

## **DEVELOPMENT OF COUPLED DTRAN/CQL3D CODES FOR RUNAWAY ELECTRON QUENCH STUDIES**

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### **ABSTRACT**

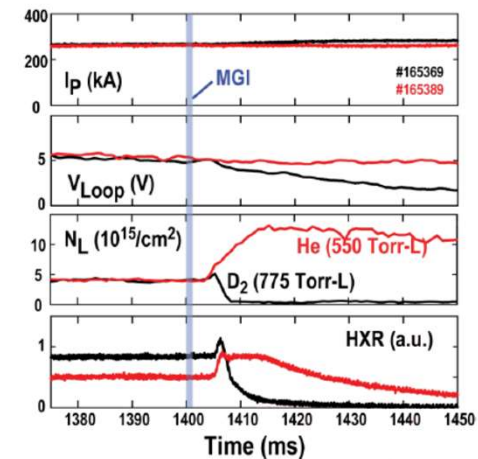
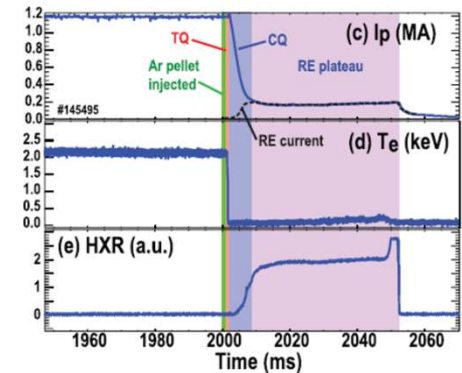
Generation and kinetics of runaway electrons (RE) in disruption and disruption mitigation events depend strongly on the rapid change in the plasma parameters, impure plasma ion composition, and electro-magnetics, whereas the RE in turn have crucial impact on plasma current, plasma conductivity and heating. For self-consistent plasma/RE studies, we are developing DTRAN/CQL3D package, in which kinetic Fokker-Planck code CQL3D is coupled to macroscopic plasma transport code DTRAN. This is a multi-element, multispecies, 1-D (radially), magnetic flux surface averaged parameters, diffusive-convective transport code. The code solves a system of strongly coupled equations reproducing the dynamics of plasma electrons, ions, parallel electric field, ionization states of various intrinsic and extrinsic impurity species, neutral atoms and molecules. Capability of DTRAN to simulate low-temperature (down to sub-eV in afterglow phase) partially-ionized plasmas including molecular effects (MAR), interchange ion reactions, increasing ion conversion) and plasma radiation opacity of many lines will be highlighted. Results of DTRAN benchmark for disruption mitigation with Argon and D2 gas puffs will be presented

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## Motivation

- ☉ Safely quenching the plasma thermal energy (TQ), plasma current (CQ), and Runaway Electron (RE) fractions are challenging tasks.
- ☉ ITER disruption mitigation system is still under-represented and seeking for new techniques. Avoidance of runaway formation is one of the first priority tasks of ITER operation scenario and of mitigation and control systems
- ☉ It is crucial to develop predictive physics understanding and advanced simulation tools for plasma disruption/mitigation
- ☉ Improved scenarios like “Inside-out” mitigation for thermal quench are under investigation and need modelling support.
- ☉ The plasma dynamics during CQ was found to deal with developed RE component and crucially depend on impurity species.



