Simulation of the Pre-Thermal Quench Stage of Disruptions during Massive Gas Injection and Projections for ITER

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Abstract. During disruption mitigation by massive gas injection (MGI) the thermal energy is expected to be radiated with high efficiency in order to prevent excessive heat loads to first wall and divertor PFCs. The energy loss will take place in two phases: a) the so-called pre-thermal quench phase that lasts from the arrival of the first gas to the onset of increased transport due to MHD activity during b) the second phase the thermal quench (TQ). Quantification of the duration of the pre-TQ phase is essential for the design of the ITER disruption mitigation system (DMS). The DMS has to be designed such that the impurity amount accumulated during pre-TQ stage should be sufficient for re-radiation of more than 90% of heat flux at subsequent TQ phase of ITER disruption. The modeling with the code ASTRA together with ZIMPUR impurity transport and radiation code allows the description of the cooling process at the plasma edge, including the penetration of impurities and the shrinking of the current channel. Newly developed model for the gas flow at the end of delivery tube of MGI system well reproduce experimentally measured evolution. The validation of the simulation approach on available experimental data has demonstrated its ability to produce quantitative estimations of the pre-TQ stage duration and of the accumulated in the plasma amounts of noble gases and deuterium under MGI. Simulation results of the pre-TQ stage in reference ITER scenarios are presented. The ability of the ITER MGI systems to provide injection of necessary impurity amount during pre-TQ stage is discussed.

1. Introduction

During disruption mitigation by massive gas injection (MGI) the thermal energy is expected to be radiated with high efficiency in order to prevent excessive heat loads to first wall and divertor PFCs. The energy loss will take place in two phases: a) the so-called pre-thermal quench phase that lasts from the arrival of the first gas to the onset of increased transport due to MHD activity during b) the second phase the thermal quench (TQ). The duration of the first phase is determined by the process of the radiation of energy from the external region of the plasma (i.e. \( q > 2 \)) and varies with the radiation efficiency and the flow rate of the injected gas species. The gases foreseen in ITER for disruption mitigation are \( \text{D}_2, \text{He}, \text{Ne} \) and Ar [1]. Quantification of the duration of the pre-TQ phase is essential for the design of the ITER Disruption Mitigation System (DMS). The DMS has to be designed such to provide a sufficient amount of impurities in the plasma before the onset of the TQ to ensure that 90% of the thermal energy is being radiated during the TQ. This requires a high flow rate, which in turn is expected to lead to a shortening of the pre-TQ phase.

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a See the Appendix of F. Romanelli et al., Proceedings of the 25th IAEA Fusion Energy Conference 2014, Saint Petersburg, Russia

b http://www.iter.org/org/team/fst/itpa/mhd
The aim of the present study is to establish a quantitative extrapolation from existing data using 1D modeling of the pre-TQ phase. The task comprises code validation using existing data of the pre-TQ duration, identification of the scaling parameters and simulation of ITER MGI scenarios. The modeling with the code Astra [2] together with ZIMPUR [3] impurity transport and radiation code allows the description of the cooling process at the plasma edge, including the penetration of impurities and the shrinking of the current channel.

2. Brief description of the model

In this study Astra [2] transport analysis code integrated with ZIMPUR [3] impurity charge state dynamics, radiation and transport code was used for self-consistent simulations of the pre-thermal quench stage of disruptions with Massive Gas Injection, MGI.

Plasma equilibrium was calculated with use of up-down symmetric, 3 momentum, fixed boundary equilibrium solver. Standard set of transport equations for $T_e$, $T_i$, $n_d$ was solved with use of the following transport model: $\chi = D_d = D_e = D_{an} = D_0 \cdot F(\rho) F_{H-mode}$, $\chi_i = 2D_{an}$, where radial profile of transport coefficients was taken in the form: $F(\rho) = 1 + 3\rho N$, $\rho_N = \rho / \rho_{max}$. For the radial pinch velocity we assumed $V_p = D \cdot (\rho N / a^2)$. Normalization coefficient $D_0$ was adjusted to provide best possible match of simulated and experimental radial profiles of electron and ion temperatures, densities, plasma current and others just before the beginning of pre-thermal quench phase. Convective terms were taken into account in the heat transport equations in the form of $\frac{3}{2} \mathcal{T}^{\prime}$, with particle flux $\Gamma_i$. In the external transport barrier region ($\rho_N > 0.93$), providing establishment of the H-mode, the coefficient $F_{H-mode}$ was used to reduce the conductivity $\chi_e$ to the level of the neoclassical ion heat conductivity, $\chi_	ext{ineo}$, and reproduce pedestals on profiles of plasma parameters.

