

DIRECT NUMERICAL SIMULATION AND RANS MODELING OF TURBULENT NATURAL CONVECTION FOR LOW PRANDTL NUMBER FLUIDS

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ABSTRACT

Results of direct numerical simulation (DNS) of turbulent Rayleigh-Bénard convection for a Prandtl number $Pr = 0.025$ and a Rayleigh number $Ra = 10^5$ are used to evaluate the turbulent heat flux and the temperature variance. The DNS evaluated turbulent heat flux is compared with the DNS based results of a standard gradient diffusion turbulent heat flux model and with the DNS based results of a standard algebraic turbulent heat flux model. The influence of the turbulence time scales on the predictions by the standard algebraic heat flux model at these Rayleigh- and Prandtl numbers is investigated. A four equation algebraic turbulent heat flux model based on the transport equations for the turbulent kinetic energy k , for the dissipation of the turbulent kinetic energy ε , for the temperature variance $\overline{\theta^2}$, and for the temperature variance dissipation rate ε_θ is proposed. This model should be applicable to a wide range of low Prandtl number flows.

NOMENCLATURE

D Channel height.
 f_N Normalization factor.
 g Gravitational acceleration.
 k Turbulent kinetic energy.
 Pr Molecular Prandtl number, $Pr = \frac{\nu}{\kappa}$.

Pr_t Turbulent Prandtl number.
 Ra Rayleigh number, $Ra = \frac{g\beta\Delta TD^3}{\nu\kappa}$.
 p Pressure.
 t Time.
 T Temperature.
 ΔT Temperature difference.
 u_i Velocity in i - direction.
 u_0 Velocity scale, $(g\beta\Delta TD)^{1/2}$.
 X_i Coordinates in horizontal ($i = 1, 2$) and vertical ($i = 3$) directions.

Greek
 β Thermal expansion coefficient.
 Δ_x Laplace operator.
 δ_{ij} Kronecker delta.
 ε Dissipation rate of the turbulent kinetic energy.
 ε_θ Dissipation rate of the temperature variance.
 $\overline{\theta^2}$ Temperature variance.
 κ Thermal diffusivity.
 ν Kinematic viscosity.
 ρ Density.
 τ Time scale.

Superscripts
 $(\bar{\quad})$ Time averaged quantity

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1 INTRODUCTION

Turbulent heat transfer in several technical processes, like in steel casting, semiconductor production, and cooling of new liquid metal cooled nuclear reactors is of basic interest. Computational fluid dynamics (CFD) is widely applied to get more insight, to design, and to improve such processes. Common turbulent heat flux models are using the simple concept of the turbulent Prandtl number (Pr_t) based on the Reynolds analogy to model the turbulent heat transfer. This widely used $k - \varepsilon - Pr_t$ model may result in very unsatisfactory predictions, in particular for low Prandtl number flows (see e.g. [1], [2], [3]). To obtain more realistic predictions for the turbulent heat transfer, especially for flows in which buoyancy is included, models are needed, which are based on the transport equations for the turbulent heat fluxes and for the temperature variance [3].

The development of improved statistical heat flux models for engineering applications, in particular for development and analysis of the lead-bismuth cooled Accelerator-Driven-System (ADS) reactor concept, requires data from measurements of the cross-correlations between velocity and temperature fluctuations. Experimental studies in liquid lead-bismuth ($Pr \sim 0.025$) are an ongoing project in the Karlsruhe lead laboratory (KALLA) which will provide a data base for a model development of turbulent convection in PbBi, which is required for the design of the spallation target, see Knebel *et al.* [4]. However, due to the specific properties of PbBi, corrosion for example, and certain deficiencies in the PbBi technology, the experimental thermal and hydraulic investigations at the present stage are rather limited. Therefore, numerical investigations by means of direct numerical simulation (DNS) are necessary in order to get more insight into the physical mechanisms of turbulent convection in PbBi, to gain some of the required turbulence data, and to complement the experimental data basis.