Hollmann PoP 2019

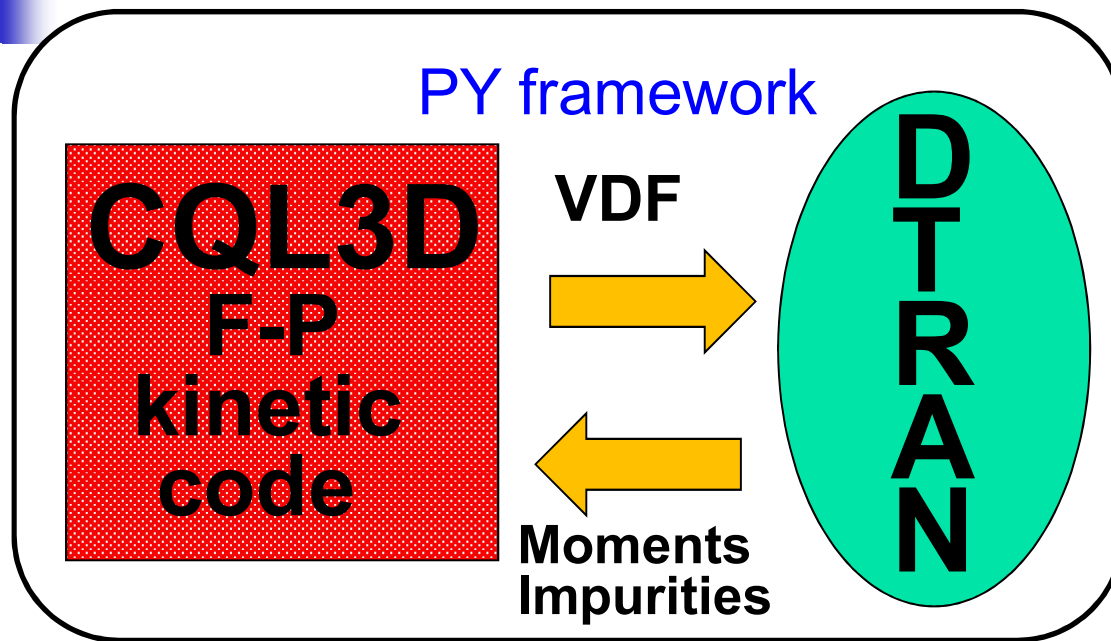


## Goals

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- ④ Develop a robust computational tool **DTRAN/CQL3D** based on coupled Fokker-Planck code CQL3D and 1D-radially plasma transport code DTRAN for self-consistent time-dependent modeling of plasma and RE formation during disruption and disruption mitigation disruptions
- ④ Understanding mechanisms leading to RE formation and ways of their avoidance. Applications to DIII-D and predictions for ITER.
- ④ Study the roles of different impurities and mixtures in TQ and CQ, safe impurity assimilation rates, and delivery scenarios. Thorough characterization of unique properties of resulting low-Te plasmas, such as RE-plateaus and afterglow plasmas.
- ④ Modeling of experimental data from various diagnostics on tokamaks and divertor simulators

## Coupled DTRAN/CQL3D model



The coupling scheme of DTRAN and CQL3D is based on two-component approximation of electron VDF, which characterize the thermalized plasma and the hot RE tail.