Plasma fuelling by gas puffing was simulated by solving the kinetic equation for neutrals in the slab approximation. Then the boundary condition, i.e. neutral density at the plasma boundary, was adjusted as to reproduce experimental plasma density profile.

Plasma temperature and density at the separatrix were taken to be equal: $T_s = 0.8eV$, $n_{de} = 0.9*10^{19} m^{-3}$. For initial conditions we assumed that plasma was already formed and steady state equilibrium configuration was established.

The NBI was simulated with use of the Fokker-Planck solver taking account of real geometry, multistep ionization of beam atoms, orbital losses, and neoclassical effects in NBCD (for details see ref. [4]).

The simulations of impurity transport and radiation were done by the ZIMPUR impurity code [3]. It allows to determine the radial distributions of impurity ions in all charge states after each temporal step. Then these distributions are used for the calculation of the impurity radiation in the plasma. Evolution of the electron density profile, $n_e(r)$, was determined by the quasi neutrality condition. The dynamics of concentrations of impurity ions in different charge states $n_k (k = 0, 1, \ldots Z)$ is represented by the set of equations balancing the elementary process rates. After the averaging over the magnetic surfaces, according to the Astra standard, they can be written in the form:

$$\frac{\partial (V' n_k)}{\partial t} + \frac{\partial}{\partial \rho} \left[ V' < (V \rho)^2 > \Gamma_k \right] = V' n_e \left[ I_{k-1} n_{k-1} - (I_k + R_k) n_k + R_{k+1} n_{k+1} \right], \quad (1)$$

where $\rho$ is the radial coordinate, $V$ is the volume inside the magnetic surface and $V' = \partial V(\rho)/\partial \rho$, the angular brackets mean an average over the magnetic surface, $\Gamma_k$ are radial fluxes of particles, $n_e$ is the electron density, $I_k$ is ionization rate, and $R_k$ is a sum of radiation
and dielectronic recombination rates. The radiation of each sort of the impurity is determined by the sum of a bremsstrahlung, linear and recombination radiation.

ZIMPUR modeling of the non-stationary processes allows to describe the cases distinguished from the coronal equilibrium, when the ionization and the recombination are unbalanced. Radial components of the ion impurity fluxes averaged over the magnetic surfaces take the form: \( \Gamma_k = V_d n_k - D_d \frac{\partial n_k}{\partial \rho}, k > 0 \). Anomalous drift velocity \( V_d \) and a diffusion coefficient \( D_d \) for impurity ions were taken the same as for the main plasma.

The presence in the ZIMPUR code of the equation for impurity neutrals facilitates the monitoring of the total impurity content in the plasma. Diffusive approximation was used for the neutral atoms of the impurity, and radial neutral fluxes were set as: \( \Gamma = -D_0 \frac{\partial n_0}{\partial \rho}; D_0 = T_0 / (m_Z n_0 T_0) \). Here \( m_Z \) and \( T_0 \) are the mass and the effective temperature of impurity atoms, which can depend on radius. Such approach allows one to take this temperature equal to the local ion temperature \( (T_0 = T_i(\rho)) \) in the plasma, where density of impurity atoms is mainly determined by recombination and ionization. On the other hand, a concentration of neutrals near the plasma edge is determined by their fluxes through the plasma boundary. Boundary conditions in the original ZIMPUR model of neutrals took the form: \( \Gamma_0 = \nu_R n_0 - G_0(t) \), where impurity source was defined as the impurity neutral flux \( G_0(t) \) through the separatrix, while the value of escape velocity, \( v_0 \), was difficult to specify within the simplified approach. Indeed, the escape velocity for the primary MGI neutrals moving inward the plasma column is close to zero, while for the secondary recombination neutrals it should be of the order of ion thermal velocity, which for the typical plasma temperature in the vicinity of the cooling front, where recombination dominates secondary impurity source, it is of the order of several km/s.

