REDUCED ENERGETIC PARTICLE TRANSPORT MODELS ENABLE COMPREHENSIVE TIME-DEPENDENT TOKAMAK SIMULATIONS

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Abstract. The inclusion of reduced-physics energetic particle (EP) transport models in the tokamak transport code TRANSP has resulted in a considerable improvement of interpretive and predictive capabilities for time-dependent simulations including the effects of EP transport by instabilities. The *kick model* has recovered the measured toroidal Alfvén eigenmode (TAE) spectrum on NSTX-U and DIII-D, and has reproduced details of the fast ion diagnostic data measured on DIII-D for EP-driven modes and tearing modes. Being able to predict the occurrence and effect of those instabilities is one of the grand challenges for fusion and a necessary step to mitigate their negative effects. The kick model has proven the potential of phase-space resolved EP simulations to unravel details of EP transport for detailed theory/experiment comparison and for scenario planning based on optimization of NBI parameters. Work is also ongoing to complement the kick model approach with the RBQ-1D model based on the resonance-broadened quasi-linear theory to develop a self-consistent, numerically efficient predictive EP transport model for integrated tokamak simulations. Both models are undergoing extensive verification and validation against analytical, numerical and experimental data to confirm their validity and identify potential applicability limitations.

1 Introduction

Validated quantitative predictions of tokamak scenarios are required to explore the operational space of fusion reactors such as ITER and DEMO. As plasma performance improves towards *burning* plasmas, the importance of predicting the behavior of highly energetic particles (EPs) - e.g. from fusion reactions, neutral beam injection (NBI) and rf waves - increases. In fact, energetic particles are expected to be the dominant source of heating and momentum for burning plasmas. Although NBI and rf waves are reliable tools for heating and current drive, the resulting EP population can destabilize Alfvénic (AEs) and other magneto-hydrodynamic (MHD) instabilities [1][2][3][4][5]. The latter typically cause a degradation in performance and, if significant EP losses are induced, can lead to damage of vacuum vessel components. As an example, results from a NSTX-U [6] discharge featuring several EP-driven instabilities are shown in Fig. 1, which is further discussed in Sec. 3.2. Considerable degradation of plasma performance can be inferred from the reduction in neutron rate, fast ion density and NB driven current with respect to *classical* simulations that do not include the enhanced EP transport by instabilities.

At present, numerical codes can predict the spectrum of Alfvénic instabilities (AEs) that is expected for a given scenario [7][4][8] and the EP transport that results from a given AE spectrum. A remaining challenge is to develop quantitative methods to compute AE stability, saturation amplitude and associated EP transport in time-dependent transport codes that are able to predict a whole plasma discharge. *Reduced* models are an effective tool to distill information from theory and first-principles codes and implement methods to investigate AE stability and fast ion transport [9][10][11][12][13][14]. Two approaches are currently being pursued at PPPL for the development of predictive, reduced EP transport models for integrated simulation codes such as TRANSP [15][16][17]. A first approach relies on numerical tools to distill information on EP transport that can then be used in TRANSP. This is the basis for the *kick model* [18][13]. A second approach is based on the quasi-linear theory for wave-particle interaction [19] extended to include the resonance frequency broadening as the mode amplitude increases [9] and the effects of multiple resonances. This approach has resulted in the development of the RBQ-1D model [14].

