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AN ALGEBRAIC HEAT FLUX MODEL IN STAR-CCM+ FOR APPLICATION TO INNOVATIVE REACTORS

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Abstract

As part of the THINS (Thermal-Hydraulics of Innovative Nuclear Systems) project, which is sponsored by the European Commission from 2010 to 2014, CD-adapco has implemented in the commercially available software STAR-CCM+ an Algebraic Heat Flux Model (AHFM). The model adopts an expression for the turbulent heat flux which is derived from the full differential transport model on the base of a local equilibrium assumption. While considerably simpler than the full differential closure this formulation retains the basic terms from the differential transport equations representing the physical mechanisms which generate the turbulent heat flux. This approach has shown a great potential, and will be object of evaluation and improvements for application to innovative reactors.

Introduction

Turbulent heat transfer is an extremely complex phenomenon which has challenged turbulence modellers for various decades. The first challenge, when trying to model this phenomenon, is related to its intrinsic coupling to the characteristics of turbulence which therefore require, as a fundamental block, the ability to accurately model the momentum transport. Such requirement is not trivial to fulfil for complex flows and has often hindered the ability to evaluate approaches for modelling the turbulent heat fluxes.

Both, turbulent momentum and heat transfer, are based on the same physical mechanism of cross-streamwise mixing of fluid elements and, as a consequence, the modellers have often assumed the possibility that turbulent heat transfer may be predicted only from the knowledge of momentum transfer, in what is known as Reynolds Analogy. While this assumption is overly simplistic it has been successfully adopted for the last two decades in the very large majority of industrial applications of CFD which are based on Eddy Diffusivity models (EDM); this success is justified by the fact that, for moderate Pr fluids, this approach has provided reasonable predictions of global parameters such as Nusselt numbers and mean temperature distributions.

For non-unity Pr fluids the limitations of the Eddy Diffusivity approach have become more evident, particularly for natural and mixed convection flows, as underlined for example by the OECD/NEA 2007 report [1] and by Grötzbach (2007) [2] which provides a comprehensive review of the topic. One of the objectives of the European sponsored projecy THINS (Thermal-Hydraulics of Innovative Nuclear Systems) [3] is to push forward the validation and adoption of more accurate closures for single phase turbulence for innovative reactors.

As part of the THINS project CD-adapco has implemented in the commercially available software STAR-CCM+ an Algebraic Heat Flux Model (AHFM) based on the model introduced by Kenjeres and Hanjalic [4]. The AHFM model adopts an expression for the turbulent heat flux which is derived from the full differential transport model on the base of a local equilibrium assumption, and which retains the fundamental production terms representing the physical mechanisms which generate the turbulent heat flux, therefore permitting to accurately model natural and mixed convection flows. The implementation and preliminary evaluation of this model are the subject of this work.

1. Model Description

While the mathematical models for turbulence and their derivations are readily available in fluid dynamics textbooks it is useful to provide here a very brief summary to describe particular aspects related to the particular model implemented in this work.

1.1 Low k-ε model

The underlying model selected for the implementation of the AHFM is based on the Low Reynolds k-ε model formulation introduced by Lien et al. [5]. The equations for the turbulent kinetic energy and it dissipation rate are as follows:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_j}\left[\rho \bar{u}_j k-\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]=P_k-\rho\varepsilon \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon)+\frac{\partial}{\partial x_j}\left[\rho \bar{u}_j \varepsilon-\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]=C_{\varepsilon 1} f_1 \frac{\varepsilon}{k} P_k-C_{\varepsilon 2} f_2 \rho \frac{\varepsilon^2}{k} \tag{2}$$

