

ADVANCES IN PREDICTION OF TOKAMAK EXPERIMENTS WITH THEORY-BASED MODELS

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Abstract

The successful validation of theory-based models of transport, MHD stability, heating and current drive, with tokamak measurements over the last 20 years, has laid the foundation for a new era where these models can be routinely used in a "predict first" approach to design and predict the outcomes of experiments on tokamaks today. The capability to predict the plasma confinement and core profiles with a quantified uncertainty, based on a multi-machine, international, database of experience, will provide confidence that a proposed discharge will remain within the operational limits of the tokamak. Developing this predictive capability for the first generation of burning plasma devices, beginning with ITER, and progressing to tokamak demonstration reactors, is a critical mission of fusion energy research. Major advances have been made implementing this predict first methodology on todays tokamaks. An overview of several of these recent advances will be presented, providing the integrated modeling foundations of the experimental successes. The first steps to include boundary plasmas, and tokamak control systems, have been made. A commitment to predicting experiments as part of the planning process is needed in order to collect real use accuracy data and evolve the models and software into a robust whole discharge pulse design simulator.

1. INTRODUCTION

The idea of an integrated Pulse Design Simulator [1] (PDS) that includes core plasma profiles, pedestal structure, boundary plasma, heating and current drive sources and tokamak control systems has a long history. Time dependent tokamak transport codes of the 1980’s had integration of heating and fueling sources, core transport and current profile evolution but the plasma transport and pedestal models were empirical or inaccurate. The two breakthroughs that launched the present rapid development of predictive integrated modeling are the gradual improvement in the validated accuracy of quasi-linear models of core turbulence transport [2, 3, 4, 5, 6] and the validated EPED theory-based model for pedestal pressure height and width [7]. The advance in quasi-linear transport models allow for accurate prediction of the core plasma profiles with neoclassical and turbulent transport as shown in Fig 1 (left). The incremental stored energy (\(W_{inc}\)) (i.e. volume integrated pressure minus the pedestal pressure) is predicted within 19% of the measured value [8] for a variety of tokamak discharge regimes. These
core transport predictions were carried out with fixed heating and fueling sources using data for the boundary condition at the 80% flux surface. The prediction of the pedestal (pressure) height by the EPED model has been extensively validated as illustrated in Fig 1 (right) [9]. The standard deviation between the EPED and measured pedestal height is 22%.

At present there are several projects developing integrated modeling workflows that couple the EPED, or similar pedestal models, to core transport and magnetohydrodynamic (MHD) equilibrium. The control system for the tokamak (coils, gas puff, external heating and current drive etc.) are beginning to be coupled to these plasma prediction workflows. A full scale PDS will require electron, ion and impurity transport, the scrape-off layer (SOL) plasma and its interaction with the wall surfaces, global MHD and energetic particle (EP) stability boundaries, and a model of the plasma control system, to simulate the whole time sequence and operational limits of the tokamak discharge.

In every domain of tokamak physics, whether it be heating sources, energetic particle stability or drift-wave turbulence there exists a fidelity hierarchy of models. The highest physics fidelity models require the most computational resources, sometimes rendering them impractical for whole discharge integrated modeling. However, the high fidelity models are essential to calibrate the accuracy of faster reduced models. With the new modular integrated modeling workflows it is possible to use high fidelity computations to check if a predicted plasma state is accurately simulated by the reduced models. Rather than continue down the fidelity pyramid with more reduction, the power of neural networks (NN), fit to reduced theoretical models, is being exploited to bridge the final gap in speed required for whole discharge modeling. Hence, a PDS system should be able to select from a library of physics models in order to perform the tasks ranging from high fidelity validation to real time prediction and control of whole discharges. Whether it be time dependent, tightly coupled, integration, or iteration of a workflow of models to a self-consistent steady state, the theory-based modeling tools are being extensively used to predict the outcome and refine the plans for present experiments. This "predict-first" methodology is allowing for highly precise targeted physics validation experiments to be performed efficiently saving tokamak operation time.

