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# DIRECT NUMERICAL AND LARGE EDDY SIMULATIONS IN NUCLEAR APPLICATIONS

G. Grötzbach, M. Wörner

Forschungszentrum Karlsruhe
Institut für Reaktorsicherheit
Postfach 3640, D-76021 Karlsruhe, Germany,
Tel. 0049-7247/824477

**ABSTRACT**

Direct numerical and large eddy simulations are powerful tools for analyses of turbulent flows at low, respectively large Reynolds or Rayleigh numbers in fundamental research. The current status of both methods and recent extensions are compiled. The progress achieved with subgrid scale models and numerics makes the method attractive for applications to nuclear research and engineering. Examples of realistic technical flows are discussed. Open problems are mainly related to more general subgrid scale models for large complex containers, to the wall and inlet conditions for high Reynolds number and buoyant flows, and to discretisation schemes for local refinement of spatial resolution. As a classical example for the use of direct simulations, results are presented for a turbulent internally heated horizontal fluid layer. The analysis of the closure terms in the transport equation of the kinetic energy demonstrates major difficulties of the conventional statistical modelling for partially stably stratified convection.

## 1. INTRODUCTION

In developing better safety features for new reactor concepts, most activity is on thermal fluid dynamics. By introducing passive auxiliary systems, i.e. which can be operated without additional power, one tries to ensure by design measures that the after heat can be removed by natural convection even in severe failure situations. The features of such new concepts are analysed by model experiments of different scales, sometimes up to 1:1, and increasingly by thermal hydraulic codes.

In this paper we begin with a description of some typical problems in nuclear thermal hydraulics which are dominated by turbulent momentum, heat, and mass transfer. The trends become obvious to apply more sophisticated turbulence models in the corresponding numerical analyses. The geometrical and physical complexity of the phenomena to be investigated necessitates more detailed prediction capabilities of the numerical models. Consequently, one finds in literature growing interest in using and improving the large eddy simulation method (LES) to nuclear problems. Next we give a description of the basics of the methods of direct numerical simulation (DNS) and large eddy simulation of turbulent flows focusing on recent developments of subgrid scale models, boundary conditions, and numerics which come mainly from basic research. More detailed discussions are given in review papers e.g. by Ciofalo (20), Ferziger (36),(37), Grötzbach (52), Lesieur & Metais (76), Mason (82), Moin & Mahesh (89), Nieuwstadt (95), and Schumann (109). Then, we will discuss some new applications of LES to nuclear problems and point out difficulties of such applications. Subsequently we will concentrate on analyses related to cooling of core melts inside the pressure vessel and in the core catcher. Finally, we will conclude on further developments which are required to get the methods of direct numerical and large eddy simulation more suited for nuclear or other technical applications.

## 2. METHODS AND TRENDS IN NUCLEAR THERMAL HYDRAULICS

Some characteristics of nuclear thermal hydraulics indicate the requirements for engineering codes which should be fulfilled for detailed quantitative analyses. The geometries to be considered range from simple channels of different dimensions over open or closed containers to large ones with complex geometrical boundaries. In large containers one has to model forced, mixed, and natural convection at large Reynolds (*Re*) and Rayleigh (*Ra*) numbers, including flows like jets or mixing layers. The complex internal structures like fuel pin bundles, guiding tubes for internal instrumentation systems, and heat exchanger bundles form small gaps which are sometimes treated by porous body models. The channel flows may extend to small *Re* and *Ra*. Thus, one finds a wide spectrum of channel dimensions, of characteristic non-dimensional numbers, and flow types in the same application.

Examples are analyses of passive decay heat removal within a complete model of the European Fast Reactor by means of the FLUTAN code by Weinberg et al. (124), investigations of thermal mixing in the upper plenum of the PHENIX reactor with the TRIO-VF code by Roubin & Astegiano (103), or investigations of local problems, like the thermal barrier in a pump housing with the N3S code by Archambeau et al. (2). Most investigations are combined turbulent momentum and heat transfer tasks in three-dimensional geometry.

Typical for nuclear safety investigations is also that one is often faced with exotic or prototypical situations: Prototypical with respect to geometry, type of fluid, and flow conditions. Therefore, there exist no validated physical models for such conditions. An important example is the cooling of a molten core inside the vessel of the reactor or in a special core catcher device. It is very hard to perform model experiments with real materials like molten $UO_2$ or steel, or with multi-phase multi-component mixtures of these fluids. In any case one would avoid using real nuclear heating to get internal heat sources in larger amounts of these fluids. Therefore, simple model fluids are used widely applying Joule heating or transient cooling down of the test fluids to mimic the internal heat sources; for an overview of recent experiments see Nourgaliev et al. (99). As such modelling of internally heated fluid layers hinders detailed local heat transfer and turbulence analyses, we have nearly no turbulence data available to develop and validate modern turbulence models locally. So, rather integral experimental information has to be used for validation of the models and codes.

The numerical models used in the nuclear field to analyse in detail turbulent heat transfer are basing on Reynolds averaged Navier Stokes equations (RANS). Most applications are run with first order turbulence models, like with variants of the $k$-$\varepsilon$ model and a turbulent Prandtl number concept (2),(103),(124). Recently a combination of the $k$-$\varepsilon$ model and a second order heat flux model was developed for forced and buoyant flows by Carteciano et al. (16). The model behaved very well in a benchmark in which blind predictions for an experiment were required (4). The problem with the first order models is that one has to classify the practical application into this or that flow type. This is mostly not possible in large containers with internal structures. Therefore, in trying to achieve more universal models with better prediction capabilities one also considers the application of full second order closure models basing on RANS. Current experience with these models is that second order models require very fine grids for practical applications (2); as a consequence wider applications can only be expected on future parallel high performance computer systems.

For these and other reasons, there is a growing interest in the nuclear field in Large Eddy Simulation (LES). This method is not based on the time-averaged equations, but on the local and instantaneous Navier Stokes equations filtered spatially, typically over the grid widths. With this method one simulates the spatially resolved scales of turbulence and uses models only for the non-resolved, hopefully more universal small scales, so-called subgrid scale models (SGS). As turbulence is time-dependent and three-dimensional, LES have to be performed always in three dimensions and time-dependent. The engineering flow problems in nuclear heat transfer or safety are also mainly three-dimensional; and according to the experience in (2), many flows become time-dependent even when stationary inlet conditions are used. Therefore, one has anyway to use three-dimensional time-dependent representations of the task, and performing an LES instead of applying a RANS-based first order turbulence model should not result in too excessive extra computing efforts. Breuer et al. (15) found the LES being a factor of eight slower than a two-layer $k$-$\varepsilon$ model for flows around surface mounted obstacles, but giving much more reliable results and more information; and Ciofalo found only a factor of two compared to a standard $k$-$\varepsilon$ model for an element of a crossed-corrugated heat exchanger (21). The results of the LES were again superior to the ones of the RANS model.

## 3. DIRECT SIMULATION METHOD

The basic equations describing laminar and turbulent flow with heat transfer are the conservation equations for mass, momentum, and energy. For a Newtonian fluid with constant material properties they can be written in terms of the primitive variables, i.e. in terms of $u_i$ for the components of the velocity vector ($i$=1,2,3), $p$ for pressure, and $T$ for temperature:

$$\partial_i u_i = 0 \qquad (1)$$

$$\partial_t u_i + \partial_j (u_i u_j) = \partial_j (1/\sqrt{Gr}\ \partial_j u_i) - \partial_i p - (T_{ref} - T)\ g_i/|g| \qquad (2)$$

$$\partial_t T + \partial_j (T u_j) = \partial_j (1/(\Pr \sqrt{Gr})\ \partial_j T) + Q \qquad (3)$$

The symbols are $t$ for time, $g_i$ for components of the gravity vector, $Q$ for dimensionless specific internal heat source, $Gr$ for Grashof number $|\underline{g}|\beta\ \Delta T_w\ D^3/\nu^2$, $\beta$ for volumetric expansion coefficient, $\Delta T_w$ for difference between wall temperatures, $D$ for channel height, $Pr$ for Prandtl number $\nu/\alpha$, ν and α for the diffusivities of momentum respectively heat, and $T_{ref}$ for reference temperature. The validity of the Boussinesq approximation is assumed in the buoyancy term. Eq. (1 to 3) are normalised by the channel height $D$, velocity $u_o = \left(|\underline{g}|\beta \Delta T_w D\right)^{1/2}$, time $D/u_o$, and temperature difference $\Delta T_w$.