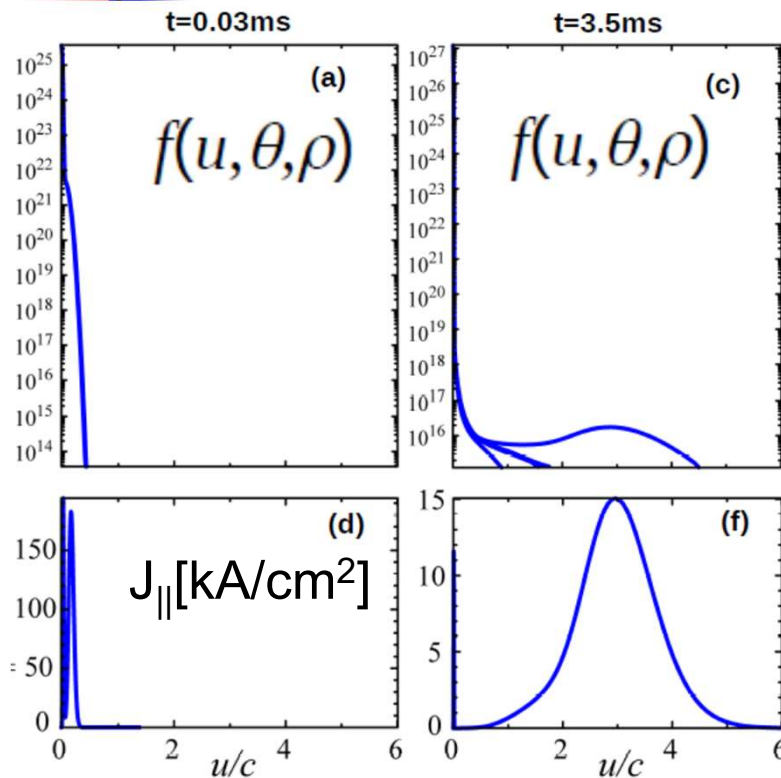
## CQL3D Fokker-Planck code

**CQL3D**: Collisional/Quasi-Linear 3D code (2 momenta, 1 general radius) See <http://www.compxco.com/cql3d.html>

### CQL3D features:

- ⊗ Solves a Bounce-Averaged Fokker-Planck eqn in Toroidal Geometry
- ⊗ 6D phase space eqn reduced to 3D averaging over toroidal angle, gyro-phase, and bounce-period (assuming  $t_{\text{bounce}} < \tau_{\text{coll}}$  ).
- ⊗ Electrons and multi-species ions.
- ⊗ Collisions, RF/neutral beam sources & applied toroidal electric field.
- ⊗ Fully- or quasi- relativistic nonlinear collision term (generalized RMJ)
- ⊗ Radial transport.
- ⊗ Fully-implicit, also in 3D. Steady-state and time-dependent solutions are supported.
- ⊗ Main applications: RF+NBI heating and current drive, and REs.
- ⊗ Coupled to Ampere-Faraday equations for self-consistent  $E_{\phi}(\rho, t)$
- ⊗ Collisional operators were recently upgraded to include electron-impurity interactions calculated by DTRAN.

## Two-component electron VDF (hot tail)



Results of CQL3D modeling of RE formation after KPAD pellet. VDF shown for different  $\theta$

CQL3D simulations show distinct hot tail associated with RE, ECH.

The robust way of CQL3D modeling is the temporal evolution of initially Maxwellian plasma

DTRAN/CQL3D uses two simple criteria to split between hot tail and thermal plasma:

$$u > \alpha * v_{\text{thermal}}$$

$$\alpha = 3 \text{ for } f_{\text{tail}}/f_{\text{max}} \sim 10^{-5}$$

$$\alpha = 4 \text{ for } f_{\text{tail}}/f_{\text{max}} \sim 10^{-8}$$

and

$$u/c > [E/E_{\text{crit}} - 1]^{-1/2}$$

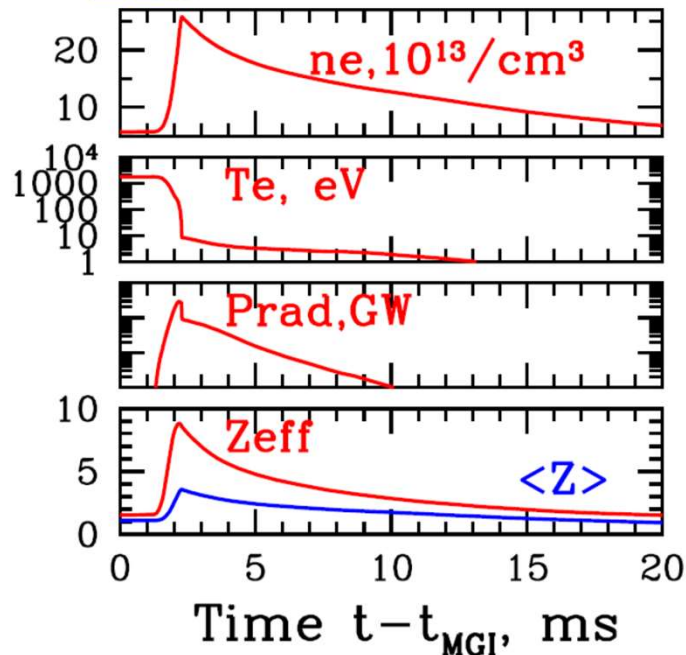


## DTRAN summary

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- ⌘ This is newly developed, multi-element, multispecies, 1-D (radially), magnetic flux surface averaged parameters, diffusive-convective-reaction transport code.
- ⌘ The code solves a system of strongly coupled equations reproducing the dynamics of plasma electrons, ions, parallel electric field, ionization states impurity species, neutral atoms and molecules.
- ⌘ Modelled species include all hydrogenic species: H(n), H<sup>+</sup>, H<sup>-</sup>, H<sub>2</sub>, H<sub>2</sub><sup>+</sup>, H<sub>3</sub><sup>+</sup>, H<sub>5</sub><sup>+</sup>, H<sub>3</sub><sup>-</sup>; and two impurity species (intrinsic [He, C] and extrinsic [Ar, Ne], all charge and molecular states. For example, Ar(n), Ar<sup>+1</sup>-Ar<sup>+18</sup>, ArH<sup>+</sup>, ArH<sub>2</sub><sup>+</sup>, Ar<sub>2</sub><sup>+</sup>, ArH<sub>2</sub><sup>++</sup>).
- ⌘ Chemical kinetics model of DTRAN is capable of simulating the chains of reactions leading to Molecular Assisted Recombination (MAR), interchange ion reactions, and increasing conversion for negative and positive ions (including Van-der-Waals clusters)
- ⌘ Reduced sub-models (1+1/2)-D for time-dependent particle sources/sinks describing the MGI and pellet ablation.
- ⌘ Magnetic equilibrium evolution will be added at final stage of DTRAN development

## Impurity dynamics and TQ plasma collapse



DTRAN test modeling of neutral impurity Argon pellet as uniform volume source with initially flat plasma profiles. Transport of all species is turned off.

The test results highlight a capability of DTRAN to simulate the Thermal Quench dynamics mimicking a shell pellet scenario for time-dependent local source of Argon impurities.

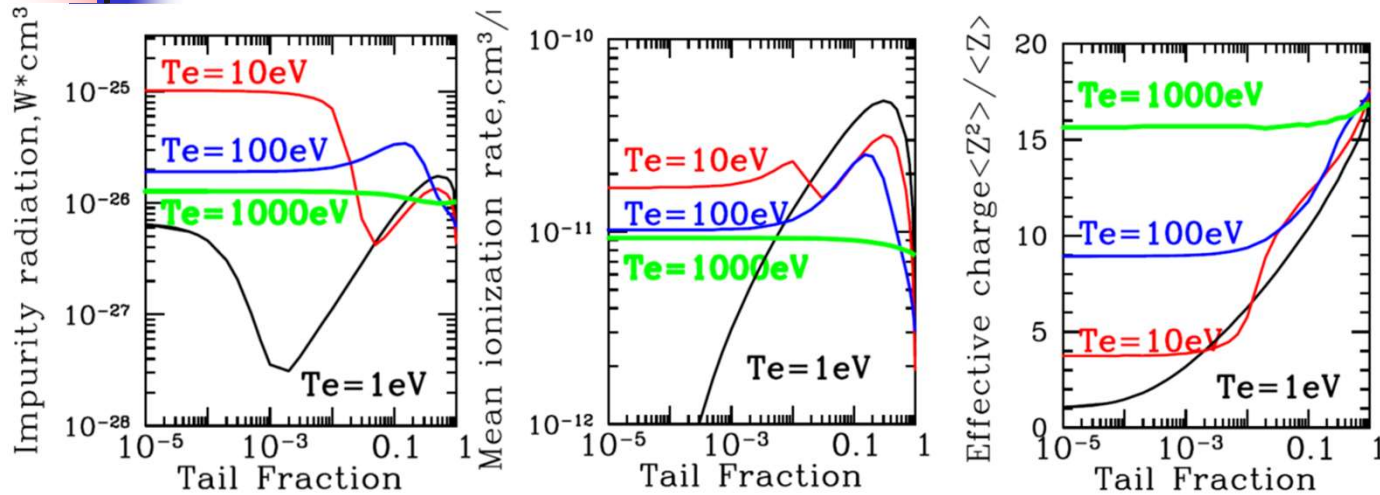
DTRAN simulates non-coronal, non-LTE impurity dynamics of multi-element impurity mixture Ar+C

Modeling was done with two-component electron VDF (RE+ THE) as will be discussed in detail in other slides.

DTRAN captures a sharp  $\sim 1$  ms drop in plasma Te during TQ via impurity ionization and radiation and slow low-Te plasma evolution during CQ phase.

