

GA-A26127

# **3D-DIVIMP MODELING ANALYSIS OF METHANE INJECTION INTO DIII-D USING THE DIMES POROUS PLUG INJECTOR**

by

**Y.R. MU, A.G. McLEAN, J.D. ELDER, P.C. STANGEBY, B.D. BRAY, N.H. BROOKS,  
J.W. DAVIS, M.E. FENSTERMACHER, M. GROTH, C.J. LASNIER, D.L. RUDAKOV,  
J.G. WATKINS, W.P. WEST, and C.P.C. WONG**

**June 2008**



## **DISCLAIMER**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

# 3D-DIVIMP MODELING ANALYSIS OF METHANE INJECTION INTO DIII-D USING THE DIMES POROUS PLUG INJECTOR

by

Y.R. MU,\* A.G. McLEAN,\* J.D. ELDER,\* P.C. STANGEBY,\* B.D. BRAY, N.H. BROOKS,  
J.W. DAVIS,\* M.E. FENSTERMACHER,† M. GROTH,† C.J. LASNIER,† D.L. RUDAKOV,‡  
J.G. WATKINS,# W.P. WEST, and C.P.C. WONG

This is a preprint of a paper to be presented at the Eighteenth International Conference on Plasma Surface Interactions, May 26-30, 2008, in Toledo, Spain, and to be published in the *J. Nucl. Mater.*

\*University of Toronto Institute for Aerospace Studies, Toronto, Canada.

†Lawrence Livermore National Laboratory, Livermore, California.

‡University of California-San Diego, La Jolla, California.

#Sandia National Laboratories, Albuquerque, New Mexico.

Work supported in part by  
the U.S. Department of Energy  
under DE-FC02-04ER54698, DE-AC52-07NA27344,  
DE-FG02-07ER54917, and DE-AC04-94AL85000

GENERAL ATOMICS ATOMICS PROJECT 30200  
JUNE 2008





## ABSTRACT

A self-contained gas injection system for the Divertor Material Evaluation System (DiMES) on DIII-D, the porous plug injector (PPI), has been employed for *in-situ* study of chemical erosion in the tokamak divertor environment by injection of  $\text{CH}_4$  [A.G. McLean, et al., these proceedings]. A new interpretive code, 3D-DIVIMP-HC, has been developed and applied to the interpretation of the CH, CI, and CII emissions. Particular emphasis is placed on the interpretation of 2D filtered-camera (TV) pictures in CH, CI and CII light taken from a view essentially straight down on the PPI. The code replicates sufficient measurements to conclude that the basic elements of the controlling physics and chemistry have been identified and incorporated in the code-model.



## I. INTRODUCTION

Carbon plasma-facing surfaces in tokamaks are subject to chemical erosion due to hydrocarbon formation. Laboratory measurements of erosion yields cannot be applied with full reliability to tokamaks due to various tokamak-specific mechanisms, such as the prompt redeposition of hydrocarbon fragments. Understanding chemical erosion and molecular breakup in current tokamaks is important for making projections of tritium inventory in ITER due to codeposition. This understanding can be developed by applying models of hydrocarbon breakup and transport to the interpretation of spectroscopic observations of emissions resulting from hydrocarbons entering the plasma. This task was made easier by the development of a gas injection system on DIII-D which can simulate chemical sputtering by introducing a known quantity of hydrocarbon gas.

A Porous graphite Plug gas Injector (PPI) was developed by A.G. McLean and J.W. Davis [1] for use with the Divertor Material Evaluation System (DiMES). The objective is to admit methane (or other hydrocarbon gases) through a porous graphite surface, so that the molecular interaction with the plasma closely approximates a hydrocarbon molecule released from a carbon surface by chemical erosion. Injecting methane at a known rate provides direct calibration of spectroscopic signals from the Multichord Divertor Spectrometer (MDS) and the DiMES TV camera which view DiMES from above. The porous surface is designed such that size and spacing of the holes [ $\sim 1000$  holes, 0.25 mm (0.010 in.) diameter, 0.8 mm (0.032 in.) spacings] is on the order of the mean-free-path of  $\text{CH}_4$  in an attached divertor plasma. The holes comprise  $<10\%$  of the surface area so that the probe closely approximates a solid surface. Flow rate corresponds to 1%-3%  $\text{D} \rightarrow \text{C}$  erosion yield over the holed surface area for typical low density, attached conditions in DIII-D, namely  $\sim 1-7 \times 10^{17}$   $\text{CH}_4$  molecules/s (0.02 torrL/s,  $\sim 2$  sccm). Further details are provided in [2]. A DiMES TV picture of the PPI in CH/CD light, with puff on, is shown in Fig. 1.