The method of direct numerical simulation of turbulence is directly based on eq. (1 to 3). Since the turbulent fluctuations carrying the kinetic energy are mainly produced at large scales, but this energy is dissipated at small scales, the method has to be based on the full conservation equations for mass, momentum, and energy. All scales have to be resolved by the grid, from the largest macroscopic structures of the flow down to the smallest scales of turbulence. The features of turbulence require to solve these equations always in three dimensions and in time.

If these requirements are met in the simulations, no subgrid scale models and no wall models are needed. Such simulations do not depend on any model coefficient. The first direct simulations were those by Orszag & Patterson (100) for decaying isothermal isotropic turbulence, those by Lipps (78) for weekly turbulent and those by Grötzbach (46) for fully turbulent Rayleigh-Bénard convection of air, and those by Kim (69) for forced convection in channels with heat transfer. Overviews on more recent direct simulations are given by Kasagi (64) and Moin & Mahesh (89). Examples for direct simulations of compressible flows are those e.g. by Friedrich & Bertolotti (38) and of purely buoyant flows by Wörner & Grötzbach (132).

## 4. LARGE EDDY SIMULATION METHOD

### 4.1. Separation of resolved and subgrid scales

To derive equations for large eddy simulations, one has to separate the flow variables in a resolved and an unresolved part. This can be done by applying a low-pass filtering procedure as introduced by Leonard (75) and non-linear or linear filter functions, or by using the formal volume integration method as applied by Schumann (108). The more general method is the filtering approach, because the actual grid width $\Delta x_j$ and the width of the filter can be chosen separately (82). The filtered field $\overline{f}$ for a quantity $f = \underline{u}, p, T$ is defined by the spatial filtering procedure:

$$\overline{f}\left(\underline{x},t\right) = \int f\left(\underline{y},t\right) G\left(\underline{x}-\underline{y}\right) d\,\underline{y} \tag{4}$$

Here we split the quantity *f* in its filtered large scale part $\overline{f}$ and in its subgrid scale fluctuation part *f'* by $f = \overline{f} + f'$. Using non-linear filter functions *G(y)*, like the widely applied Gaussian filter, the filtered non-linear terms in the Navier Stokes or thermal energy equations take the following form:

$$\overline{u_i\, u_j} = \overline{u}_i\, \overline{u}_j + \overline{\overline{u}_i\, u_j'} + \overline{\overline{u}_j\, u_i'} + \overline{u_i'\, u_j'} \tag{5}$$

$$\overline{u_j\, T} = \overline{u}_j\, \overline{T} + \overline{\overline{u}_j\, T'} + \overline{\overline{T}\, u_j'} + \overline{u_j'\, T'} \tag{6}$$

The first term on the right hand side represents the resolvable part of the instantaneous local turbulent shear stresses and heat fluxes, the last term represents the subgrid scale contributions which have to be modelled. The filtered non-linear terms look formally like the Reynolds terms which are deduced by time-averaging. The main difference is that time-averaging is replaced by filtering over typically mesh cell volumes *V*. Therefore, the meaning of the unknown terms is different from those in RANS models: they do not contain the complete momentum and heat exchange due to the turbulent fluctuations, but only that part corresponding to the unresolved small scales. This means, for decreasing grid width and hence for better spatial resolution, the models for the subgrid scale terms have to converge to zero, i.e. to a direct simulation.

The second and third terms on the right hand side in eq. 5 and 6 result from using non-linear filters and contain filtered cross-products between filtered resolved and unresolved quantities. They vanish when linear filters like the box filter are used. Germano (40) shows that details of the filters are not important compared to the importance of the subgrid scale models. Indeed it was shown on the basis of simulation results for complex channels by Neto et al. (94) that the cross-products can be neglected. Recently Härtel & Kleiser (57) found theoretically that in inhomogeneous flows near walls the energy transfer between grid scales (GS) and subgrid scales (SGS) is independent on the type of filter applied. Nevertheless, Ghosal & Moin (42) developed a filter method with variable filter width to improve accuracy for inhomogeneous flows in complex geometries.

### 4.2. Subgrid scale models

In LES the dissipation of turbulent kinetic energy is partly in the unresolved scales, whereas the production is in the resolved scales. The SGS models become more important with increasing Reynolds number or increasing grid width, and have to model more of the total dissipation. In the coarse grid limit the subgrid scale models should account for about the complete turbulence like the models used for the Reynolds terms. Accordingly, most existing subgrid scale models are formally deduced from statistical models. The main difference is that the length scale is not the mixing length as used in Reynolds models, but it is a representative for the local grid width, because this is a measure for the unresolved turbulent exchange of momentum and heat.

#### 4.2.1. Algebraic SGS models

Most subgrid scale models are first order models because they are based on an eddy diffusivity concept, introducing an effective eddy diffusivity and conductivity for the subgrid scales:

$$\overline{u_i'\, u_j'} = 2\ \upsilon_t\ S_{ij} \tag{7}$$

$$\overline{u_j'\, T'} = a_t\ \partial\overline{T}/\partial x_j \tag{8}$$

where $S_{ij} = 0.5\left(\partial\overline{u}_i/\partial x_j + \partial\overline{u}_j/\partial x_i\right)$ is the local and instantaneous deformation rate of the resolved flow field.

The first subgrid scale model introduced for the momentum fluxes is the still widely used Smagorinsky model (115). It incorporates the mean grid width $h = V^{1/3}$ as a length scale for the subgrid scale diffusivity and a coefficient $C_S$,

$$\upsilon_t = \left(C_s\ h\right)^2\ S \tag{9}$$

where $S = \sqrt{S_{ij} S_{ij}}$ . The model was first used by Deardorff (26) for channel flows. Following the ideas of Schumann (108) it was later extended by Moin & Kim (87) to include the van Driest damping function to reduce SGS contributions near walls. Examples for newer applications to slightly complex flows are those for a crossed corrugated heat exchanger element (21), for the flow around a cylinder to determine the forces on an off-shore platform by Lu et al. (80), and for a turbulent plane jet by Weinberger et al. (125).

The Smagorinsky model became more attractive again when Germano et al. (41) developed a method to calculate dynamically the local coefficient $C_S$ from the actually simulated resolved scales by applying a test filter which is typically two times coarser than the one used to separate the SGS from the GS. This dynamic model gets the subgrid scale contributions down to zero in those areas in which the resolution allows for direct simulations. In principal, this dynamic calculation of the instantaneous model coefficients can be combined with any SGS model. An analysis of the dynamic Smagorinsky model on anisotropic grids was performed by Scotti et al. (111). An anisotropic dynamic model in tensor form was developed by Abbà et al. (1) to improve the accuracy in channel flows near walls.

