AMMONX: a kinetic ammonia production scheme for EIRENE implementation

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ABSTRACT

Until recently the EIRENE suite handled hydrogen chemistry (i.e. H atoms, H_2 molecules and molecular ions, and their isotopomers). Extensions also existed for C_xH_y species (H is any hydrogen isotope) chemistry, but no kinetic scheme including NH_x chemistry had been implemented. After a benchmarking of available schemes and kinetic data, a reduced scheme including 50 reactive processes is presented here, implying a large set of N-bearing species (N, N_2, N_2^+, NH_x radicals and ions). This mechanism is a part of a more complete scheme of 130 processes also including the metastable states of N_2 and N. After validation of this scheme by comparison with experimental works of the literature, it was used in the Eirene suite to model the evolution of the plasma phase during N_2 injection in the area under the divertor and to follow the possible NH_3 formation.

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STEPS OF BUILDING AMMONX

Main sources of the review

1. AMJUEL data file for EIRENE from D. Reiter version : March 2016
2. Sode et al.[2] and Carrasco et al.[1] experimental/modeling works for N_2/H_2 plasmas
3. LxCat database for cross section of collisional processes with electrons
4. Anicich reviews and Umist database for ion/neutral processes
5. Works of Capitelli and al. [3] and NIST database for neutral processes

Database of 130 processes

✓ 20 species taken into consideration:
H_2, H, H^+, H_2^+, H_3^+, N_2, $N_2(A)$, N_2^+, N, $N(^2D)$, N^+, NH, NH^+, NH_2, NH_2^+, NH_3, NH_3^+, NH_4^+, N_2H^+, e-

Database includes following processes :
- ✓ Ionization by e-/neutrals collisions
- ✓ Neutrals dissociation by electron-impact
- ✓ e-/ions dissociative recombinations
- ✓ Ion/neutrals processes
- ✓ N_2, N and H_2 metastable-states chemistry
- ✓ Neutral/neutral chemistry

Process of scheme

1. One production and one consumption process must exist for each species
2. Comparison between diffusion characteristic times of the species to the surface in Tokamak conditions and reacting frequency in the plasma allow disregard of almost all the processes involving only neutrals
3. Only processes with characteristic times comparable to the predominant production and consumption processes identified in step 1 are selected. (Processes with only radicals have been neglected)

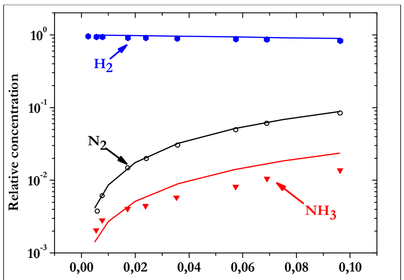
Scheme A containing 40 plasma processes without metastable states chemistry *
+
Surface/wall recombination of ions and radicals (one per actives species)
Scheme available in AMDS format for SOLPS-ITER users

Scheme B containing 50 plasma processes with metastable states chemistry*
+
Surface/wall recombination of ions and radicals (one per actives species)
Scheme available in AMDS format for SOLPS-ITER users

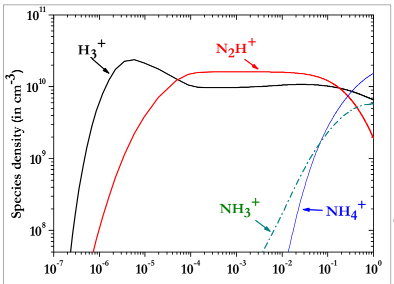
[1] M. Sode et al. Journal of applied physics **117** (2015) 083303
[2] E. Carrasco et al. Phys. Chem. Chem. Phys. **15** (2013) p.1699
[3] M. Capitelli et al. in Plasma Kinetics in Atmospheric Gases, Springer-Verlag Berlin Heidelberg (2000)

* Both A and B schemes are available on LSPM web site http://www.lspm.cnrs.fr/ammonx

VALIDATION OF THE SCHEME A BY 0D MODELING



Evolution of main by-products relative concentration as a function of initial N_2 fraction (symbols are expt. results from Carrasco et al. [2])