Where

$$P_k=-\rho\overline{u_i u_j}\frac{\partial u_i}{\partial x_j} \tag{3}$$

and

$$\mu_t=f_\mu \frac{C_\mu \rho k^2}{\varepsilon} \tag{4}$$

The user has the option in STAR-CCM+ to either adopt the simple Boussinesq approximation for the turbulent stresses or to select a Non-Linear Constitutive relations to account for anisotropy of the turbulence (quadratic terms) and further the influence of curvature and rotation (cubic terms). While the results presented in this paper all adopt the Boussinesq approximation, future work will also include the evaluation of nonlinear stress strain correlation. The stress strain correlation have the following form:

$$\rho\overline{u_i u_j} = \frac{2}{3}\rho k\delta_{ij} - \mu_t S_{ij} + C_1\mu_t \frac{k}{\varepsilon}\left[S_{ik}S_{kj} - \frac{1}{3}\delta_{ij}S_{kl}S_{kl}\right] + C_2\mu_t \frac{k}{\varepsilon}\left[\Omega_{ik}S_{kj} + \Omega_{jk}S_{ki}\right] + C_3\mu_t \frac{k}{\varepsilon}\left[\Omega_{ik}\Omega_{jk} - \frac{1}{3}\delta_{ij}\Omega_{kl}\Omega_{kl}\right]$$

$$+ C_4\mu_t \frac{k^2}{\varepsilon^2}\left[S_{ki}\Omega_{lj} + S_{kj}\Omega_{li}\right]S_{kl} + C_5\mu_t \frac{k^2}{\varepsilon^2}\left[S_{kl}S_{kl} - \Omega_{kl}\Omega_{kl}\right]S_{ij} \tag{5}$$

In order to account for near-wall effects, damping functions are introduced which are shown in the formulation of the ε-equation (f_1, f_2 in Eq. (2)) and in the expression for the turbulent viscosity ($f\mu$ in Eq. (4)). The damping functions adopt the following form:

$$f_1 = \left(1 + \frac{P_k'}{P_k}\right) \tag{6}$$

with

$$P_k' = 1.33\left[1 - 0.3e^{-R_t^2}\right]\left[P_k + 2\mu\frac{k}{y^2}\right]e^{\left(-0.00375Re_y^2\right)} \tag{7}$$

and

$$f_2 = \left(1 - 0.3e^{-R_t^2}\right) \tag{8}$$

with

$$R_t = \frac{k^2}{\nu\varepsilon} \tag{9}$$

$$Re_y = \frac{y\sqrt{k}}{\nu} \tag{10}$$

while for the turbulent viscosity

$$f_\mu = 1 - \exp[-\left(C_{d0}\sqrt{\mathrm{Re}_y} + C_{d1}\,\mathrm{Re}_y + C_{d2}\,\mathrm{Re}_y{}^2\right) \tag{11}$$

where $C_{d0} = 0.091$, $C_{d1} = 0.0042$, $C_{d2} = 0.00011$.

If we now introduce the Reynolds-averaged energy equation this takes the following general form:

$$\frac{\partial\rho c_p T}{\partial t} + \frac{\partial\rho c_p T u_i}{\partial x_i} + \frac{\partial\rho c_p \overline{\theta u_i'}}{\partial x_i} = \frac{\partial}{\partial x_i}k\frac{\partial T}{\partial x_i} \tag{12}$$

The quantity $\overline{\theta u_i'}$ is called the Turbulent Heat Flux, and is the Reynolds-average of the fluctuating velocity-temperature correlation. As mentioned in the introduction this is most commonly represented by the simple Eddy-diffusivity model, which is based on the Reynolds analogy between the transport of momentum and heat and is expressed as:

$$\overline{\theta u_i'} = -\frac{\nu_t}{\sigma_T}\frac{\partial T}{\partial x_i} \tag{13}$$

where σ_T is called the turbulent Prandtl number and has usually the value of 0.9. As discussed, for moderate Pr fluids this approach has provided reasonable predictions of global parameters such as Nusselt numbers and mean temperature distributions, and these agreements justify the success of this simple method.