In this paper, the turbulent heat flux and the temperature variance for the natural convection are analyzed using the results of the new DNS for $Pr = 0.025$ (lead-bismuth) at $Ra = 10^5$. The DNS evaluated turbulent heat flux is compared with the DNS based results of a standard gradient diffusion turbulent heat flux model and with the DNS based results of a standard algebraic turbulent heat flux model. The influence of the turbulence time scales on the predictions by the standard algebraic heat flux model at these Rayleigh- and Prandtl numbers is investigated. An improved statistical turbulent heat flux model is developed. This new modeling approach is based on the transport equations for the turbulent kinetic energy k , for the dissipation of the turbulent kinetic energy ε , for the temperature variance $\overline{\theta^2}$, for the temperature variance dissipation rate ε_θ , and on the new modeling formulation for the turbulent diffusion in $\overline{\theta^2}$ developed in [2] which explicitly considers molecular fluid properties.

2 DNS and statistical analysis of Rayleigh-Bénard convection

A simple physical model for the investigation of heat transfer by natural convection is the Rayleigh-Bénard convection. It is given by an infinite fluid layer which is confined by two rigid horizontal isothermal walls. The lower one is heated and the upper one is cooled. The physical problem is characterized by two dimensionless numbers: The Rayleigh number $Ra = \frac{g\beta\Delta TD^3}{\nu\kappa}$, and the Prandtl number $Pr = \frac{\nu}{\kappa}$, where g is the gravity; β is the thermal expansion coefficient; ΔT is the wall temperature difference; D is the distance between the two horizontal walls; ν is the kinematic viscosity; and κ is the thermal diffusivity. An additional dimensionless number is the Grashof number $Gr = \frac{Ra}{Pr}$. Direct numerical simulation is a method in which the three dimensional conservation equations for mass, momentum and energy are solved numerically such that all relevant physical processes are resolved by the grid and by the computational domain. This means that the mesh size is fine enough to resolve the smallest scales of turbulence and to resolve the viscous and thermal boundary layers in the near wall region. In particular the periodicity lengths which define the size of the computational domain must be large enough to resolve the largest scales of turbulence. Meeting both requirements determines the huge computational effort for such DNS, especially for convection in liquid metals.

The simulations of Rayleigh-Bénard convection are performed with the TURBIT code (Grötzbach [5], Wörner [6]). It is a finite volume code which allows for direct numerical simulations of turbulent heat and mass transfer in simple channel geometries. The governing equations are solved in dimensionless form where the following normalization is used: channel height D , velocity $u_0 = \sqrt{g\beta\Delta TD}$, time D/u_0 , pressure ρu_0^2 , and difference between the temperatures of the two walls ΔT . The boundary conditions are periodic in both horizontal directions, whereas at the lower and upper wall the no slip condition and constant wall temperatures are specified.

In the following analysis we will use data from a new DNS for $Pr = 0.025$ and $Ra = 100,000$. Simulations for this flow at sufficiently large turbulence levels became only recently feasible because this flow requires the resolution of very small velocity scales with the need for recording long-wave structures for the slow changes in the convective temperature field. The new simulation is started from an earlier simulation by Bunk and Wörner [7]. The simulation is performed on a mesh with $400 \times 400 \times 75$ cells within the horizontally periodic domain of size $8 \times 8 \times 1$ on a VPP5000 computer. It covers about 24 000 statistically relevant time-steps for analyzing the results. In the following we assign a time averaged quantity with $\bar{\cdot}$. Numerically $\bar{\cdot}$ is determined by averaging the data over both homogeneous horizontal directions and over time.

Fig. 1 shows the vertical profiles of the temperature root-mean-square values and of the turbulent heat flux. The results

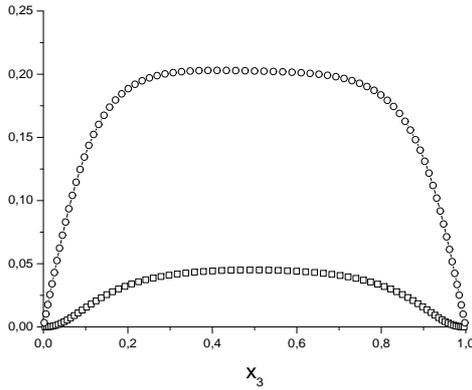


Figure 1. DNS EVALUATED VERTICAL PROFILES OF $\sqrt{\theta^2}$ -O- AND $u_i\theta$ -□-, at $Pr = 0.025$, $Ra = 100,000$.

indicate thick thermal boundary layers and the dominance of the large structures at $Ra = 100,000$, $Pr = 0.025$. Due to the large thermal diffusivity in comparison to the kinematic viscosity, temperature fluctuations are rapidly damped so that large structures dominate the temperature field. These results show that the temperature field is influenced by conduction and by convection at these Rayleigh- and Prandtl numbers. The temperature fluctuation profile and turbulent heat flux profile show only one broad maximum (Fig. 1); it is expected, that with increasing Rayleigh number two maxima will be formed with a local minimum in the middle in the temperature variance profile.

