevance of these strong variations depends on the parameter range of application. One may expect that the strong dependence on *Re* and *Pr* at low *Pr* may be of less relevance so far as the expected normalised eddy conductivity ε_h/a is around one or below; see the discussion of Figure 2. From both figures it gets obvious that the influence of *Pr* is important. The relevance of the spatial variation is as usual in channel flows: The influence of an eddy diffusivity or eddy conductivity model is largest where the corresponding gradients of the mean fields are largest; this is usually at the first few y^+. For the heat flux in low *Pr* fluids this is a less critical area because the large conductivity dominates the turbulent flux in a much thicker wall layer. The turbulent scalar fluxes are dominant in the thermal buffer layer up to the area where the scalar fluctuations are largest, Figure 3, and where at the same time the gradients of the scalar are still large, Figure 1: Thus, accurate models are needed up to about ½ y^+_{max} or y^+_{max}; this is for *Pr*=0.025 up to y^+=100 to 200, increasing with *Re*. There, $1/Pr_t$ is strongly changing. For *Pr*=0.71 accurate models are strongly required up to about y^+=25; there the spatial variation of $1/Pr_t$ is less distinct. And for *Pr* above one the Pr_t value becomes important in an ever thinner layer because the temperature difference between wall temperature and bulk temperature is built up in a thin layer of thickness of order y^+_{max}.

The current treatment of the heat flux determination by means of the Reynolds analogy by most CFD users is that mostly a spatially constant value of Pr_t=0.9 is applied for all types of flows, for all Prandtl numbers, and for all shear stress models. This assumption is also included in Figure 6; it deviates quite considerably in the sensitive area from the expected non-constant distribution. Even rather sophisticated anisotropic shear stress models, like non-linear Eddy Viscosity Models (EVM) or even full 2nd order Reynolds Stress Models (RSM) are combined with the simple isotropic Reynolds analogy using a constant Pr_t value. The influence of non-constant distributions and differing correlations for Pr_t is practically analysed and evaluated on the basis of recent CFD data in [46] at this conference. It is found that the computed temperature differences really profit from the non-constant distributions when high-quality velocity field modelling is used.

One of the more urgent remaining challenges of modelling turbulent heat fluxes in non-unity Prandtl number flows by the turbulent Prandtl number concept is to get more accurate and consistent experimental data from non-adiabatic LM channel flows. This is tedious work because Pr_t depends on the gradients of the mean fields and on turbulence data which have to be determined with high temporal and spatial resolution. For low-*Re* flows there are already quite accurate DNS data available, see above. For high-*Re* LM flows combined LES of the velocity field and DNS of the thermal field could also provide sufficient data. Such combined LES-DNS were already used in [26] over a wide range of practically relevant Reynolds numbers. Depending on the practical experience with the relevance of locally varying Pr_t modelling from [46] one should develop improved turbulent Prandtl number correlations for local use. Another challenge is the modelling of anisotropic heat fluxes in bundle flows by Reynolds analogy. It may turn out that e.g. hot spot analysis in fuel bundles with grid spacers may require more sophisticated anisotropic heat flux modelling, like algebraic or second order heat flux models. These will be discussed in the next chapter. A minor problem is the selection of adequate thermal wall functions, if at all required. The Kader correlation [25] became a standard for applications over wide ranges of *Pr*. On the other hand, in nuclear applications to LM flows one can mostly discretise down into the conductive sublayer so that applications of thermal wall functions can widely be avoided.

3.2 Transport equation based heat flux models

The methods to be discussed in this chapter aim on adequate description of following issues which are often safety and lifetime related: Insufficient mixing, especially at low flow rates, may lead in horizontal piping to thermal stratification causing thermal shocks and thermal fatigue, see e.g. [22]. Such buoyant flows are widely three-dimensional, time dependent and show per se anisotropic turbulent fluxes. This holds especially for buoyancy influenced or governed convection in large pools and plena. Examples are the studies of the backflow from the immersed coolers into the breeder elements in the Japan Sodium Fast Reactor JSFR [47] and the analyses of thermal striping in the control plug above the core for PFBR [48]. Even non-buoyant flows may show strongly anisotropic heat fluxes like in the mixing of differentially heated interacting jets [49]. And the highly anisotropic flow in fuel bundles with tight lattice becomes unsteady due to the coherent structures moving in the narrow gaps betweens the pins [14].

The current treatment of such problems by CFD with the large commercial or special codes from the nuclear community is on a roughly acceptable basis only regarding the calculation of the momentum fields, because the highly anisotropic or buoyant flows may be modelled by non-linear EVM or full second order RSM. As mentioned above, buoyancy is formally treated so far as explicit buoyancy terms appear in the solved transport equations, but not the buoyancy hidden in closure terms, see e.g. the *k*-diffusion [40]. In contrast in the heat flux modelling one mainly finds applications of isotropic versions of the Reynolds analogy, i.e. of simple Pr_t assumptions. The experience with such strange model combinations is rather contradictory: In analysing sodium experiments to model the thermal stratification in the upper plenum of an FBR it is found that a standard k-ε model gave insufficient results to reproduce the temperatures in an interconnected pool-channel system, but that a RNG-k-ε model and a RSM model (obviously combined with a constant Pr_t value) gave temperature gradients at the stratification interface within 10% of the measured ones [50]. Other applications, like those of the Pr_t concept combined with a standard k-ε model to large pools of core melt, even show a complete failure in predicting the temperature differences and wall heat fluxes in a fluid with *Pr* near one [51]. Indeed it is well known and understood that standard eddy conductivity models, and this means also the Pr_t concept, are inadequate for extended pools and fluid layers [52]. So, from the current expectations in the accuracy of CFD one may assume that such concepts may be acceptable for buoyant flows with a boundary layer character like in vertical channels, tilted pools, connected domains, but that they fail in buoyancy governed convection in large pools in which the flow is dominated by thermals or plumes.

