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Validation of SOLPS-ITER simulations with kinetic, fluid, and hybrid neutral models for JET-ILW low-confinement mode plasmas

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\begin{abstract}
For JET L-mode plasmas in low-recycling conditions (electron temperature at the outer strike point, $T_{\text{e,ot}} \geq 30$ eV), SOLPS-ITER simulations agree within the error bars for the experimental profiles at the low-field side (LFS) divertor target. The peak Balmer-$\alpha$ ($\text{D}_\alpha$) emission in the LFS divertor agrees within the error bars of the KS3 filterscope diagnostic, but is approximately 30\% lower than the peak value of the KTI spectrometer. Simulations have been performed with fluid, kinetic, and hybrid models for the neutrals. The large fluid-kinetic discrepancies of more than a factor 2 are successfully corrected by using a hybrid fluid-kinetic approach, for which kinetic atoms are transferred to the fluid population when the local Knudsen number of the atom becomes smaller than a user-defined transition Knudsen number $K_{\text{tr}}$. The hybrid-kinetic discrepancies are limited to a few \% for $K_{\text{tr}} \leq 100$. When increasing the upstream density to high-recycling conditions, at the onset of detachment ($T_{\text{e,ot}} \approx 5$ eV), the simulations predict more than a factor 2 lower peak ion saturation current to the LFS divertor than the experiments. Also the $\text{D}_\alpha$ emission is underpredicted with approximately a factor 2. For these high-recycling conditions, the fluid-kinetic discrepancies are limited to maximum 50\%, which are again corrected by using the hybrid approach.
\end{abstract}

\section{Introduction}
Experimental validation of plasma edge codes for nuclear fusion devices is essential to employ them for the interpretation and development of operational scenarios, and for the design of future reactors. Experiments at multiple fusion devices are used to validate many different analysis and modeling tools. In this paper, we validate the widely used SOLPS-ITER code suite [1] for JET ITER-like wall (JET-ILW), low-confinement mode (L-mode) plasmas.

The emphasis is on the validation of simulations with different models for the neutral particles, i.e., hydrogenic atoms and molecules. Although a kinetic description (typically solved with a Monte Carlo (MC) procedure, e.g., with the EIRENE code [2] in SOLPS-ITER) is the most accurate, simulations with a kinetic neutral model can take up to several weeks for reactor-scale devices in detached conditions due to the increased amount of ion-neutral interactions [3]. Therefore, fluid neutral models have been developed in the past decades [4–6]. The accuracy of these fluid models has been significantly improved in the past years by making the transport coefficients and boundary conditions consistent with the underlying kinetic description [7,8]. These improved fluid models are called advanced fluid neutral (AFN) models. In addition, a hierarchy of hybrid fluid-kinetic neutral models has been developed to increase the accuracy of a purely fluid approach, but with a reduction in computational cost compared to a fully kinetic treatment [9–12]. In this paper, we focus on the validation of simulations with a purely kinetic neutral model, an AFN model, and the advanced spatially hybrid approach from Ref. [13], which combines the spatially hybrid approach from Refs. [10,14] with the possibility of transitioning particles from the kinetic to fluid population in the plasma edge domain by means of a so-called condensation process [9].

\section{Validation}

For JET L-mode plasmas in low-recycling conditions (electron temperature at the outer strike point, $T_{\text{e,ot}} \geq 30$ eV), SOLPS-ITER simulations agree within the error bars for the experimental profiles at the low-field side (LFS) divertor target. The peak Balmer-$\alpha$ ($\text{D}_\alpha$) emission in the LFS divertor agrees within the error bars of the KS3 filterscope diagnostic, but is approximately 30\% lower than the peak value of the KTI spectrometer. Simulations have been performed with fluid, kinetic, and hybrid models for the neutrals. The large fluid-kinetic discrepancies of more than a factor 2 are successfully corrected by using a hybrid fluid-kinetic approach, for which kinetic atoms are transferred to the fluid population when the local Knudsen number of the atom becomes smaller than a user-defined transition Knudsen number $K_{\text{tr}}$. The hybrid-kinetic discrepancies are limited to a few \% for $K_{\text{tr}} \leq 100$. When increasing the upstream density to high-recycling conditions, at the onset of detachment ($T_{\text{e,ot}} \approx 5$ eV), the simulations predict more than a factor 2 lower peak ion saturation current to the LFS divertor than the experiments. Also the $\text{D}_\alpha$ emission is underpredicted with approximately a factor 2. For these high-recycling conditions, the fluid-kinetic discrepancies are limited to maximum 50\%, which are again corrected by using the hybrid approach.