3 Algebraic heat flux models

3.1 Overview

We denote with $U = \bar{U} + u$, $T = \bar{T} + \theta$ and $P = \bar{P} + p$ the Reynolds decomposition of velocity, temperature and pressure. Transport equations for the heat fluxes can be derived from the momentum and energy equations (see i.e. Hinze [8]):

$$\begin{aligned} \frac{\partial \overline{u_i \theta}}{\partial t} + \overline{U_j} \frac{\partial \overline{u_i \theta}}{\partial x_j} = & - \frac{\partial}{\partial x_j} \left(\overline{u_i u_j \theta} + \frac{1}{\rho} \delta_{i,j} \overline{p \theta} - \kappa u_i \frac{\partial \overline{\theta}}{\partial x_j} - \nu \theta \frac{\partial u_i}{\partial x_j} \right) \\ & - \left(\overline{u_i u_j} \frac{\partial \bar{T}}{\partial x_j} + \overline{u_j \theta} \frac{\partial \bar{U}_i}{\partial x_j} \right) - \beta g_i \overline{\theta^2} \\ & + \frac{1}{\rho} \overline{p} \frac{\partial \overline{\theta}}{\partial x_i} - (\nu + \kappa) \frac{\partial u_i}{\partial x_j} \frac{\partial \overline{\theta}}{\partial x_j}, \end{aligned} \quad (1)$$

where δ_{ij} is the Kronecker delta.

The simplest form of two equation eddy diffusivity model is

$$\overline{u_i \theta} = - \frac{C_\mu}{Pr_t} \frac{k^2}{\epsilon} \frac{\partial \bar{T}}{\partial x_i}, \quad (2)$$

here the standard coefficients $C_\mu = 0.09$ and $Pr_t = 0.9$ are used. Unlike in isothermal flows, the application of the model (2) to buoyancy driven flows is insufficient, since it fails to account for the intensive turbulent heat flux in conditions where the mean temperature may be uniform, or its gradient may have the same direction as the heat flux vector, as pointed out by Hanjalić [9]. In the following we assign the model (2) as simple gradient diffusion model (SGD).

The buoyancy term in the heat flux equations includes the temperature variance $\overline{\theta^2}$. In analogy to the turbulent kinetic energy k the temperature variance $\overline{\theta^2}$ is a measure for the temperature fluctuations. Gibson and Launder [10] formulated an algebraic heat flux model, which includes buoyancy effects to overcome a deficiency of the gradient models for buoyant flows. This model assumes a constant turbulence time scale ratio to predict $\overline{\theta^2}$. Chung and Sung [11] introduced a four equation heat flux model solving modeled equations for the turbulent kinetic energy k , the dissipation rate of the turbulence kinetic energy ϵ , the temperature variance $\overline{\theta^2}$, and the temperature variance dissipation rate ϵ_θ . The models by Gibson and Launder and Chung and Sung introduce the mechanical time scale $\frac{k}{\epsilon}$. This time scale is traditionally used in algebraic heat flux models. Since the mechanical time scale enters into the model and not the time scale of the temperature field this description may be physically insufficient, in particular for buoyant flows, see Hanjalić [9]. Considering only the mechanical time scale in algebraic heat flux models may also be physically insufficient if the molecular Prandtl number strongly deviates from one. The appropriate choice of the turbulence time scales is of great importance for modeling of the turbulent heat fluxes, as pointed out by Elghobashi and Launder [12]. Using a thermal time scale or some combination of thermal and mechanical time scales may improve the modeling of the turbulent heat transport, particularly in buoyancy dominated flows, but there is little evidence in support of this; mainly because most reported tests were performed for equilibrium flows where the ratio of the time scales does not vary appreciably, as pointed out by Hanjalić [9].

