Multi-objective training of an algebraic heat flux model to cure model-data inconsistencies in the momentum treatment

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ABSTRACT

Machine learning is gaining importance in fluid dynamics to exploit large databases and solve complex regression problems. One of the major fields of application is modelling turbulence, which asks advanced machine learning tools to construct new closures that overcome traditional modelling assumptions. Improvements in traditional turbulence closures are especially needed in the context of liquid metal heat transfer. The low Prandtl numbers of liquid metals make the similarity between momentum and thermal fields less justified. Consequently, traditional closures based on the eddy diffusivity concept (Reynolds analogy) show severe limitations when applied to non-isothermal liquid metal flows.

The work of M. Fiore et al. [1] was aimed at developing an Algebraic Heat Flux Model (AHFM) based on the analysis of the high-fidelity data collected in several European collaborative projects (SESAME, MYRTE [2]) and the application of artificial neural networks (ANN) for a wide and efficient mapping. The data-driven AHFM was developed with a "frozen" training approach, i.e. the ANN was trained with averaged DNS data for several flow configurations. The model was validated against canonical flows within and outside the training range and combined with Reynolds Stress Models (RMSs) and less expensive momentum models based on the Boussinesq approximation. The results highlighted the impact of the momentum turbulence model on the predictions of the AHFM. This behaviour is illustrated in Figure 1, where the data-driven AHFM is applied in the case of non-isothermal turbulence channel flow in combination with the Elliptic Blending RSM and the Launder-Sharma k-epsilon model.

This work further investigates the impact of the momentum closure on the AHFM and identifies possible training strategies that allow the AHFM to interface with both RSMs and eddy viscosity-based momentum closures. First, we analyzed the high-fidelity and RANS 10dimensional input spaces for the same flow configurations. The Principal Component Analysis (PCA) of the model inputs revealed three clusters related to thermal, isotropic and anisotropic momentum parameters. The separation between the DNS and RANS inputs was evident from the distance between the data in the third cluster, suggesting that the ANN could distinguish the nature of the input data and handle both. The network was then trained with a hybrid DNS-RANS database in a multi-objective optimization framework in which the cost function weights the performances on the two sets of inputs. The training campaign produced the Pareto front by varying the weights between the objectives (Figure 2), relating the heat flux error achieved with high-fidelity and RANS inputs. The sharpness of the Pareto Front near (equal importance) shows that the network can provide accurate heat flux predictions with both categories of inputs, detecting their nature and compensating for the missing information related to the Reynolds stress anisotropy. A sensitivity analysis with the Shapley value algorithm was conducted to better understand the new model behaviour. The inputs were grouped into four categories, and the sensitivity of the heat flux predictions to each of them

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was computed in the presence of DNS and RANS inputs. The computed values (Figure 3) show that the model learned to reduce the sensitivity when modelled input data are detected, thus being a more robust thermal model in the presence of low-order momentum turbulence models. The new data-driven AHFM was implemented and validated in OpenFoam to verify its better performance in turbulent channel flows, non-isothermal backwards-facing step flow, and impinging jets. To better understand the new model behavior, a sensitivity analysis with the Shapley value algorithm was carried out. The inputs were grouped into four categories and the sensitivity of the heat flux predictions to each of them was computed in presence of DNS and RANS inputs. The computed values (Figure 3) show that the model learned to reduce the sensitivity when modelled input data are detected, thus being a more robust thermal model in presence of low order momentum turbulence models. The new data-driven AHFM was implemented and validated in OpenFoam to verify its better performance in case of turbulent channel flow, non-isothermal backward facing step flow and impinging jets.



Fig.1 Comparison of heat flux predictions when the thermal models are combined with the RSM (left) and the k-epsilon model (right).

Fig 2. Pareto front resulting from the training campaign ($\alpha = \frac{L_{RANS}}{L_{DNS}}$).



Fig 3. Shapley values obtained for DNS (solid line) and RANS (dashed line) input data. **REFERENCES**

[1] Fiore, Matilde, et al. "Physics-constrained machine learning for thermal turbulence modelling at low Prandtl numbers." International Journal of Heat and Mass Transfer 194 (2022): 122998.

[2] Shams, Afaque, et al. "A collaborative effort towards the accurate prediction of turbulent flow and heat transfer in low-Prandtl number fluids." Nuclear Engineering and Design 366 (2020): 110750.