This overview highlights the recent progress in predictive theory-based modeling. In Section II: Physics validation of theory-based models, three examples will be given. The first is the dramatic demonstration that local transport models can reproduce the seemingly non-local phenomenon observed after laser blow off cooling of the plasma edge. The second is the designed experimental demonstration that the super-H mode branch of the pedestal can be achieved in DIII-D in a shape compatible with JET constraints. The third example is the proof that an integrated modeling workflow can predict energy confinement in ASDEX Upgrade H-mode plasmas more accurately than an empirical global confinement database scaling law. In section III: Predictive modeling for experimental design, three examples are given. The first is the prediction, and validation of the impact of a new off-axis Neutral Beam Injection (NBI) system on DIII-D on the current and pressure profiles and global MHD stability. The second is the extensive predictive modeling in preparation for the D-T campaign on JET. The third is the predictive modeling being used to optimise high $\beta_p$ fully non-inductive discharges on EAST. In section IV: Progress towards a pulse design simulator, the advances in integrating plasma and tokamak control simulations are highlighted. First, the integrated plasma modeling workflow TRIASSIC [10] is presented as an example of a plug and play library of modeling tools with a flexible interface. Second, the emerging integration of tokamak control systems with plasma prediction by several teams is summarized. The concluding section V: Predict-First Initiative, gives a perspective on what is needed, beyond the tools, to develop a complete PDS capability with quantified uncertainty in time for...
use in planning ITER discharges.

2. PHYSICS VALIDATION OF THEORY-BASED MODELS

2.1. Cold pulse propagation in tokamaks

The fast response of cold pulses due to impurity injection in tokamaks, with an inversion of the inward electron temperature pulse from decrease to increase, has long been argued to be inconsistent with a local transport paradigm [11]. The first demonstration that the cold pulse temperature response could be captured by a local turbulence transport model (TGLF [4]) was performed for the Alcator C-MOD tokamak [12, 13]. Only electron and ion temperatures were predicted in these first cases, with the density profile being evolved in a prescribed way. It was found that the inversion of the electron temperature pulse from decrease (outer radii) to increase (inner radii) was caused by the stabilization of the trapped electron mode (TEM) through the flattening of the electron density profile. In discharges where the TEM mode was not dominant there was no inversion, in agreement with experiment. The transport model was then used to predict the cold pulse response and design experiments for [14] the DIII-D tokamak. The very fast, high spatial resolution, density profile data on DIII-D confirmed the speed of the prescribed density response and the electron temperature response predictions were observed. The final step was to prove that the TGLF model could predict the fast density response to the impurity injection. This required adding the injected impurity density to the transport modeling. This integrated modeling was performed for experiments on the ASDEX Upgrade tokamak [15]. The predicted electron temperature response is compared with data in Fig. 2. It was found that the transient destabilization of ITG modes in the plasma periphery, by the laser ablated impurities, produces a fast inward propagation of the impurity density, consistent with the increase of the ion transport coefficients for hollow impurity profiles in the presence of ITG [16]. Deeper into the plasma, the consequent sudden flattening of the electron density profile leads to fast stabilization of the TEM that produces electron heat transport in the plasma core. Thus, the speed of the combined electron, ion, and impurity, temperature and density pulses were accurately modeled and new physics insights were discovered. This is a convincing proof that local turbulence transport can account for the seemingly paradoxical cold pulse phenomenon.

![FIG. 2. Time evolution of the central (a) and peripheral (b) electron temperature measured (red) and simulation (blue) with ASTRA/STRAHL/TGLF. Fig 12. from ref [15]](image)