1.2 Algebraic Heat Flux Model

In order to improve the fidelity of the turbulent heat flux, full second order closures can be derived in a similar fashion to what is done for momentum closures. Such closures are attractive as they model the turbulent heat fluxes with separate transport equations, therefore trying to account for the complex creation and dissipation mechanisms, but their derivation requires assumptions which often do not find a physical support, leading to lack of generality. A more promising approach is represented by the AHFMs, which are obtained from the simplification of the full second order differential equations on the base of a local equilibrium assumption. The expression adopted in the STAR-CCM+ implementation is as follows:

$$\overline{\theta u_i} = -C_0^{\theta u}\tau^*\left(C_1^{\theta u}\overline{u_i u_j}\frac{\partial T}{\partial x_j} + C_2^{\theta u}\overline{\theta u_j}\frac{\partial U_i}{\partial x_j} + C_3^{\theta u}\beta g_i\overline{\theta^2}\right) \tag{14}$$

While considerably simpler than the full differential closure this formulation retains all three production terms from the differential transport equation representing the physical mechanisms which generate the turbulent heat flux due to:

- non-uniformity of the mean thermal field
- mechanical deformation (mean rate of strain)
- amplification/attenuation of turbulence fluctuations due to the effect of buoyancy.

It should also be noted, that consistently with the original work of Kenjeres, an additional term related to the molecular dissipation of $\overline{\theta u_i}$ that often appears in equation 14 is omitted as negligible at high Ra numbers.

In order to complete the closure 2 more equations need to be solved, which represent the temperature variance and its rate of dissipation:

Temperature Variance

$$\frac{\partial \rho\overline{\theta^2}}{\partial t} + \frac{\partial \rho\overline{\theta^2}U_k}{\partial x_k} = 2\rho P_\theta - 2\rho\varepsilon_\theta + \frac{\partial}{\partial x_j}\left(\frac{k}{c_p} + \frac{\mu_t}{\sigma_{\overline{\theta^2}}}\right)\frac{\partial\overline{\theta^2}}{\partial x_j} \tag{15}$$

Temperature Variance Dissipation Rate

$$\frac{\partial \rho \varepsilon_\theta}{\partial t} + \frac{\partial \rho \varepsilon_\theta U_k}{\partial x_k} = \frac{\partial}{\partial x_j}\left(\left(\frac{k}{c_p} + \frac{\mu_t}{\sigma_{\varepsilon_\theta}}\right)\frac{\partial \varepsilon_\theta}{\partial x_j}\right) + \frac{\varepsilon_\theta}{\overline{\theta^2}}\left[C^\theta_{\varepsilon_1}\rho P_\theta + C^\theta_{\varepsilon_2}\rho P_\theta \frac{\varepsilon}{\varepsilon_\theta}\frac{\overline{\theta^2}}{k} + C^\theta_{\varepsilon_3}\rho P_k \frac{\overline{\theta^2}}{k} - C^\theta_{\varepsilon_4}\rho \varepsilon_\theta - C^\theta_{\varepsilon_5}\rho \varepsilon \frac{\overline{\theta^2}}{k}\right] \tag{16}$$

where the coefficients suggested from Kenjeres and Hanjalic are shown in table 1.

Table 1 Model Coefficient (Kenjeres and Hanjalic [4])

$C_{\varepsilon 1}{}^{\theta}$	$C_{\varepsilon 2}{}^{\theta}$	$C_{\varepsilon 3}{}^{\theta}$	$C_{\varepsilon 4}{}^{\theta}$	$C_{\varepsilon 5}{}^{\theta}$	$\sigma_{\theta 2}$	$\sigma\varepsilon_{\theta}$
1.3	0.0	0.72	2.2	0.8	1.0	1.3

2. Model Implementation

The model described in the previous paragraph has been implemented in the commercially available STAR-CCM+ software and is accessible as an optional treatment for temperature flux. The model is implemented in conjunction with STAR-CCM+ segregated solver which is based on a large body of work by Peric, Demirdzic and colleagues [6][7][8]. Given the target of the THINS project to evaluate and possibly improve the predictive capabilities of the proposed model its coefficient will need to be evaluated and are therefore open to the user and easily accessible as shown in Fig.1.