In principle, there are better suited models available, but not in the large commercial codes. A short summary of better modelling is given in [24]. All the better models increase the sophistication on the thermal side by adding separate transport equations for some statistics of the thermal field. All use as a counterpart to the k-ε equations at least a transport equation for the temperature varianc $\overline{T'^2}$, and if fluids with Prandtl numbers different from unity are involved, also a transport equation for its dissipation ε_θ. Among the first order or gradient models the 2+2 or 4-equation models should be suitable for a wide range of molecular Prandtl numbers, because they introduce separate time scales for the velocity field, k/ε, and for the temperature field, $\overline{T'^2}/\varepsilon_\theta$, where ε is the dissipation of kinetic energy. Variants which are in some terms adapted to the requirements of variable Prandtl number flows are provided e.g. in [53] using mixed time scales. The model is investigated in [54] in its tensorial form as proposed by [55]. This allows for better anisotropic transport features:

$$\overline{u_i' T'} = -C_{k\theta} \sqrt{\frac{k}{\varepsilon} \frac{\overline{T'^2}}{\varepsilon_\theta}}\, \overline{u_i' u_j'} \frac{\partial \overline{T}}{\partial x_j} \tag{4}$$

The Algebraic Heat flux Models AHM introduce additional terms which help to get rid of the gradient assumptions which hinder good modelling in convection types in which gradients become approximately zero or in which counter-gradient fluxes occur. RANS models of this type were deduced in [56], [57], or [58]. In starting from the transport equations for the turbulent heat fluxes, assuming fully developed flow and local equilibrium, the latter author deduced the following algebraic heat flux model, in which the mixed time scales from [53] are in addition implemented as in [54] to allow for variable Prandtl number:

$$\overline{u_i' T'} = -\sqrt{\frac{k}{\varepsilon}\frac{\overline{T'^2}}{\varepsilon_\theta}}\left[C_1 \overline{u_i' u_j'}\frac{\partial \overline{T}}{\partial x_j} + C_2 \overline{u_j' T'}\frac{\partial \overline{u_i}}{\partial x_j} + C_3\, g_i \beta \overline{T'^2} + \varepsilon_{\theta i}\right] \tag{5}$$

Here g_i is the component of the gravity vector, β is the volumetric expansion coefficient, and $\varepsilon_{\theta i}$ is the destruction term in the transport equation of the turbulent heat flux. In pure buoyant flows the term involving the coefficient C_3 is the dominant one in this anisotropic model. Therefore, a comparison between eq. 4 and 5 indicates that AHM models form the minimum standard for a meaningful modelling of strongly buoyancy influenced flows.

Full second order heat flux models are based on the transport equations for the turbulent heat fluxes and at least for the temperature variance $\overline{T'^2}$. Of course, a large number of closure terms appear. Modelled forms of these equations are discussed e.g. in [59], [60], and with the focus on liquid metal heat transfer modelling in [61]. The latter model, called the Turbulence Model for Buoyant Flows (TMBF), was developed to get in a first step an improved treatment of the turbulent heat flux in buoyant flows. The TMBF is the combination of a low Reynolds number k-ε model with a full second order heat flux modelling involving the temperature variance equation and as an option also the dissipation equation for the thermal variance ε_θ. So, it uses 4 or 5 equations for modelling the heat flux vector. The heat flux modelling is suited for anisotropic and buoyant flows and it is in many terms adapted to liquid metal convection; some of these model contributions are deduced from our DNS data, e.g. from [62] or [63]; the latest model version of the TMBF is given in [49].

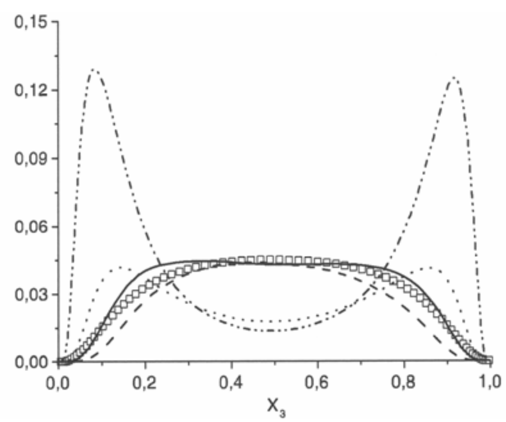

Figure 7 DNS data for vertical distribution of turbulent heat flux (-□-), for its prediction by a k-ε-Pr_t model (-¨-), by the AHM model eq. (5) (—), by (5) with velocity time scale (¨¨), and by (5) with temperature time scale (---) for RBC, $\varepsilon_{\theta i}$=0, *Ra*=10^5 and *Pr*=0.025 [54].

With detailed statistical analyses of our DNS data for Rayleigh-Bénard convection (RBC) at different Prandtl numbers and for an internally heated fluid layer (IHL) we contributed to a better understanding of all of these models and proposed model improvements. An overview of proposals for nuclear application relevant improvements regarding the influences of anisotropy, buoyancy and Prandtl number is given in [24]. The influence of the buoyancy contribution to the modelling in AHM models is compared in Figure 7 to the k - ε - Pr_t approach with a constant Pr_t value of 0.9. For the analysis of all curves $\varepsilon_{\theta t}$ was neglected in eq. (5). It gets evident that the Pr_t concept fails to approximate the heat flux distribution. Any time scale in eq. (5) gives better results. The hidden influence of the buoyancy contribution to the modelling of the triple correlation $\overline{u_3'^2 T'}$ in the diffusion term of the vertical heat flux equation was also investigated. By analysing the complete transport equation for this triple correlation, an improved model could be deduced [64]. The standard Daly and Harlow model (DH) gives inadequate contributions to the heat flux diffusion in IHL and problematic ones in RBC, whereas the buoyancy extended model (DHE) gives qualitatively improved contributions, Figure 8. Further buoyancy related analyses were concentrating on the destruction term $\varepsilon_{\theta t}$ of heat flux transport equation [63]. The developed model improvements were already implemented in the TMBF model and used.

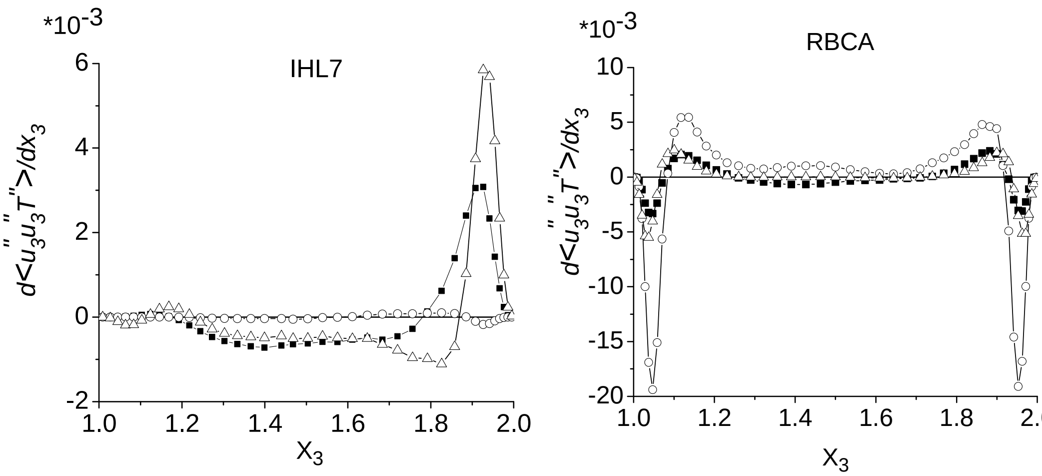

Figure 8 : Profiles of the partial derivatives of triple correlation $\overline{u_3'^2 T'}$ and its modelled values for IHL and RBC analyzed from DNS; DNS (▪), DH (○) and DHE (△) [64].