\section{Conclusions}

The emphasis is on the validation of simulations with different models for the neutral particles, i.e., hydrogenic atoms and molecules. Although a kinetic description (typically solved with a Monte Carlo (MC) procedure, e.g., with the EIRENE code [2] in SOLPS-ITER) is the most accurate, simulations with a kinetic neutral model can take up to several weeks for reactor-scale devices in detached conditions due to the increased amount of ion-neutral interactions [3]. Therefore, fluid neutral models have been developed in the past decades [4–6]. The accuracy of these fluid models has been significantly improved in the past years by making the transport coefficients and boundary conditions consistent with the underlying kinetic description [7,8]. These improved fluid models are called advanced fluid neutral (AFN) models. In addition, a hierarchy of hybrid fluid-kinetic neutral models has been developed to increase the accuracy of a purely fluid approach, but with a reduction in computational cost compared to a fully kinetic treatment [9–12]. In this paper, we focus on the validation of simulations with a purely kinetic neutral model, an AFN model, and the advanced spatially hybrid approach from Ref. [13], which combines the spatially hybrid approach from Refs. [10,14] with the possibility of transitioning particles from the kinetic to fluid population in the plasma edge domain by means of a so-called condensation process [9].

\section{Acknowledgments}

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\section{References}


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hybrid approach is the furthest in development and is trivial to apply from a user’s perspective.

For the first time, we compare the results of simulations with different neutral models with experimental data, focusing on measurements at the low-field-side (LFS) midplane, LFS divertor target, and spectroscopic measurements of Lyman and Balmer series deuterium emission. This thorough validation will give critical information on the validity of plasma edge simulations and the range of applicability of a fluid or hybrid neutral approach, which is essential for their use in designing future reactors.

2. Overview of the fluid and hybrid neutral models in this paper

The details of the AFN model can be found in Ref. [7]. It consists of a continuity and parallel momentum equation with the assumption that the neutrals have the same temperature as the ions. The improved accuracy compared to older fluid neutral models is achieved by imposing particle and momentum fluxes at the boundaries. These fluxes are derived from the assumption that the particle velocity distribution of incident neutrals is a truncated Maxwellian. The recycled distribution is then calculated with the help of the TRIM reflection database [15].

A major shortcoming of the AFN model is that a fluid approximation is not valid across the entire computational domain due to possibly long mean free paths of the neutral particles. In addition, whereas the hydrogen atoms reach the fluid limit in some regions, the molecules (H₂) and non-hydrogenic atoms typically still behave kinetically. These two issues are solved by using a spatially hybrid approach, where the AFN model is combined with a kinetic model for the atoms sampled at interfaces in the scrape-off-layer (SOL) and private-flux (PF) regions. In principle, the user is free to choose the location of these interfaces, but it is convenient to let them coincide with SOLPS-ITER’s existing plasma–void interfaces, which delimit the plasma grid (see Fig. 1). The void regions (blue regions in Fig. 1) are assumed to be vacuum. The kinetic treatment in the void regions allows us to take into account geometrically complex wall geometries, including solid structures such as a dome and radiation shields (louvres). In addition, the hybrid model for the atoms is coupled to a kinetic model for the molecules in the entire computational domain, which is essential to obtain accurate results for detached conditions and is another important shortcoming of the AFN and other fluid neutral models.