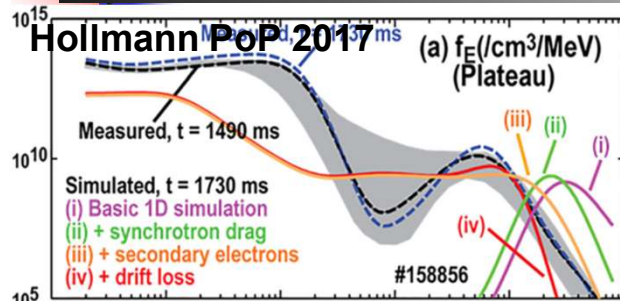


## Hot RE tail strongly impacts the impurity radiation and distribution over ionization states

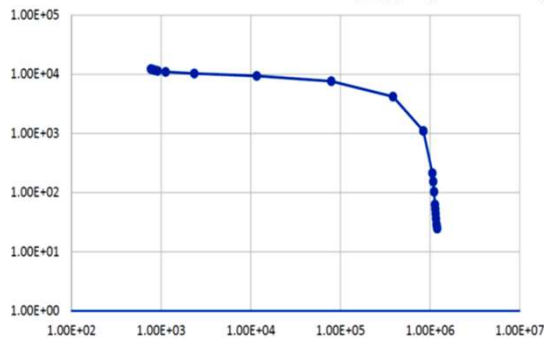


- ⌚ **DTRAN** implements for impurity modeling the atomic rate coefficients ADP a version of ADPAK. Here ADP calculates **collision-radiative equilibrium (CRE)**.
- ⌚ The ADP code includes additional terms describing electron-impact collisions with atoms/ions associated with the hot tail of electron VDF
- ⌚ The ADP results show high sensitivity of CRE to hot tail parameters. For CQ  $T_e < 10\text{ eV}$ , even small tail fractions  $10^{-4}$ - $10^{-3}$  1MeV beam affects the impurity CR kinetics

## Form of hot tail is significant for low-Te plasma



Electron energy (MeV)

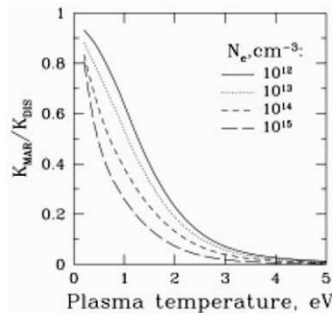
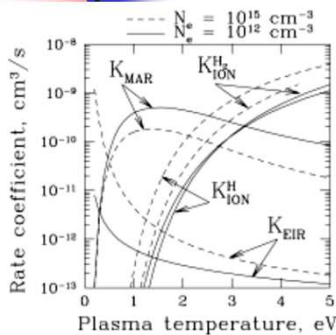


Hydrogen atom ionization cross-section averaged over the VDF tail normalized to 100 A/cm<sup>2</sup> for a set of VDF with different mean energies

☯ The form of hot tail and its parametric dependence are not well known and are the subject of future studies. With account of secondary electrons it can stretch over the wide range

☯ At fixed RE current, significant ionization and radiation losses may come from secondary electrons in 0.1-1 keV range compared to MeV RE.

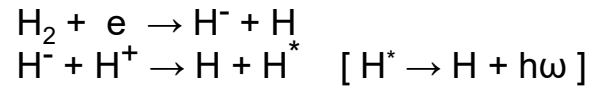
## Molecular Activated Recombination (MAR)



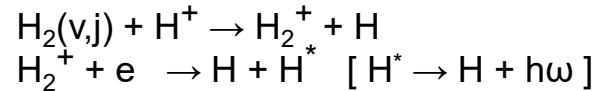
- K<sub>MAR</sub> rate coefficient is relatively high ~4x10<sup>-10</sup>cm<sup>3</sup>/s
- K<sub>MAR</sub> involves ro-vibrational kinetics of molecular species
- K<sub>MAR</sub> depends strongly on Lyman series opacity
- MAR has been shown to be important in detached divertor plasma and linear divertor simulators, ion sources

MAR proceeds via the following reaction chains:

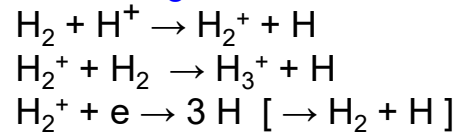
Chain #1: Mutual ion-pair neutralization



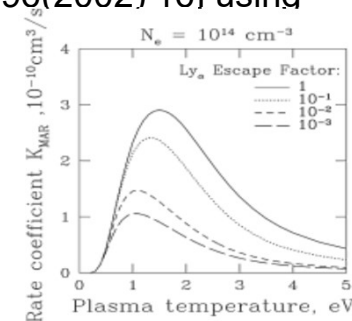
Chain #2 Atomic-to-molecular ion conversion