Further improvements can be achieved by introducing backscatter of kinetic energy from the small scales to the large scales, which was found to occur within the buffer layer in plane channel flows, e.g. by Piomelli et al. (101), or in stably stratified fluid layers, e.g. by Kaltenbach et al. (63). It is argued that in such cases a stochastic backscatter is necessary (82). There exist proposals for backscatter models in (56),(74),(83),(109). Successful applications of dynamic SGS models are numerous, e.g. those by Breuer & Rodi (14) and by Jones & Wille (62). There seem to occur some problems with coarse grids and large Reynolds numbers, see Sullivan & Moeng (117), and with transitional flow in flat plate boundary layers, see Voke et al. (123). Combinations of dynamic models with backscatter also exist, e.g. the model by Mason included in the code comparison of Nieuwstadt et al. (96). Such comparisons as well as the one in (62) and especially the experience by Breuer (11) with applications to the flow past a cylinder indicate that for practical high Reynolds number LES the influence of changing the type of a model is considerably less than of changing the spatial discretisation scheme.

4.2.2. Transport equation based SGS models

More sophisticated first order models aim to provide some decoupling of the subgrid scales from the local grid scales in time or in space. Examples for one-equation models based on a transport equation for the kinetic energy in the subgrid scales are the one for channel flows at high Reynolds numbers (108), or that for moderate Reynolds numbers including rough walls (53). Those authors use the theory of isotropic turbulence to calculate all local coefficients of their models. The calculation accounts for the local grid details including the actual finite difference approximation, the resolution capability, and the grid anisotropy. Such one-equation models allow to treat backscatter in a natural manner. Corresponding methods and tests are given in Ghosal et al. (43) and Davidson (25).

Full second order models do not apply eq. (7,8), but solve modelled transport equations for the cross-correlation terms. Such a model was developed and used by Deardorff (28). From the knowledge and computing capabilities available at that time he concluded that full second order SGS models do not give any advantage over simpler models. Just recently Fureby et al. (39) reconsidered a simplified version of Deardorff's model. Contrary to Deardorff they found major advantages of their second order model regarding the treatment of turbulence anisotropy in channel flows near walls. Their promising model does not need any information on the distance to the next wall.

A good compromise between first and second order modelling was found e.g. by Schemm & Lipps (104), Sommeria (116), and Schmidt & Schumann (105). They use algebraic simplifications of the second order equations together with a one- or two-equation model. These models, which reproduce meteorological flows quite well, are the counterparts to the so-called algebraic stress models, ASM, in Reynolds modelling.

4.2.3. Subgrid scale heat flux models

The turbulent subgrid scale heat flux, eq. (8), is often calculated by using a turbulent Prandtl number $Pr_{tSGS}$ for the subgrid scales:

$$a_t = \upsilon_t / Pr_{tSGS} \qquad (10)$$

The values to be used for $Pr_{tSGS}$ are about 0.4, see e.g. (20),(28),(53). The values have to be modified slightly when e.g. backscatter models are included (109). The small value means that at small scales the transfer of heat is much more intensive than that of momentum. It is found for fluids with molecular Prandtl numbers of about one that modifications of the value of $Pr_{tSGS}$ do not change simulation results too much for forced flows at large Reynolds numbers (53). This approach is often used in meteorology, e.g. by Deardorff (27), Moeng (86), and also in applications of LES to technical flow problems, e.g. by Ciofalo & Collins (22), Neto et al. (94), Murakami et al. (91), by Voke & Gao (122), by Braun & Neumann (12), and by Grand et al. (44).

More complicated subgrid scale heat flux models also exist, similar to the first order and second order SGS shear stress models discussed above. The conclusions on the necessity and relevance of these models are the same, because all these investigations, except (39), (108), were performed for flows with heat transfer.

Careful comparisons of four codes using different subgrid scale models and different numerics show that their results agree quite well for simple meteorological conditions (96); this points to the robustness and universality achieved currently with the method of LES at least for simple meteorological conditions.

The influence of the type of fluid, i.e. the molecular Prandtl number *Pr*, needs special discussion. The form of the spectra of temperature fluctuations at small scales strongly depends on the Prandtl number. For highly viscous fluids, this is for large values of *Pr*, the temperature spectra extend to much smaller scales than the velocity spectra, whereas fluids with small values of *Pr,* e.g. liquid metals, effectively filter off small scale fluctuations so that the smallest scales in the temperature field are much larger than in the velocity field. This behaviour could be treated by applying the dynamic filtering of Germano to the heat flux model, see e.g. (20) and with the self-adaptive subgrid scale heat flux model of (45). The latter uses a one-equation model in combination with the extended theory of (108) to calculate the model coefficients by using the theory of isotropic turbulence and the local value of the time averaged dissipation $< \varepsilon >$. This model and the calculation of the coefficients were successfully used to perform simulations for forced convection in plane channels and annuli at Reynolds numbers from some $10^4$ to some $10^5$ and for fluids with Prandtl numbers from 0.007 to 7 (45),(49). This theory, applied to the SGS shear stress and heat flux models, is also used to judge in advance on the suitability of grids for adequate direct simulations (48),(49). This SGS model was extended for stably stratified flows by applying modified length scales, Seiter (112).

#### 4.2.4. Other subgrid scale treatment

The SGS models discussed above are applied in physical space. Models were also developed for spectral methods; they model the subgrid scale contributions in wave number space. Such models, like that by Chollet & Lesieur (19), are based on the Eddy Damped Quasi Normal Markovian (EDQNM) theory by Kraichnan (71). Because of their complexity from the point of view of an engineer these models are not widely used. Such models were e.g. applied to study the diffusion in isotropic turbulence (77) or by Naitoh & Kuwahara (93) to study the flow in a cylinder of a piston engine. A version for applications in physical space is the structure function model by Normand & Lesieur (97). The selective structure function model is applicable to highly intermittent, transitional, and separated flows, and the filtered structure function model to spatially developing flows. These models, which were also extended for irregular grids, are now more often used; applications are given in the overviews (44),(76).

All subgrid scale models, which were discussed above, explicitly introduce physical assumptions to model the momentum and heat fluxes by the unresolved scales. To minimise numerical diffusion one usually uses numerical discretisation methods in space which are of second or fourth order. There are also methods which do not involve subgrid scale models, instead the numerical scheme has sufficient numerical diffusion or damping to mimic the effective diffusion due to the subgrid scales. In using third order upwind schemes, like the one introduced by (66), one can successfully simulate many turbulent flows without using SGS models, like the impinging wall jet by Muramatsu (92) and the flow around and through cars by Hashiguchi (58). Similarly Boris et al. (11) found that the Piecewise Parabolic Method (PPM) also has intrinsic SGS features. Of course, the numerical diffusion does not always sufficiently meet the requirements of the subgrid scales; therefore, all results gained from such pseudo-direct simulations have to be checked carefully.

## 5. BOUNDARY CONDITIONS

Formulating boundary conditions for DNS or LES is a more serious problem than with Reynolds models, because one needs time-dependent wall conditions and inlet or outlet conditions which account for realistic local turbulent fluctuations.

No-slip wall conditions and prescribed wall heat fluxes or surface temperatures can be discretised without further approximations when the viscous and conductive wall layers are resolved by the grid. Corresponding spatial resolution criteria were specified and tested from an engineering point of view (48),(49). To analyse terms of statistical models near walls from the results of direct simulations, much finer grids are required than the specified two to three mesh cells to be used in the viscous and conductive wall layers. At large turbulence levels and with coarse grids near walls, suitable time-dependent formulations of wall laws have to be applied. Methods for high Reynolds number flows are the one in (108) for shear stresses and in (53) for heat fluxes at different Prandtl numbers and wall roughness. Universal extensions for pure buoyant convection can hardly be determined (112). These approximations relate the instantaneous local shear stresses and heat fluxes to the velocity and temperature fluctuations in the next fluid mesh cell by using time-averaged wall laws. Therefore, this approach is only applicable to fully developed statistically stationary flow. The same restriction holds also for the two-layer model by Manhart & Wengle (81) which uses a power law velocity distribution. Other approximations were developed, but it turned out to give no significant improvement in practical applications (20).