The influence of the Prandtl number on the modelling in any of the here discussed heat flux models is investigated by analysing all terms in the transport equation for temperature variance $\overline{T'^2}$ for buoyant flows [62]. It was found that the ratio between kinematic k/ε and thermal $\overline{T'^2}/\varepsilon_\theta$ time scales strongly depends on *Pr.* To avoid application of models for this dominating but problematic time scale ratio to calculate ε_θ from ε, one should use a separate transport equation for ε_θ. It was also found that non-equilibrium phenomena make the turbulent diffusion in such buoyant flows important. The developed model improvement was in a modified form also implemented and used in the TMBF [49]. A more recent promising extended diffusion approach for the $\overline{T'^2}$ equation was deduced by the two-point correlation technique [65]. In studying the influence of the chosen time scale on the AHM it turned out that neither the kinematic time scale, nor the thermal one gives adequate vertical heat fluxes, but that the mixed time scale as used in eq. (5) gives the best reproduction of the DNS data [54], Figure 7.

The challenges which are remaining for improvement are obvious: We need better models in the commercial codes which are applicable with sufficient accuracy to buoyant flows and to LM flows. Adapco is coming up with a code version containing somewhat like the Kenjeres model [58]. ANSYS has since years a β-release of a full second order heat flux model. The many already developed single model improvements for buoyant and low-*Pr* flows may not fit together; so there is some work to be done to adapt, test, calibrate, and validate the models for wide application fields. Experiments with LM are usually not suited to determine higher order closure terms in the models as discussed here. The reason is the insufficient resolution in time and space of those sensors which are available for LM. Therefore, we need DNS for higher, more relevant values of *Re* and *Ra*. Part of those simulations should be performed on somewhat more realistic channel geometries; the problem is, that the coding to analyse all the closure terms in such transport equations is lengthy and complicated. Therefore it was only developed for a few fundamental research codes. This deficit in adequate turbulence data is one of the reasons, why for a long future, still experiments are required in combination with models for convection in large and complex containers, as was also stated for other reasons in [22]. It may be that plume dominated convection in large pools, i.e. the convection in pools which are much larger than the macroscopic wavelengths of the coherent plume-like structures, can never be sufficiently calculated by URANS, but will need some kind of LES. Finally, buoyant flows are sometimes robust against changes in boundary conditions, sometimes they are very sensitive like in the analysis for an alternative sump cooling concept for EPR in which it was necessary to treat the conjugate heat transfer in the fluid and in the structures [66]. So it is hard to decide in advance when conjugate heat transfer is required or when the conduction in the enclosing solid structures needs not to be calculated. Such modelling or simplification decisions are the reason why it will always be necessary to have some prototypic more or less realistic model experiments to validate not only the models and codes, but also to validate the assumptions made by the CFD code users.

4. DNS or LES-based CFD and HYBRID Methods

There are simulation issues which cannot be solved by RANS and URANS because Reynolds time-averaging leads to unsuited variable definitions or problematic interpretation of the closure models and of the results. To the first class belong time-dependent three-dimensional flows in which the time scales of interest are near to or inside the upper part of the turbulence spectra representing the large scales or low-frequent changes of the field variables. An example is the above mentioned natural convection in large pools [51], [52]. The method which is in principle thought to be suitable for such problems is the Large Eddy Simulation LES. It may be due to similar reasons that there are also flows which are up to now a challenge for URANS like the velocity fields in detached and reattaching flows and flows with spontaneous unsteadiness, i.e. unsteadiness which is not due to time-dependent boundary conditions [67]. In addition there are especially in the nuclear field sometimes complex prototypical flows with several interacting physical processes, so that the flow type or the underlying flow regime cannot be easily classified to select an adequate model according to the best practice guidelines [34]. In such cases one usually expects higher accuracy and reliability from LES. A well experienced team from Tokyo Institute of Technology states e.g. that DNS is the adequate tool to investigate not understood mechanisms, similarly LES, whereas RANS is the tool for analysing well understood mechanisms [15]. Indeed, LES is increasingly used in the nuclear field due to the reasons mentioned above. Unfortunately, the numerical effort is enormous. Currently it is a matter of research and development to find more universal and numerically more efficient methods. Solutions are to be expected in the field of the HYBRID methods combining computational areas in which RANS models are applied with areas in which LES is used, like the Detached Eddy Simulation (DES) [68] or the Scale-Adaptive Simulation (SAS) method [69]. Some of the challenges from above may profit from such recent methods and developments. Therefore, in the following chapters some peculiarities are discussed for application of LES to nuclear LM flows, like on resolution criteria, on the turbulent Prandtl number for the subgrid scales, on extended subgrid scale heat flux modelling, and some on the HYBRID methods.

