Turbulent transport model validation at JET using integrated modelling enhanced by Gaussian process regression

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To have confidence in the predictions of any given model in unproven conditions, it must first be rigourously tested to show it behaves as expected and to understand its range of validity, through a process called *model verification and validation (V&V)*. However, with a complex non-linear system, such as a tokamak plasma device, the interpretation of experimental data and the V&V of any resulting models becomes increasingly difficult [1], though no less important.

This study proposes a more rigourous approach to profile fitting, through the use of *Gaussian* process regression (*GPR*) techniques [2, 3], and outlines the consequent improvements it brings to V&V within the field of nuclear fusion research. In particular, this procedure was applied to the JETTO transport code [4], which solves the mass, momentum, heat and current transport equations, coupled with the QuaLiKiz quasilinear turbulent transport code [5, 6]. A demonstration of this GPR fitting and improved validation process was performed on JET-ILW discharge #92436, a high-power H-mode baseline scenario plasma, with $B_T = 2.73$ T, $I_p = 2.98$ MA, and 28 MW neutral beam injection (NBI) and 5 MW ion cyclotron (IC) auxiliary heating applied. This discharge is of particular interest as it is the JET-ILW baseline with the highest D-D neutron flux to date and is the subject of extrapolation towards a D-T plasma. The input data used to generate these fits were averaged over a 0.5 s time window, specifically from 9.75 s – 10.25 s, with additional data filters applied based on physical constraints and known limitations.

Within this study, the primary inputs under investigation are the electron density, n_e , electron temperature, T_e , ion temperature, T_i , and toroidal flow angular frequency, Ω_{tor} , profiles. These *kinetic profiles* were evolved in time simultaneously and evaluated over ~ 10 τ_E to reach steady-state, due to the high sensitivity of the simulation on these quantities at the simulation boundary, especially on T_i/T_e [7]. These inputs are typically expressed on the *square-root nor-malized toroidal flux* coordinate, or simply *toroidal rho*, $\rho_{tor} = \sqrt{\psi_{tor}/\psi_{tor, LCFS}}$, where ψ_{tor} is the toroidal magnetic flux passing through the flux tube defined by the magnetic geometry, and LCFS is the last-closed-flux-surface. It is stressed that routine inclusion of momentum transport



Figure 1: Comparison of GPR fits (green line) and error (green shaded region) for JET #92436 against JETTO + QuaLiKiz output (blue line), using the GPR fits as the initial / boundary conditions and the base scenario parameters. The mean output (red dashed line) and output distribution (red shaded region) was determined from a Monte Carlo sampling of the four respective initial / boundary conditions simultaneously, with 100 sample points. Left quad: Kinetic profiles. Right quad: Derivative of kinetic profiles. For each quad, the following description applies: Upper left: Electron density profiles. Upper right: Electron temperature profiles. Lower left: Ion temperature profiles. Lower right: Toroidal angular frequency profiles.

prediction in multi-channel flux-driven transport modelling is non-standard, facilitated here by recent developments within the QuaLiKiz model [5].

After the extraction of experimental measurements of these quantities, they were processed by the GPR1D tool, which applies the GPR fitting technique (now available on a public GitLab repository, https://gitlab.com/aaronkho/GPR1D.git). The resulting fitted profiles, along with their associated derivatives, were then used as inputs for the integrated model. The uncertainties of the GPR fit, which are themselves derived from the measurement uncertainties, allowed for more rigourous sensitivity studies regarding the impact of the boundary conditions of the simulation, set at $\rho_{tor} = 0.8$ within the simulations performed in this study.

Figure 1 compares the GPR fit and the results from the JETTO + QuaLiKiz integrated model, including a Monte Carlo study of the boundary conditions performed using the GPR uncertainties. Although excellent agreement was achieved overall, the Monte Carlo study, facilitated by having the fit uncertainties, provided more quantitative insight into this statement. The overprediction in n_e was deemed less significant due to the large sensitivity of the model in predicting this quantity given the input uncertainties, but the T_i underprediction remained significant. Due to the known dependency of the EM-stabilisation effect on large fast ion pressure gradients [8, 9], generated in this discharge by IC heating, the ad-hoc electromagnetic (EM) stabilization factor, provided currently by an implementation based on $W_{\rm th}/W_{\rm tot}$, may have underestimated the magnitude of this stabilisation effect. However, the quantification of this shortcoming is outside the scope of this study and deeper investigations are left as future work.

