2022 AIP Congress

Monte Carlo Simulation of Electron Dissociation of H_2 Gas

Reese Horton*, Liam Scarlett, Igor Bray, Dmitry Fursa

Curtin University, Perth, Western Australia

*reese.horton@postgrad.curtin.edu.au

December 12, 2022

Australian Government

PAWSEY supercomputing centre

Curtin University

Introduction and Motivation

- Accurate MCCC cross sections exist for modelling.
- Much recent modelling makes use of old/outdated data.
- MCCC data gives significantly improved results.

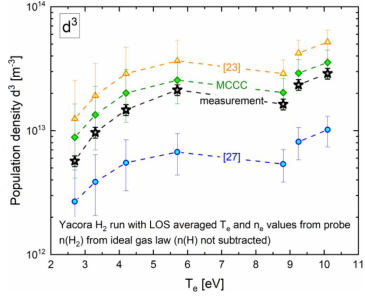

Figure 1: Comparison of $d\,^3\Pi_u$ population densities of H_2 calculated in a collisional radiative model using several different H_2 data sets, produced by Wunderlich et al *[J. Phys. D (2021), 54(11):115201]*.

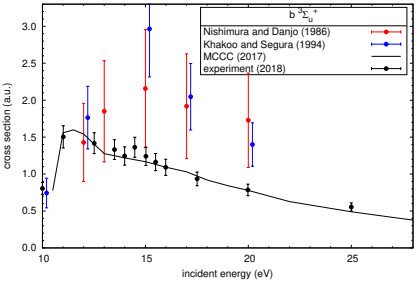

Figure 2: MCCC $b\,^3\Sigma_u^+$ excitation cross sections compared with experiment of Zawadski et al *[Phys. Rev. A (2018), 98(6):062704]*.

Aims

- Aim: develop a simulation of energy deposition in gasses using modern MCCC data.
- Extend the research group's area of work to include simulation, rather than just producing scattering data.
- Produce energy deposition parameters describing ionisation and dissociation for use in astrophysics and plasma modelling.

Simulation Outline

- Specify incident energy of primary electron.
- Randomly sample scattering process using CCC cross sections and structure model, update energy.
- Add secondary electrons to list if ionisation occurs.
- Follow until all electrons fall below cutoff energy.

Current Work - Molecular Dissociation and Ionisation

- Extend to include vibrationally resolved data.
- Aim to calculate number of dissociations and heat released.
- Used a method equivalent to sampling kinetic energy release distributions to model dissociative excitations.

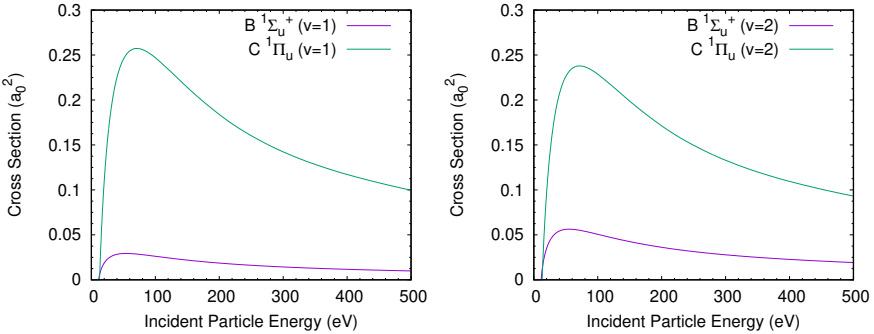

Figure 3: Excitation cross sections for $v = 1$ and $v = 2$ vibrational levels of the $B\,^1\Sigma_u^+$ and $C\,^1\Pi_u$ states of H_2. Taken from *MCCC Database, mccc-db.org*.

Electronic States

- Model includes 21 spectroscopic electronic states, for which the mean number of dissociations can be obtained.
- A larger number of bound pseudostates are used to model the remainder of the spectrum.

Table 1: Bound spectroscopic electronic states of H_2 treated in the MCCC monte carlo model.

$R = 0$ Limit	Electronic State
$n = 1$	$X\,^1\Sigma_g^+$
$n = 2$	$b\,^3\Sigma_u^+$ $a\,^3\Sigma_g^+$ $c\,^3\Pi_u$ $B\,^1\Sigma_u^+$ $EF\,^1\Sigma_g^+$ $C\,^1\Pi_u$
$n = 3$	$e\,^3\Sigma_u^+$ $g\,^3\Sigma_g^+$ $d\,^3\Pi_u$ $Bp\,^1\Sigma_u^+$ $h\,^3\Sigma_g^+$ $K\,^1\Sigma_g^+$ $i\,^3\Pi_g$ $Q\,^1\Pi_g$ $j\,^3\Delta_g$ $J\,^1\Delta_g$ $GK\,^1\Sigma_g^+$ $D\,^1\Pi_u$ $H\,^1\Sigma_g^+$ $I\,^1\Pi_g$

Results - Mean Energy Per Ion Pair

- As a 'litmus test', calculated the mean energy per ion pair, presented in a recent paper *[Horton et al, Plasma Sources Sci. Technol. (2021), 30(11):115004]*
- Compared results with Dalgarno et al *[ApJS (1999), 125(1):237-256]* and ICRU *[Bichsel et al, ICRU Report 31 (1979)]* experiments.
- Excellent agreement using vibrationally averaged data.