4.1 Resolution criteria

Before discussion of the modelling which is used in LES applications to nuclear LM issues, one should shortly consider some of the spatial resolution requirements for adequate resolution of turbulence in DNS and LES. Theoretical criteria can be found in textbooks, but the criteria found in practical DNS and LES applications differ from these quite considerably. Practically relevant criteria for the velocity field are well established in academia since decades, like the criteria for simulating temperature fields in flows of different *Pr* [26], [70], [71]. The criteria were revisited in the light of the extensive published practical experience and summarised for applications of DNS and LES in nuclear engineering in [32]:

The basic requirement for a DNS is to resolve in space and time all relevant scales of turbulence in the velocity field, pressure field, and in all involved scalar fields. Thus one would have to resolve all scales from much above the macroscopic length L in Figure 4 down to the smallest scales in the velocity field, which is characterised by the Kolmogorov length $\eta = \left(\nu^3/\varepsilon\right)^{1/4}$, or in the temperature field, which is characterised in low-*Pr* flows by the temperature microscale $\eta_T = \left(a^3/\varepsilon\right)^{1/4} = \eta/\mathrm{Pr}^{3/4}$. Insufficient resolution of the large scales is rather critical as these carry most turbulence energy. The practically found required resolution of small scales does not reach the specified microscales; it is much coarser: In most applications it is found sufficient to resolve only part of the small scales, so far as the dominant coherent structures are resolved. The mean grid width $h=(\Delta x_1\ \Delta x_2\ \Delta x_3)^{1/3}$ should be:

$$h \ \leq\ 6.26\left(\nu^3/\varepsilon\right)^{1/4} = 6.26\,\eta \qquad (6)$$

As the discretisation in time is coupled to the one in space, more than 3 orders of magnitude in computing time can be saved. A full small scale resolution may only be required for some analysing purposes, e.g. when the dissipation should be determined with high accuracy. This modest sensitivity at small scales is due to the small energy content in those scales. Where the acceptable resolution limits really are, this depends on the numerics of the code. In case of even coarser grids, when the limiting wave number $k_{max}=\pi/h$ of the grid is far inside the spectrum, SGS models have to be introduced to perform LES instead of DNS. In the spectra sketched in Figure 4, an LES is only required for the velocity field.

The influence of *Pr* on the temperature spectra is strong, as well as the dependence on *Re* and on the wall distance *y*. At low *Pr* it may be possible to resolve the complete temperature spectra, as indicated in Figure 4. The validated limit for a DNS of the temperature field is:

$$h \;\leq\; 3.45\left(a^3/\varepsilon\right)^{1/4} = 3.45\,\eta_T = 3.45\,\eta\,/\,\mathrm{Pr}^{3/4} \tag{7}$$

As the dissipation is a local value depending on *Re* and on wall distance *y*, the required mean grid width for a 'thermal DNS' depends on *Re*, *Pr* and *y*. Indeed, the first LES for channel flows with low-*Pr* fluids showed that even on coarse grids full resolution, i.e. thermal DNS, is achieved for sodium over a wide range of technically relevant *Re*, whereas for PbBi or Hg the temperature field is only in some parts of the channel fully resolved, in other parts it needs small SGS contributions [26], [71]. A SGS heat flux modelling which is suited for simulations in the transition range between DNS and LES with automatic adaptation to the local resolution is discussed in the next chapter.

There seems also to be a small influence of *Pr* on the size of the large scales in the temperature field [32]. With decreasing *Pr* the streamwise two-point correlations of *T'* extended in some simulations over larger distances, or larger periodic computational domains were required in other simulations to get domain-independent results. This request for larger computational domains is only relevant if part of a channel is simulated; it is of no relevance for simulating convection in closed containers.

An advantageous feature of low-*Pr* simulations is that the strong conductivity leads to thick thermal wall layers, Figure 1. Like in RANS there is usually no serious problem with formulating the wall conditions for the temperature field, because the conductive wall layer is usually also well resolved, independent whether the velocity field applies wall functions or not. So, thermal wall functions are seldom required at low-*Pr* flows. Thus, one may achieve at low *Pr* LES with or without wall functions for the velocity field combined with DNS of fully resolved temperature fields without wall functions. This means, there may be no modelling parameter at all in the thermal field.

4.2 Pr_{tSGS} -based SGS heat flux models

In this chapter the LES simulation method is discussed in the variant which uses the turbulent Prandtl number concept to approximate the SGS heat fluxes. Applications of this method aim on adequate and reliable modelling of many locally time-dependent issues in flows of different *Pr*; many examples are discussed e.g. in [22]. To those flow problems belong the mixing, stratification and thermal striping issues in large plena, in which URANS is of limited accuracy [50] or the mixing problems in T-junctions for which LES seems to be now the accepted standard method [72], [73]. Other tasks for LES are in some decay heat removal conditions in large pools cooled by buoyant convection where URANS may fail [51], [52], or the unstable und unsteady impinging jet flows in ADS target window cooling.

The scalar SGS flux modelling, which is mostly available in the CFD codes, is basing on the turbulent Prandtl number concept. Similar like in RANS, see equations (1, 2), a SGS eddy conductivity is introduced for the volume or surface averaged SGS fluxes, which is calculated by means of a prescribed turbulent Prandtl number for the SGS, Pr_{tSGS}. Its value for common fluids with *Pr* around one is quite different to the value used in RANS. Starting from the early LES work in meteorology [74] to later fundamental research work [75] and first technically oriented applications [71], values for Pr_{tSGS} from 0.4 to 0.5 are well established. Nevertheless, the RANS value of 0.9 is sometimes erroneously applied in LES. The problem of choosing an adequate value can roughly be avoided by using dynamic determination of the value of Pr_{tSGS} [75].

For low-*Pr* flows it could be concluded from the energy spectra, Figure 4, that even at high *Re* the total resolution of *T'* may be possible. From the figure it follows that this strongly depends on *Re*, *Pr*, wall distance *y*, and on the local resolution by the grid $k_{max}=\pi/h$. Thus, there will be a wide parameter range in which an LES of the velocity field can be combined with a DNS of the temperature field. So, the turbulent Prandtl number depends also an all those parameters; it is the regulating parameter to adapt the SGS heat flux model to full resolution of *T'*, to local partial resolution, and to full LES.

A model, which considers all these parameters, is the one-equation SGS heat flux model in [26]. In [76] a concept was developed to calculate the model coefficients of a one-equation SGS shear stress model by means of the theory of isotropic turbulence and by using the Kolmogorov spectra as the only empirical input. Following this concept, a theory could be developed to calculate also the coefficients of the SGS heat flux model [77], [78]. The theory contains all above discussed influences and is applicable from DNS, through the DNS-LES transition, up to full LES. The results were validated for many such mixed DNS/LES and full LES over a wide parameter range of technical interest [26], [71]. The theory for the coefficients of both model parts, for the momentum and for the scalar flux model, were combined and simplified for isotropic grids [79]. The resulting model indeed gives a correlation $Pr_{tSGS} = f(Re, Pr, y, h)$ which can reproduce the resolution behaviour as discussed on the basis of the spectra [32].