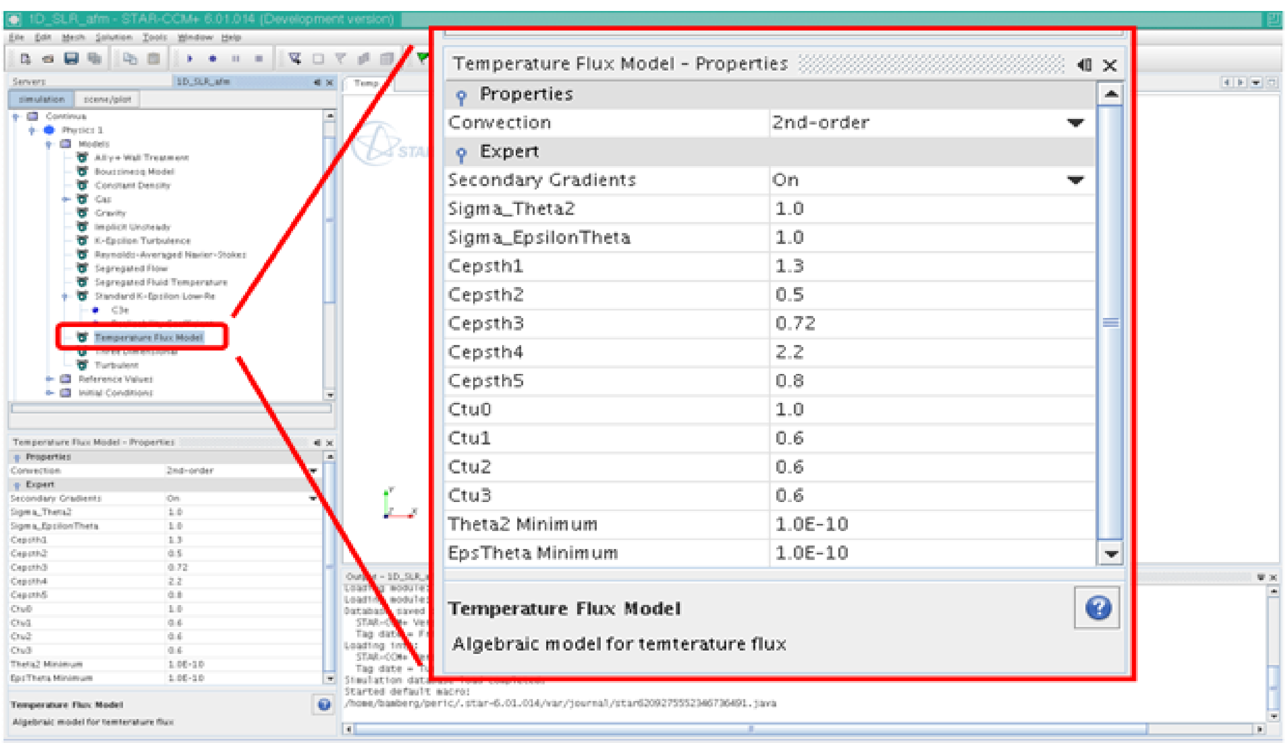


Figure 1 AHFM Implementation and access to its coefficients in STAR-CCM+

2.1 Model Preliminary Verification

As a necessary part of the implementation work, a preliminary verification of the model has been performed to confirm that it provides rational predictions and in particular that it shows the potential for the expected improvement in heat transfer predictions.

2.1.1 Horizontal Cavity Heated from Below

The first test for the model is the capability of reproducing the roll patterns inside a two-dimensional 1:4 aspect ratio enclosure. Kenjeres and Hanjalic showed how the eddy diffusivity assumption fails in reproducing the correct roll patterns and even in some cases cannot capture the turbulent behaviour but predicts laminar conditions.