Channels with an inlet and an outlet require specifications for all physical variables for every mesh cell on such a boundary at each time. Currently no sufficient theoretical tools are available to formulate such boundary conditions for realistic turbulent flows. Therefore, periodic boundary conditions are applied in the mean flow direction when ever possible. When real inlet and outlet conditions have to be considered, approximations have to be chosen.

For the inlet, several procedures of different complexity were realised, depending on the physical problem to be considered. Surle et al. (118) used constant values at the inlet. Constant radial profiles from separate calculations with a Reynolds model were taken in (92). To get time-dependent inlet values Dai et al. (24) used constant values superposed by sinusoidal fluctuations, and Neto et al. (94) superposed fluctuations with white noise features. Some methods to access the tremendous problems with such conditions are discussed in a recent overview (89). When real turbulent inlet signals are required, the only available solution is to perform a separate DNS or LES for a periodic channel with roughly the required flow parameters and store the results for one plane perpendicular to the mean flow direction at each time step. These data are used as time-dependent inlet conditions. Realisations of this method are reported e.g. in (14),(91),(122). By analysing a turbulent plane jet the latter method was found superior to using artificial inlet conditions (125).

Approximations for the outlet are either to assume that all gradients normal to the outflow surface are zero. This works roughly with incompressible flows, see Schmitt & Friedrich (107). However, it might become problematic due to reflections in case of compressible flows. The more accepted method is to apply a convective outflow condition, like in (11), but serious problems were reported from applications to backward facing steps by Bärwolff et al. (3) and to mixing chambers by Moin & Kravchenko (88). Both apply additional buffer regions to decouple the upstream area from the distortions at the outlet. Non-reflecting new outlet conditions were developed (1).

## 6. NUMERICS

So far it looks like the progress of LES towards engineering applications would strongly depend on the availability of adequate subgrid scale models and boundary conditions. In fact, real retardation comes mainly from the numerics because one needs the combination of accurate discretisation and integration schemes in combination with large numerical efficiency, especially as regards to the solvers for the system of equations. The solvers are the dominant part which in complex geometries determine the computational costs. They are not discussed here, because they would require a separate careful evaluation.

Accurate discretisation and solution algorithms are required to solve the basic equations or the filtered equations including the respective SGS models in space and time. Of course, spectral schemes are very accurate, and are therefore used for simulations of the transition from laminar to turbulent flow in channels, see e.g. Kleiser & Zang (70) and the comparison in (110). However, they cannot be applied to an arbitrary, complex geometry. For simple channels they are often used in combination with finite difference schemes, like in the models or applications in (69),(77),(86). Thus, for engineering applications one has to rely on finite volume or finite element based discretisations.

For spatial discretisation, mainly finite difference and finite volume schemes are used. They are efficient and flexible, especially for structured non-orthogonal grids (23),(14). Higher order schemes have been shown to need less nodes than lower order schemes to gain the same spatial resolution of the smallest scales (89). The order of the schemes must be even to have small numerical diffusion. The numerical diffusion must be much smaller than the diffusion introduced by the SGS model. This obviously holds only for fourth and higher order schemes, but the accuracy of the lower order schemes can be improved by using pre-filtering with a filter width of $2\Delta x$ (88). Third order schemes are widely used in Japan; their inherent numerical diffusion mimics SGS features implicitly and without any control, see remarks above. They were recently extended to a multi-directional finite difference scheme for skewed flow (58). Among the upwind schemes the second order QUICK scheme has unacceptable strong diffusive features (14). Higher order upwind-biased schemes, which are designed to have reduced aliasing, are even worse than second order central schemes, Kravchenko & Moin (72). In comparing central and upwind schemes of several orders for the flow past a cylinder, strong influences of the scheme were found e.g. on the separation length and on the turbulence level (11). It is concluded that for an LES the numerical dissipation produced by a scheme is more crucial than its formal order of accuracy, and these influences are much stronger than those from using different subgrid scale models.

More efficient spatial discretisation in critical areas, e.g. in the layer near solid surfaces, is recently achieved with finite volume schemes by introducing local grid refinement methods. Deck (30) used it to resolve the details of the flow around a square cylinder and Fureby et al. (39) in the sublayer of a channel flow. Multi-block grids are realised in the pseudo-DNS which are extensively used in the Japanese automotive industry for the flow around cars, through the interior, or through the engine compartment (58). Moving multi-block grids are applied on curvilinear coordinates for pseudo-DNS of the vortex formation in a 4-valve piston engine by Meinke et al. (85). The step to use hybrid unstructured grids is also gone by Ducros et al. (33) in an LES of a pipe flow. Zonal grid embedding by using B-splines looks promising because it is of high accuracy order and it conserves energy even for incompressible flows, but it seems currently to require too much computational effort (88).

The finite element method is the most flexible, but less computationally efficient method to discretise spatially a complex flow domain. The large flexibility to concentrate the elements where they are needed lets one expect to get practically efficient and accurate simulations. The method was used with a Smagorinsky model for an unsteady wake behind a cylinder by Kato & Ikegawa (65). Special test filters were developed to make the method applicable with the dynamical model on parallel computers, and LES-suited mesh generators, see Jansen (61). An application of the finite element based multi-purpose code N3S to the square cylinder benchmark is evaluated in Rodi et al. (102).

For integration in time, schemes are required for the convective terms which are at least of second order. A DNS as well as a LES has to capture all resolved fluctuations in time, because one does not want to filter off the highest spatially resolved frequencies. Therefore, usually all convective terms are treated by explicit methods, like by the Euler-leapfrog method or the Adams-Bashforth scheme. The Courant stability criterion ensures a sufficient resolution in time.

Nevertheless, there are reasons to use implicit schemes for some terms. With DNS one uses fine grids near walls, but there the viscous terms become dominant over the convective terms. When the diffusion terms are treated explicitly, their stability limit strongly reduces the time step width. This is avoided by using implicit time integration of the diffusion terms like the Crank-Nicholson scheme (69). The same arguments hold for the energy equation, especially with liquid metals; there, it is only the implicit treatment of the thermal diffusion which enables such simulations on current computer systems (126). Another example is the implicit treatment of terms with azimuthal transport in pipe flows because the azimuthal grid width goes to zero near the axis, whereas the others remain finite and determine the resolved scales, Eggels et al. (34). Sometimes even the convective terms are treated implicitly in LES when one accepts to lose the highest resolvable frequencies only locally in those areas in which the grid is locally refined (21),(89).

## 7. SOME REACTOR RELATED SIMULATIONS

As in other research and application fields, there were large expectations on the possibilities of DNS and LES growing up in nuclear thermal hydraulics. From a methodological point of view and from the rapidly increasing computational power, one could expect around '90 that it should be possible and reasonable to modify newer multi-purpose codes to analyse prototypical three-dimensional time-dependent engineering problems by means of LES (51). And after first promising results in several groups, in '95 even expectations were formulated that this could also be a method to access two-phase problems, Hassan et al. (60).

### 7.1. Applications of increasing complexity

#### 7.1.1. Channel and bundle flows

Going back to the roots of large eddy simulation in Europe, one should remember that Schumann started his developments in 1970 in the Institute for Reactor Development at the Nuclear Research Centre Karlsruhe, now Institute for Reactor Safety. After having set up a model and code basis, we were rather early using our first LES, and later also our DNS, to investigate problems motivated by actual nuclear applications. Of course, for a long time these investigations were bound to simple geometries. E.g., LES were used to study pressure fluctuation induced forces on the inner rod in axial forced flow through an annulus, to study anisotropic eddy diffusivities in channels with secondary currents or spanwise thermal inhomogeneity, and to clarify the principal mixing capabilities in a strongly buoyancy influenced vertical flow in the downcomer of the HDR-reactor. Combined LES of the momentum field and DNS of the thermal field helped to improve eddy conductivity concepts for liquid metal forced convection in channels. Compilations and discussions of this work are given in (49),(110).