$$\mathrm{Pr}_{tSGS} = \frac{0.226\ \left(1-11.535\ \mathrm{Re}_0^{\ -1}\ (h/l_0)^{-4/3}\ \varepsilon_0^{\ -1/3}\right)}{1/2-2.606\ \left(\mathrm{Re}_0\ \mathrm{Pr}\right)^{-1}\ (h/l_0)^{-4/3}\ \varepsilon_0^{\ -1/3}} \qquad (8)$$

With $l_0=D$ and $u_0=u_\tau$ the Re_0 becomes Re_τ and the non-dimensional local dissipation $\varepsilon_0(y)$ becomes $\varepsilon^+(y)$; *h* is the local mean grid width *h*(*y*). On coarse grids or high *Re* and *Pr* the correlation gives Pr_{tSGS}=0.452, which is within the published experience. Similar to equation (2) for RANS, the SGS heat flux is proportional to 1/ Pr_{tSGS}. The evaluation of equation (8) for two Re_τ, two grids with different resolution *h*, and two positions in the channel y^+ in Figure 9 shows, at small *Re* the SGS heat flux is zero on the fine grid up to large *Pr* values, in this example up to around *Pr*=0.4. The values for the fine grid and for the lowest *Re* go for large *Pr* beyond 1/0.452, and for y^+=200 up to infinity, because the velocity field is nearly completely resolved and thus the turbulent Prandtl number concept is no longer applicable. The ten times larger Re_τ allows for thermal DNS on the fine grid up to *Pr* around 0.02. On the four times coarser grid the SGS heat flux reaches at this Re_τ already its full value as it is used in LES at high *Re* or high *Pe*. The SGS contribution is largest near the wall at y^+=30 and becomes smaller for larger wall distance, as expected from the behaviour of the *y*-dependent spectra. As mentioned above, the underlying SGS model including the theory to calculate its coefficients was validated over a wide parameter range by practical DNS and LES applications; and thus this universal and flow independent correlation for Pr_{tSGS} is also well validated.

In [80] the dynamic one equation SGS shear stress model of the code OpenFOAM is combined with a turbulent Prandtl number concept for the SGS heat flux. The resulting heat flux model can be considered as a simplified form of the LM version of the one-equation SGS heat flux model used in [26]. A method was introduced to calculate the coefficient of the scalar flux model by means of assumptions for time scales and spectra. From this the following correlation can be deduced: $1/Pr_{tSGS}=(4\alpha/\beta)^{1/2}Pr^{4/9}$, where the Kolmogorov constant is chosen to be α=1.6 and the Batchelor constant β=1.3. This correlation approximates roughly the behaviour of equation (8) at low *Re*, Figure 9. Due to the missing dependence on *Re* and on the resolution by the grid, the correlation cannot predict full resolution at low *Re* and at medium LM Prandtl numbers when very fine grids are used. At technically more relevant large *Re* and for coarse grids the predicted Pr_{tSGS} values may be too inaccurate because the SGS heat flux is e.g. for *Pr* around 0.02 seriously underestimated. Thus, even the qualitative behaviour of $1/Pr_{tSGS}$, as it is expected from the spectra in Figure 4, is not reproduced.

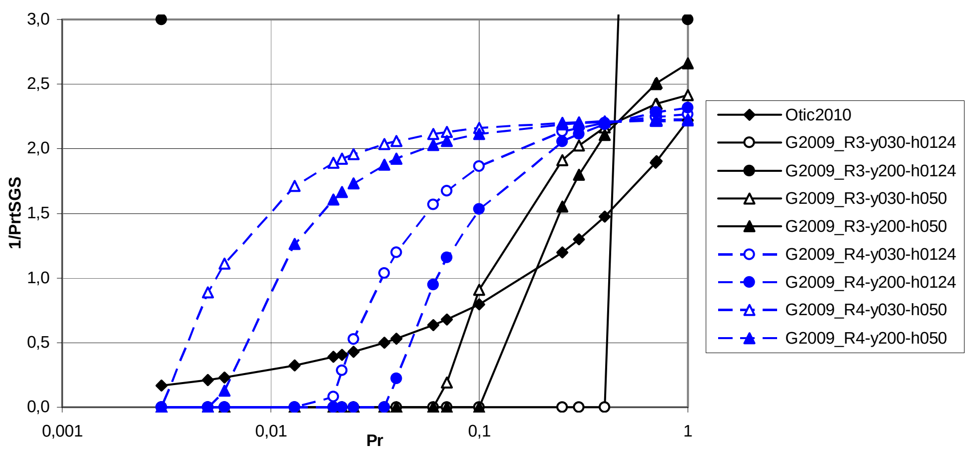

Figure 9 :Inverse of turbulent SGS Prandtl number Pr_{tSGS} over *Pr* for Re_τ=1000 (R3, solid lines) and 10,000 (R4, dashed lines), wall distance y^+=30 (y030, open symbols) and 200 (y200, full symbols), and resolution *h/D*=0.0124 (h0124, circles) and 0.050 (h050, triangles) analyzed from the correlations by Otic [80] and by the author [79].

Like in RANS, one may expect that also nuclear LM applications of LES may be very insensitive against modifications of the SGS heat flux model coefficients. In [80] an insensitivity against Pr_{tSGS} was concluded from low-*Re* simulations for *Pr*=0.022. An analysis of the used grids by means of the above given resolution criteria shows that even the velocity field has near-DNS resolution and thus the temperature field will be fully resolved. This total resolution is confirmed by Figure 9 because the low-Re_τ data used to analyse equation (8) are roughly the ones from those simulations. Thus, such a insensitivity concluded from near-DNS simulations may be misleading, but indeed, there are LM channel flow simulations at higher *Re* from the transition range between DNS and LES which show strong insensitivity against heat flux model coefficients [26]. Similar robust behaviour was found e.g. in buoyancy and surface tension-driven flows in a rotating Czochralski-apparatus at *Pr*=0.013 [81]: Changing Pr_{tSGS} from 0.4 to 0.9 had no effect on the results. The influence of the coefficients of the heat flux model is obviously much smaller than the influence coming from numerics, because it is also found that a 2nd order upwind scheme leads to inadequate results.