The DIVIMP impurity production and transport code is 2D (poloidal/parallel and radial directions) [3]. The interpretation of DiMES impurity experiments requires 3D analysis and 3D-DIVIMP-HC has been developed from DIVIMP, including a hydrocarbon breakup module, and applied to the PPI experiments. 3D-DIVIMP-HC is a Monte Carlo modeling code which launches individual  $\text{CH}_4$  molecules uniformly across the holed-portion of the DiMES surface. The particles are tracked in 3D as they experience the breakup processes tabulated in the Janev-Reiter (JR) [4,5] model/database. The simulation proceeds using a fixed time step which is chosen to be smaller than the characteristic times of any process which the particle experience.

For charged particles (molecular ionic fragments,  $C^+$ , etc), the 3D motion is followed along the field lines allowing for diffusion (with imposed diffusion coefficients) in the radial and poloidal/diamagnetic directions; parallel motion is governed by parallel diffusion, the electric field force, electron and ion temperature gradient forces and friction force due to collisional-coupling with the background (fuel ion) plasma flow. These forces depend on background plasma conditions which are input to the code based on measurements from Langmuir probes and divertor Thomson scattering.

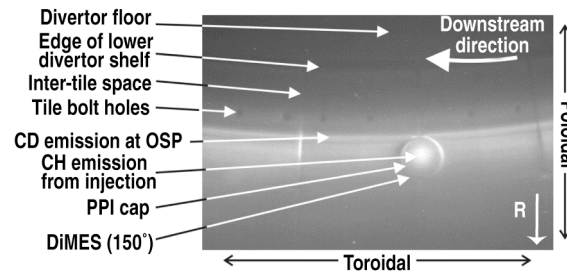


Fig. 1. DiMES TV view of the PPI in CH/CD light showing the light from the puff, at the center of DiMES. The bright arc at the upstream edge of the DiMES head is due to a slight vertical misalignment.

In addition to these general plasma forces there are also near-surface effects that need to be included. 3D-DIVIMP-HC includes a model for the magnetic pre-sheath (MPS) electric field from work by J. Brooks [6]. This electric field can be substantial in the near surface region and can have a significant effect on loss of atomic and molecular ions from the plasma. In addition, 3D-DIVIMP-HC implements a range of surface interaction models for the hydrocarbon fragments. These options range from the ability to have all fragments stick to surfaces or reflect from surfaces. The experimental measurements from Jacob [7] were used here.

To make comparisons with spectroscopic measurements, the 3D spatially distributed emission of the atomic lines and molecular bands of interest are calculated based on the recorded density of each state. Photon emissivity coefficients from ADAS [8] for the atomic emission lines and HYDKIN [9] for the CH 0-0 band are used to calculate the emission from each cell of the modeling grid. The calculations here assumed that particles are in the ground state when excited by electron impact; this is not necessarily the case since molecular breakup can produce excited states; in future analysis this aspect will be further investigated. The total emission, integrated along the required line-of-sight through the modeling grid is calculated and compared to the experimental value. The line-of-sight and viewing cone are chosen to match the experimental diagnostic.



## II. MODELING AND RESULTS

The 3D-DIVIMP-HC code was used to examine the CH, CI and CII emissions measured during the 2007 PPI experiment. This experiment was performed in an attached L-mode plasma with  $T_e = 20$  eV and  $n_e = 1.2 \times 10^{19} \text{ m}^{-3}$  at the PPI location. We report here on (a) the spatial distribution of HC fragments and carbon particles, and (b) the absolute emission intensity of the following spectral measurements: CH 0-0 band, CI 909 nm and CII 427 nm, 514 nm and 658 nm. Data from four separate shots, found to be reproducible within the minimum range of error possible, were used to gather these data.

The CD/CH distribution measured by DiMES TV in shot #129689 is shown in Fig. 2. The edge of the PPI and the emission from the puffed  $\text{CH}_4$  are clearly visible in the middle. In addition, emission coming from the strike point region where the plasma surface interaction is the strongest and at tile edges is clearly visible. There is an observable emission from the upstream edge of DiMES due to a small misalignment of the sample holder. This makes it easy to correctly orient the images for comparison to the modeling results. The 3D-DIVIMP-HC simulation of the CH 430 nm band emission is shown in Fig. 3. This result models only the puffed  $\text{CH}_4$  and so does not reproduce the band of naturally occurring emission corresponding to the strike point position or tile edges. In order to make quantitative comparisons of the toroidal profile through the center of the emission cloud, a toroidal arc (the black band in Fig. 2) composed of 8 pixels in the radial direction in the DiMES TV picture ( $\sim 6$  mm wide) is extracted, averaged and plotted against the 3D-DIVIMP-HC emission for the same region. In addition a background signal measured after the discharge is subtracted from the experimental profile prior to comparison. In Fig. 4, the 3D-DIVIMP-HC result (red) is seen to match the measured profile (black) fairly well.