Recent LES in literature are for increasing geometrical complexity. By using an LES for two parallel rectangular channels coupled by a narrow gap Biemüller et al. could show experimentally and by LES, coherent periodic vortices travel along the gap causing these systematic fluctuations (10). Investigations for heat exchanger tube bundles in cross-flow are performed by Hassan & Lee (59). For single pins they determined the spectra of the drag and lift forces from 2d and 3d simulations by using the GUST code. Recent simulations for bundle flows and comparisons between RANS models and LES are presented at this conference, Laurence (73).

#### 7.1.2. Convection in pools

The direct numerical simulations in the nuclear field concentrated, as in other fields, on providing data for statistical turbulence models, here especially for buoyant convection. The first applications were motivated by core catcher investigations for Fast Breeder Reactors (47). Results of recent simulations for internally heated fluid layers will be discussed later. The simulations for Rayleigh-Bénard convection first focused on learning to perform adequate DNS (48), because this convection type is experimentally well investigated, in contrast to the internally heated fluid layer. Later simulations aimed at investigating and improving statistical turbulence models for pure buoyant convection. The temperature variance equation was analysed for air (54) and for sodium (129), the transport equation for the destruction of temperature variances for both fluids (130), and the heat flux budget (127). The terms in the kinetic energy equation were analysed (128) and the differences of the pressure transport in Rayleigh-Bénard and internally heated convection layers (132). Some of the analyses resulted in proposals for model improvements, like for the dissipation by Ye et al. (134), some were realised in the multipurpose code FLUTAN (16). Turbulence data for calibration of second order turbulence models are also provided by pseudo-direct simulations with FLOW-3d for a cubical box (98).

### 7.1.3. Thermal striping

Meanwhile, multi-purpose codes are available which are extended for LES. Thus, the geometrical complexity of the investigated problems increases. A series of separate effect analyses for isolated problems from complex nuclear flows are performed with the TRIO-VF code and variants of the structure function model (44),(76). These investigations mainly concentrate on the thermal interaction of temperature fluctuations with solid structures (thermal striping). This is a serious problem in large reactor systems because it may limit the lifetime of components by thermal fatigue. Coherent vortices are simulated in the mixing layer behind a backward facing step in (94). Fallon et al. (35) investigate the influence of thermal stratification on the formation or suppression of these vortices. A jet impinging on a wall is investigated with the Smagorinsky model (122) and with the aid of the third order upwind scheme with the AQUA code (92). The mixing in round jets as a model to mimic the exit from single subassemblies at the core outlet is investigated with the filtered and selective structure function model with the TRIO-VF code and a special purpose code, Urbin et al. (120). Good agreement between the results of both codes was found except for steeper spectra from TRIO, because with this code coarser grids have to be used. The transfer conditions of special model experiments with model fluids to sodium conditions was also analysed with TRIO, Tenchine & Moro (119), and good agreement between measured and simulated temperature fluctuations was found.

For a more quantitative analysis of thermal striping it is necessary to treat the turbulent convective heat transfer coupled with the thermal conduction in the solid structures. This is achieved in the applications by Ushijima & Tanaka (121) to the upper plenum flow including the instrumentation plug, in the applications of the finite element code N3S using a dynamic Smagorinsky model to the flow in the thermal barrier in a pump shaft (2), and in the applications of the STAR-CD code using unstructured grids and no SGS model to the flow through a T-junction, Simoneau et al. (114). Of course, with this task LES is superior to any RANS based calculation because the dynamics of interest are a result of the large scale structures and are without additional modelling a direct outcome of a simulation.

Thermal striping investigations for the upper plenum with its complex internal structures are currently at the limit of the computational possibilities. The simpler model experiment CORMORAN was investigated with TRIO with the k-ε model and with the structure function model (118). This holds also for the upper plenum simulation for the PHENIX reactor, in which every subassembly exit was resolved with a grid of 233,000 cells, except that the selective structure function model is applied (103). The time mean results of the statistical and LES modelling types agree well, but the LES offers additional data on the temperature fluctuations as they are necessary for the designer.

### 7.1.4. Two-phase flows

Two-phase or multi-phase flows are those with the highest geometrical and physical complexity. In nuclear engineering and safety they occur frequently, in particle or gas transport in fluids, in phase change phenomena by freezing or boiling, in stratified liquid pools with free surfaces or swimming crusts, up to the challenging problem of jet fragmentation and droplet formation combined with the rapid heat transfer and phase change which may lead to vapour explosions. There is work going on to improve current methods or to develop new ones treating the interfacial phenomena explicitly.

Some applications, in which turbulence has to be included, belong to the area of flows with homogeneously distributed separated phases. The common tools for such flows are multi-field multi-fluid models assuming interpenetrating fields. Turbulence modelling is widely done by zero-dimensional physical models; this means, the interfacial momentum, heat, and mass transfer is modelled by friction factors, Nusselt numbers, and Sherwood numbers respectively. This modelling becomes inadequate at higher void fractions when the topology of the phases develops towards heterogeneous distributions. Similarly, the treatment of turbulence at large scale interfaces is up to now included only in form of such simple models. The use of standard RANS based turbulence models is hindered by the poor knowledge basis we have on turbulence in two-phase flows. Thus, progress is mandatory and there is a good chance for the DNS and LES community to fill this tremendous gap and to provide methods for detailed local analyses in multi-phase flows. However, as the problem is challenging, we are still at the begin of a long development, and the following literature does not always belong to the nuclear field.

Simulations for dispersed phases started early in history of LES with studies of the transport of passive particles in channels, Deardorff & Peskin (29). Recent work on particle dispersion in channel flows is e.g. by Dehning (31) using a one transport equation subgrid scale model. Now, somewhat more complex flows are possible and Chen & Pereira (17) study with the structure function model the particle dispersion in a plane mixing layer. Such numerical investigations require DNS or LES because of the flow instabilities. Similarly, Maxey & Chang (84) treat micro-bubbles passively, this means the bubbles have no consequences on the velocity field. The authors study by DNS and an Eulerian treatment of the bubbles how small scale vortices of isotropic turbulence interact with the bubbles and modify their mean rise velocity.

Simulations of turbulence at free interfaces is a growing subject. The interfaces in the first simulations for sheared and unsheared flow are kept plane, see Banerjee (5) and Lombardi et al. (79). The investigations concentrate on the turbulence statistics in the boundary layers near interfaces and on the mechanisms causing these statistics. For the sheared cases situations are found similar to the ones near solid walls with ejection and sweep cycles, whereas for unsheared cases long living roughly two-dimensional upwellings are observed. Work on wave formation is discussed at this conference, Banerjee (6).

Developments of methods for direct and large eddy simulations of turbulent bubbly flows are ongoing in the authors team. The basic ideas of LES are applied to the turbulence in the liquid phase and also to the phase topology in dispersed two-phase flows. Thus, in a separated phase treatment the large scale interfaces will be resolved and calculated by adequate numerical schemes, whereas the small scale part will be treated by an interfacial area concentration equation. Accordingly, the interfacial exchange terms consist of resolved parts and subgrid scale parts. In a first step we consider DNS and LES of bubbly flows in simple geometries. Finally, the method will be implemented in a code for technical applications. This work is basing on supporting experiments on statistical and local turbulence in bubbly flows, Cherdron et al. (18).

So far we saw that DNS and especially LES is increasingly supplementing research engineers in the nuclear field in those areas in which statistical models have serious problems with accuracy, reliability, prediction capabilities, or even fail from a methodological point of view. This holds mainly for three-dimensional time-dependent flows in complex geometries and with local instabilities. All applicators state that the larger computational expense for LES is compensated by the gain of more information from the simulations.