In the original spatially hybrid approach from Ref. [10], kinetic atoms launched at the plasma–void interfaces were followed in the MC part until they were absorbed. Consequently, the simulations were slowed down when the atoms reached high-collisional regions. On the other hand, all recycled atoms at the divertor targets were approximated as fluid, which is potentially invalid near the outermost flux surfaces where the collisionality is typically low. These issues are circumvented by combining the spatially hybrid approach with the approach from Ref. [9], as successfully demonstrated for an ITER case in Ref. [13]. One of the approaches in Ref. [13] is to launch all particles at both targets and plasma–void interfaces kinetically. Their initial position and velocity are sampled from the incident ion and fluid neutral distributions. Both the incident ion and fluid neutral distributions are assumed to be truncated Maxвелlians. For the ions, sheath acceleration is added at the target plates. At each charge-exchange (CX) collision event, the particle Knudsen number \( K_n \) is calculated as

\[
K_n = \frac{\Delta \nu_{\text{CX}}}{L}
\]

(1)

with \( \Delta \nu_{\text{CX}} \) the CX mean free path of the particle in the MC simulation, and \( L \) a macroscopic length scale, which is fixed and imposed by the user. The value of \( L \) is typically determined by the length scale of the steepest plasma density or temperature gradient of the problem. Hence, it scales with the machine size and it is typically smaller for H-mode compared to L-mode. When \( K_n \) is smaller than a user-defined transition Knudsen number \( K_n^t \), the particle is transferred to the fluid population by means of sources in the fluid neutral model. Atoms resulting from volumetric recombination (3-body and radiative) are treated as a fluid, which is justified by the low temperatures of the recombination region (\(< 1 \text{ eV}\)). Hence, the hybrid approach converges to a fully kinetic treatment for \( K_n \rightarrow 0 \) (except for a small error due to the fluid treatment of atoms from volumetric recombination), whereas it tends to the purely fluid solution for \( K_n \rightarrow \infty \). The only difference with the purely fluid model is that first-flight effects are still taken into account for the hybrid model with \( K_n \rightarrow \infty \). In this paper, we evaluate the accuracy of this so-called advanced spatially hybrid method for different values of \( K_n^t \).

The AFN and spatially hybrid neutral models were implemented in the new extended grid version of SOLPS-ITER [16], which contains a 9-point stencil for a correct discretization for cells not perfectly aligned to the magnetic field and non-orthogonal cells. This improved numerical treatment is essential for an accurate description of the isotropic behavior of fluid neutrals [17]. In this paper, we use the extended grid version for all our simulations. For simulations with fully kinetic neutral model, we study the effect of electromagnetic drifts. The simulations with fluid and hybrid neutral models are always run without drifts, but with parallel currents that determine the electric potential. The validity of the AFN model in the presence of drifts is the topic of Ref. [18]. Although the extended grid version allows a flexible choice of the location of the fluid-kinetic interfaces for the spatially hybrid approach, we still let them coincide with the plasma-void interfaces. These interfaces are still present in our simulations, because the grid is directly converted from previous simulations with the structured SOLPS-ITER version.

3. Case description

We consider two types of purely deuterium plasmas: (i) a low-recycling case from JET campaign C28 in 2011; and (ii) a high-recycling case at the onset of detachment from C38 in 2019. The line-averaged densities in the LFS edge of the main plasma ((\( \bar{n}_e \text{edge} \)) are approximately \( 1.4 \cdot 10^{19} \text{ m}^{-3} \) and \( 2.6 \cdot 10^{19} \text{ m}^{-3} \) for case (i) and (ii), respectively. The magnetic configuration is shown in Fig. 1. The plasma current and the toroidal magnetic field at the magnetic axis are
2.5 MA and 2.5 T, respectively, with the ion $\mathbf{B} \times \nabla B$ vector pointing into the divertor. The total heating power (ohmic and neutral beam) is approximately 2.9 MW. About 0.7 MW is radiated in the core, resulting in 2.2 MW crossing the separatrix, which we assume equally distributed over the ions and electrons. Further details of the case can be found in Ref. [19].

To obtain the same upstream conditions in the simulations as in the experiments, the electron density at the outer midplane (OMP) separatrix position $n_{e,\text{sep},m}$ is controlled by means of a feedback gas puff in the PF region, which injects $D_2$ molecules. The gas puff location is indicated in Fig. 1. According to Ref. [20], $n_{e,\text{sep},m} \approx 0.5 \times n_e(\text{edge})$. Hence, we use $n_{e,\text{sep},m} = 0.7 \times 10^{19}$ m$^{-3}$ and $n_{e,\text{sep},m} = 1.3 \times 10^{19}$ m$^{-3}$ for the low- and high-recycling case, respectively. The gas puff for the purely fluid simulations is represented by a particle flux at the inner PF boundary. The radial transport coefficients are taken from Ref. [19] and plotted in Fig. 2. For the hybrid simulations, we assume a macroscopic length scale $L = 0.1$ m in Eq. (1). Finally, impurity sputtering from the wall is not taken into account in the simulations. This simplification is justified by measurements of the effective charge state, which is between 1.0 and 1.2.