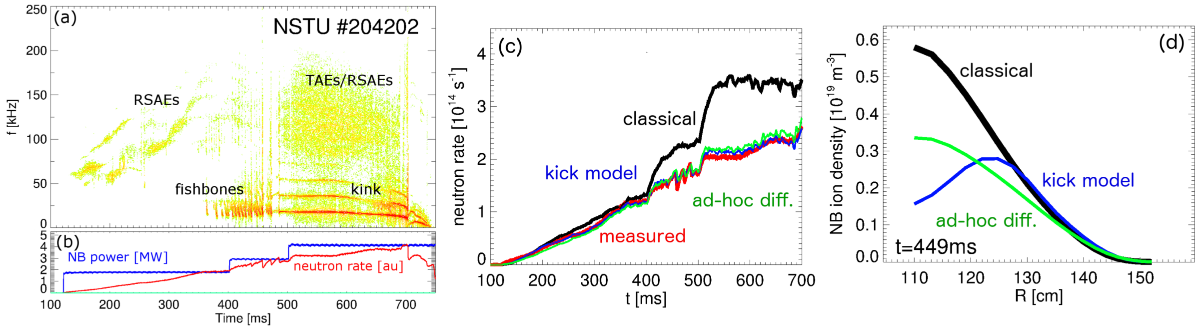

FIG. 1: (a) Magnetic fluctuations spectrum from NSTX-U discharge #204202. Several types of EP-driven instabilities are observed. (b) Waveform of injected NB power and measured neutron rate. (c) TRANSP results for classical simulations (black) and simulations including the effects of instabilities. The measured neutron rate is shown in red. (d) Profiles of fast ion density around $t = 450$ ms.

Initial studies with kick and RBQ-1D models have highlighted the importance of including EP phase space effects to analyze and interpret the stability properties of Alfvénic modes. For example, the competition between gradients in the EP distribution along both energy and canonical angular momentum cannot be captured by simpler models solely based on AE drive by radial gradients of the EP population (so-called *critical gradient models* [10][11]) or gradients in the velocity variable only [20][21]. The latter effects are especially important in plasmas with NB injection - such as those of NSTX-U, DIII-D [22] and most present-day tokamaks - due to the strongly non-isotropic EP distribution. Phase space resolution is also crucial for a quantitative validation of the models against fast ion diagnostics, e.g. Fast Ion D-Alpha (FIDA) and neutral particle analyzers (NPA).

In the remainder of this work, recent advances in the modeling tools are first introduced in Sec. 2. Section 3 presents examples of the application of those tools to interpret discharges from NSTX-U and DIII-D, including a discussion on their application for *predictive* analysis (Sec. 3.3). The main results of this work are summarized in Sec. 4.

2 Modeling tools for interpretive EP transport analysis

Kick model. Fast ion physics is simulated in TRANSP through the NUBEAM Monte Carlo module [16][17], which includes classical phenomena such as collisional scattering and slowing-down, and atomic physics (e.g. charge-exchange and neutralization reactions). In recent years, NUBEAM has been updated to include a physics-based reduced model to account for resonant EP transport by instabilities. The *kick model* [18][13] introduces a transport probability matrix in NUBEAM. The matrix is defined over phase-space constant of motion variables E, P_ϕ and μ that represent the EP energy, toroidal angular momentum and magnetic moment [23][24]. For each (E, P_ϕ, μ) region, the matrix contains a probability $p(\Delta E, \Delta P_\phi)$ which represents the probability of correlated fast ion energy and P_ϕ changes (or *kicks*) caused by the instabilities. Each probability matrix is associated with either a single mode or a set of modes. The kick matrix is computed via particle following codes such as ORBIT [25], using mode structures computed through MHD codes such as NOVA/NOVA-K [26][27][28] (see Appendix of Ref. [13] for more details).

RBQ-1D resonance-broadening quasi-linear model. The RBQ-1D model [14] is capable of evolving the fast ion distribution function while self-consistently evolving the amplitude of modes. The code is presently under development in its one-dimensional version, with the distribution function relaxation happening along the toroidal canonical momentum P_ϕ. (Resonant wave-particle interactions are still resolved in terms of the three constants of motion defining the fast ion phase space). Significant reduction of the AE amplitude is observed in simulations when the actual AE radial displacement structure is included in RBQ-1D to realistically evaluate the wave particle interaction bounce frequency. The reduction of RSAE and TAE amplitudes is two or three times in comparison with simplified model simulations assuming no radial dependence of the mode structure [9]. RBQ-1D is interfaced with the NOVA/NOVA-K codes,