Validation of the simulation model against JET experiments (see Section 3) demonstrated the key role of accurate modeling of the neutral losses. Then ZIMPUR neutral model in this study has been generalized by separate treatment of the primary (cold MGI) and secondary (thermal) neutral dynamics. The algorithms of the impurity neutral dynamics mostly repeats that of recently developed diffusive model for the hydrogen neutrals [5]. In this model neutral energy range is split for several, \( i \), energy groups to solve the system of coupled equations

\[
\frac{1}{V'} \frac{\partial (V' n_{i0})}{\partial t} = \frac{1}{V'} \frac{d}{d \rho} \left( V' \left< \frac{\partial}{\partial \rho} \right>^2 > D_{i0} \frac{dn_{i0}}{d \rho} \right) - n_i n_{i0} + G_i; \tag{2}
\]

\[
G_i = n_i g_i \left\{ \nu_R + \sum_{j=0}^{\infty} n_j \sigma [\sigma V]_{CX}^j \right\}, \tag{3}
\]

\[
D_{i0} = \frac{2E_i}{3m_Z \nu_i}, \quad \nu_i = \nu_i + n_i \left\{ \sum_{j=1}^{\infty} g_j [\sigma V]_{CX}^j \right\} \tag{4}
\]

Here \( \nu_R \) and \( \nu_i \) are recombination and ionization frequencies independent of the neutral energy. Indexes in the charge exchange rates \([\sigma V]_{CX}^j\) correspond to the charge exchange of the neutrals from energy group \( 'j' \) with ions of group \( 'l' \), \( g_i \) is a ion fraction within the energy group. The boundary conditions take the form

\[
\left\{ \frac{V_i}{2} n_i + D_{i0} \frac{dn_i}{d \rho} \right\} = 0, \quad V_i = \sqrt{\frac{2E_i}{m_Z}}. \tag{5}
\]

Evolution of the primary neutral density is governed by the equations
\[
\frac{1}{V'} \frac{\partial (V'n_{00})}{\partial t} = \frac{1}{V'} \frac{\partial}{\partial \rho} \left[ V' < (\nabla \rho)^2 > D_{00} \frac{\partial n_{00}}{\partial \rho} \right] - (v_j + v_{CX0}) n_{00}, 
\]

(6)

\[
V' < (\nabla \rho)^2 > D_{00} \frac{\partial n_{00}}{\partial \rho} = -G(t),
\]

(7)

where \( G(t) \) is the primary neutral flux due to MGI.

For calculating \( G(t) \) new phenomenological model describing the gas flow from the MGI valve through the delivery tube into tokamak has been developed [6]. Simulation results are in a good agreement with experimental measurements of the gas density along the delivery tube of MGI injector of the tokamak JET [7,8]. The model provides accurate simulation of the gas flow accounting for the depletion of MGI reservoir during injection. Input parameters for the gas flow simulations are gas pressure and composition in MGI reservoir, reservoir volume, orifice diameter and delivery tube diameter and length.

3. Simulation of JET Discharges

In ASTRA-ZIMPUR simulations we started with adjusting model parameters to reproduce desirable stationary regime. Then auxiliary heating was switched off and MGI valve opened (t=0 at the figures below). After gas propagation through MGI system delivery tube (Time of Flight, TOF) gas front reached plasma surface and accumulation of the impurity at the plasma periphery started. When impurity content reached an amount sufficient for radiative energy loss to overpower Joule heating the cooling front begun to propagate inward accompanied by the plasma current contraction. Sharp peak of the skin current formed at the edge of the current channel. When perturbation due to this peak reached \( q=2 \) surface Thermal Quench started. Then transport coefficients were raised to \( \sim 30 \text{ m}^2/\text{s} \). Simultaneously with fast decrease of plasma temperature the peak of Ar concentration spread rapidly provided Ar penetration into the central plasma. When central temperature, \( T_c(0) \), fall by \( \sim 25\% \) the "mixing" phase started. In our model this "mixing" was simulated by further 10 times increase of the transport coefficients. Then plasma thermal energy decreased and impurity distribution in the plasma became almost uniform.

Calculated Pre-TQ duration time, \( \tau_{pTQ} \), at MGI of Ar (10%) + D2(90%) gas mix into JET plasma [8] is shown in Fig.1. Red points were obtained in simulations with original ZIMPUR model of neutrals assuming extremely low loss velocity, \( v_0=7.5\text{m/s} \) for all Ar atoms and ions. One of the principal targets in this series of calculations was to increase as much as possible the amount of injected gas. However, as it is seen from the red line corresponding to D2+10%Ar gas mix injection, the maximum achieved injected (and for this particular case also assimilated) amount is much smaller than it was in experiment. Extensive series of calculations with variation of transport coefficients for impurity demonstrated that duration of the pre_TQ stage:

- Weakly affected by the increase of Ar ion diffusion coefficient. Strongest effect was seen when Ar ion diffusion was taken 10 times higher than that for the main plasma at the cold plasma region behind the cooling front.
- Weakly affected by the 2-3 times increase of all transport coefficients for both main plasma and impurity ions.
- Sensitive to the neutral diffusion rate \( D_0(T_0) \) (it was suggested that lowering this coefficient should prevent primary neutrals from deep penetration through the cold plasma region)
Most sensitive to (actually depends on) the impurity neutral loss rate, i.e. to the “escape” velocity $v_0$. Good match with experimental data (with largest injected impurity amount) was obtained for $T_0=0.6$eV, $v_0=5$km/s.