In addition to using the GPR fit uncertainties to vary the boundary conditions, non-statistical sensitivity studies were performed using the JETTO + QuaLiKiz simulation to determine the possible physical phenomena repsonsible for achieving the record conditions in JET #92436. These sensitivity studies can still be evaluated against the fit uncertainties provided by the GPR. The additional sensitivities performed include: removing electron temperature gradient (ETG) scale turbulence in QuaLiKiz; removing an ad-hoc EM-stabilization factor based on W_{th}/W_{tot} from QuaLiKiz; removing the linear contribution of fast ions from QuaLiKiz; switching off the rotational contributions in QuaLiKiz; and adjusting the fitted angular rotation, Ω_{tor} , profile within $\pm 2\sigma$ to have a steeper or shallower gradient at the simulation boundary.

Figure 2 compares the results of these sensitivity studies to the fitted experimental profiles and their uncertainties. From these studies, a few points of interest to the turbulent transport physics community can be highlighted. The exclusion of ETG scale turbulence from QuaLiKiz yields a significantly higher T_e profile within the simulation of this discharge, likely due to the supression of electron heat transport generated by the ETG instabilities. Although the rudimentary multiscale component of the QuaLiKiz ETG model [8] is not fully verified against nonlinear multiscale simulations [10, 11], the excellent agreement in T_e here provides a compelling case for further nonlinear investigation of ETG impact in this discharge. However, such an investigation is outside the scope of this study. The impact of rotation shear in QuaLiKiz appears primarily in n_e within the simulation of this discharge, which is attributed to a strong $E \times B$ shear stabilisation effect on ITG instabilities within QuaLiKiz. Despite the fact that ITG instabilities also drive ion heat transport, this effect is not as prevalent in T_i likely due to compensating effects from the increasing density gradient. Additionally, the sensitivity of density peaking to the rotational shear is consistent with previous works [12, 13], although a more detailed transport analysis of this effect is recommended and left for future work.

Overall, a novel implementation of model validation incorporating the use of GPR techniques in profile fitting has been proposed and demonstrated in JETTO integrated modelling of JET-ILW discharge #92436, coupled with the QuaLiKiz quasilinear turbulence model. A comparison between the fitted and simulated profiles showed that an excellent level of agreement was achieved, with discrepancies in both the core n_e and T_i profiles. The n_e overprediction was deemed statistically insignificant due to the sensitivity of the model to the simulation boundary conditions and the T_i underprediction was suspected to be the result of an incomplete description of the fast ion contributions to the instabilities driving turbulent transport. It was also shown that the Ω_{tor} profile was crucial to the accuracy of integrated modelling results of JET discharges and that QuaLiKiz was capable of providing reasonable momentum flux predictions within the studied plasma regime. This capability is expected to be important for extrapolating to future scenarios, such as D-T plasmas.

As a final note, the proposed fitting procedure lends itself well to automatisation, and future



Figure 2: Results of the listed sensitivity studies (see legends), where the input profiles (green lines) are compared against the output profiles and the base case scenario (blue line). Left quad: Studies regarding the addition or inclusion of known physical phenomena. Right quad: Studies regarding toroidal rotation profile modifications. For each quad, the following description applies: Upper left: Electron density profiles. Upper right: Electron temperature profiles. Lower left: Ion temperature profiles. Lower right: Toroidal angular frequency profiles.

work is foreseen in applying this procedure to similar data from other tokamak devices, such as ASDEX-Upgrade, Alcator C-Mod, and WEST, with the aim of developing a large database of discharges suitable for performing model V&V studies on various gyrokinetic codes. Furthermore, large database of model inputs and outputs can be used to generate training sets for neural networks, allowing for the development of extremely quick and reliable model emulators for use in scenario optimization and tokamak controller design.

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