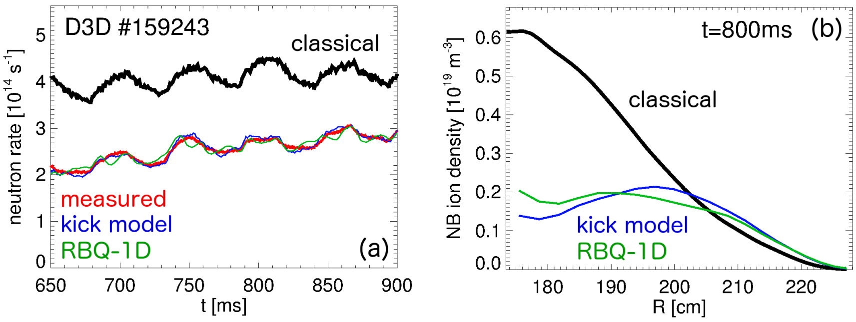

FIG. 2: Benchmark between interpretive analysis of DIII-D discharge #159243 with kick and RBQ-1D models. (a) Neutron rate from TRANSP compared to the measured rate. (b) Fast ion density profiles at $t = 800$ ms, showing good consistency between kick and RBQ-1D models. (Adapted from Ref. [14]).

which provide radial mode structure, damping rate and resonant surfaces for candidate unstable modes. Numerical outputs from RBQ-1D have been verified against known analytical solutions of the pitch angle scattering operator for simplified test cases. Both the resonant and the collisional diffusive operators within the code have been verified.

Reduced EP transport models in TRANSP. The kick model has been expressly developed to fit within the Monte Carlo implementation of NUBEAM. As described in detail in Ref. [13], wave-particle interaction processes are distilled (through ORBIT modeling) into *kick probability matrices*, $p(\Delta E, \Delta P_\zeta | E, P_\zeta, \mu)$. Each probability matrix can represent a single perturbation or a set of perturbations with similar temporal evolution. Information on magnetic equilibrium, plasma profiles and heating sources is passed from TRANSP to NUBEAM at the beginning of a NUBEAM time step k. Inputs from the kick model (probability matrices and amplitude evolution) are also loaded. From step k to step $k+1$, a representative ensemble of fast ions is evolved. The particle ensemble is updated based (primarily) on active NB sources and sinks, such as losses, re-neutralization and thermalization. In addition, particle variables are mapped in phase space to compute the kick model corrections to the particle's orbit. Knowing its (E, P_ζ, μ) variables, kicks ΔE and ΔP_ζ are sampled randomly from each transport probability matrix. The evolution of the fast ion ensemble under classical physics and kick model effects is repeated until the end of step k, at which time quantities such as fast ion density, power from thermalization, NB-driven current are computed. TRANSP parameters are then updated, for instance by recomputing the magnetic equilibrium based on total current evolution, and made available for the next NUBEAM step.

A comparison between kick and RBQ-1D models for a DIII-D discharge featuring unstable AEs is shown in Fig. 2 [14]. Both models are used here in interpretive mode, in which the mode amplitude is provided as input (e.g. from experimental measurements). The measured neutron rate shows a $\approx 40\%$ deficit with respect to classical predictions that do not account for enhanced EP transport by instabilities. The reduced models recover the measured deficit well within the typical uncertainty of $\pm 10\%$ in the neutron rate measurements, see Fig. 2a. Moreover, both models result in a similar radial NB ion density profile (Fig. 2b), in spite of the different methods used to infer the EP transport coefficients. In general, the initial benchmark between the two model shows reasonable agreement even at the level of the fast ion distribution function modified by the EP interaction with instabilities [14]. The comparison is being recently extended to the use of the models in *predictive* mode, cf. additional discussion in Sec. 3.3.

3 Analysis of fast ion transport in NSTX-U and DIII-D plasmas

Confinement of energetic particles can be affected by a variety of instabilities. The following sections discuss examples of the analysis of NSTX-U and DIII-D plasmas, including the corresponding physics insight that can be achieved through the use of reduced EP transport models.

Starting from instabilities with frequencies comparable to the local plasma rotation frequency, tearing