Computed profiles of main ions for 0.5% of N_2 in initial mixture

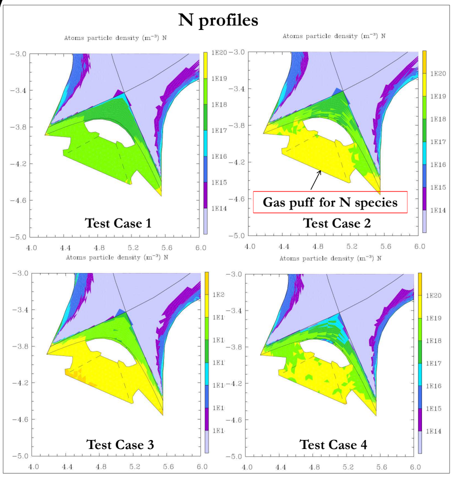
Simulated conditions

Parameter	*Value*
Power density	25 kW.m^{-3}
Neutral pressure	10 Pa
Plasma temperature	2.8 ± 0.5 eV
Electron density	3.0 ± 0.5 × 10^{16} m^{-3}
Surface temperature (Assumed to be saturated with H and N).	350K
N_2 percentage in H_2	0.5 to 10%
Residence Time	0.5 s

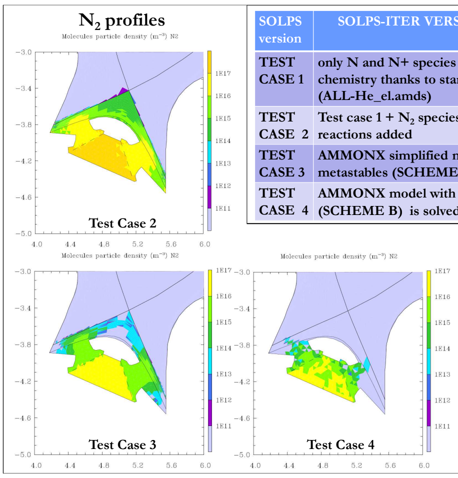
- ☞ Comparison between experimental results of Carrasco et al. [2] and results of simulation with scheme A show a good agreement, even if the production of NH_3 is slightly overestimated by the model (less than factor 3)
- ☞ The scheme A can be used with good confidence for the processes of NH_3 production in conditions close to tokamak edge plasma
- ☞ Effects of plasma phase secondary processes (ignored in the reduced mechanisms in a first approximation) in possible ammonia production has to be studied

EIRENE MODELING

N profiles



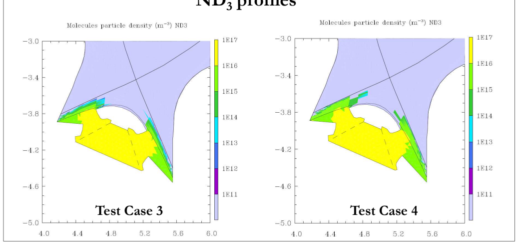
N$_2$ profiles



SOLPS version	SOLPS-ITER VERSION 3.0.6-51 (master)
TEST CASE 1	only N and N+ species are included in EIRENE chemistry thanks to standard model AMJUEL (ALL-He_el.amds)
TEST CASE 2	Test case 1 + N_2 species and its chemical reactions added
TEST CASE 3	AMMONX simplified model without metastables (SCHEME A) is used
TEST CASE 4	AMMONX model with metastables (SCHEME B) is solved

A simplified surface mechanism has been implemented for surface processes under following hypothesis :
- All ions are neutralized by collision with the wall
- ND_x radicals are recombining through one process giving the following distribution 10% of N_2, 30% of ND, 30% of ND_2 and 30% of ND_3

ND$_3$ profiles



☞A new test case is proposed (based on ITER test case ITER_2588_D+He+N) with N_2 gas puff injection under the divertor

☞ Taking into account the metastable species reduces the N_2 diffusion above the divertor

☞For cases 3 and 4, after implementation in Eirene suite, first simulations show clearly ammonia formation in too high amounts under the divertor – Studies on ND_3 formation on the surface are still in progress

CONCLUSIONS

1. A new database named AMMONX including NH_X formation processes has been achieved based on AMJUEL formalism
2. Two reduced schemes of 40 and 50 processes respectively are proposed to model NH_3 formation in plasma edge conditions under the divertor area and have been validated by model/experiment comparison
3. After implementation in Eirene suite, first simulations predict clearly ammonia formation in high amounts under the divertor
4. Study of respective roles of the plasma phase and the surface mechanism in NH_3/ND_3 formation are still under progress

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