2.2. Super-H regime

The EPED model [17] for H-mode pedestal structure computes the pressure at the top of the edge transport barrier (pedestal) and the width of the barrier by taking into consideration two constraints. The stability boundary of kinetic ballooning modes (KB) (a kinetic-MHD instability that is localized within the edge barrier) and the peeling ballooning modes (PB) (an MHD mode that spans the transport barrier width). The EPED model has been extensively validated with experimental measurements from a large number of tokamaks worldwide [7, 9, 18, 19, 20, 21]. The EPED model predicts that there are two stable branches to the pedestal structure under certain conditions. Experiments on DIII-D confirmed the existence of these two branches [19]. The higher pressure branch is called the super-H mode. The world record pedestal pressure was achieved on the Alcator...
C-MOD tokamak [20] and record D-D fusion gain was achieved on DIII-D [9] in the super-H regime. After installation of the ITER like wall (ILW) on JET the pedestal pressure was reduced compared to what was found with a carbon wall. This is, at least in part, due to the need to run JET at higher density in order to prevent influx of tungsten from the divertor to the core plasma. The normal H-mode branch has a reduction in the pedestal pressure at high density but the super-H pedestal pressure rises with density. The super-H regime holds promise for achieving high fusion performance on JET. This motivated exploring if the super-H regime could be accessed by JET. Due to interactions with parts of the vessel wall, the JET triangularity is limited to $\delta \leq 0.4$ for a lower single null divertor plasma. EPED predictions, shown in Fig. 3 for JET (left) were performed and it was found that super-H access at low density was possible for $\delta > 0.4$. An single day experiment on DIII-D [21], in a shape and aspect ratio similar to JET, confirmed the predicted super-H (SH) access shown in the red box of Fig. 3 (right).

2.3. Data free predictive modeling

With an integrated modeling workflow that includes core transport, pedestal structure, and an MHD equilibrium solver, it is possible to produce a prediction of the plasma, out to the separatrix, without a boundary condition taken from data. Even without a SOL model of the separatrix boundary conditions, prediction of energy confinement time for H-modes can be made. For a limited set of DIII-D H-modes this data-free prediction has been found to be quite accurate [23].

The Integrated Modeling based on Engineering Parameters (IMEP) workflow [24] uses the ASTRA transport code [25, 26] to predict the core plasmas profiles. A pedestal model is included based on the idea that PBM limit the pedestal (like EPED), but differs from EPED in that it does not assume a KBM scaling of the transport connecting pedestal width and height. Instead, the particle fueling and a constraint on the electron temperature gradient is employed. An empirical model for the boundary plasma provides a separatrix boundary condition. The negative effect of fuelling on the pedestal top pressure is better predicted by this approach than the KBM constraint. This workflow yields a prediction of global energy confinement time for a data set of 50 ASDEX Upgrade H-modes that is significantly better than the IPB98(y,2) [27] empirical scaling law as shown in Fig. 4. A power law cannot capture the variations in the energy confinement with operational parameters (e.g. fueling) as well as the integrated theory-based model. The IMEP-ASTRA workflow used TGLF.
for core turbulent transport, NCLASS [28] for the neoclassical transport and MISHKA [29] for the PBM stability.

3. PREDICTIVE MODELING FOR EXPERIMENTAL DESIGN

3.1. Design of off-axis neutral beam current drive system on DIII-D

The neutral beam injection (NBI) heating systems on DIII-D have made upgrades to their positioning capability in recent years. One upgrade was to enable positioning of the NBI line of sight to be tilted to match the pitch of the magnetic field at an off-axis location. This was predicted by theory to increase the off-axis current drive capability of the NBI [30]. These major changes to the NBI systems were motivated by modeling predictions with the state of the art Integrated Plasma Simulator IPS-FASTRAN workflow [31]. The predicted off-axis current driven by the NBI is shown in Fig. 5 (left). The predicted plasma profiles, including the current density, are

![Deposition profile of the off-axis NBI predicted and measured](image1)

![Change in the $\beta_N$ required for full non-inductive operation and the global MHD limit](image2)

FIG. 5. (left) deposition profile of the off-axis NBI predicted and measured. (right) Change in the $\beta_N$ required for full non-inductive operation and the global MHD limit [31]

a steady state self-consistent IPS-FASTRAN solution of the pedestal structure (EPED) (height and width), core transport (TGLF+NCLASS), MHD equilibrium (EFIT) and NBI heating and current drive (NUBEAM) using validated theory-based models. The modeling predictions for the off-axis neutral beam current drive have now been confirmed with experiments as shown in in Fig. 5 (left). In the right panel of Fig. 5 are shown the predicted increase in the MHD stability limit ($\beta_N$) (red) for fully non-inductive current discharges ($f_{NI} = 1$) (black) at higher safety factor ($q_{95}$). These predicted stability limits have also been validated with experiments [31]. Use data on the accuracy of these predict first method simulations are a valuable start on quantifying the uncertainty in the IPS-FASTRAN workflow predictions. The IPS-FASTRAN workflow was the first integrated modeling tool that iterated, core transport, the EPED model and the MHD equilibrium to steady state. It has been the main contributor to the experimental planning of the DIII-D advanced tokamak program. This tool was used for a tokamak design project that identified a candidate for a compact net electric tokamak fusion pilot plant [32] taking advantage of the advance tokamak regime.