![FIG.1 Simulation results of the Pre-TQ stage in JET. Red points - no Ar losses, green stars - adjusted neutral model with $v_0=5$km/s, $T_0=0.6$eV, blue triangles – improved neutral transport model, blue squares - $\tau_{pTQ}$ vs. assimilated Ar quantity. Black circles - experimental data.](image1)

![FIG.2 Dependence of total number of injected (accumulated) Ar particles into the plasma during preTQ time vs number of particles in the volume of MGI system. Points here correspond to the red squares excluding the leftmost at Fig.1](image2)

Important finding of the simulations was the fact that $\tau_{pTQ}$ is almost independent of the D$_2$ influx and determined by the accumulation of radiating impurity only. Results of simulations with constant total amount of Ar+D$_2$ particles in MGI reservoir ($N_V$), but different fraction of Ar presented in the Table 1. From the third column of this table one can see that during pre-TQ time almost the same amount of Ar, $N_{pl}=(17\pm18)*10^{20}$ was accumulated in the plasma. When this “critical” amount of Ar is accumulated in the plasma periphery, cooling front propagates inward with almost the same speed reaching q=2 surface after 1.07-1.08 ms.

**TABLE 1: DURATION OF PRE-TQ STAGE vs. Ar FRACTION IN GAS MIX.**

<table>
<thead>
<tr>
<th>Ar fraction</th>
<th>$N_V$ ($10^{20}$)</th>
<th>$N_{pl}$ ($10^{20}$)</th>
<th>$\tau_{pTQ}$ (TOF)</th>
<th>$\tau_{pTQ}$ -TOF (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>60</td>
<td>16.8</td>
<td>2.45 (1.38)</td>
<td>1.07</td>
</tr>
<tr>
<td>0.5</td>
<td>60</td>
<td>18.2</td>
<td>3.82 (2.74)</td>
<td>1.08</td>
</tr>
<tr>
<td>1.0</td>
<td>60</td>
<td>17.5</td>
<td>5.75 (4.68)</td>
<td>1.07</td>
</tr>
</tbody>
</table>

The difference in total pre-TQ phase durations relates to the difference in Time of Flight only (shown in parenthesis in the Table 1). The latter evidently increases with rise of the effective mass of the gas mix associated with increase of Ar fraction.

Also it was found that rising the gas pressure in MGI reservoir does not change much the accumulated Ar quantity but shortens time of injection only. The existence of such a critical Ar amount apparently sets the upper limit on accumulated Ar quantity during pre-TQ stage. Dependence of the accumulated Ar amount on total number of Ar particles in MGI reservoir is shown in Fig.2. One can see that accumulated amount reaches saturation with increase of
the pressure in MGI reservoir. It is explained by the corresponding shortening of the injection time.

The injection of Ar quantity less than or about $5 \times 10^{20}$ (leftmost red point in Fig.1) was shown to prevent contraction of the plasma current and TQ, while significant fraction of plasma thermal energy losses ($>80\%$) still provided by radiation (soft termination). The transition from such soft termination to forced TQ has threshold character.

Calculated duration of the pre-TQ stage, $\tau_{pTQ}$, agree well with experimental data if low assimilation, less than 10%, of Ar impurity is suggested. Introduction of Ar atom losses in the model results in slower accumulation of Ar provided good agreement between simulated and experimental pre-TQ duration. Best fit with experimental data was achieved with setting $D_0(T=0.6\text{eV})$, $v_0=5\text{km/s}$ (green stars at Fig.1). Then assimilation of Ar was found to be of the level $\sim5\%$ of injected amount. It should be noted that DINA simulations of the Current Quench stage of the disruptions in these JET pulses revealed that measured plasma current decay is well reproduced in assumption of exactly the same, 3-5%, assimilation of Ar.

Details of the simulation results for 77808 shot with maximum injected Ar quantity (Rightmost green star at Fig.1) are shown in Figs. 3 & 4.

FIG.3 Time traces of various simulated parameters for discharge with injection of the mixture of Ar and D$_2$ gases ($N_{Ar}$ tot in the plasma $\sim2.4 \times 10^{20}$; 58.7 $10^{20}$ injected particles with $\sim10\%$ of Ar and $\sim90\%$ of deuterium): $0$- is the time of the opening of gas valve.