Nagano and Kim [13] developed a gradient ansatz model for the turbulent heat flux vector which accounts better for the influences of the molecular Prandtl number considering the mixed mechanical- and temperature time scale. Recently Kawamura and Kurihara [14] proposed a transport model for the turbulent heat flux where the effects of Prandtl number and the turbulent Reynolds number are also taken into account.

Models which consider the mixed time scale assuming the

Table 1. TIME SCALES τ , NORMALIZATION FACTORS f_N , AND VALUES OF f_N FOR $Ra = 100,000$, $Pr = 0.025$

τ	f_N	Value of f_N
$\frac{k}{\varepsilon}$	\sqrt{Gr}	2000
$\frac{\theta^2}{\varepsilon_\theta}$	\sqrt{GrPr}	50
$\sqrt{\frac{k}{\varepsilon} \frac{\theta^2}{\varepsilon_\theta}}$	\sqrt{GrPr}	316

gradient transport of the turbulent heat flux are developed and improved e.g. in [15], [16], and [17].

Starting from the high-Reynolds-number heat flux equations Sommer and So [18] developed an explicit algebraic heat flux model for buoyant flows, which introduces a mixed time scale. Recently Shikazono and Kasagi [19], Wörner, Ye and Grötzbach [20], and Otić, Grötzbach and Wörner [2] derived turbulence models which consider mixed turbulence time scale and it is found that the mixed time scale is more suitable for low Pr flows.

3.2 Model analysis and development of a new model

Launder [21] simplified the transport equations for the heat flux (eq. (1)) to give an algebraic heat flux model as:

$$\overline{u_i \theta} = -C f_N \tau \left[\overline{u_i u_j} \frac{\partial \overline{T}}{\partial x_j} + \overline{u_j \theta} \frac{\partial \overline{U}_i}{\partial x_j} + \frac{g_i}{|g|} \overline{\theta^2} \right], \quad (3)$$

here C is an empirical coefficient; f_N is the normalization factor due to the normalization introduced in section 2 (see table 1); τ is turbulence time scale. The model developed by Sommer and So [18] is similar to the above model. Notice that the first term on the right of the model (3), $(C f_N \tau \overline{u_i u_j} \frac{\partial \overline{T}}{\partial x_j})$, is the gradient diffusion approximation of $\overline{u_i \theta}$. For buoyancy-driven flows at sufficiently large Rayleigh numbers and apart of the channel walls, i.e. for vanishing mean temperature or velocity gradients, the model (3) may be reduced to

$$\overline{u_i \theta} = C f_N \tau \overline{\theta^2} \frac{g_i}{|g|}, \quad (4)$$

where the model takes the positive sign for the buoyancy-driven flow.

In the following we analyze the influence of the time scale on predictions of the turbulent heat flux by the model (3) using the DNS results for the Rayleigh-Bénard convection at $Ra = 10^5$, $Pr = 0.025$, while considering the mechanical time scale $\frac{k}{\varepsilon}$, the thermal time scale $\frac{\theta^2}{\varepsilon_\theta}$, and the mixed time scale $\sqrt{\frac{k}{\varepsilon} \frac{\theta^2}{\varepsilon_\theta}}$ (see table 1). In Rayleigh-Bénard convection the mean velocity is zero

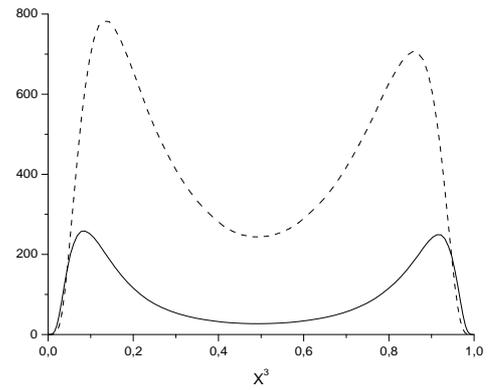


Figure 2. DNS BASED RESULTS OF THE SGD MODEL (2) — AND OF THE MODEL (3) - - - USING $\tau = \frac{k}{\varepsilon}$, FOR $Pr = 0.025$, $Ra = 100,000$.