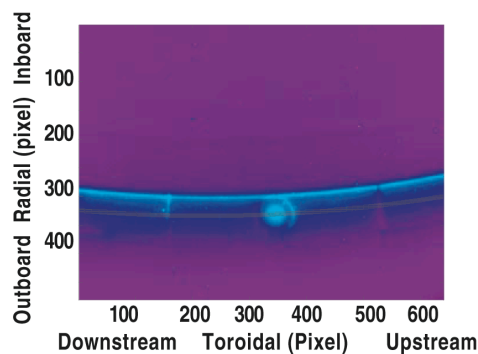


Fig. 2. CD/CH 2D TV picture with the toroidal arc region where the measured and calculated emission is compared (Fig. 4).

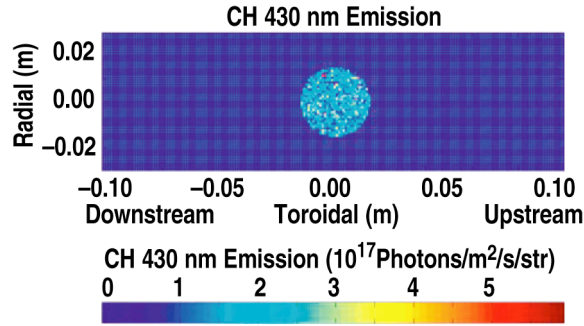


Fig. 3. CH 4300 A band emission 2D simulation from 3D-DIVIMP-HC.

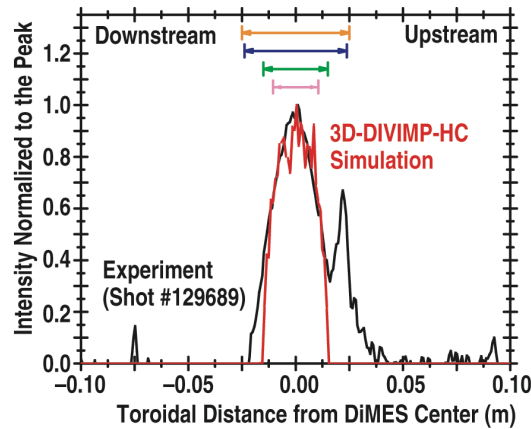


Fig. 4. CH comparison. Experiment: black; code: red. Dashed lines indicate the DiMES hole region (orange), the PPI head region (blue), the PPI holed region (green), and the MDS L5 view region (pink). CD +  $D_{\gamma}$  filter used for shot #129689. The  $\text{CH}_4$  was launched vertically with speed 650 m/s.  $D_{\perp} = 1 \text{ m}^2/\text{s}$ . The same simulation assumptions are used for Figs. 5 and 6.

The CI 909 nm distribution is measured by DiMES TV in shot #129060. The same process was applied to the analysis of this result as the CH measurement. The toroidal profile of this emission (black) is then compared to the 3D-DIVIMP-HC results (red) in Fig. 5. 3D-DIVIMP-HC matches experimental shape fairly well, although it appears to be somewhat narrower than the measured experimental profile. Due to the interaction at the upstream edge it is difficult to determine if the profile is just too narrow or does just not match the downstream tail of the CI profile. The CII distribution is measured by DiMES TV in shot #129691. Toroidal profiles are compared in Fig. 6. The code-calculated profile (red) has a FWHM (full width at half maximum) which matches that of the experimental but its peak is shifted downstream and it exhibits a tail on the downstream side than experiment. There are several variables that affect the length of the tail. These include the efficiency of coupling the  $\text{C}^+$  to the background plasma flow as well as the effect of the MPS E-field and the radial and diamagnetic diffusion coefficients. All

of these will affect the loss rate of carbon particles and the amount of time they have to couple to the background plasma flow. These dependencies are the subject of continuing investigation.