FIG.4 Radial profiles of plasma parameters just before TQ of discharge with injection of the mixture of Ar and D$_2$ gases ($N_{Ar}$ tot in the plasma $\sim2.4 \times 10^{20}$; 58.7 $10^{20}$ injected particles)

It should be noted, however, that in the whole the calculated evolution is very similar to previously obtained without Ar losses, but with injection of much smaller quantity of the impurity. By another words, experimental data can be in principle well reproduced by setting the appropriate value of “assimilation factor”, $R_g=N_{\text{accumulated}}/N_{\text{injected}}$. However, such an approach has low predictive capability. Adjusting the values of impurity atom escape velocity
\(v_0 \sim v_{i,ch}\), where \(v_{i,ch}\) is a ion thermal velocity in the vicinity of the sharp cooling front, and of diffusion coefficient \(D_0\) in original ZIMPUR model is more accurate but still leaves some freedom in their particular choice. While improved model for impurity neutral transport Eqs.(2-7) has no free parameter. Then assimilation factor, \(R_g\), becomes the result of calculations but not an assumption made.

Results of calculations with use of the improved neutral transport model are shown in Fig.1 by blue triangles. Blue squares in Fig.1 are the same results but with respect to assimilated impurity amount. In this series of calculations the assimilation of Ar impurity was found to be very close to or a little bit higher (4\%5\%) than in calculations with fitted values of \(v_0, D_0\). However, values of \(\tau_{pTQ}\) became of about 30-50\% higher. The difference came from change of the Ar impurity profile (lower concentrations in the vicinity of cooling front in case of improved neutral transport model). Nevertheless, the agreement with experimental data is still sufficiently good, as higher accuracy is hardly expected from simplest 1D modeling where enhanced ion transport on destroyed magnetic surfaces behind the cooling front, loss of injected atoms in SOL, 3D effects etc are beyond of the consideration.

4. Pre-TQ stage in ITER

TQ thermal load mitigation (TM) sub-system of the ITER DMS according to the conceptual design [9] consists of 4 similar valves of \(0.2 \times 10^{-3} \text{m}^3\) each with total gas inventory up to \(4 \times 2 \text{kPa} \times \text{m}^3\). Two options for the valve location are considered. The first (in-port) one is close to the plasma with delivery tube of \(L_d = 1 \text{m}\) length and the second one with \(L_d = 8 \text{m}\). Orifice and delivery tube diameters in gas flow simulations were taken to be of \(d = 28 \text{mm}\) and \(D = 2d = 56 \text{mm}\), respectively. ASTRA-ZIMPUR simulation results for Ar and Ne injection from all 4 simultaneously launched TM valves are shown in the Fig.5. The ratio of assimilated to injected noble gas quantity, \(R_g\), and duration of the pre-TQ stage, \(\tau_{pTQ}\), are given under the graphs. All simulations for ITER were done with improved neutral transport model.

*FIG.5 Pre-TQ stage in ITER with Ar and Ne MGI*

It was shown previously [10] that for successful TM the total assimilated quantity of radiating impurity should exceed \(\sim 2.0 \times 10^{22} \text{ Ne or } \sim 1 \times 10^{22} \text{ Ar}\). One can see, that both variants of positioning valves in ITER TM DMS system are capable in providing accumulation of necessary impurity amount. In-port location of TM valves, however, along with rather short
response time has significant reserve. Even launching single valve with 2 kPa\*m$^3$ Ne, yields fast ($t_{\text{pTQ}} \sim 3.52 \text{ ms}$) assimilation $\sim 3.25 \times 10^{22}$ of Ne particles. Response time for remote location of TM valves can be shortened with use of the Ar, Ne + D$^2$ gas mix. However, even for pure noble gases estimated assimilation efficiency gives accumulated impurity quantities close to the target for TM values. Thus in-port location seems to be more preferable.

5. Summary

ASTRA – ZIMPUR simulations clearly demonstrated that radiating impurity neutral dynamics plays the dominant role in the pre-TQ stage in MGI mitigated disruption scenarios. Separate treatment of the primary MGI neutral penetration and secondary recombination neutral transport/losses realized in improved ZIMPUR neutral transport model allows sufficiently accurate estimation of the impurity assimilation under MGI into the hot plasma. Validation of the simulation model against available JET data demonstrated reasonably good agreement between simulation results and experimental data. Application of the model to ITER gives favorable predictions on the capabilities of ITER TM DMS. In-port positioning of the TM valves is shown to be preferable providing very short, of few ms, response time and 2-3 times more effective delivery of the radiating impurity into plasma for mitigation of the heat loads on the plasma facing components during TQ stage of disruption.

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References