Abstract

Computational Fluid Dynamics (CFD) has become an essential tool in the analysis, design, and optimisation of complex engineering systems involving coupled physical phenomena such as fluid flow, heat transfer, species transport, multiphase effects, and electrochemical reactions. However, the increasing complexity of these models requires a rigorous assessment of their predictive capability, particularly when they are applied to design support or safety-critical contexts. In this framework, the Verification and Validation (V&V) methodology provides a structured approach to quantify numerical and modelling uncertainties and to assess the credibility of simulation results with respect to experimental or reference data. This work applies a comprehensive V&V framework to four representative case studies of increasing physical complexity: TPMS structures for heat transfer applications, a V-rib turbulence promoter, tritium transport in confined environments, and a Proton Exchange Membrane Fuel Cell (PEMFC) as a fully coupled multiphysics electrochemical system. Each case is used to investigate different dominant sources of uncertainty, ranging from geometric and manufacturing effects to turbulence modelling, transient flow behaviour, and electrochemical closure relations.

The first case study considers TPMS (Triply Periodic Minimal Surface) structures for heat transfer enhancement and pressure drop characterisation. The objective is the development of empirical correlations based on validated CFD simulations. The analysis combines grid convergence studies and experimental validation to quantify discretization and modelling uncertainties. Results show that model performance strongly depends on the TPMS orientation and operating conditions. While some configurations exhibit good agreement with experimental data within uncertainty bounds, others show systematic deviations attributable to manufacturing imperfections introduced by additive manufacturing, including surface roughness and geometric deviations from the idealised computational model. In addition, at low Reynolds numbers the relative importance of measurement uncertainty increases,

leading to larger discrepancies between numerical and experimental results. Overall, the TPMS study highlights the importance of accounting for geometric variability when developing reduced-order predictive models.

The second case study focuses on a V-rib configuration used as a turbulence promoter in conjugate heat transfer applications. The presence of ribs induces complex flow structures characterised by separation, reattachment, and secondary motion, which significantly enhance heat transfer while increasing pressure losses. Two turbulence modelling approaches are investigated: a lagged eddy-viscosity model and a Reynolds Stress Model (RSM). The V&V analysis shows that numerical uncertainty is strongly dependent on both mesh resolution and turbulence closure. The RSM provides improved predictions for thermal fields, accurately capturing the temperature evolution and characteristic trends observed experimentally, while the simpler model shows better robustness for hydraulic quantities. Validation against experimental data confirms that both models reproduce the main physical behaviour of the system, although discrepancies remain in regions dominated by strong anisotropy and thermal gradients. The study also identifies the assumption of simplified thermal boundary conditions as a relevant source of epistemic uncertainty.

The third case study addresses tritium transport in confined environments, where the objective is to assess the capability of CFD models to predict the dispersion and accumulation of radioactive species under complex flow conditions. This application is particularly relevant for safety assessment, as even moderate modelling inaccuracies may lead to significant deviations in predicted concentration levels in localised regions. The analysis reveals that the system is strongly influenced by transient flow structures and turbulence-driven mixing processes. In the absence of detailed experimental data, the assessment is based primarily on solution verification and sensitivity analysis. The results show that numerical predictions are highly sensitive to modelling assumptions related to turbulence representation and boundary conditions. In this context, the V&V framework is used to quantify numerical robustness and to identify the limits of applicability of the model rather than to perform strict validation. The study highlights that in safety-critical applications involving radioactive species such as tritium, uncertainty quantification is essential to ensure conservative and reliable interpretation of CFD results.

The fourth case study concerns a PEMFC, which involves strongly coupled electrochemical, thermal, and multiphase transport phenomena. The V&V analysis

is performed across different CFD platforms and modelling strategies, including ANSYS Fluent, STAR-CCM+, and OpenFOAM. Significant differences in numerical robustness and predictive accuracy are observed depending on the multiphase formulation and electrochemical implementation. Euler–Euler multiphase approaches exhibit numerical instability under certain conditions, while simplified formulations provide more stable but less detailed representations of the physical processes. Validation is performed using current density data, as no experimental measurements are available for liquid water saturation. The results show that discrepancies between numerical predictions and experiments are strongly influenced by differences in electrochemical modelling, interface treatment, and phase interaction assumptions. In particular, the kinetic-dominated regime exhibits larger deviations, highlighting the sensitivity of the model to the formulation of reaction source terms.

Across all four case studies, several general conclusions emerge. First, model-form uncertainty is consistently identified as the dominant contributor to the overall error budget once a sufficient level of grid refinement is achieved. Second, model performance is strongly dependent on the operating regime, with specific flow or transport conditions leading to a degradation of predictive accuracy. Third, the V&V framework proves essential not only for quantifying numerical and modelling uncertainties, but also for identifying the physical origins of discrepancies between simulations and experimental data. The results demonstrate that CFD model credibility cannot be defined in absolute terms, but must be assessed relative to a specific context of use and a quantified uncertainty range. Depending on the application, the same model may be suitable for engineering correlation development, design support, qualitative trend prediction, or only indicative analysis. This perspective is particularly relevant for multiphysics systems, where no single modelling approach is universally valid across all operating conditions. Overall, this work demonstrates that a systematic V&V methodology is essential to ensure that CFD simulations provide not only physically consistent results, but also quantitatively reliable information for engineering decision-making and safety assessment. By explicitly distinguishing between numerical errors, modelling assumptions, and experimental uncertainties, the proposed framework enables a transparent and robust interpretation of simulation results across a wide range of complex engineering applications.