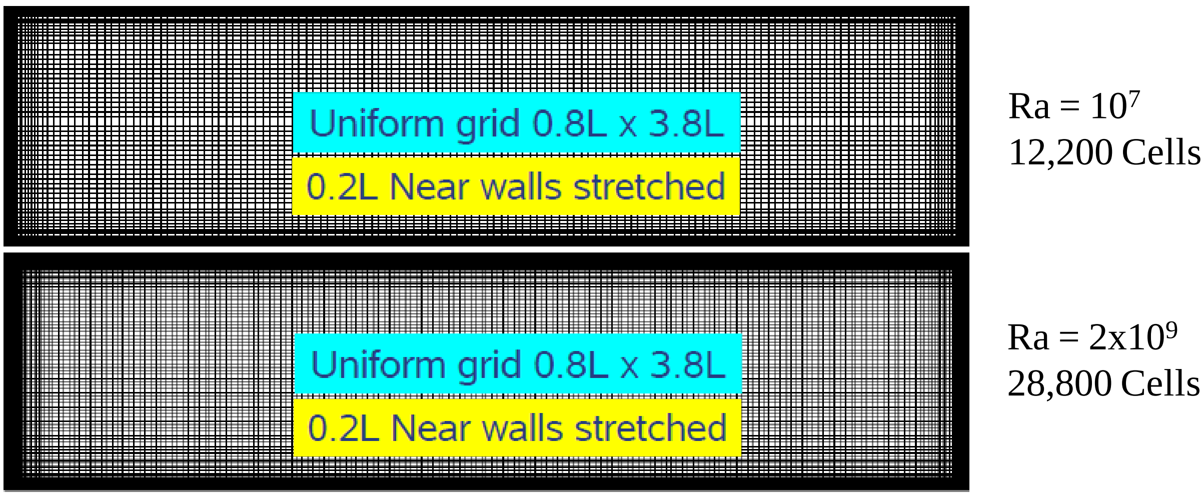


Figure 2 Computational grids for 1:4 aspect ratio enclosures

Two tests are performed for different Ra numbers, Ra=10^7 and Ra=$2x10^9$. The grids adopted for the computations are shown in Fig. 2, while uniform in the bulk the grids are then stretched in the near wall region, and contain respectively 12,200 and 28,800 cells.