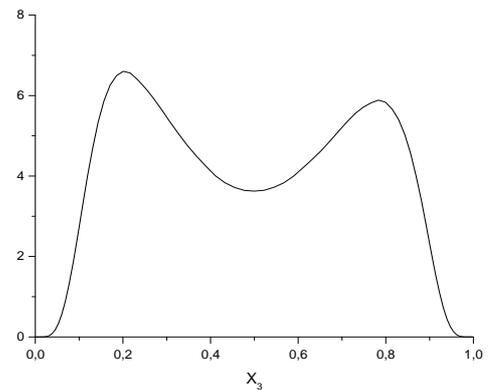


Figure 3. DNS BASED RESULTS OF THE MODEL (3) USING $\tau = \sqrt{\frac{k}{\varepsilon} \frac{\theta^2}{\varepsilon_\theta}}$ —, AT $Pr = 0.025$, $Ra = 100,000$.

and mean temperature gradient has the same direction as the heat flux vector. Therefore, the Rayleigh-Bénard convection is a good test case to point out some characteristics of the standard models when applied to buoyancy-driven flows. Fig. 2 shows a comparison of the DNS based predictions by the SGD model (2) and by the model (3) considering the mechanical time scale in (3). Fig. 3 shows the DNS based predictions by the model (3) considering the mixed time scale. Fig. 4 shows a comparison of the DNS results for the turbulent heat flux $\overline{u_i \theta}$ with the DNS based predictions by the model (3) considering the thermal time scale in (3) and by the model (4) considering the mixed time scale in (4). We intentionally fix the empirical coefficient $C = 1$ in the

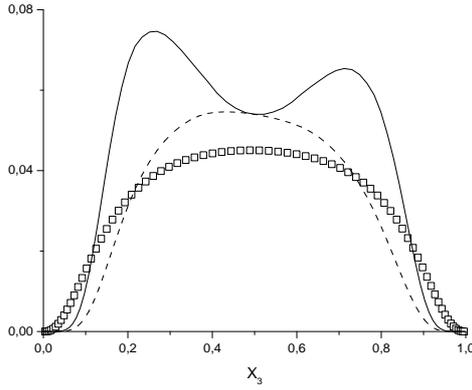


Figure 4. DNS EVALUATED TURBULENT HEAT FLUX \square , DNS BASED RESULTS OF THE MODEL (3) USING $\tau = \frac{\overline{\theta^2}}{\varepsilon_\theta}$ —, AND DNS BASED RESULTS OF THE MODEL (4) USING $\tau = \sqrt{\frac{k}{\varepsilon} \frac{\overline{\theta^2}}{\varepsilon_\theta}}$ ---, AT $Pr = 0.025$, $Ra = 100,000$.

models (3) and (4) for all comparisons, since the qualitative and quantitative differences are tremendous. Using only the mechanical time scale results in the over-predictions by the model (3) up to four orders of magnitude. The model (3) performs considerably better when the mixed or the thermal time scale is used (Fig. 3 and Fig. 4). The major deficiency of the models (2) and (3) in this flow type is due to the fact that the direction of the mean temperature gradient is the same as the direction of the heat flux vector, resulting in the prediction of a local minimum in the channel center where the heat flux should reach its maximum. For buoyant flows the simple model (4) gives qualitatively much better results, but the results also show insufficiency of the model in the near wall region (Fig. 4). This analysis shows the importance of the appropriate choice of the time scales in modeling of the flows with $Pr \ll 1$. Analogous results may be expected for flows with $Pr \gg 1$.

These results indicate that a good approximation of the temperature variance $\overline{\theta^2}$ is necessary for convective low Prandtl number flows. The transport equations for the temperature variance $\overline{\theta^2}$ can be derived from the energy equation:

$$\frac{\partial \overline{\theta^2}}{\partial t} + \overline{U_i} \frac{\partial \overline{\theta^2}}{\partial x_i} = \underbrace{-\frac{\partial}{\partial x_i} \left(\overline{u_i \theta^2} - \kappa \frac{\partial \overline{\theta^2}}{\partial x_i} \right)}_{D_\theta} \quad (5)$$

$$\underbrace{-2\overline{u_i \theta} \frac{\partial \overline{T}}{\partial x_i}}_{P_\theta} - \underbrace{2\kappa \frac{\partial \overline{\theta}}{\partial x_i} \frac{\partial \overline{\theta}}{\partial x_i}}_{\varepsilon_\theta}$$