Thus, among the remaining challenges there is one that the insensitivity against heat flux model coefficients, which is found in many academic near-DNS simulations applying Pr_{tSGS}, may be very limited. That in some parameter ranges even coefficients are acceptable which are wrong by factors, this is promising. Nevertheless, there exists no systematic analysis whether this holds also for technically more relevant high-*Re* simulations and for simulations on coarser grids. Other challenges are not directly through the Pr_{tSGS} problem, but are at large *Pe* and medium size LM-Prandtl numbers on coarse grids due to the need of thermal wall functions, which cannot always be avoided. Using wall functions for thermal striping issues leads to reduced *T'* at walls [73], [82]. So, improved wall modelling is required to allow for more realistic transfer functions of thermal fluctuations from the fluid to the walls like in [83]. This is one of the issues which is still thought to require model experiments for validation. For this purpose one may use some model fluids [10], or one needs realistic geometries and realistic fluids [22]. To provide the instrumentation for gaining the required validation data is a further challenge because LES needs more detailed turbulence statistics with sufficient resolution in space and time than RANS needs.

4.3 Extended SGS heat flux models

LES is thought to be rather powerful and reliable for predicting or reproducing complex physical phenomena in complex geometries. Nevertheless, there are physical phenomena which may not only be dominated by the resolved scales, but which may also be relevant in the SGS. Examples for such nuclear issues may be the strongly anisotropic shear stresses [84] and heat fluxes in strong mixing, or in the local temperature distributions in fuel bundles with spacers [85]. Others are the strong buoyancy influences with stable stratification in pools, e.g. of core melt [51], and in horizontal pipes [22]. When such issues shall be solved by LES, currently the only available tool for the scalar fluxes in the large codes is the concept of SGS turbulent Prandtl number, which is an isotropic flux modelling, but more sophisticated models may be needed.

There are some analyses and model developments available to improve LES methods to allow for full anisotropy of the momentum and scalar fluxes. Like in RANS, the transport equations for all second moments are used, i.e. for all components of the SGS shear stress tensor and of the SGS heat flux vector (SGS-RSM and SGS-RHM = SGS Reynolds Heat flux Models). As in RANS there also exist models in which the transport equations for the second moments are reduced to algebraic expressions by assuming local equilibrium. These SGS-ASM (SGS Algebraic Stress Models) and SGS-AHM models enable to some extend for anisotropy. For neutrally stratified meteorological conditions (*Pr*=0.7) it is found in [86] by systematically reducing the complexity of the equations that the algebraic SGS models are an acceptable and necessary compromise to mimic the required anisotropic SGS fluxes. Accordingly, a later developed meteorological model, basing on algebraic SGS fluxes, was quite successful [87]. The first full second order SGS-RSM and SGS-RHM was also applied to neutrally stratified meteorological conditions [88]. It was concluded from coarse-grid simulations with wall functions, that such a tremendous effort would not be required. Nevertheless, this model was extended by a moisture transport cycle and cloud formation and used as a powerful tool to study the physical processes in the planetary boundary layer [89]. In [90] it is shown that the combination of SGS-RSM and well resolved wall layers leads to a superior method to reproduce the anisotropy near walls. And just recently in [91] such a model is extended to a non-zonal hybrid RANS/LES method which gives convincing results for the anisotropy in channel flows.

The analyses and experience of simulating strong buoyancy influences with unstable and stable stratification indicate the same required sophistication of modelling. Standard dynamic formulations of the Smagorinsky model were found inadequate for neutral meteorological conditions and needed model improvements [92]. Applying a dynamic Smagorinsky model with a Pr_{tSGS} based heat flux model to a weakly stratified open channel flow shows that stratification effects become more dominant in the velocity field with decreasing *Pr* [93]. This experience indicates that like in RANS it has to be expected from the SGS analogue of eq. 5 that for buoyant flows at least an SGS-AHM model with a transport equation for the SGS temperature variance ${}^{V}\overline{T'^2}(\underline{x},t) = 1/2\ {}^{V}\overline{\left(T - {}^{V}\overline{T}\right)^2}$ will be necessary (superscript v- means average over mesh cell volume and ' means deviation from volume mean, i.e. fluctuation in the SGS). In combination with the transport equation for the SGS kinetic energy ${}^{V}\overline{E'}\,(\underline{x},t)$ this may also help to have in low-*Pr* fluids different SGS fluctuation time scales in the velocity and in the temperature fields.

The objective of a research project at IKET was to develop such a two equation algebraic SGS heat flux model which accounts for the anisotropy of the scalar fluxes, for the influence of the Prandtl number of the fluid, and for the influence of arbitrary thermal stratification [94]. Thus the model should consist of an algebraic SGS heat flux approach and the transport equations for SGS kinetic energy and SGS thermal variance. Such a model should considerably improve the critical situation mentioned above. Basing on analyses of DNS data, firstly some RANS counterparts of the critical terms in SGS models were investigated and some improvements for RANS models were developed, see chapter 3.2. Finally the RANS models were transformed in accordance with the above mentioned historic literature to corresponding SGS models and were implemented in the SGS temperature variance equation from [88]. The proposed final model (in enclosure 22 of [94]) consists of a two-equation SGS counterpart of equation (5). There, the standard modified high-*Re* Rotta model was introduced for the SGS-dissipation ${}^{v}\overline{\varepsilon}$ and the model from [88] for the dissipation of thermal variance ${}^{v}\overline{\varepsilon_\theta}$. As a consequence the temperature variance cancels out from the mixed time scale. This limits the applicability of the algebraic model to large *Re* and, more serious, to *Pr* around one. In [68] and in [77] it became obvious that the destruction or dissipation models are the most sensitive ones in one-equation SGS models. Therefore, often improved dissipation modelling is used, like in [95] for a wider *Re* range and for including additional physical influences, like from wall roughnesses. In addition the dissipation of thermal variance depends on *Pr*. Therefore, other than in [94], here it is recommended to use the complete SGS counterpart of equation (5) and to introduce in the mixed time scale the results of the actually applied dissipation models for ${}^{v}\overline{\varepsilon}$ and the *Pr*-dependent one for ${}^{v}\overline{\varepsilon_\theta}$:

$$ {}^{v}\overline{u_i' T'} = -\sqrt{\frac{{}^{v}\overline{E'}}{{}^{v}\overline{\varepsilon}}\frac{{}^{v}\overline{T'^2}}{{}^{v}\overline{\varepsilon_\theta}}}\left[C_1\ {}^{v}\overline{u_i' u_j'}\frac{\partial\ {}^{v}\overline{T}}{\partial x_j} + C_2\ {}^{v}\overline{u_j' T'}\frac{\partial\ {}^{v}\overline{u_i}}{\partial x_j} + C_3\, g_i \beta\ {}^{v}\overline{T'^2} + {}^{v}\overline{\varepsilon_{\theta i}}\right] \qquad (9) $$