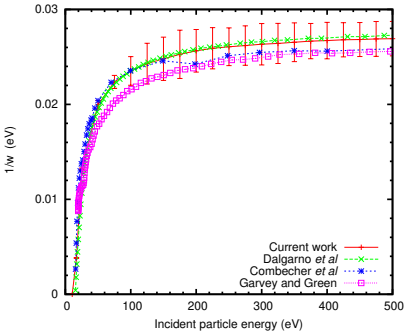

Figure 4: Inverse of the mean energy per ion pair, compared with the work of Dalgarno et al.

Results - Mean Numbers of Excitations

- Obtained results for mean number of excitations of specific electronic states per ion pair.

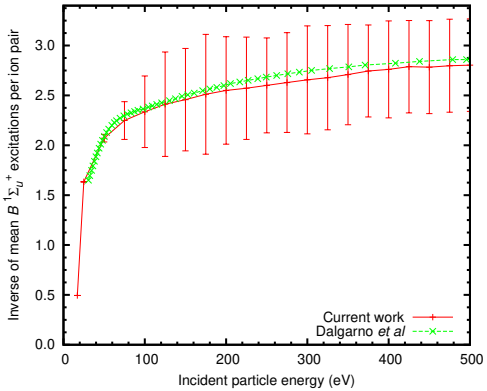

Figure 5: Inverse of the mean number of $B\,^1\Sigma_u^+$ excitations per ion pair, compared with Dalgarno et al.

Results - Mean Numbers of Dissociations

- Ran calculations with increasing numbers of states.
- Obtained expected 'step like' behaviour for $b\,^3\Sigma_u^+$ only model.
- Inclusion of ionisation leads to final two peaks at low energies.

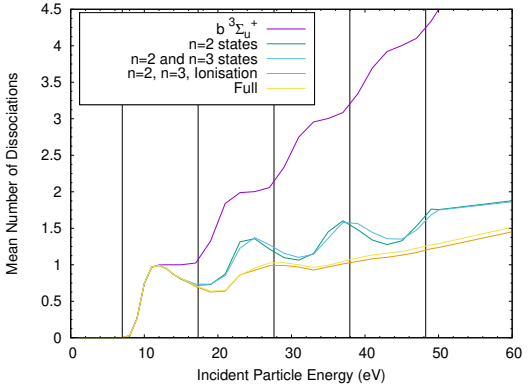

Figure 6: Mean number of dissociations as a function of incident particle energy.

Results - Dissociations of Specific States

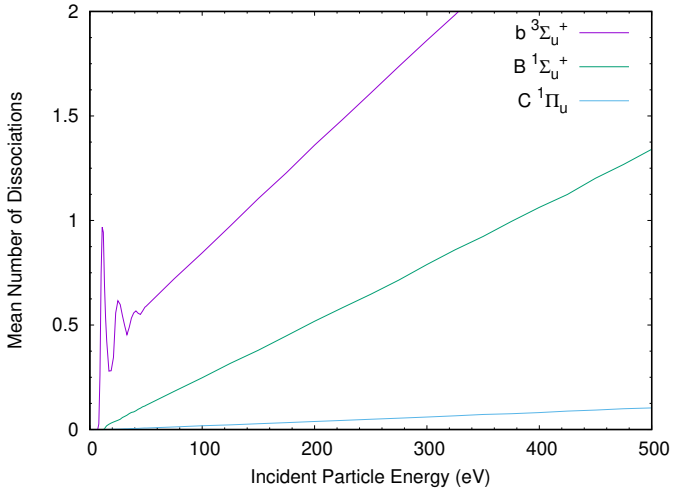

Figure 7: Mean number of dissociations of specific states of H_2.

Conclusions

- Distributions for radiative decay dissociation to be included to allow modelling of gas heating via molecular dissociation.
- Currently working to model external electric field: drift velocity, fluid parameters, etc.
- Currently working to include positron scattering.

Conclusions

- Distributions for radiative decay dissociation to be included to allow modelling of gas heating via molecular dissociation.
- Currently working to model external electric field: drift velocity, fluid parameters, etc.
- Currently working to include positron scattering.

THANK YOU!