Based on the DNS results it is shown [2] that the diffusion term D_θ in the temperature variance equation (eq. (5)) is of great importance for the balance of the above transport equation. The triple correlation $\overline{u_i \theta^2}$ may be modeled using a simple gradient ansatz, but only if $Pr \sim 1$. For low Pr the new model is more suitable because it accounts for the molecular fluid properties [2]:

$$\overline{u_i \theta^2} = -C_\theta \left[\frac{2}{\sqrt{GrPr}} \sqrt{\frac{k}{\varepsilon} \frac{\overline{\theta^2}}{\varepsilon_\theta}} \Delta_x \overline{\theta^2} + \frac{k^2}{\varepsilon} \frac{\partial \overline{\theta^2}}{\partial x_j} \right], \quad (6)$$

where C_θ is an empirical coefficient $C_\theta = 0.11$ and Δ_x is the Laplace operator.

A model for the temperature variance dissipation rate may be given as follows:

$$\frac{\partial \varepsilon_\theta}{\partial t} + \overline{U_i} \frac{\partial \varepsilon_\theta}{\partial x_i} = -C_{P1} \frac{\varepsilon_\theta}{\overline{\theta^2}} \overline{u_i \theta} \frac{\partial \overline{T}}{\partial x_i} - C_{P2} \varepsilon_\theta \frac{\partial \overline{U_j}}{\partial x_j} - C_{D1} \frac{\varepsilon_\theta^2}{\overline{\theta^2}} - C_{D2} \frac{\varepsilon_\theta \varepsilon}{k}, \quad (7)$$

where C_{P1} , C_{P2} , C_{D1} , and C_{D2} are empirical coefficients as determined in [13].

Equations (3) – (7) together with the equations for the turbulence kinetic energy k and for the dissipation rate of the turbulence kinetic energy ε yield a new four equation algebraic heat flux model for forced and buoyant flows applicable to a wide range of low Pr flows.

A slight numerical disadvantage of the model is induced by the term $\Delta_x \overline{u_i \theta^2}$ since the eq. (6) is implicit in the triple correlation and because second derivatives necessitates finer grids. Accuracy and numerical stability of the model are discussed in [2].

4 Conclusions

Results of a new direct numerical simulation of turbulent Rayleigh-Bénard convection for $Pr = 0.025$, $Ra = 10^5$ are used for an analysis of the temperature variance and of the turbulent heat flux. These results show that the temperature field at these Prandtl and Rayleigh numbers is still considerably influenced by conduction and by convection, since the temperature fluctuations are damped strongly in low Prandtl number flows.

The DNS evaluated turbulent heat flux is compared with the DNS based results of a standard gradient diffusion turbulent heat flux model using a turbulent Prandtl number and with the DNS based results of a standard algebraic turbulent heat flux model. These results show that, the major deficiency of these models is due to the fact that the mean temperature gradient and the heat flux vector are in the same direction in this flow type, which results in qualitatively and quantitatively wrong predictions in this

flow type and at these Rayleigh and Prandtl numbers.

The influence of the turbulence time scale on the predictions by the standard algebraic heat flux model is investigated. The results support the conclusion that an appropriate choice of the time scale is of great importance in a simple modeling of the turbulent heat flux and indicate that for the buoyancy-driven low Prandtl number flows the thermal time scale may be more appropriate in the heat flux ansatz. A simple model which correlates the turbulent heat flux with the temperature variance is suggested and compared with the DNS evaluated turbulent heat flux. This simple model performed qualitatively better than the gradient diffusion or algebraic models but with considerable deficiencies in the near wall region.

These results indicate that a good approximation of the temperature variance is necessary for low Prandtl number flows especially if those are influenced by buoyancy. With this extended modeling a four equation algebraic turbulent heat flux model is developed, which is based on transport equations for the turbulent heat fluxes, for the turbulent kinetic energy k , for the dissipation of the turbulent kinetic energy ϵ , for the temperature variance $\overline{\theta^2}$, and for the temperature variance dissipation rate ϵ_θ . In low Prandtl number buoyant flows and in the forced flows we expect good results from this model, since the model is based on the transport equations while considering explicitly the molecular fluid properties in the turbulent diffusion term of $\overline{\theta^2}$. The generality of the model can only be proven when successfully applied to different types of problems, for example in flows in more complex domains. Implementation, calibration, and validation of the new model is a part of the ongoing project on the thermal and hydraulic investigations of the lead-bismuth cooled ADS nuclear reactor concept.

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