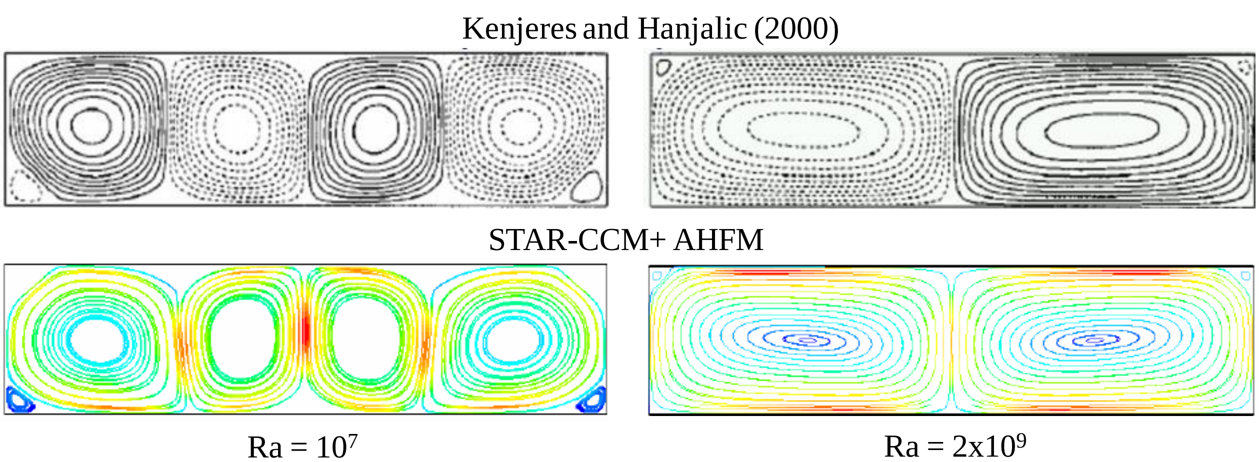


Figure 3 Roll structures represented by velocity streamlines

Looking at the results in Fig. 3, the implemented model confirms the predictions from Kenjeres and Hanjalic, where for the higher Ra number, $2x10^9$, the flow patterns consist of 2 large rolls and 2 very small corner rolls on the top, while the lower Ra case, $1x10^7$, shows 4 large and 2 small rolls in the bottom corners, which eddy-diffusivity models are known to not reproduce. The local Nu numbers along the horizontal wall are also shown for the 2 analysed cases in Fig. 4, again showing consistent predictions to the results of Kenjeres and Hanjalic. The roll structures cause strong periodic variations of the local Nu numbers, with maximum points in the stagnation regions. Also the absolute values predicted by the present implementation are in reasonable agreement with previous results; in particular for the lower Ra case the predicted average Nu = 18, typical of a turbulent regime, shows the expected increase in heat transfer that the eddy diffusivity assumption cannot capture.

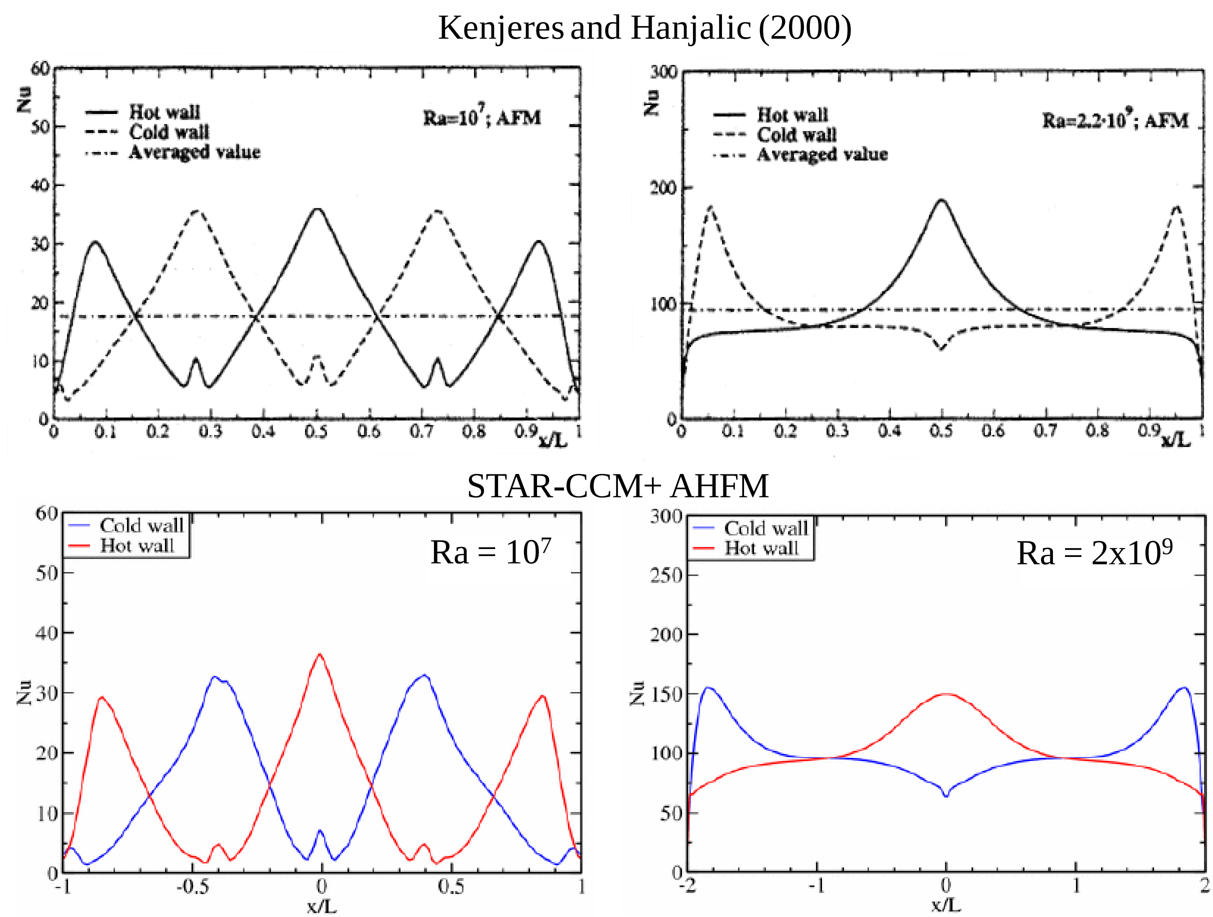
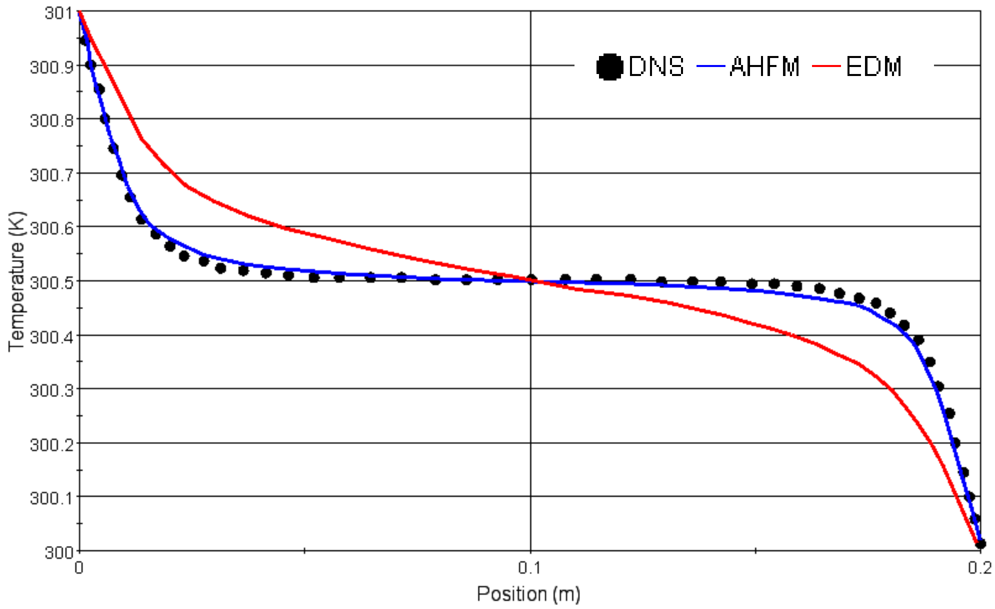