We validate the simulations for several important diagnostics, which are indicated in Fig. 3.

4. Results

4.1. OMP plasma profiles

All simulations are within the error bars of the experimental data in the OMP SOL ($R - R_{\text{sep}} > 0$) (Fig. 4). The statistical error of the measurements here and in upcoming figures is visualized by plotting the measured data during a certain time interval. Hence, the difference between the minimum and maximum measured value at a certain location gives the range of the statistical error. By comparing different diagnostics, we get a rough estimate of possible systematic errors. It should be noted that all simulations in this figure and upcoming figures are without drift contributions, except for the blue dashed lines that represent the solutions of simulations with fully kinetic neutrals with $E \times B$, diamagnetic, and inertial drifts turned on. Comparing the blue solid and dashed lines in Fig. 4 reveals the limited effect of drifts on the upstream profiles.

Slight improvements of the radial transport coefficients are possible to improve the fit for $n_t$ between the kinetic and hybrid simulations and RCP and Li beam data in the SOL for $n_t(\text{edge}) \approx 1.4 \times 10^{19}$ m$^{-3}$ (Fig. 4a). However, fitting the transport coefficients manually is a time-consuming process. An automatic fitting procedure with Bayesian inference has been recently developed for SOLPS-ITER [29], but is presently only available for simulations with a purely fluid neutral model. In the SOL, the OMP profiles of the purely fluid simulations are already within the uncertainty intervals of the measurements (green lines in Fig. 4). In addition, it is not expected that these slight improvements significantly influence the plasma state in the divertor. Similarly, the profiles of $n_t$ inside the separatrix ($R - R_{\text{sep}} < 0$) could be improved for $n_t(\text{edge}) \approx 2.6 \times 10^{19}$ m$^{-3}$ (Fig. 4c). However, the divertor conditions are almost unaffected by the plasma profiles in the core region. The feedback gas puff guarantees the same values for $n_{e,\text{sep},m}$ in the different simulations, which leads to similar divertor conditions for all models. We illustrate the independence of the divertor conditions on the profile of $n_t$ inside the separatrix by reducing $D_2$ from Fig. 2 to 0.1 m$^2$/s for $R - R_{\text{sep}} < 1$ cm. Fig. 5 shows that the varied profile of $n_e$ in the OMP core region does not significantly influence $n_t$ and $T_e$ at the LFS target plate.

Finally, Fig. 4 shows that $K n_t$ in the hybrid simulations can become large (> 100) without introducing significant hybrid-kinetic discrepancies. Even for $K n_t \rightarrow \infty$ (red pluses in Fig. 4), the maximum hybrid-kinetic discrepancy stays within 10%, indicating the importance of first-flight effects. Due to the high temperatures, upstream particle sources are almost completely determined by atoms that ionize immediately without undergoing CX collisions. Hence, the first-flight trajectory of an atom is almost equivalent to its full trajectory and the hybrid results for $K n_t \rightarrow \infty$ approach the solutions with fully kinetic neutrals within 10% at the OMP.

4.2. LFS target profiles

Whereas the simulation results with kinetic and hybrid neutral models are within the uncertainty bars of the LPs at the LFS divertor target for low-recycling conditions (Fig. 6a–c), the simulations underpredict

![Fig. 2. Radial profiles of the particle ($D_\perp$) and thermal ($\chi_e$ and $\chi_i$ for the ions and electrons, respectively) diffusivities, where $R - R_{\text{sep}}$ corresponds to the radial distance from the separatrix at the OMP.](image)