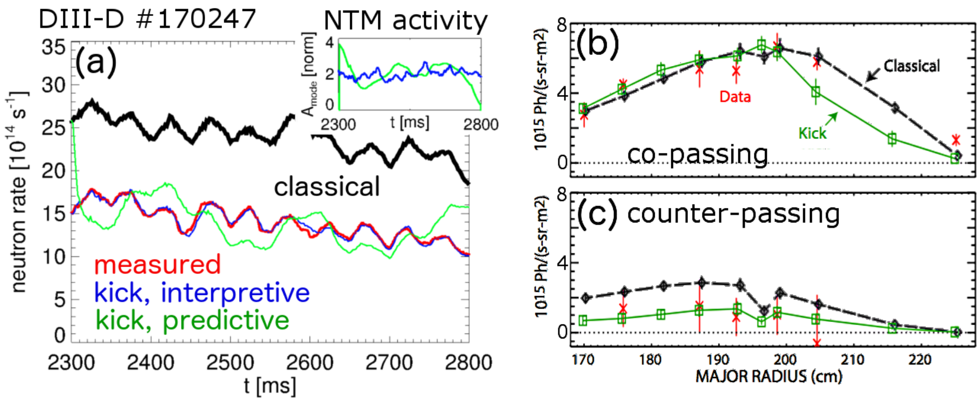

FIG. 3: Analysis of DIII-D discharge #170247. (a) Neutron rate from TRANSP modeling compared to the measured rate. The inset shows the mode amplitude inferred from the interpretive kick model analysis (blue) and from measurements of the NTM island width (green). (b-c) Radial profiles of FIDA signal for co- and counter-passing fast ions from TRANSP (lines) and from experimental data (red symbols). (Adapted from Refs. [29][30]).

modes (TMs), kink modes and sawteeth are well known to enhance EP transport. Examples from NSTX and DIII-D discharges with unstable fishbones and neoclassical TMs (NTMs) are discussed in Sec. 3.1. At higher frequency, Alfvénic instabilities (toroidal and reversed-shear AEs, TAEs and RSAEs) dominate the fluctuation spectrum. Examples of their effect on fast ion transport and associated TRANSP analysis are also discussed in Sec. 3.1. Unlike the examples in Sec. 3.1, in many practical scenarios multiple types of instabilities can be simultaneously present. The example shown in Fig. 1 is further discussed in Sec. 3.2 to illustrate the complexity of such multi-mode cases and how reduce models can address them.

3.1 Single-mode scenarios

Figure 3 shows simulation results for a DIII-D discharge aimed at investigating fast ion transport by NTMs [29]. The discharge was specifically designed to sustain large $(m, n) = (2, 1)$ NTMs, where m, n are the poloidal and toroidal mode numbers. The deviation between measured and (classically) simulated neutron rate (Fig. 3a) indicates substantial fast ion transport.

Results from two simulations with the kick model are also shown in Fig. 3a. For the first simulation, the NTM amplitude in the kick model is adjusted until satisfactory agreement with the measured neutron rate is achieved. In the second simulation, the NTM island width is inferred from experimental data from electron-cyclotron emission (ECE) and magnetic pickup coils [31][32], then converted into the input mode amplitude for the kick model. The overall reduction in neutron rate is comparable for the two cases. In fact, the mode amplitude used for the interpretive simulation is quite close to the one directly inferred from the experiment, see inset in Fig. 3a.

Figures 3b-c show Fast-Ion D-Alpha measurements [33] compared to reconstructed signals based on the TRANSP output processed through the FIDAsim code [34]. The comparison reveals important features of fast ions in phase space. For co-passing fast ions, both experimental data and simulations indicate a weak effect of the instability. FIDA signals are close to those from the classical simulation over most of the minor radius. Counter-passing fast ions, in turn, are strongly affected by NTM. The simulated reduction in FIDA signal of $\sim 50\%$ is consistent with the measurements.

Single-mode analysis has also been applied to NSTX discharges with unstable fishbones. For all models, transport levels are adjusted to bring the simulated neutron rate in agreement with the experiment. The main difference among models is how different regions of fast ion phase space are affected by the fishbones. In the TRANSP fishbone model [36], the fraction of fast particles redistributed by the mode can be set as input. Under the assumption that the main (bounce) resonance driving the mode involves trapped fast ions, only deeply trapped particles are affected for smaller fractions. In this analysis, a fraction of 25% gives a reasonable agreement in terms of measured vs simulated neutron rate. The second model uses a radially uniform, time varying diffusivity to enhanced fast ion transport. In

