Benchmarking kinetic and fluid neutral models for attached and detached state

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Kinetic neutral model and fluid neutral model have been benchmarked under the attached and detached state, using the SOLPS code. To attain the attachment and detachment condition, we changed the value of the core boundary D+ density in a wide range. To benchmark the profiles at the divertor region, the upstream profiles are carefully fitted. In the SOL region, no significant differences were observed in the plasma profiles. However, in the divertor region, large differences were observed in the plasma profiles. The neutral density from the kinetic neutral model is higher near the separatrix, considering the molecules. Therefore the kinetic neutral model is easier to realize the detached condition. Also the tendency of the neutral density differed, even if we use the common background plasma profile. More optimization of the fluid neutral model should be performed. Otherwise kinetic neutral model should be used to analyze the divertor region.

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1. Introduction

Neutral behavior has an important role in the transport simulations of the edge plasma. Most of the edge plasma transport codes treat neutral particles by a simple fluid model or a kinetic model. The kinetic treatments by the Monte-Carlo method are more exact than the fluid model. However, the kinetic model introduces the issue to the Monte-Carlo noise and raises the question of proving convergence. In addition, the simulation cost will be massive. On the other hand, the fluid model is easier to prove convergence, and faster than the kinetic model.

2-D edge plasma code SOLPS [1], consists of a fluid code B2.5 [2], coupled to a Monte-Carlo neutral code EIRENE [3]. Benchmarks of the kinetic neutral model (B2.5-EIRENE), and the fluid model (B2.5) are done in Ref. [4,5]. However, the benchmark studies of neutral model were limited to the detach case.

In the previous study, the kinetic neutral model and the fluid neutral model were benchmarked only in the detach state in Ref. [5]. In this study, benchmark has been made in detach and attach state, using SOLPS. To consider both detached and attached case we changed the value of the core boundary D+ density in a wide range.
2. Simulation Model

The simulation model used in this research is the same as Ref. [5]. The B2.5 multi fluid code simultaneously solves the particle balance, parallel momentum balance, ion and electron energy balance and the current continuity equations. The deuterium ions, D+, and all the carbon ions, C+-C6+, are described by the fluid approximation in B2.5. The detailed description of these basic equations and the expression for the radial and poloidal velocity components are given in Ref. [6]. The transport coefficients are chosen based on the comparison between the simulation results and the experimental data in the previous study. Figure 1 shows the numerical mesh generated from the JT-60U MHD equilibrium.

In the kinetic neutral model, Monte-Carlo neutral code (EIRENE) is coupled to B2.5. The B2.5 treats the ions and EIRENE treats the neutrals. In the EIRENE code, essential features of neutral dynamics for D, D2, and C are considered. In the fluid neutral model, the neutral species, D and C, are treated just like ion species by B2.5. Although the atomic and molecular processes are very important for the neutral dynamics in the divertor region, the molecules are not considered. Also neutrals are assumed to have the same common temperature as all other ion species. The pressure-driven diffusion coefficient for the neutrals are given by

\[ D_n = \frac{v_{th,n}^2}{(K_{CX}n_i + K_n)T_n} \]

where, \( v_{th,n} \) is the neutral thermal velocity, \( T_n \) is the neutral temperature shared with ions, and the density of ion and electron are \( n_i \) and \( n_e \). The rate coefficients for the charge exchange and ionization are \( K_{CX} \) and \( K_i \). The thermal diffusivity is assumed to be

\[ \chi_n = \frac{v_{th,n}^2}{(K_{CX}n_i + K_n)T_n} \cdot \]

The boundary conditions are as follows: at the core boundary the ion density is given, and the total energy input 2.5 MW is equally split between the ions and electrons channels. The net particle fluxes across the core boundary are assumed to be zero for all the ion species. For the boundary condition at the wall side, a radial decay length of 1 cm for the densities and temperature of ions and electrons is used. Also the feedback boundary condition is used in the fluid model to adjust the incoming neutral flux from the wall to fit the electron density of the outer-midplane separatrix.