The SGS heat flux destruction term ${}^{V}\overline{\varepsilon_{\theta i}}$ follows from [88]; the low-*Pr* adapted term could e.g. be taken from [96]. The formally deduced transport equation for the SGS temperature variance ${}^{V}\overline{T'^2}(\underline{x},t)$ is taken from [77]. The modelled form of the equation follows the one in [88]; the turbulent diffusion could be replaced by an adaptation of the new Helmholtz equation model which was deduced for RANS by the two-point correlation technique in [65]; the thermal dissipation uses the model from [88] with adaptation to variable *Pr*, or the thermal dissipation is approximated by the dissipation of kinetic energy with the use of the time scale ratio *R*. Unfortunately, this ratio of the thermal and momentum time scales is at low *Pr* in forced flows [29] and in buoyant flows [62] strongly dependent on *Re* or *Ra*, on *Pr*, and on wall distance *y*. An adaptation of the new RANS model for thermal dissipation [54] for application in the SGS model was not considered. All the model adaptations for variable Prandtl number have still to be verified and the complete model has still to be validated. Therefore, it has to be checked whether this extended model meets its expectations.

The remaining challenges of this chapter are obvious: There are nuclear issues which require such extended SGS models. How urgent this necessity is, this may change with time, because on one hand side an increasing accuracy is requested, on the other hand side the practical resolution of LES is increasing due to larger available computing performance and thus more and more of the complex physics is included in the resolved scales. Nevertheless, like in RANS, such numerically efficient and robust models are currently needed in the large CFD codes to get better LES modelling of anisotropic and stratified flows in fluids of different *Pr*. The adaptation of the SGS models to low-*Pr* fluids is more rudimental than really settled, so contributions from academia are still welcome.

4.4 HYBRID methods

There are issues remaining, which may not be solved with the requested accuracy or reliability by RANS or URANS, and some which can up to now not at all be simulated by LES with adequate numerical detail. Examples for the first category according to [67] are massively detached flows. Such flows occur in bents, T-junctions, or behind strong cross section changes like in diffusers, behind spacers in fuel bundles, or in the cross flow in heat exchangers. To achieve more accurate secondary currents due to anisotropy effects is also relevant in many industrial applications [97]. These are usually not the applications in which LES would be routinely applied in the nuclear community because too fine grids are required to simulate such flows adequately.

Related to the second category is the simulation of large buoyant pools and plena, which is mostly at the limits or beyond the requested resolution of LES. This holds especially for any analysis of the hydrogen transport in the geometrically complex reactor containments. Even the recalculation of corresponding much smaller benchmark experiments is a real issue [98]. In such nuclear applications to large or huge computational domains exists a wide range of flow length scales. Thus LES applications are mainly at or beyond the limits of current computer power. So the HYBRID methods combining LES and RANS with suitable anisotropic modelling in both model parts could be a solution. The issue to model more accurately the correct *Pr* dependence of the heat transfer is a minor one compared to these more serious problems.

The development of HYBRID methods is a rapidly emerging field [99], because it allows for many model combinations on the RANS side and on the LES side. It lets expect promising progress. On the other hand, getting an overview is itself a challenge. E.g. zonal methods, which means in each zone a certain model is applied, and non-zonal methods, in which the application domain of the different methods is not fixed, are compared in [100]. It is concluded that zonal models may be more suited to complex flows because they need no special adaptations of the used SGS models. The computing effort is drastically reduced by HYBRID methods down to about 1% of that one of pure LES. In a recent review [101] the methods are classified in blending turbulence models, in interfacing RANS and LES, and in second generation URANS models. The Detached Eddy Simulation DES [68] belongs to the interfacing models. In its original version it uses a highly specialised RANS model for air foil applications. The performance in such applications is promising; therefore it is applied also to many other flows and variants of the method are made available in the large commercial codes. The Scale-Adaptive Simulation method SAS [69] belongs to the second generation URANS models. The turbulent time scales which can be simulated are beyond those resolvable by URANS and below those resolvable by LES. This rather young method is also already made available for industrial application in a commercial code.

The potential of HYBRID methods shall be demonstrated by two examples which are related to the issues mentioned above. For a 3d diffuser a HYBRID method was compared with LES in [102]. Despite being much less computing intensive, the results for the separation pattern and turbulence data of the HYBRID method compared well with those of the LES, and both compared well with DNS and experiments. In thermal convection at high Rayleigh numbers it is found in [103] that HYBRID methods give a wider fluctuation spectrum than a specific 3-equation URANS. In addition, the energy transfer between potential and kinetic energy is more realistic. This energy exchange is found to become more important at lower *Pr* [93]. This promising behaviour of HYBRID models in really challenging flows shows why it is concluded in [97] that the method will find its place in industrial applications and that some kind of HYBRID will be the turbulence model in the next CFD code generation. There will be very different combinations of RANS and LES; SAS will be one of those.

Of special interest for the discussed nuclear issues are HYBRID methods in which anisotropic modelling is used in the RANS and/or in the LES part. Simple and numerically efficient anisotropic RANS models are the non-linear EVM and Explicit Algebraic Stress Models EASM. According to the classification in [104] they are a link between isotropic EVM and RSM models. Consistently formulated EASM URANS models are in general found to be robust and efficient [105]; thus they should be suitable for a combination with LES to a HYBRID model. Indeed, the HYBRID method with a non-linear EVM in the RANS part shows good results in a 3d diffuser application near walls where the anisotropy is largest [106]. In [107] an EASM-RANS and LES combination is applied to the separated flow over periodic hills in which a new dynamic treatment of the interface between LES and RANS is used. Also this model gives a good reproduction of the anisotropy near the walls as found in the benchmark results. Thus, the extremely fine grids which would be needed by LES near walls can be replaced by coarser ones in the near-wall RANS zone. An example with an anisotropic SGS model is the newly developed Partially Integrated Transport Modelling PITM [91]. This continuous approach with seamless coupling was investigated for a 2-equation SGS model, and for a full RSM SGS model with an additional transport equation for the dissipation in the SGS. The simulations for channel flows showed anisotropic turbulence in good agreement with DNS data.