### 7.2. Experiences and open problems

The subgrid scale models for nuclear flows, especially in large components, should be as universal as possible. Existing models reach a high degree of perfection at low Reynolds numbers, but at Reynolds numbers and flow types of interest it is found necessary to choose certain models. E.g. Voke et al. (123) prefer the Smagorinsky model with manually adapted local coefficients for a transitional stratified flat plate boundary layer, and Fallon et al. (35) prefer the selective structure function model for a backward facing step. Barsamian and Hassan (7) decided to develop a new modelling of the filtered cross-products for cross-flow through heat exchanger bundles. Thus, models which have no wall distances as length scales, as the one in (39) are not yet common and need further assessment.

The wall condition formulation should not depend on the type of flow. For high Reynolds numbers we still have to use modelled wall conditions in which the wall shear is approximated instead of using the no-slip condition. All wall laws hold only for fully developed statistically stationary forced flows. Therefore, wall approximations cannot be applied to separated flows (35). On the other hand, there is a small sensitivity against the type of wall condition applied even in geometrically determined flows (21). If the tendency towards transport equation subgrid scale models holds on, the problem with the wall conditions will grow because wall conditions for higher order models can hardly be formulated. Thus, a solution can only come from the numerical side, i.e. to use efficient discretisation methods, e.g. with local grid refinement or with unstructured grids, which allow to resolve the viscous and thermal wall layers.

Finite channels with a turbulent inlet flow need meaningful time-dependent turbulence data at the inlet plane. This is found in many investigations to be a sensitive requirement, e.g. in (113),(114),(125). Existing approximate methods do not seem to get rid of the problem (89). Thus, the only possible, but expensive solution is still to use simulation data from a separate simulation with periodic boundary conditions for a similar flow. The outlet conditions are less serious, but need some more improvements.

The spatial discretisation schemes should show very small numerical diffusion and should allow for an accurate and efficient discretisation of the geometry. Regarding numerical diffusion and accuracy, many of the single-purpose simulation codes reach a very high academic standard, but this cannot be expected from the robust multi-purpose codes. The quite common QUICK scheme turns out be inappropriate to LES; it damps out all turbulence (11). And second order central schemes do not always guarantee sufficiently small numerical diffusion, as it is shown by the pseudo-direct simulations with the STAR-CD code (114). So, one has to expect that the coefficients of subgrid scale models depend on the discretisation and integration schemes actually used in the codes. On the other hand, the large flexibility and accuracy to correctly reproduce complex geometries is an advantage of the new code generation with unstructured grids. Convincing examples are those by Simoneau et al. (114) who use STAR-CD for a T-junction, those first demonstrations of the capabilities of TRIO_U, but obviously in the structured mode, by Barsamian et al. (9), or those with the finite element code N3S (2). Proceeding to unstructured grids needs special care with the widely used dynamic model because extended test filters have to be applied (61).

Time integration schemes should be applied so that the Courant number is below one in most areas, because otherwise spatially resolvable high-frequent fluctuations are filtered out. Courant numbers slightly above one may only be acceptable locally, where grids are strongly refined (21). As implicit time integration schemes are found in most multi-purpose codes, it is left to the user to choose the adequate Courant number range; the large damping found with the STAR-CD code may come from allowing Courant numbers up to ten (114).

The solution algorithms and solvers used in such codes are optimised for large robustness, often at the expense of efficiency. On the other hand, an LES needs about the same spatial discretisation as a good RANS calculation, but it needs more time steps (103). With the current computer generation we are at the limits of what can be realised with RANS models. Thus, many users try to simplify the problem when it shall be investigated also by LES.

Using coarser grids is a dangerous simplification, because multi-purpose codes have non-negligible numerical diffusion. This may lead on coarse grids to time-independent results, as observed with the first T-junction calculations (113). A reduction of the problem to two dimensions is also found; e.g. the cross-flow simulations for heat exchanger bundles with the GUST code are performed in 2d (8). Such simulations should be interpreted with special care because 2d and 3d turbulence behave different; e.g., 3d treatment is necessary even when the mean flow stays rather 2d in the transitional flow behind a circular cylinder (11).

Symmetry is also sometimes assumed as a measure to save CPU-time. All upper plenum simulations were performed with azimuthal symmetry, e.g. with 60° symmetry (121), 90° symmetry (103), and 180° symmetry (119). From these simulations, as well as from the results for the flat plate boundary layer (123) it is concluded that the symmetry assumption leads to insufficient results. The only rule which can be given here is, the macroscopic length scale of the flow must be much smaller than the periodicity or symmetry length chosen (48),(49).

## 8. CONTRIBUTIONS BY DNS TO COOLING OF CORE MELTS

In giving some example results we come back to the classical field for DNS applications in simple geometries, i.e. the analysis of turbulence data for flows or for parameter ranges for which no other sources of data are available to improve statistical turbulence models.

### 8.1. Problem

Single-phase convective cooling of an internally heated fluid was intensively investigated by model experiments in the seventies for fast breeder reactors; now, for new water cooled reactors, the parameter range has to be extended to larger Rayleigh numbers $Ra = g\beta Q D^5/(\nu\alpha\lambda)$ and other geometry. In addition, detailed turbulence data are needed to provide adequate computational tools. An overview of experiments is given in (99). The experiments mainly aim on determining the heat fluxes across the boundaries, dependent on Rayleigh number and surface position. Temperature data are provided seldom; turbulence data were only determined by Kikuchi et al. (67),(68) for the untypical case with an adiabatic lower boundary.

The first consistent set of turbulence data for this flow were provided by direct simulations for a periodic channel with small horizontal extensions (47),(49). They show that the lower 80% of the layer is stably stratified and about half the height therein is dominated by a counter gradient heat flux. Thus, statistical turbulence models using gradient assumptions are not adequate for this type of flow; this was also confirmed by practical applications of such models by Dinh & Nourgaliev (32). Turbulence data for calibration of second order turbulence models are also provided by those simulations, as well as by pseudo-direct simulations with FLOW-3d for a cubical box (98). The earlier simulations are verified by a simulation in a channel with large horizontal extension (50). These results, and those by the LES in (112) confirm that this flow shows the seldom feature of a decreasing macroscopic wavelength with increasing Rayleigh number. This allows for a reduction in the size of the computational domain and consequently for finer grids at large *Ra*.

Recent DNS reach Rayleigh numbers as high as $Ra=10^9$, and are therefore suited to analyse higher order turbulence models. The mechanisms in the flow are investigated in (106) and their interaction with the pressure diffusion in (132). The following analysis of the k-equation is taken from the detailed statistical analyses in (133). Most of the statistical results of this simulation series will be included in the WWW databank (131).

### 8.2. Case specifications

The convection in an internally heated fluid layer is characterised by the Rayleigh number $Ra = Gr \cdot Pr$, the Prandtl number, and the Damköhler number $Da = Q D^2/(\lambda \Delta T_{\max})$, where $Q$ is the specific internal heat source and $\Delta T_{\max}$ is the maximum temperature difference between fluid and wall. For normalisation we use the channel height $D$, the velocity scale $u_0 = (g\beta \Delta T_{max} D)^{1/2}$, and the temperature scale $\Delta T_{\max 0}$. As a result we get the non-dimensional equations (1) to (3) in which the dimensionless heat source is equal to $Da_o/(Pr\ Gr^{1/2})$. To get the non-dimensional temperature maximum close to one, $Da_o$ is determined from the energy balance $Da_o=Nu_b+Nu_t$ by initial guesses for the Nusselt numbers at top and bottom. Here we consider the model fluid water, $Pr=7$, in the fully turbulent regime at $Ra=10^8$. Following experimental correlations for $Nu$ we choose $Da_o=35$ for this Rayleigh number. The bottom and top wall are kept at Temperature $T_w=0$.