3.2. JET D-T campaign

The JET tokamak program has been preparing for its second deuterium-tritium (D-T) operational campaign, begun in March 2021, for the last several years. Part of this preparation has been to extensively model the best experimental target discharges and use the transport modeling to predict the fusion power production that JET can achieve. The modeling effort has also included validation of the transport models for conditions found in JET high performance discharges using both reduced models and gyrokinetic turbulence simulations.

The installation of the ITER-like wall (ILW) in JET resulted in constraints to the operation of JET that lowered H-mode energy confinement [33]. When operating with the ILW, JET has observed that the pedestal height is, in some cases, reduced from similar cases with the carbon wall. An extensive set of comparisons of more than 200 JET-ILW discharges to the EPED model [34], [35] has explained some of the observations in JET-ILW discharges, but significant mysteries remain, including pedestal and ELM behavior with strong gas puffing, and the effects of impurities on the pedestal. Recent studies (e.g., [36], [37]) have further clarified aspects of pedestal MHD
FIG. 6. The shaded area represents the GPR confidence interval, with the experimental data averaged between 9.5s < t < 10.15s. The solid line is the JINTRAC-QuaLiKiz prediction for density and temperature profiles before the first pellet (t = 10.18s), after 2 particle confinement times of relaxation. The dotted lines show the profiles just after the first pellet injection (t = 10.19s) [47]

stability in JET-ILW discharges. Although EPED has been shown to have good agreement with experiment across a number of machines, including JET; some characteristics of metal wall tokamaks that have been found to impact pedestal structure have only recently been included in the model and not extensively compared to experiment. The strong hydrogenic gas puffing that is used to lower the divertor temperature, to reduce sputtering, results in increased separatrix relative to pedestal density [34]. The high gas puffing was also found to lead to decrease in the edge rotation frequency, thereby slowing down the core rotation and degrading the core confinement [38].

The tungsten divertor of the ILW was also observed to generate a strongly peaked tungsten accumulation in the core of low density JET H-modes. The transport physics of this peaking has been extensively modeled with neo-classical transport and turbulence simulations including toroidal rotation velocities larger than the tungsten thermal velocity. Using the NEO code with full sonic rotation physics [39], neo-classical transport has been shown to be the cause of the peaking of the metal impurity density profile in the center of the plasma in strongly rotating ASDEX Upgrade and JET discharges. Super-thermal tungsten toroidal rotation was found to enhance both the diffusive and convective components of the tungsten radial particle flux by more than an order of magnitude. As a consequence, the neo-classical ion transport (as opposed to the ion scale turbulent transport) dominates the central part of the plasma inside $r/a < 0.3$. This differs from the case of the main hydrogenic species that has sub-thermal rotation. The results were validated [40, 41, 42] by comparing soft x-ray (SXR) emission tomography and predicted SXR emission forward-modeled from the two-dimensional tungsten density computed using the neo-classical transport from NEO and the turbulent transport from the gyrokinetic code GKW [43] that also includes sonic rotation effects. However, in addition to neo-classical transport, it was also recently found that toroidal rotation with moderate rotation shear, relevant for the pedestal, can lead to enhanced ion scale turbulent transport that dominates over the neo-classical transport at low collisionality [44]. The turbulent transport of electron particles also plays an indirect role in the tungsten accumulation. The electron density peaking is determined by the turbulence, since neo-classical electron particle transport is very small. Peaking of the electron density increases the neo-classical particle pinch of the tungsten. Additional electron heating can flatten the electron density [45], by exciting electron modes in the turbulence. This is consistent with the observation that additional central electron heating helps prevent the accumulation of metal impurities. This screening effect has been demonstrated to be effective in D plasmas [46]. Ultimately, for modeling impurity accumulation, both the neo-classical and turbulent transport must be considered. Inclusion of sonic rotation effects, neglected in most theoretical models, is also important.