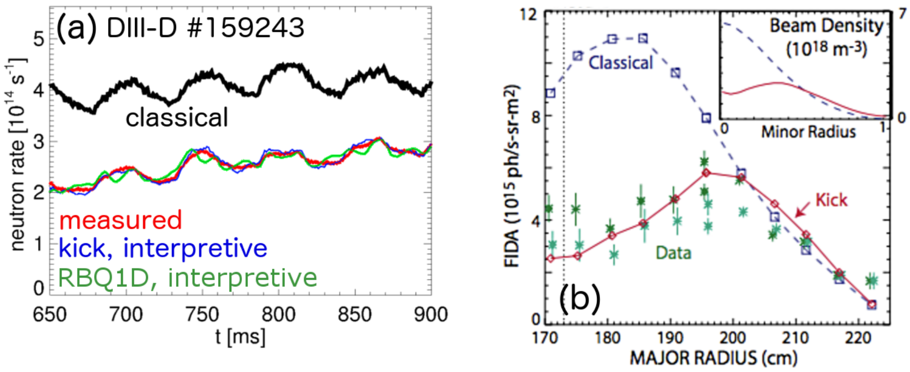

FIG. 4: Analysis of DIII-D discharge #159243. (a) Neutron rate from TRANSP modeling compared to the measured rate. (b) Radial profiles of FIDA signal from kick model analysis (line) and from experimental data (green symbols). The inset show the fast ion density from TRANSP. (Adapted from Ref. [35]).

its simplest implementation (adopted here), the model acts on all fast ions independently of their phase space localization. A diffusivity of up to 1 m^2/s is required to match the measured neutron rate. In the kick model, fishbones are modeled with an analytical hat-like radial structure. Toroidal and poloidal mode numbers are $n = 1$ and $m = 1$. ORBIT simulations produce the transport probability used in NUBEAM/TRANSP. ORBIT shows that both trapped and co-passing particles can drive the mode, in agreement with previous studies [37]. Mode amplitudes $\delta B/B \sim 1 - 5 \times 10^{-3}$ give reasonable match with the measured neutron rate. (δB is the perturbed radial magnetic field).

All three models can recover (by design) the measured neutron rate decrease, but the inferred NB ion density and NB driven current profiles typically differ. Profiles from the ad-hoc diffusivity run simply resemble those from the classical run rescaled by $70 - 80\%$. Because of their selectivity in phase space, the fishbone and kick model show more variability. However, density and NB driven current profiles are very different. For example, since the fishbone model only redistributes deeply trapped particles that contribute very little to the toroidal current, its NB driven current profile almost overlaps that from the classical run. In contrast, the kick model is also redistributing co-passing particles, which results in a decrease of the core NB driven current.

The analysis of scenarios with NTMs or fishbones is simplified by the reduced number of instabilities that have to be simulated. In contrast, scenarios with unstable AEs typically have to include a much larger number of modes, from 3-4 up to $\sim$ 20 or more. This translates to a very large number of (possibly overlapping) resonances that populate the fast ion phase space. Examples from a DIII-D plasma with unstable AEs are shown in Fig. 4. (Details on the experimental scenario can be found in Refs. [35][38]). Interpretive analysis with the kick and RBQ-1D models achieves a good match with the measured neutron rate. For this case, a detailed comparison with FIDA signals has been performed [35], see Fig. 4b. TRANSP computes a slightly hollow fast ion density profile (see inset in Fig. 4b) and a corresponding hollow FIDA brightness profile as a function of radius. Simulated FIDA features are in excellent quantitative agreement with the measurements. Given the complexity of the AE transport matrices once all resonances are included, it can be concluded that kick and RBQ-1D models are capturing the relevant wave-particle interaction and transport physics.

3.2 Multi-mode scenarios

The successful use of the reduced EP transport models in the analysis of cases with a single type of instabilities is promising. A more challenging task is the analysis of scenarios with multiple instabilities simultaneously affecting fast ions. So far, this capability has been tested only for the kick model. (RBQ-1D relies on the theory of quasi-linear EP transport specifically developed for Alfvénic instabilities). Figure 1 shows an example of a NSTX-U discharge with coexisting AEs, fishbones and kink modes. The transport probabilities for each type of mode are computed through ORBIT. For AEs, radial mode