Sufficient experience and some experimental information is available to specify adequate grids and to validate the results (49),(50). Nevertheless, an extensive discretisation study was performed investigating all spatial parameters including theoretical expressions for smooth vertical grid width distributions (106). We use $X_{1,2} = 4$ for the horizontal extensions of the control volume to which periodic boundary conditions are applied. The numbers of mesh cells are $N_{1,2}=160$ and $N_3=55$. The vertical grid widths are $\Delta x_{3wt}=0.0057$ and $\Delta x_{3wb}=0.012$.

The simulation with the computer code TURBIT was started on a coarser grid from artificial initial values with zero velocities, with a roughly trapezoidal vertical mean temperature profile, and with random temperature fluctuations superimposed to it. When the simulation reached a steady state in a statistical sense, the results were interpolated to a finer grid. After repeating this procedure, the simulation was continued on the finest grid to obtain results for a certain time interval in which the flow is statistically stationary and which can be used for statistical analysis.

### 8.3. Flow structures

The temperature profile has the minima at both walls and a maximum near the upper wall. This indicates the following mechanisms: The fluid is stably stratified throughout the channel height except for the thin upper layer with cold, heavier fluid. From this layer plumes or thermals develop due to Rayleigh-Taylor instability which move cold fluid into the heated core.

The isosurface for a temperature value of $T = 0.88$ is given in Fig. 1 for an arbitrary time. It shows in only ¼ of the computational domain the principal phenomena and intermittent character of this flow. $T = 0.88$ is found very near the upper cold wall, because the boundary layer is very thin their, and in a larger distance to the lower cold wall, because the boundary layer is thick there. From the temperature profile it is known that hotter fluid is between both isosurfaces. The upper and lower isosurfaces are connected by some plume-like structures in which cold fluid is very fast plunging downward. Plumes with downward movement concentrate in knot-like structures. The plumes are horizontally connected by thin spoke patterns with slower fluid. The spoke patterns exist only in a thin near-wall layer. The colour code marks the values of the dynamic pressure. The pressure values are on average larger near the upper wall; there, negative deviations are found in the spoke areas where e.g. larger negative vertical velocities occur. They are smaller on average near the lower wall; there positive pressure deviations occur where the larger negative vertical velocities exist, i.e., where the plumes plunge down. From such figures one can deduce conclusions on the mechanisms forming the cross-correlations in the transport equation models (132).

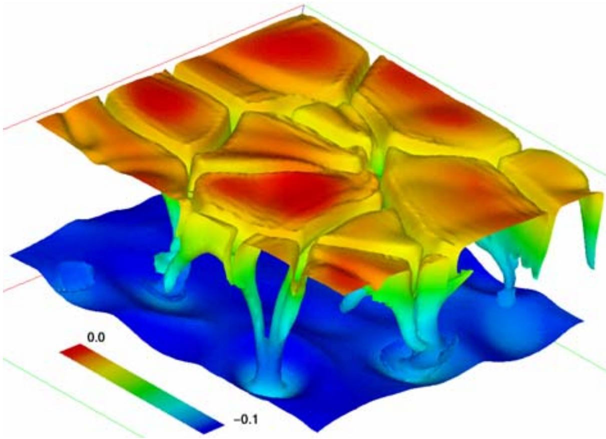


Fig. 1: Isosurface for instantaneous temperature $T = 0.88$, colour code for dynamic pressure, $Ra = 10^8$. One quarter of horizontal cross-section.

The structures found in this simulation have also been found in our earlier simulations and are verified for smaller $Ra$ by comparisons to experiments e.g. in (49),(50). The macroscopic length scale is determined by the typical horizontal extension of the cell-like structures or by the distances between the knots. Figure 1 makes obvious that the cell size is much smaller than the computational domain and that the flow will not be limited by the horizontal size of the periodic domain.

The dynamics of this flow is analysed for several $Ra$ by means of movies. The spoke pattern like structures are attracted by the few dominant plume areas. By withdrawing spokes, small cells contract to knots and remaining cells are enlarged. Within these calm areas new spokes develop due to local Rayleigh-Taylor instabilities. They grow to slice like spokes, match with other spokes, and divide existing larger cells. The plumes don't appear regularly, but some plume areas move slowly in the horizontal direction. Some plumes merge and may form new knot-like plume centres. The dynamics of the flow found here is comparable to that found at a smaller Rayleigh number (50), except that at larger $Ra$ more and more plumes detach from the wall, degenerate to thermals, and do not penetrate deeply into the lower boundary layer (133).

### 8.4. Balance equation of turbulent kinetic energy

The standard turbulence model in most engineering codes is any variant of a $k$-$\varepsilon$ model. It is a first-order model because it is based on eddy diffusivity assumptions for turbulent shear stresses and heat fluxes. As we already saw, the eddy conductivity concept is not adequate for the thermal energy equation, we want to study here the diffusion assumptions in the kinetic energy equation. For fully developed convection in an infinite horizontal fluid layer, the transport equation for $k = 1/2\langle u_i' u' \rangle$ reduces to:

$$0=\frac{\partial}{\partial x_3}\left[-\left\langle u_3' \frac{u_i'u_i'}{2}\right\rangle - \langle u_3' p' \rangle + \frac{1}{\sqrt{Gr}}\frac{\partial k}{\partial x_3}\right] + \langle u_3' T' \rangle - \frac{1}{\sqrt{Gr}}\left\langle \frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}\right\rangle$$

$$D_k \qquad\qquad G_k \qquad\qquad \varepsilon$$

Here $D_k$ denotes the diffusion of $k$, consisting of a turbulent part $D_{k,t}$ and a molecular part $D_{k,m}$. Responsible for the production $G_k$ is the buoyancy force represented by the turbulent heat flux. The dissipation is $\varepsilon$. The prime *Y'* for any variable *Y* denotes in this chapter deviations from the time mean value *<Y>*, i.e. the fluctuation in the Reynolds sense.

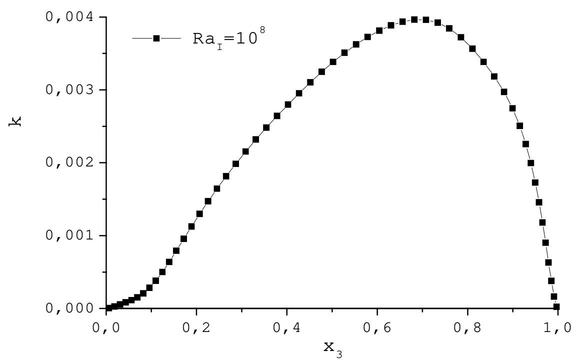


Fig. 2: Vertical profile of the kinetic turbulence energy, *Ra=10*$^8$.

The vertical kinetic energy profile analysed from the simulation results shows an increase from the lower wall at $x_3 = 0$ to a wide maximum value at about 70% channel height, followed by a rapid decrease to the upper wall at $x_3 = 1$, Fig. 2. The position of the maximum is below the one of the heat flux maximum, which is contained as the production term in the analysed energy budget, Fig. 3.

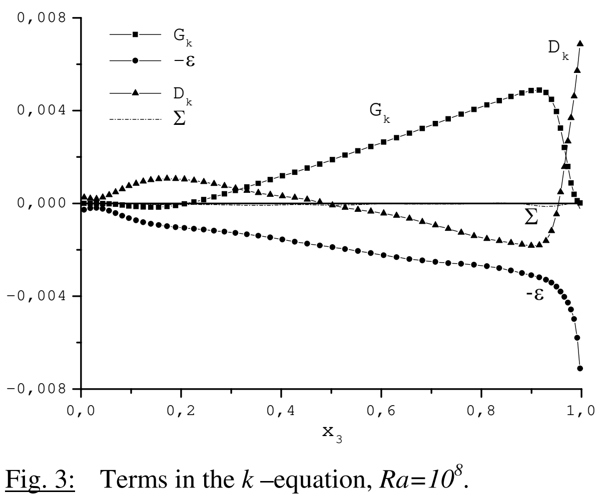


Fig. 3: Terms in the *k* –equation, *Ra=10*$^8$.