The impact of the main ion species on energy confinement in JET has been the focus of experiments [48] and modeling [49, 50, 51, 52]. The ion species dependence of the core transport was well predicted by quasi-linear models [50] but, as was also experimentally observed in 1997 JET DT campaign [53], most of the species dependence in H-mode comes from the pedestal which is being investigated with gyrokinetic simulations.

The JINTRAC integrated modelling framework, with the quasi-linear model QuaLiKiz [5] as the turbulent transport model and HIPI2 [54] as the pellet deposition model, successfully reproduced observations over multiple pellet cycles in JET mixed-isotope experiments. The modeling of the impact on the plasma profiles of one pellet in the
series is shown in Fig. 6. The electron density profile becomes quite hollow transiently after the pellet injection (D pellet in H plasma). The hollow density profile has a stabilizing effect on trapped electrons well captured by QualiKiz. The concomitant local modification of the temperature profile is destabilizing and maintains inward particle transport. The predicted relaxation time of this density hill and inward penetration of deuterium agrees with the JET experiment.

The accuracy of transport modeling prediction of 80 JET H-mode discharges has been validated [55] and TGLF for turbulent plus NCLASS [28] for neoclassical transport was found to be an accurate predictor of ion temperature profiles in the core plasma. This provided a baseline validation of the transport models for JET. A large effort is being made to make predictions of the two highest performance regimes in JET. Based on the good reproducibility of the reference D discharges, the DT predictive modelling results are being used to provide guidance for planning the ongoing second D-T campaign experiments.

3.3. High poloidal beta regime in EAST

The EAST tokamak research program is focused on demonstration of steady state tokamak operation [56]. The current in the plasma must not be driven by induction (ohmic) for true steady state. The EAST tokamak has external current drive from Electron Cyclotron Heating (ECH) and Lower Hybrid Wave (LHW) sources. At high poloidal beta ($\beta_P$) much of the current is self-generated (bootstrap current) by the particle drifts in the inhomogeneous magnetic field. The EAST modeling team has undertaken predictive integrated modeling, including core transport, pedestal structure, and MHD equilibrium, to optimize the use of the external current drive sources to achieve a fully non-inductive discharge. The STEP integrated modeling workflow [57] is used (with TGLF, NEO, EPED, EFIT). An example of this modeling [58] is shown in Fig. 7. The predicted electron (a) and ion (b) temperatures profiles agree well with the EAST measurements even though the plasma is in a high $T_e/T_i$ regime with energy confinement a factor of 1.3 higher than the IPB98(y,2) empirical scaling. The components of the current driven by all of the sources (c) show good agreement with the integrated model. This demonstrates that the errors in the predicted plasma profiles do not become amplified by the current drive source calculation. The high $\beta_P$ regime has energy confinement that can be more than 1.5 times the empirical scaling. The higher safety factor of this regimes provides lower disruptivity and higher bootstrap fraction compared to other advanced regimes making it an attractive steady-state tokamak fusion reactor regime [59].

![Integrated modeling prediction of a fully non-inductive high $\beta_P$ regime discharge on EAST](image)

FIG. 7. Integrated modeling prediction of a fully non-inductive high $\beta_P$ regime discharge on EAST [58]. Electron temperature (a), ion temperature (b) and current density components (c)

4. PROGRESS TOWARDS A PULSE DESIGN SIMULATOR

4.1. Integrated plasma modeling workflows

The ITER Integrated Modeling and Analysis Suite (IMAS) [60] has set standards for data structure and communication between codes that are being used to build workflows. The STEP workflow [57] being developed at DIII-D can interface with a wide range of transport, MHD equilibrium, MHD stability, pedestal, heating and current