![Fig. 3. Principal diagnostics: a reciprocating probe (RCP) [21], a lithium beam system [22], a high-resolution Thomson scattering (HRTS) system [23], an array of target Langmuir probes (LP) [24], high-resolution poloidally scanning mirror spectrometers (KT1 [25] and KT3 [26]), and a low-resolution photo-multiplier tube filterscope using optical fibers (KS3) [27]. In addition, we use data from a tangentially viewing camera in the divertor region (KL11) (not shown) [28].](image)
the peak ion saturation current density \(j_{\text{sat}}\) by more than a factor 2 in high-recycling conditions (Fig. 6d). LP data become unreliable for measuring temperatures for \(T_e < 5\) eV. Hence, we use the line-averaged \(n_e\) and \(T_e\) across the LFS divertor leg obtained by the KT3 spectrometer for \(\langle n_e \rangle_{\text{edge}} \approx 2.6 \cdot 10^{19} \text{ m}^{-3}\) (Fig. 6e-f). The line-averaged \(n_e\) and \(T_e\) are inferred using Stark broadening of the Balmer-\(\delta\) line and using the fitted continuum emission of the Balmer series, respectively [30,31].

It is clearly seen that the simulations underpredict the temperature with approximately a factor 2 for high-recycling conditions (Fig. 6f). The simulation-experiment discrepancies are barely reduced when including the drifts (blue dashed lines in Fig. 6). Finally, we conclude that the hybrid simulations with \(Kn^t = 100\) (red circles) are accurate
for low-recycling conditions (Fig. 6a–c), and give a maximum hybrid-kinetic discrepancy of 20% for high-recycling conditions (Fig. 6d–f). The fluid error is already significantly reduced for the hybrid model with $Kn' \to \infty$ (red pluses in Fig. 6) due to the correct treatment of first-flight effects.

### 4.3. Lyman and Balmer series emission

Spectroscopic measurements provide crucial information on the plasma state inside the volume. To compare the simulations with the experiments, we calculate the emission along the different diagnostic chords as a post-processing step in the simulations. For each simulation (with kinetic, fluid, or hybrid neutral model), we run a single fully kinetic EIRENE iteration on the (statistically) converged plasma state. The first step of this EIRENE iteration is recalculating the neutral properties for the provided plasma state. For simulations with fluid and hybrid neutral model, this kinetic recalculation leads to an improved accuracy of the neutral state at an almost negligible cost, because a fully kinetic MC treatment is only used for a single iteration. In addition, molecular contributions are explicitly added to the simulations with purely fluid neutral model by this kinetic post-processing phase. In a second step, EIRENE calculates the line integrals of the deuterium line radiation along the diagnostic chords, using the AMJUEL-HYDHEL databases [32,33]. These databases include contributions from the molecules and molecular ions to the Lyman and Balmer emission.

For high-recycling conditions, the Lyman and Balmer series emissions from simulations with purely fluid neutral model already agree within 25% of accuracy with simulations with fully kinetic neutral model, as shown in Figs. 7b–c and 8c–d. The simulation with fluid neutral model is relatively accurate due to the fact that the neutral state is recalculated with a fully kinetic EIRENE iteration. Whereas the simulation with drifts correctly predicts the Ly-β emission for $\langle n_e\rangle_{\text{edge}} \approx 2 \cdot 10^{19}$ m$^{-3}$ (blue dashed line in Fig. 7c), all simulations overestimate the Ly-α emission (Fig. 7b). This observation suggests the importance of Ly-α opacity in JET plasmas [34], which is neglected in the simulations. The drifts play an important role in the Ly-β emission profile in the LFS divertor (Fig. 7c).

The simulation-experiment agreement of the target profiles for low-recycling conditions in Fig. 6a–c is also visible in the Balmer-α ($D_\alpha$) and Balmer-β ($D_\beta$) emission profiles (Fig. 8a–b). Although simulations with kinetic and hybrid neutral models agree with the KS3 data for $D_\alpha$, KT1 predicts a 30% higher peak value (Fig. 8a). Similarly, for high-recycling conditions, the simulation-experiment discrepancies for the target profiles (Fig. 6d–f) are also observed for the $D_\alpha$ and $D_\beta$ emission (Fig. 8c–d). The increased asymmetry between the high-field-side (HFS) and low-field-side (LFS) divertor for $D_\beta$ compared to $D_\alpha$ indicates the increased importance of volumetric recombination in the HFS divertor, which is not correctly captured in the simulations. The KL11 data are obtained by taking the line integrals along the KT1 chords in the tomographic reconstructions of the camera data. The reduced peak emission for KL11 in the HFS divertor compared to KT1 and KS3 is due to the correction for the reflections in the KL11 post-processing phase. These reflections are especially important for the vertical HFS target. The hybrid approach successfully corrects the fluid-kinetic errors in both low- and high-recycling regimes. Even for $Kn' \to \infty$, the maximum hybrid-kinetic discrepancy for Lyman and Balmer emission profiles remains below 25%.
4.4. Performance of the hybrid method