The production is zero at both walls, is positive and increasing in the upper part of the channel, and is negative in the lower part of the channel. The dissipation is increasing throughout the channel, forming a sharp peak next to the upper wall. There are only two vertical positions where local equilibrium exists; elsewhere, the diffusion term redistributes the energy. Next to the upper wall it has completely to balance the dissipation. As all terms are analysed independently, the small value of the out-of-balance term $\Sigma = G_k + D_k - \varepsilon$ is a measure for the accuracy of the analysis and indicates that the flow is sufficiently developed.

Terms that have to be modelled in the *k* equation are the cross-correlations in the diffusion term and the dissipation. Here we consider closure assumptions for the diffusive transport. The velocity triple-correlation is the dominant one, Fig. 4; it is large and has large gradients. The pressure velocity cross-correlation is comparably small and has a large gradient only next to the upper wall. The areas in which the pressure correlation is positive or negative are consistent with the discussion of Fig. 1. In contrast to this result, the turbulent diffusion in Rayleigh-Bénard convection is dominated by the pressure diffusion; the reasoning is discussed in (132). Both terms change sign at different positions and can therefore not be modelled together as it is usually done.

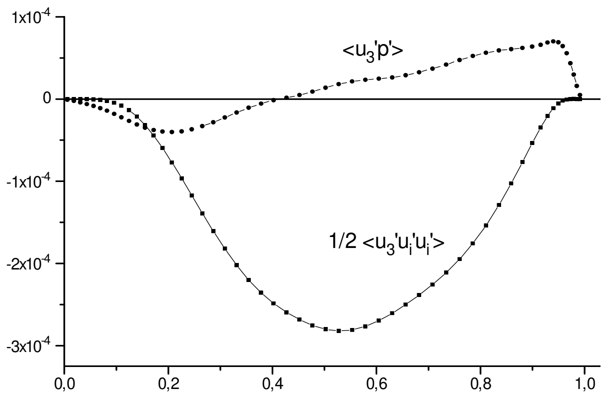


Fig. 4: Terms from turbulent diffusion $D_{k,t}$ for *Ra=10*$^8$.

The model commonly used for closure of turbulent diffusion in the k-equation is:

$$-\left\langle u_3' \frac{u_i'u_i'}{2}\right\rangle - \langle u_3' p' \rangle = \frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_3} \qquad (11)$$

where $\nu_t$ is the turbulent diffusivity for momentum calculated from the standard *k-ε* model,

$$\nu_t = C_\mu k^2/\varepsilon \qquad (12)$$

and $\sigma_k$ is a turbulent Prandtl number for kinetic energy. In analysing the right hand side of equation (11) from the simulation results we use the common coefficients $C_\mu$=0.09 and $\sigma_k$=1. In considering the sign, the left hand side of eq. 11 shows downward directed energy fluxes for the lower 85% of the channel height and upward directed fluxes for the upper 15%, Fig. 5. As the energy maximum is found in Fig. 2 to be at 70% height, a counter-gradient flux occurs between 70% and 85%. Indeed, the modelled term deviates qualitatively in this area from the correct right hand side values. Quantitatively, both curves deviate drastically: the cross-correlations reach values beyond $10^{-4}$, the model reaches values somewhat above $10^{-6}$. Drastically corrected values of the turbulent Prandtl number would be required to correct for this quantitative difference, but such a measure is of course not meaningful.

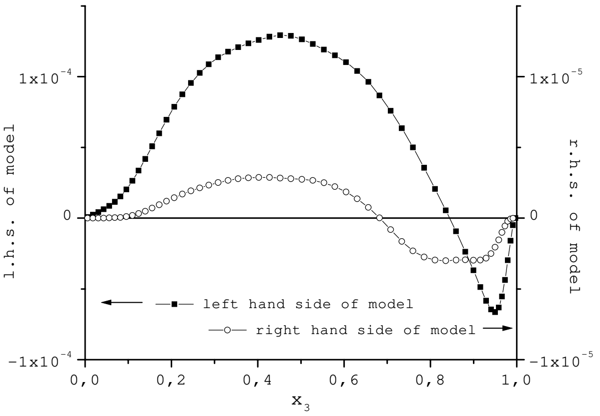


Fig. 5: Left and right hand side of the diffusion model eq. 11, $Ra=10^8$.

From the temperature profile it is known that using eddy conductivities is not practicable with this partially stratified convection; from the *k*-budget it follows that also simple gradient diffusion concepts fail to model the turbulent diffusion of *k*. As a consequence one tends towards second order closures, but there gradient diffusion is used again for closure. At least for the turbulent heat flux equation we already showed that those closure terms are also problematic (133). The relevance of these conclusions has to be checked by careful practical applications of such models.

## 9. CONCLUSIONS

The methods of direct numerical and large eddy simulation are powerful tools to analyse turbulent flows in detail. With increasing progress in numerical methods and with the rapid growth of the computational power, the methods become more attractive and applicable to a wider community. In nuclear reactor research and engineering the methods are nowadays used for similar tasks as in other disciplines, but they may be of different importance.

The DNS method is used in fundamental research to study mechanisms in certain flows. Here, in the nuclear field, we have sometimes to rely on numerical methods because the fluids, like liquid metals, are scarcely accessible for local measurements. DNS is also used for the determination of turbulence statistics to develop special features of statistical turbulence models. The core melt investigations are an example for a fluid of comparable limitations; so DNS is the only method which up to now could contribute reliable and detailed data to the necessary improvements of turbulence models. Results of such simulations were also discussed in this paper. DNS is also a data source to improve existing and to develop new subgrid scale models for low-Reynolds number flows.

The large eddy simulation is the method to access high Reynolds or Rayleigh number flows. Usually, in switching over from Reynolds models to LES, one aims at increased accuracy, at better predictability, and sometimes also at using the time-dependent features to study flows with instabilities. In the nuclear field full advantage of LES is taken by applying it intensively to the thermal fluid-structure interaction problem. Conventional theoretical methods rely heavily on input from special purpose experiments, whereas LES produces the temperature fluctuation data required for thermal fatigue analyses without any additional modelling. In this context we find realisations of the method in multi-purpose codes and recent impressive applications to complex geometries like to the upper plenum of a large reactor with internal structures.

Two-phase or multi-phase multi-component flows are a challenge to any numerical model. Again, natural features of LES could simplify the physical modelling of the geometrically and physically complex flow. Ongoing developments are related to fundamental aspects of the flow at interfaces and to the interface-turbulence interaction. Work on this topic is of tremendous interest, but we are far from having the methods and tools available to access technical problems right now.

The increasing importance of LES in nuclear applications does not mean that the existing modelling is ideal. There are a number of accurate subgrid scale models for low-Reynolds number flows, like variants of the dynamic model or the structure function model, but when changing from one flow type to another, other models have still to be selected. Existing models need to be improved and assessed for high Reynolds number flows, e.g. to be independent on the wall distance and to remove the turbulent Prandtl number problem. There is obviously a new tendency towards transport equation models. Existing wall conditions allow only for rough approximations; they fail e.g. for separated and purely buoyant flows. A solution may come from the numerical side with the ability to resolve the sublayers by local grid refinement or by unstructured grids. Turbulent inlet conditions still remain expensive, because they can only be provided by separate periodic simulations. Here the community should form an adequate data base. Second order spatial schemes are academically not accepted, but they are standard in many codes for complex geometries. The robust upwind-schemes turn out to be inadequate for LES. The progress in numerics, especially in the efficiency of the solvers, made it possible to widely apply LES methods in multi-purpose codes and to investigate geometrically complex flows. The number of nodes which can be used is still below what is needed. The trend towards finite element and unstructured grid discretisations may help to save computing effort and will accelerate the trend towards practical applications of LES in engineering.

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