Some of the remaining challenges to solve the discussed flow issues by HYBRID methods are as expected for a rather new method: The method helps to make LES possible at all for some geometrically or physically complex flows; of course, now one expects that the numerical efficiency is increased to enable also parametric use. Some of the underlying URANS models are strongly oriented to special applications, like in the original DES; thus, the implementation of more universal models would help to reduce the additional scientific knowledge which CFD users should have to ensure adequate numerical modelling of their issue. The coupling at the interface between RANS area and LES area needs improved methods to generate the turbulence at the LES boundaries. There may be some *Pr*-dependence in the coupling when the scalar fields are added. Experience with passive and active scalar fields has to be increased. The resolution requirements have to be reconsidered because one is now much more asking, how coarse may a grid be; a first step in this direction for HYBRIDs is given in [108]. We are just at the begin of a development which gives a qualitative increase in computability and which is surprisingly rapidly entering the industrial application field. This also extends the request for much more detailed validation experiments. The degree in measured detail should fit in minimum to the degree of the numerical representation. So, not only highly resolved local turbulence data are needed, but also field data are of highest interest to complete the knowledge on the involved flow mechanisms so that no important questions are left open. To gain field data in the opaque LM remains a challenge.

5. Conclusions

Most of the issues in CFD applications to nuclear heat transfer are due to complex geometries or due to complex involved physical phenomena. Thus, like in other CFD applications, the availability of a universal modelling cannot be expected. E.g., even in simple channel flows there is contradicting experience with the heat transport in low Prandtl number fluids: In many cases there is a small sensitivity detected against model parameters in the used RANS models; but there exist also parameter ranges in which the scalar flux models react more sensitive. The reason can be understood by considering that nuclear CFD applications with liquid metals or especially with heavy liquid metals operate in a transition zone between two parameter ranges with different scaling laws. So, there will be no simple universal heat flux modelling, but it is required to ensure reliability under all conditions. Accordingly, the Reynolds analogy does not work in this transition range, so that more complex turbulent Prandtl number formulations are required. There are some available for simple channel flows and variable Prandtl number. It became obvious that local applications of such correlations only lead to an increase in quality when the velocity fields are also adequately reproduced. Thus it should still be investigated which correlation has the better reliability in local applications and how sensitive the thermal results are against crude velocity field modelling.

More improved RANS-models are required when the nearly always present anisotropy in the turbulent fluxes becomes important and when strong buoyancy is involved. Heat transfer issues, in which this is relevant, are discussed in the paper. In such cases, a more sophisticated flux modelling like a non-linear eddy viscosity model or an Algebraic Stress Model ASM combined with an Algebraic Heat flux Model AHM including an additional transport equation for the temperature variance is the lowest adequate model degree. Many of the known model terms in transport eq. models need better adaptation to low-*Pr* and buoyancy influenced flows. Some related DNS-based model extensions were shown or mentioned. An improved heat flux model with such features should be made available in the major commercial CFD codes.

LES seems better to be suited for nearly all issues, but for cost reasons it is only for a few applied; some are listed. The discussion of the resolution criteria shows that the simulation of the turbulent temperature fields in low-*Pr* fluids in nuclear apparatuses also operates in a transition range; i.e. the transition between Direct Numerical Simulation DNS and LES. Near the DNS limit the results are highly insensitive against wrong SubGrid Scale (SGS) heat flux coefficients, whereas near the LES limit a stronger influence has to be expected, but it will remain under that found in RANS. A universal correlation for the turbulent SGS Prandtl number is given which covers the complete range from DNS to LES for all types of flows. It depends on the local grid resolution, *Re*, *Pr* and a local turbulence quantity. Issues in which LES for buoyant flows on coarser grids is applied need extended SGS flux models. Adequate models like SGS-ASM and SGS-AHM or even full second order flux models exist in meteorology. Their adaptation to low-*Pr* fluids can be done consistent with the corresponding models in RANS. A first step towards such an SGS-AHM model is discussed. Further research and development is needed before making such models available in the major codes.

There are promising developments going on in the field of hybrid LES-RANS methods. It may be expected that the HYBRIDs make LES more attractive and make it practicable for a wider application field. Some LES applications to large flow configurations will only become practicable in the context of a HYBRID realisation, but flows in the reactor containment will remain a challenge for some more time. With these methods one gains comparable accuracy to pure LES for about only 1% of computing effort. This indirect gain in accuracy asks of course for more accurate modelling so that only higher level models like the above mentioned anisotropic models should be implemented in the RANS part and in the LES part. The correct representation of variable *Pr* shall be a minor problem because it can be widely taken from the used basic model parts.

The adequate application of LES or DNS, and also of HYBRIDs, may be a challenge for some CFD users because it requires much more detailed basic knowledge in turbulence. Thus, the competence of CFD users is more indispensable than before and determines the quality of the results much more than in RANS. The education at our universities should much more consider these methods. Not all the problems with CFD are due to insufficient modelling or meshing; part of the problems in CFD are user-made: E.g. inadequate models may be selected in RANS: So sometimes still isotropic models are applied to fuel bundle flows. Or there are seriously wrong applications of DNS and LES, especially when inadequate boundary conditions are selected at open boundaries. So, the development of best practice guidelines for low-Prandtl number flows and for buoyant flows could help to improve the situation. Nevertheless, uncertainties will remain. E.g., a CFD can never reproduce the complete reality. The user has to introduce simplifications to get a numerical counterpart and has to combine adequate physical models. This all leads to the fact that we need not only a validation of the models, solvers, and codes, but also a validation of the decisions of the code users, i.e. of the users in engineering.

The experiments which are needed to gain data for any kind of validation and benchmarking should be consistent in their resolution with that in CFD. As the resolution in CFD is permanently increasing, not only in space and time, but also in capturing more and more physical phenomena, that one of the experiments should simultaneously increase to gain a higher degree of details, accuracy and amount of data. Especially field data become more important, but providing these is a real challenge in liquid metal flows, like the complete instrumentation to determine highly resolved local flow variables. Thus, even simple experiments with LM may be problematic because the actual geometry or exact positions of sensors cannot be proven or the velocity field statistic is not sufficiently known. Large experiments may have too sparsely distributed instrumentation. So, not only benchmark exercises for large experiments, like for plena, sump cooling, and containment flows, sometimes pass into experiment evaluation workshops, but also those for simple LM flows. Thus, there is also a strong need for validation of experimental data, especially of data from LM flows. Due to the needed improved education of the CFD users, to validate their simplification of the physical problem to a numerical counterpart, we always will need detailed and highly instrumented experiments for each new prototypic flow configuration and for each new combination of involved physical phenomena.

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