Chain #3 Increasing molecular ion conversion

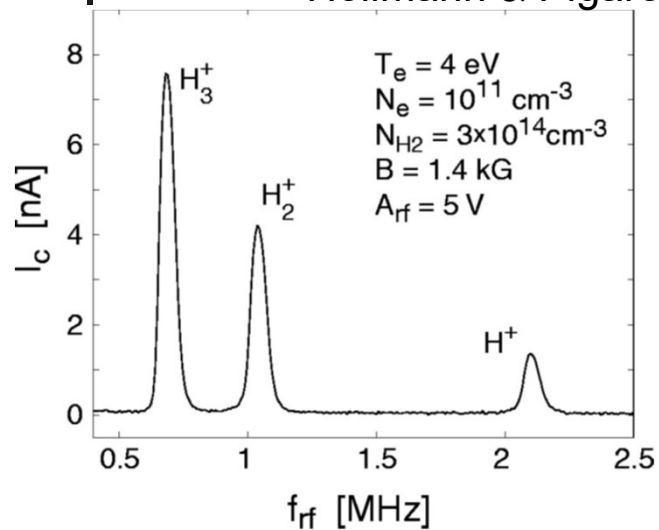


These processes have been studied [A. Pigarov, Phys. Lett A822 (1996) 251; Phys. Scripta T96(2002) 16] using collisional-radiative CRAMD

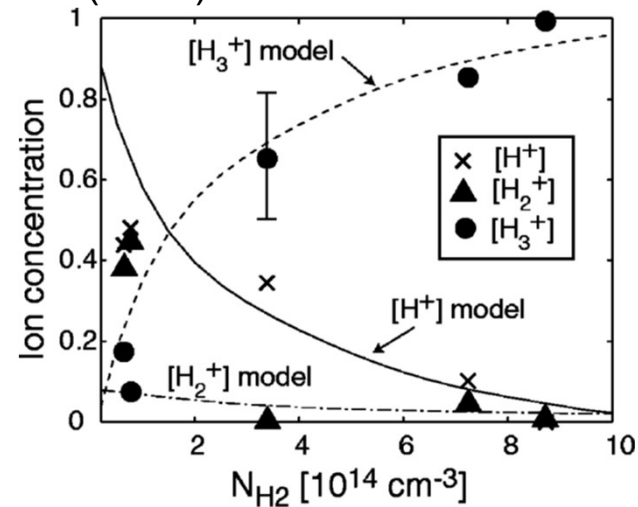


## Usual PISCES-B plasma

Hollmann & Pigarov PoP (2002) 4330

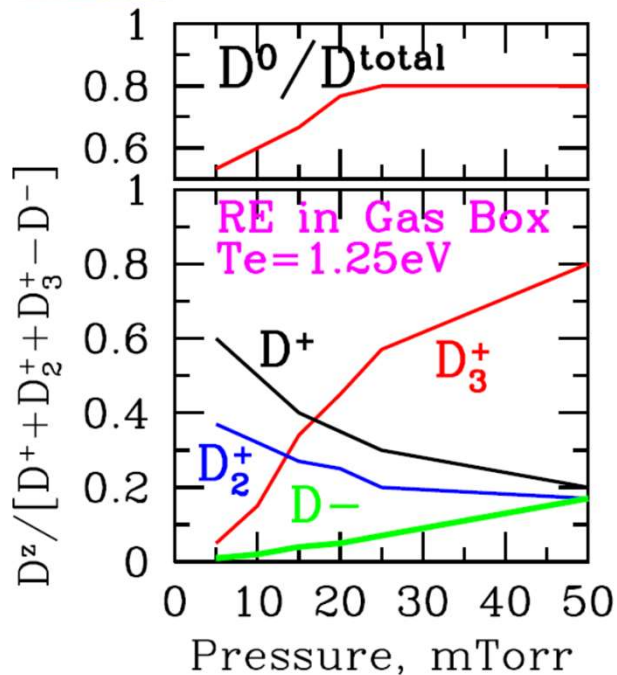


Mass spectrometer (omegatron) measurements showed that dominant ion is  $H_3^+$ . The measured vibrational temperatures  $>4500$  K