Figure 4 Local Nusselt number predictions

2.1.2 Rayleigh-Bernard convection

Another important verification has been performed for predictions of Rayleigh-Bernard convection. The DNS data from Bunk and Woerner [9] are used as reference and the non-dimensional results have been scaled to the RANS test case conditions with $Ra=6.3x10^5$, air as fluid $Pr=0.71$, cavity size $L=0.2m$ and temperature difference of 1K.



Computed
Nusselt Number

	Nu
EDM	3.706
AHFM	6.874

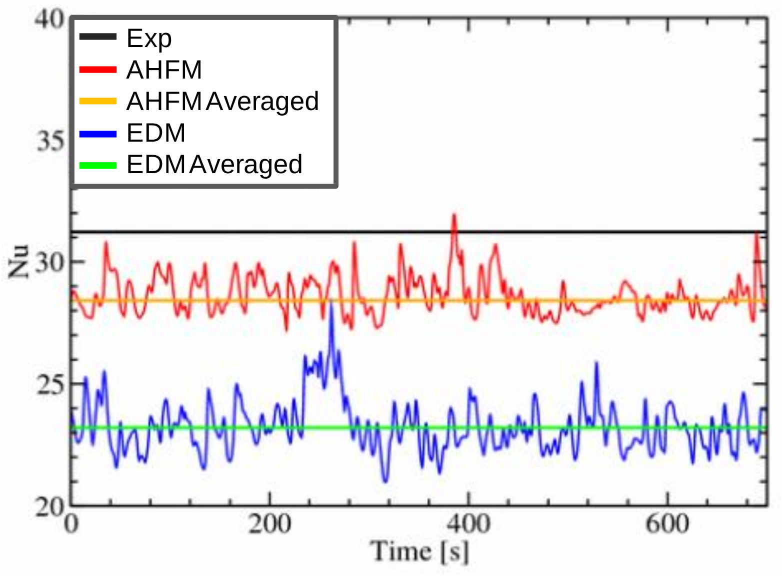
Figure 5 Rayleigh-Bernard convection predictions