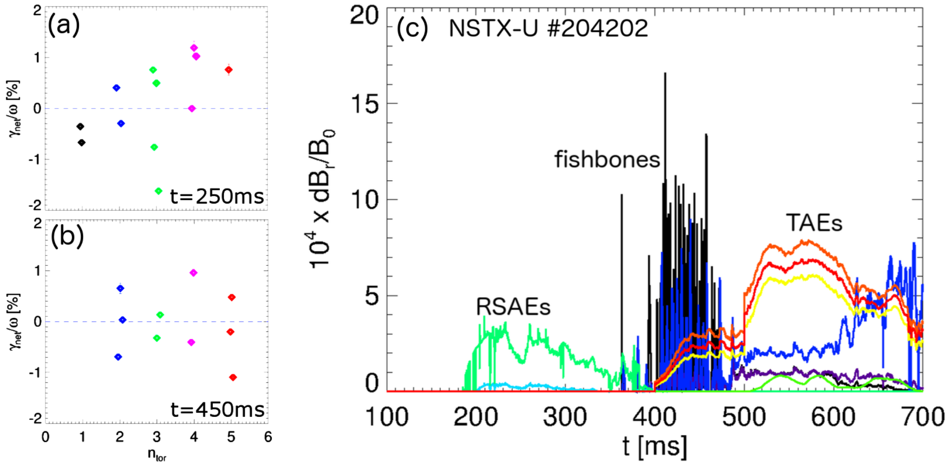

FIG. 5: Estimate of mode stability and saturated amplitude for NSTX-U discharge #204202. (a-b) Net growth rate for AE modes around $t = 250$ ms and $t = 450$ ms. (c) Peak $\delta B/B$ results for mode amplitude at saturation.

structure is inferred from NOVA-K analysis at two times ($t = 250$ ms and $t = 450$ ms). Simple analytical expressions are used for kink and fishbones.

Even for interpretive analyses, the challenge for the TRANSP/kick model simulation is to consistently adjust the mode amplitudes, possibly as a function of time. The procedure adopted in this work already hints at a possible use of the kick model (and, by extension, of RBQ-1D) for predictive analysis. For AEs, NOVA-K provides the damping rate in addition to the radial mode structures. Since the power exchanged between fast ions and the $k-$th mode, $P_{EP,k}$, can be calculated from the kick model, it is assumed that the saturated mode amplitude is such that $P_{EP,k}$ equals the power dissipated through damping, $P_{damp,k}$.

The linear growth rates inferred from the kick model for the case in Fig. 1a are shown in Fig. 5 for all candidate eigenmodes with $n = 1 - 6$ from NOVA-K. Modes with positive (linear) growth rates are retained for the following analysis, in which mode amplitude is gradually increased in a sequence of TRANSP runs and adjusted in time until the condition $P_{EP,k} = P_{damp,k}$ is verified at all times. This provides the expected AE saturation amplitude, cf. Fig. 5. Once AE amplitudes are known, fishbone and kink modes are added to the simulation. Their amplitude is rescaled until good agreement with the measured neutron rate is achieved. TRANSP results for the neutron rate are shown in Fig. 1c. As a comparison, the neutron rate obtained using a radially uniform, time dependent ad-hoc diffusivity for fast ions is also shown. Figure 1d illustrates the resulting fast ion density at the end of the fishbone sequence, $t = 450$ ms. As in the previous examples, the ad-hoc diffusivity results in a uniform decrease of the profiles with respect to classical simulations. The kick model predicts a larger effect of the instabilities in the core region, where fishbone amplitude is largest, and only negligible effects outside mid-radius.

3.3 Outlook of predictive use of the reduced models

The examples discussed in Sec. 3.1 are mostly limited to the interpretive use of the kick and RBQ-1D models. A central issue in the development of *predictive* capabilities is to infer the stability properties and resulting saturated amplitudes of the instabilities. A first example has been discussed in Sec. 3.2 for NSTX-U discharge #204202, cf. Fig. 5. A second example is shown in Fig. 6 for an ensemble of discharges from NSTX, NSTX-U and DIII-D. Results from predictive kick model analysis are summarized in Fig. 6a, showing that the analysis can recover the measured neutron rate typically well within $\pm 10\%$. Overall, results are also in good agreement with those from interpretive simulations, see Figs. 6b-c showing the predicted reduction in NB current drive efficiency with respect to classical simulations.