C-R modeling confirmed that  $H_3^+$  is dominant ion and MAR is the dominant plasma recombination process in PISCES-B plasmas

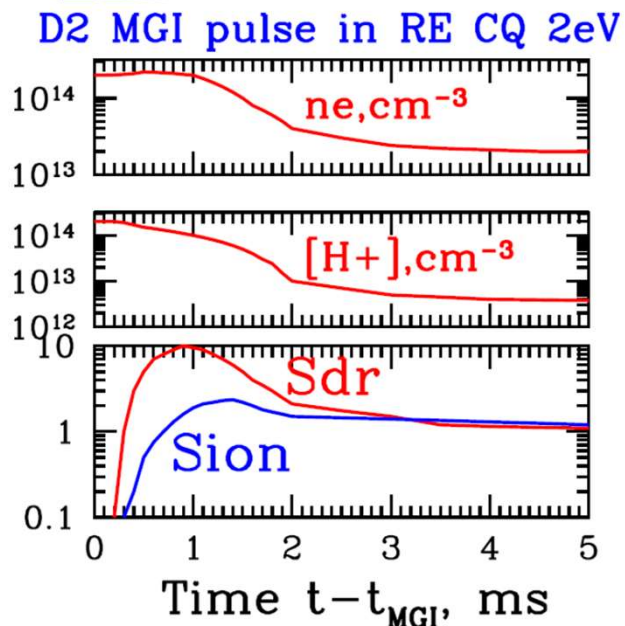
## CR kinetics of Deuterium Low-Te plasma in CQ



DTRAN results on afterglow D plasma maintained by  $1\text{kA/cm}^2$   $1\text{MeV}$  RE. Thermal electron  $T_e$  profile is fixed. Closed Gas Box recycling model

- ☉ Very high degree of  $\text{D}_2$  gas dissociation. Atomic  $[\text{D}]$  increases with pressure up to 80%
- ☉  $\text{D}_3^+$  is the main ion species for  $>20$  mTorr.
- ☉  $\text{D}^+$  is the dominant ion species at low pressures.
- ☉ Increasing ion-to-molecular ion conversion is the leading effect. Van-der-Waals clusters  $\text{H}_5^+$  and  $\text{H}_3^-$  are expected at 1 Torr.
- ☉ High atomic  $\text{D}_0$  to molecular  $\text{D}_2$  conversion at walls is needed to maintain large volume  $\text{D}_2$  source.
- ☉ CR kinetics includes reactions of RE tail with all bound electrons.

## MGI of D2 into CQ causes rapid plasma recombination due to MAR



Results of DTRAN modeling for 0.5 ms pulse of D2 MGI into fully ionized D+ plasma. Sdr is total DR rate compared to total ionization source via 100A/cm<sup>2</sup> 1 MeV RE beam plus thermal electrons

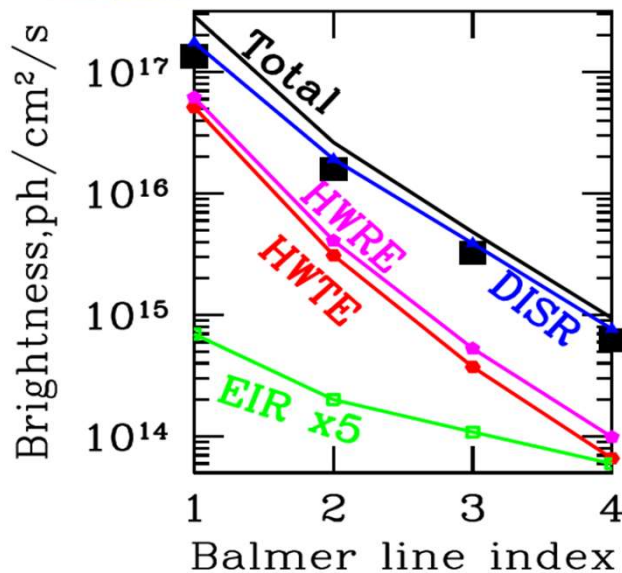
- Experimentally shown [see Hollmann 2019, poster BP10.32] that short MGI pulse of D2 gas into Ar-pellet created CQ low-Te plasma results in rapid plasma recombination in contrast to the case of He MGI.

