Progress on kinetic modeling of lithium transport with MCI

T. E. Evans and R. Deranian General Atomics

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MCI is being modified for kinetic impurity transport studies in the SOL and divertor of ITER

- Goal → integrate a structured 2D grid representation of the ITER pedestal, SOL and divertor plasma into the Monte Carlo Impurity (MCI) code:
 - Simulate kinetic transport properties associated with impurity ionization/recombination, thermalization, transport and radiation
 - Compare kinetic simulations with analytic models
 - Study the sensitivity of kinetic simulations to changes in plasma parameters and atomic data
- The results will be used to validate fundamental impurity transport models in low collisionality ITER relevant plasmas



A new 2D grid generator is being implemented in MCI for ITER simulations



Thermal impurity neutrals such as Li, Be will be launched from the wall (B) and ionized/transported through the SOL, divertor and private flux region (PFR) to the target plate (A), symmetry plane (c) and core (D)

- Particles are reflected at C and D (flux conservation) but stick at A (sink)



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Background plasma parameters from UEDGE are loaded into the 2D MCI grid



- Background plasma parameters e.g. T_e, T_i, n_e, n_i, and v_{II} calculated with a fluid code (*i*.e. UEDGE) are loaded into the MCI grid
- These parameters are used to calculate grid specific atomic data such as ionization and recombination rate coefficients and to carry out kinetic impurity (Li, Be, etc.) transport simulations





Impurity neutrals are launched along the wall with a thermal Maxwellian velocity distribution

- Impurity neutrals enter the plasma with 3D ballistic trajectories
 - cosine distribution in ϕ and θ
 - − ionization mean free path (λ_{ionization}) is determined by the initial launch trajectory, velocity (V₀) and local plasma parameters (n_e and T_e → ionization rate coefficient)

$$\lambda_{ionization} = v_0 / n_e \overline{\sigma v(T_e)}$$



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Impurity ion transport and thermalization is calculated using three characteristic frequencies

$$ds = s_{i+1} - s_i = v_{\parallel,i} \Delta t + C_i \left(\Delta t\right)^2 / 2 \pm \sqrt{2D_{\parallel,i} \Delta t} \qquad D_{\parallel,i} = 1.22 \times 10^8 \left(T_{imp,i} / m_{imp} v_{\parallel}\right) \\ dv_{\parallel} = v_{\parallel,i+1} - v_{\parallel,i} = C_i \Delta t \qquad T_{imp,i+1} = T_{imp,i} + \left(T_{b,i} - T_{imp,i}\right) \Delta t v_{SE}$$

Where:

$$C_{i} = \frac{eEZ_{imp}}{m_{imp}} + (v_{b,i} - v_{ll,i})v_{sl} + \frac{1}{m_{imp}} \left[0.71Z_{imp}^{2} \frac{dT_{e}}{ds} + \beta_{imp} \frac{dT_{b}}{ds} \right]$$
$$\beta_{imp} = \frac{3\left[\mu_{m} + 7.07Z_{imp}^{2} \left(1.1\mu_{m}^{5/2} - 0.35\mu_{m}^{3/2}\right) - 1\right]}{5.4\mu_{m}^{2} - 2\mu_{m} + 2.6}; \mu_{m} = \frac{m_{imp}}{m_{b} + m_{imp}}$$

$$\upsilon_{\parallel} = \frac{6.8 \times 10^4 n_b Z_b^2 Z_{imp}^2 \ln \Lambda}{m_{imp} T_{imp} (T_b/m_b)^{1/2}} \quad \upsilon_{sl} = \frac{6.8 \times 10^4 (1 + m_b/m_{imp}) n_b Z_b^2 Z_{imp}^2 \ln \Lambda}{m_{imp} T_{imp} (T_b/m_b)^{1/2}} \quad \upsilon_{SE} = \frac{1.4 \times 10^5 n_b Z_b^2 Z_{imp}^2 \ln \Lambda}{m_{imp} T_b (T_b/m_b)^{1/2}}$$

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Magnetic data is used to calculate the position of the impurity ions after each transport step



• MCI typically gets magnetic data from an EFIT equilibrium file but for ITER simulations the magnetic data will be imported from UEDGE

- subroutines to replace EFIT data with UEDGE data and calculate dh and dw are needed



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Background plasma parameters are used to calculate impurity ionization, thermalization and transport processes

UEDGE T_e and n_e data on MCI grid



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Atomic data from ADAS is directly integrated into MCI and updated frequently with each new ADAS release



 Recent improvements in the accuracy of the ADAS Li ionization data have resulted from better fundamental data and the ADAS GCR modeling project

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MCI Li transport modeling in DIII-D plasmas provides us with a good set of benchmarks for the ITER simulations

- Localized Li sputtering from the DIII-D DiMES probe and its transport into the core have been simulated using the MCI unstructured grid and B2.5 plasmas.
- Li simulations compared to DIII-D experimental data in order to validate MCI's transport physics models and assess sensitivities to:
 - Boundary conditions
 - Variations in background plasma solutions
 - Atomic data



B2.5 equilibrium 1 Te distribution (105508:3900)



The Li core concentration calculated with MCI is quite sensitive to small changes in divertor recycling



 A reduction in divertor recycling (a B2.5 free parameter) changes Te near the target and the core Li concentration.

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Tasks and status

- Changes in the MCI code needed to simulate impurity transport in the ITER pedestal, SOL and divertor plasmas are underway:
 - Structured 2D grid (completed)
 - Read background plasma and magnetic data from UEDGE file (completed)
 - State-of-the-art Li atomic data (completed)
 - Calculate vertical and horizontal magnetic step size for each parallel diffusion step using cell specific collision frequencies (in progress)
- Simulate Li and Be thermalization/transport low collisionality ITER plasmas and compare to MCI Li transport results in DIII-D (as well as to the DIII-D Li DiMES experimental data)
 - Preliminary Li transport modeling and experiments in DIII-D (completed)
 - Future DIII-D Li transport experiments/modeling are being proposed to simulate Be transport in ITER (JET)
 - Li^{1+} ionization data is very similar to $Be^{1+}above 30 eV$