7
drive, and boundary models from high physics fidelity codes to neural networks. It is a flexible tool for planning experiments on DIII-D [61]. The KSTAR team is developing a similar suite called TRIASSIC (Tokamak Reactor Integrated Automated Suite for Simulation and Computation) [10]. The structure of TRIASSIC is illustrated in Fig. 8. The library of Fortran codes communicate with each other through the IMAS data structure wrapped in a Python interface. This suite can be iterated by an external controller to find a steady state self-consistent with all of the included physics modules. The IPS-FASTRAN [31] and IMEP-ASTRA [24] workflows also work in a similar way. The TRIASSIC workflow is proving successful at modeling KSTAR discharges. It is being used to find optimum profiles of magnetic shear over safety factor ($s/q$) for higher energy confinement in Hybrid regime discharges [62]. For the validation of TRIASSIC, a database of about 50 stationary discharges of various KSTAR scenarios was established. First, they conducted interpretive simulations to compare plasma stored energy which can be calculated by using plasma density, temperature, and fast ion energy by TRIASSIC or from the experiment by EFIT [63] relying on magnetic diagnostics. Comparison [10] of energy calculated by TRIASSIC with EFIT yields a low standard deviation of 8%. The TRIASSIC predicted stored energy in high $\beta_P$ discharges, with energetic particle (EP) instabilities was too high. This indicates that a model for the transport of fast ions due to EP modes is needed.

FIG. 8. The structure of the integrated suite of code, TRIASSIC. Equilibrium, transport, heating and current drive, grid, neutral modules separately access to the IMAS data structure via the Python interface. Each plasma analysis codes, originally coded in the Fortran language, was wrapped by the F2PY wrapper which enabled direct access via Python interface. [10]

4.2. Integration of plasma control system

The tokamak plasma control system (PCS) has to be robustly engineered for reliable operations. Coupling of the PCS to an integrated model of the plasma equilibrium and transport is the next step towards a PDS. The control of the plasma position and shape by the PCS system [64] is accomplished with a real time free boundary MHD equilibrium calculation using the magnetic probe signals and the EFIT code [65]. A kinetic equilibrium reconstruction (KER) includes measurements of the plasma pressure and safety factor profile. Using a KER in the PCS requires real time plasma profile prediction. The pressure and safety factor evolution by the RAPTOR transport code [66], with a simple transport model, has been coupled to the free-boundary equilibrium code LIUQE [67] to compute KERs that are used by the PCS system of the TCV tokamak [68].

An project to include the KSTAR (PCS) coupled to the TRANSP code [69, 70] simulation of the plasma and MHD equilibrium is underway [71]. At present only highly reduced models of the plasma fit to predictive TRANSP simulations are used in the control coupling.

The “flight simulator” FENIX [72] is being developed to simulate the plasma discharges before their execution. A flight simulator has to predict the plasma discharge and the control system behaviour with reasonable accuracy according to the pulse schedule to detect possible errors in pulse design. The FENIX simulator is built using the ITER PCS Simulation Platform [73] with ASTRA and the 2D equilibrium solver SPIDER [26]. The FENIX simulator has been validated with ASDEX Upgrade discharges [74] with a primitive transport model.

5. PREDICT FIRST INITIATIVE

The new integrated modeling and predictive control workflows are an exciting step towards a critical requirement for tokamak reactors of the future. Tokamak discharges must be shown, by predict-first modeling, to have controlled operation of the whole discharge with a quantified margin away from operational limits. The whole time history of the discharge and the plasma control system must be simulated. A fast pulse design simulator (PDS)
G. M. Staebler

[1] that can run simulations of a range of scenarios, including unplanned actuator faults, exploring the range of plasma control responses is within reach using neural networks fit to QuaLiKiz [75] or TGLF and EPED [76]. However, a PDS is much more than a software project. Achieving this capability requires a dedicated effort, in today’s machines, to routinely use predict-first simulations in the planning of experiments and to collect data on the accuracy of the predictions. This will drive improvements in the models and methodologies, and will provide the experience based data to confidently quantify the uncertainty of the PDS. Experience on smaller tokamaks, that can exceed operational limits without damage, is the only way to validate a PDS. The use of the evolving models for experimental design will provide the benefit of more efficient use of tokamak operational time by identifying problems with the run plan.

We have not yet begun this predict-first initiative in a serious way on any tokamak, let alone on a worldwide bases, but this is what is required for sufficient experience data to be collected in time for ITER operations. It is time the fusion energy community commit to a coordinated, intense focus on the goal of developing this validated PDS capability.

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