- DTRAN simulations demonstrate that in the case of D2 MGI the Molecular Activated Recombination (MAR) is the dominant recombination process. It is capable of reducing thermal electron density by 10X

- A quasi-equilibrium is obtained for  $t - t_{\text{MGI}} > 2\text{ms}$ , where ionization of D0, D<sub>2</sub>, D<sub>2</sub><sup>+</sup>, D<sub>3</sub><sup>+</sup> by RE beam is compensated by Dissociative Recombination of ions.

- The D→D<sub>2</sub> conversion in plasma-gas interaction with wall should be high. Wall is in net outgassing regime releasing D<sub>2</sub>.

## CQ plasma spectroscopy shows signatures of RE tail and molecular effects



The Balmer brightnesses were calculated by CRAMD code as chord average over the plasma profiles obtained by 1-D radial transport code. See poster BP10.32 by E.M. Hollmann

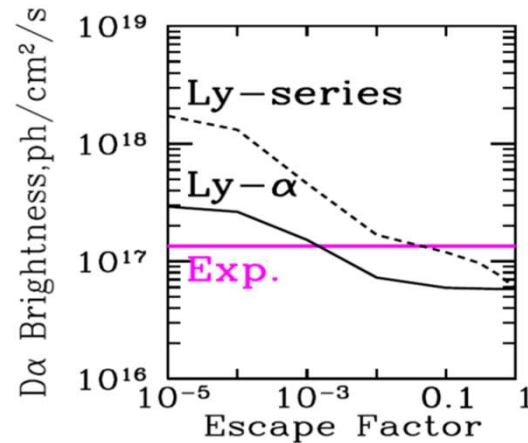
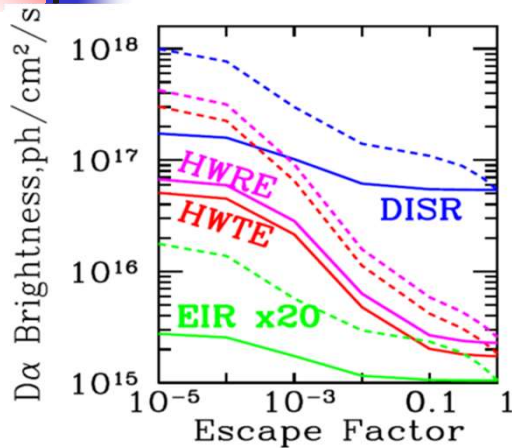
The main contribution to synthetic Balmer spectrum from CQ plasma gives dissociative recombination (DISR) of D2+ and D3+.

Only DR matches well the slope of Balmer ratios.

Thermal and hot-tail electron-impact excitation contribute equally to and together give at least 25% of Balmer- $\alpha$  line intensity.

Other processes, e.g. EIR, has small contributions

## Impact of radiation opacity on CQ plasma



- ⊗ It is widely acknowledged that radiation of Lyman series lines is largely trapped and changes the I&R rate coefficients.
- ⊗ An opacity model based on calculations of opacity factors for many lines of deuterium and impurities is under development for DTRAN.
- ⊗ This effect is highlighted by CRAMD code calculations where opacity of Lyman series is able to change the Blamer lines emissivity by an order of magnitude.





## Conclusions and plans

- ⌘ We are developing **DTRAN/CQL3D** code based on the coupled Fokker-Planck code CQL3D and 1D-radially plasma transport code DTRAN for self-consistent time-dependent modeling of plasma and RE formation during disruption and disruption mitigation disruptions.
- ⌘ The coupling scheme of DTRAN and CQL3D code is based on two-component approximation of electron VDF, which characterize the thermalized plasma and the hot RE tail.
- ⌘ The VDF components are strongly interacting each other. The collisional-radiative kinetics of impurity ionization states, radiation and ionization rates, plasma resistivity, and Ohmic heating in DTRAN depend largely on the hot tail modeled by CQL3D, whereas initial Maxwellian and characteristics of numerous inelastic electron collisions depend on plasma state calculated by DTRAN.
- ⌘ The DTRAN results presented here include: impurity dynamics in TQ, hot tail impact on CR rates and radiation of impurities, properties of RE-plateau plasma and its recombination dynamics during D2 MGI, and spectroscopic modeling confirmation on the roles of DR and radiation opacity.