Mean temperatures for the Rayleigh-Bernard convection case are shown in Fig. 5, and while the present results only represent a preliminary qualification of the model, one important observation can be made: the AHFM seems to much better capture the DNS temperature distribution, thanks to the improved prediction of the heat transfer phenomena and therefore of the local Nu values, while the EDM, as expected, considerably underpredicts the Nu values; this behaviour is consistent with expectations and provides a first confirmation of the potential of the model.

2.1.3 Cube cavity heated from below

The last verification presented in this work has been performed on a 3-dimensional geometry, trying to verify the behaviour of the model on complex, unsteady 3-D turbulence. The selected case is based on the work of the Leong et al. [10] where heat transfer is computed in a cube cavity heated from below, with $Ra=1.0x10^8$, air as fluid Pr=0.71, cavity size L=0.5m and temperature difference of 10K. Unsteady calculations are performed for 700s with a time step of 0.1s,

The computational results as well as the grid are presented in Fig. 6. The comparison again shows the potential of the AHFM to more accurately predict the heat transfer phenomenon and produce results that are closer to the experimental values.



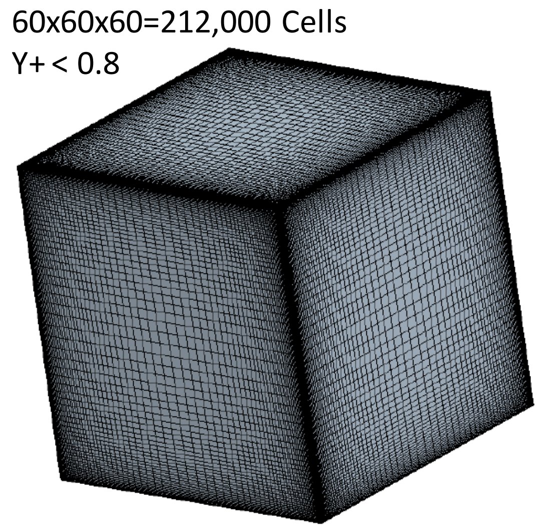


Figure 6 Cube cavity predictions and computational grid

In this particular tests anyhow, while the AHFM predictions show a clear improvement, the absolute value of the average Nusselt number still underpredicts the experimental value. The under-predictions are believed to be related to the simplified boundary conditions which do not exactly represent the experimental configuration but more investigations are needed to clarify these findings.

Table 2 Averaged Nusselt number for cube cavity

	***Nu* (Nusselt Number)**
Experiment (Leong et al. [10])	**31.22**
EDM	**23.16**
AHFM	**28.42**

3. Conclusion

As part of the THINS project, sponsored by the European Commission, CD-adapco has implemented in the commercially available software STAR-CCM+ an Algebraic Heat Flux Model (AHFM) which retains the basic terms from the differential transport equations representing the physical mechanisms which generate the turbulent heat flux.

This work has introduced the details of the model and its implementation and has presented and discussed the results of the preliminary validation. The model has been tested on 3 different cases: an horizontal cavity heated from below, the classic Rayleigh-Bernard convection, and a 3-D cube cavity. In all three cases the AHFM model has shown the potential to improve the predictions of heat transfer, and qualitatively reproduce the expected behaviours. Moreover the verification has shown satisfactory prediction of quantitative heat transfer in the 3 selected cases.

The present model implementation will constitute the base for validation and improvement of the AHFM model during the remainder of the THINS project.

4. Acknowledgement

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