A challenge in the predictive simulations is the calculation of stability and saturation levels over time scales of the order of - or longer than - typical fast ion slowing down times (from 10's of milliseconds to seconds). To this end, the analysis should take into account self-consistently possible variations of the background plasma profile, for example density and temperature (also affecting the damping rate) or

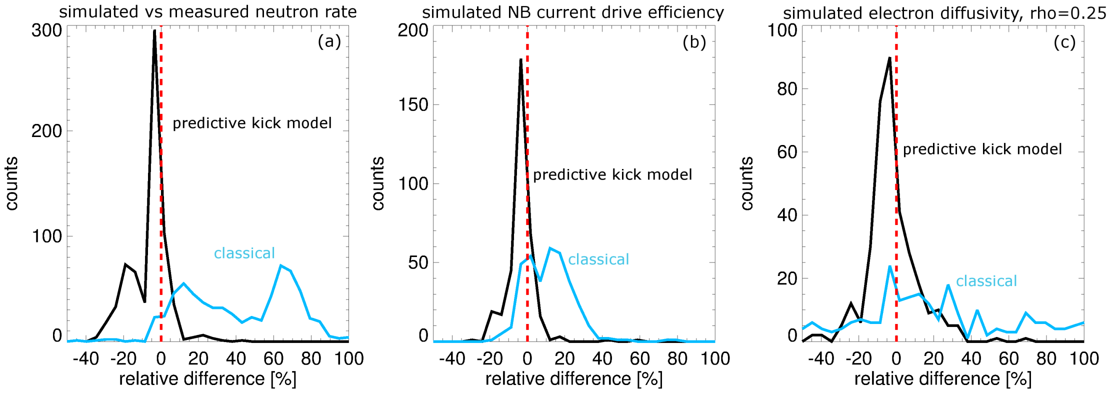

FIG. 6: (a) Relative difference between measured and simulated neutron rate using predictive kick model analysis (black) and classical runs (cyan). (b-c) Relative difference between predictive (black) and classical (cyan) simulations with respect to interpretive analysis for NB current drive efficiency $\eta_{Jnb} = I_{NB}/P_{NB}$ *(ratio of NB current over injected power) and electron thermal diffusivity at normalized radius* $\rho = 0.25$.

q-profile (affecting the radial mode structure). Simulations that recompute the mode properties as time evolves are still computationally very expensive [39][40][41][42]. A reduced approach for codes such as TRANSP is presently under consideration. In spite of these difficulties, reduced models already represent an effective alternative to first-principles codes for scenario development, when accuracy in the prediction of EP-driven instabilities and associated transport is sacrificed in favor of the integration of those effects into the bigger picture of *integrated modeling* [43].

4 Conclusions

The inclusion of reduced EP transport models in TRANSP is resulting in improved interpretive and predictive capabilities for long time scale time-dependent integrated tokamak simulations. Including the effects of EP transport by instabilities is crucial for the accurate, quantitative computation of the heat and momentum sources, which also affect thermal transport calculations and predictions.

Over the last few years, the kick model has been successfully applied to analyze EP transport on NSTX/NSTX-U and DIII-D. Its integration with the TRANSP code has made continuous progress, along with the development of diagnostics tools in TRANSP to facilitate the comparison between code predictions and experimental data. Work is also ongoing to complement the kick model approach with the RBQ-1D model based on recent improvements to the original quasi-linear theory. RBQ-1D is based on the resonance-broadening quasi-linear theory and can address the need for a self-consistent, predictive transport model for integrated simulations. Initial benchmark between kick and RBQ-1D models shows good agreement in terms of predicted EP transport. Recent efforts are extending the kick model capabilities to account for MHD instabilities other than Alfvénic modes, e.g. NTMs, kinks, fishbones and sawteeth. Validation across multiple devices is ongoing and will be reported in future publications. In general, enhancements to TRANSP by including reduced EP transport models have already enabled scenario development and predictions that include a realistic treatment of fast ion transport by instabilities.

Acknowledgements

The NSTX-U and DIII-D Teams are gratefully acknowledged for their support in all experimental aspects of the research presented in this work. This manuscript is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences, and has been authored by Princeton University under Contract Number DE-AC02-09CH11466 with the U.S. Department of Energy. Neither the United States Government nor any agency thereof, nor any of their employees, makes any

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