Neutral gas modelling

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BOUT++ Workshop 16th September 2014

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- Neutral gas and plasma turbulence
- Neutral gas physics: Cross-sections and mean free paths
- Typical length-scales
- Approaches used in BOUT++
- Discussion

Neutrals and plasma turbulence (1/2)

- 2D transport codes include molecular and atomic physics \rightarrow Essential for e.g. divertor physics, detachment
- 3D turbulence codes have typically assumed fully ionised, single ion species plasma

Strong motivations for including neutral gas physics in 3D code:

O Effect of neutrals on turbulence

- Sources and sinks of density and momentum
- Damping from ion-neutral interactions
- Electron-neutral interaction may have more complex effect on drift-wave stability

Neutrals and plasma turbulence (2/2)

2 Effect of turbulence on neutrals

• Ion-neutral cross-sections are strongly nonlinear:

$$\overline{n\langle\sigma v\rangle}\neq\overline{n}\overline{\langle\sigma v\rangle}$$





2D ITER simulations with and without synthetic fluctuations¹ Caused by hardening of CX neutral spectrum

¹S.Mekkaoui

Neutral gas processes

Several processes involved:

- Charge Exchange (CX) $H + H^+ \rightarrow H^+ + H$
- Ionisation (electron impact) $H + e^- \rightarrow 2e^- + H^+$ Also produces radiation through excitation
- Recombination has several pathways:
 - Radiative recombination: $e^- + H^+ \rightarrow H + h \nu$
 - Three-body recombination: $e^- + e^- + H^+ e^- + H$
 - Negative-ion mediated recombination (MAR):

$$e^- + H_2 \rightarrow H_2^- \rightarrow H + H^-$$

 $H^+ + H^- \rightarrow H + H$

• Ion-conversion mediated recombination (MAR):

$$\begin{array}{rrrr} H^+ + H_2 & \rightarrow & H + H_2^+ \\ e^- + H_2^+ & \rightarrow & H + H \end{array}$$

¹EIRENE: http://www.eirene.de/

²KN1D: http://www.psfc.mit.edu/labombard/KN1D_Source_Info.html

Interaction cross-sections

 Analytic forms used for ionisation, recombination, and charge exchange cross sections²



¹Thanks to Eva Havlickova, CCFE

Interaction mean free paths

- Mean free paths shown for a 300K (0.025eV) neutral gas atom using a crude analytical model for cross-sections
- Often a 3.5 eV "Frank-Condon" energy is assumed instead
- Charge exchange results in a population of fast neutrals, which can have much longer m.f.p.



BOUT++ neutral models

Three approaches being followed to neutral modelling

- Simple drag model for CX in LAPD¹
- Pluid modelling²
 - Valid for short mean-free-path interactions
 - Conputationally lower cost than Montecarlo methods
- Montecarlo modelling
 - Can be applied when m.f.p is long
 - Much more expensive computationally, but parallelises very well
 - Coupling to EIRENE
 - Currently testing in linear geometry³





³S.Mekkaoui et al. PSI conference 2014

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¹P.Popovich, M.V.Umansky, T.A.Carter and B.Friedman arXiv:1005.2418 (2010)

²Z.H.Wang, X.Q.Xu, T.Y.Xia, T.D.Rognlien Nucl. Fusion 2013

- Sensitivity of turbulence to neutral gas studied in LAPD simulations¹
- Treat charge-exchange as a sink of vorticity with ion-neutral collision rate $\nu_{in} \sim 10^{-3} \Omega_{ci}$

$$\partial_t \omega = \ldots - \nu_{in} \omega$$



¹P.Popovich, M.V.Umansky, T.A.Carter and B.Friedman arXiv:1005.2418 (2010)

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Fluid neutral model

Fluid model developed¹ which takes into account dissociation and ionisation:

$$H_2 \rightarrow 2H^0 \rightarrow 2H^+ + 2e$$

and charge-e Currently models neutrals along a 1D beam (SMBI). Provides a source of density for fuelling



¹Z.H.Wang, X.Q.Xu, T.Y.Xia, T.D.Rognlien Nucl. Fusion 2013

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Ongoing work with neutral fluid models

- 1D modelling of detachment fronts
 - At high density (low divertor temperature), volume recombination can detach plasma from the target plates
 - Ionisation-recombination front can move upstream
 - Stability and control of this front is essential



Ongoing work with neutral fluid models

• 1D modelling of detachment fronts

- At high density (low divertor temperature), volume recombination can detach plasma from the target plates
- Ionisation-recombination front can move upstream
- Stability and control of this front is essential
- 2D modelling of plasma turbulence
 - neutral gas interactions
 - Diffusive model for neutral gas
 - So far low power cases → small variation in density



BOUT++ / EIRENE coupling

Work ongoing to couple $\mathsf{BOUT}++$ to EIRENE

- Starting in linear geometry (LAPD, PSI-2, Magnum-PSI)
- Technical coupling completed. Both codes run in parallel (MPI), passing data in memory
- Initial turbulence simulations beginning
 - \rightarrow Some issues related to initialisation transients



- Simple models used in BOUT++ to study broad trends
- Fluid models can be run for long times relatively cheaply
- A kinetic treatment is probably needed
 - Need to capture changes in neutral energy spectrum
 - Mean-free-paths can be comparable to turbulent scales
- Ongoing work with BOUT++ and EIRENE³

³S.Mekkaoui, EFDA fellowship 2014. Poster at PSI 2014