Some parameters used in the fluid model are changed from the kinetic neutral model to fit the mid-plane profiles. Following recommendations from Ref. [4] are used to fit the mid-plane profiles: (1) use the core neutral loss boundary condition rather than the zero flux boundary condition, (2) use a neutral flux limiter. To apply the fluid model to the neutrals, the neutral mean free path needs to be smaller than plasma and neutral gradient length. Therefore, some correction for the kinetic effects, i.e., a neutral flux limiter is needed.
Electron Temperature [eV]

Distance from Separatrix [cm]

(a) 1.0x10^{19} [m^{-3}]

(b) 1.5x10^{19} [m^{-3}]

(c) 2.4x10^{19} [m^{-3}]

(d) 3.6x10^{19} [m^{-3}]

3. Results

Figure 2 shows the radial profiles of electron temperature at the outer divertor plate from the kinetic neutral model and the fluid neutral model. When the D^+ density at the core boundary is 1.0 \times 10^{19} \text{ m}^{-3}, the results from the kinetic neutral model and the fluid neutral model were both in the attached condition. However, when the core D^+ density is higher, the results from the kinetic neutral model is in the detached state with the electron temperature at the separatrix being lower than 5eV, while the fluid neutral model was still in the attached state with the electron temperature at the separatrix higher than 10eV. When the core D^+ density is 3.6 \times 10^{19} \text{ m}^{-3}, the tendency differed. The result from the fluid neutral model has a peak near the separatrix, while the kinetic neutral model has a peak at the outside of the separatrix. In experiments, a peak is recognized outside of the separatrix, in the radial profile of electron temperature at the divertor plate.
Figure 3 shows the radial profiles of poloidal energy flux from the fluid neutral model and the kinetic neutral model at the divertor plate. When the core D+ density is low, the energy flux concentrates near the separatrix in both fluid and kinetic neutral models. Also the total energy flux reaching the divertor plate is larger in the kinetic neutral model. However, as the core D+ density increases, the total energy flux significantly decreased in the kinetic neutral model compared to the kinetic neutral model. Also the peak of the energy flux moves outward in both models but the movement distance is much larger in the kinetic neutral model. In the kinetic neutral model, the value of the energy flux near the separatrix is much smaller than the fluid neutral model. Therefore, the kinetic neutral model is easier to realize the detachment condition.
Next we focused on the density profile of neutrals (deuterium atoms and molecules). Figure 4 shows the neutral densities at the divertor plate, from the fluid neutral model (B2), the kinetic neutral model without common background plasma (B2-E) and the kinetic neutral model with the background plasma common to the fluid model (E). At the divertor plate, density of molecules is higher than atoms. The effect of molecules may be more dominant than the atoms near the divertor plate. However, the fluid neutral doesn’t consider the molecules. Therefore, the kinetic neutral model is easier to realize the detachment condition, considering the molecules. The tendency of the fluid neutral model and the kinetic neutral model differs. The tendency of the fluid neutral model differs even if we use the common background plasma for the kinetic neutral model. The neutral density increases as it goes outward from the separatrix, while the kinetic neutral model decreases. In this calculation we may need to reconsider and confirm the neutral source of the fluid model to the kinetic neutral model.
4. Summary and Future Study

Kinetic neutral model and fluid neutral model has been benchmarked under the attached and detached state, using SOLPS. To benchmark the profiles at the divertor region, the upstream profiles are carefully fitted using the feedback boundary condition. At the SOL region, no significant differences were observed. However, in the divertor region, large differences were observed in the plasma profiles. The fluid model couldn’t realize the detached condition.

To consider the cause, we focused on the neutral profiles. In the divertor region, densities of molecules are higher than the density of atoms. The effect of molecules may be more dominant than the effect of atoms in the divertor region. However, the fluid neutral doesn’t consider the molecular effects. The kinetic neutral model has a higher density of neutrals near the separatrix, making it easier to realize the detachment condition. The difference in the tendency appears even if we use the same background plasma profiles. In this simulation condition that we used, we may need to reconsider about the neutral sources such as the chemical sputtering coefficients, the boundary conditions and the flux limits of ions and neutrals. We need to optimize the free plasma parameters such as the diffusion coefficients, transport coefficients and decay length for the density and temperature.

From this benchmark study, further improvement or optimization of fluid neutral model should be made to reproduce the reasonable divertor characteristics. Otherwise the kinetic model should be used for neutrals to analyze the divertor region especially in the detached state.

References