When using the same amount of MC particles in the hybrid approach as for the fully kinetic approach and distributing them according to the source strengths of the different source contributions, the hybrid approach is maximum 1.7 and 7.1 times faster than a fully kinetic treatment for the low- and high-recycling case, respectively, as illustrated by the horizontal blue and red lines in the top part of Fig. 9. These upper limits are reached when \( Kn' \to \infty \). When correcting the speed-up factors to take into account the variation in statistical error on \( n_e \) at the LFS strike point \( (n_{\text{ot}}) \) (same approach as in Ref. [14]), the maximum speed-up factors become 3.0 and 6.8, respectively (horizontal dashed lines in top part of Fig. 9). The increased contribution of the fluid neutral part reduces the statistical error for \( (n_e)_{\text{edge}} \approx 1.4 \cdot 10^{19} \text{ m}^{-3} \), and hence, the speed-up increases (blue dashed line shows a larger speed-up than the blue solid line in Fig. 9). The opposite happens for \( (n_e)_{\text{edge}} \approx 2.6 \cdot 10^{19} \text{ m}^{-3} \) (red dashed line is below red solid line). It is expected that this statistical deterioration is due to the much quicker absorption of MC particles in the hybrid approach due to the increased collisionality of the high-recycling case. The analog simulation strategy in EIRENE is not efficient for very short particle trajectories. In Ref. [35], it is shown that a statistical error reduction (for a given computational time) is not efficient for very short particle trajectories. In Ref. [35], it is shown that a statistical error reduction (for a given computational time) is not efficient for very short particle trajectories.

For \( Kn' \to \infty \), the hybrid-kinetic discrepancies for \( n_{\text{ot}} \) become approximately 28% and 24% for \( (n_e)_{\text{edge}} \approx 1.4 \cdot 10^{19} \text{ m}^{-3} \) and \( (n_e)_{\text{edge}} \approx 2.6 \cdot 10^{19} \text{ m}^{-3} \), respectively (horizontal lines in bottom part of Fig. 9), which is significantly more accurate than the simulations with purely fluid neutrals, where the errors are 59% and 41%, respectively. For accurate results (errors < 15%) with still a significant speed-up, it is recommended to use \( Kn' = 100 \). Then, the speed-up factors (with statistical error correction) become 1.6 and 5.7 for the low- and high-recycling case, respectively. It is expected that these speed-up factors further increase when moving to high-collisional detached plasmas. A similar analysis can be done for other properties than \( n_e \) but the hybrid-kinetic discrepancies are the largest for \( n_e \) at the LFS target (see Fig. 6).
asymptotic convergence to the kinetic solution for $K n_t \to 0$ for all regimes. The hybrid approach is approximately 6 times faster than a fully kinetic approach (with maximum errors within 20%) for a high-recycling case. It is expected that the performance can be further increased by optimizing the MC estimators. Additionally, we expect a performance increase for computationally costly simulations of the ITER and DEMO reactors in a detached regime due to the increased amount of CX collisions.

CRediT authorship contribution statement


Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Fig. 9. Speed-up and accuracy of hybrid approach. The solid lines in the top figure represent the speed-up without taking into account the variation in statistical error. For the dashed lines, the speed-up is corrected to get the same statistical error on $n_{e,ot}$ as for the kinetic approach. The horizontal lines show the limits for $Kn^t \to \infty$. Blue: $\langle n_{e,ot} \rangle \approx 1.4 \cdot 10^{19}$ m$^{-3}$; red: $\langle n_{e,ot} \rangle \approx 2.6 \cdot 10^{18}$ m$^{-3}$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

References