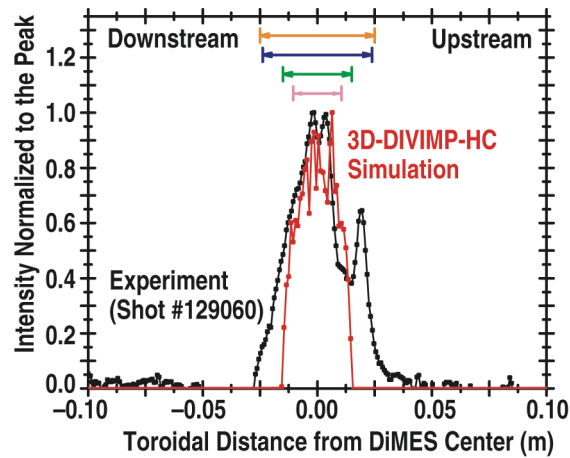


Fig. 5. CI comparison. Experiment: black; code: red. Shot #129060. Other details as Fig 4.

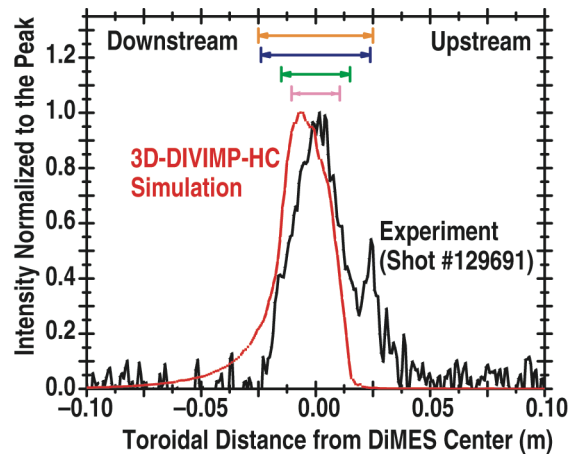


Fig. 6. CII comparison. Experiment: black; code: red. Shot #129691. Other details as Fig. 4.

Absolute emission intensities of CH, CI 909 nm, CII 427 nm 514 nm and 658 nm were measured using MDS which views a 2.1 cm diameter circle centered on the DiMES sample. The particle source on DiMES is 3cm across. As a result, the MDS views only regions which are the source of the puff. MDS background subtraction used the emission measured simultaneously on another MDS chord viewing at the same radial location but displaced toroidally. Comparisons with the code are shown in Table I. The absolute magnitudes agree to within a factor of two for CH, CI and CII-658 nm emissions. The CII-427 nm emission modeling give results significantly below the experimental values. The possibility that the CII-427 nm line is due to excited  $C^+$

created by the CH<sub>4</sub> breakup is being investigated. The background plasma conditions used in the simulations are spatial averages of the Langmuir probe and divertor Thomson scattering measurements; however, ionization rates and photon efficiencies are fairly sensitive to the local plasma density and temperature. Thus, relatively small changes in the plasma conditions might have a significant effect on the absolute emissions as well as the ratios between the lines. This effect is also currently being investigated.

**Table I. Comparison of Measured (MDS) and Code-Calculated Absolute Emissivities**

	<b>CH 4270-4315 nm</b>	<b>CI 9100 nm</b>	<b>CII 4267 nm</b>	<b>CII 5140 nm</b>	<b>CII 6580 nm</b>
MDS L5 ( $\times 10^{14}$ photons/cm <sup>2</sup> /s/sr)	1.64–2.56	1.1	1.3–2.2	2.6	1.4
DIVIMP-HC ( $\times 10^{14}$ photons/cm <sup>2</sup> /s/sr)	0.94	0.87	0.22	0.77	1.5

### III. CONCLUSION

The Janev-Reiter methane breakup model/database, combined with the neutral and ionic transport modeling in the 3D-DIVIMP-HC code, successfully replicates a number of the major features of measurements made using the porous plug injection of  $\text{CH}_4$  into an attached divertor plasma in DIII-D. It is therefore concluded that the most basic elements of the controlling physics and chemistry have been identified and incorporated in the code-modeling. A number of significant discrepancies between experiment and code-modeling have been identified and resolution of these differences is the focus of continuing code analysis.



## REFERENCES

- [1] A.G. McLean, *et al.*, J. Nucl. Mater. **363-365** (2007) 86.
- [2] A.G. McLean, *et al.*, these proceedings.
- [3] P.C. Stangeby and J.D. Elder, J. Nucl. Mater. **196-198** (1992) 258.
- [4] R.K. Janev and D. Reiter, Phys. Plasmas **9** (2002) 4071.
- [5] R.K. Janev and D. Reiter, J. Nucl. Mater. **313-316** (2003) 1202.
- [6] J. Brooks, Phys. Fluids **B 2** (1990) 1858
- [7] W. Jacob, J. Nucl. Mater. **337-339** (2005) 839-846.
- [8] H.P. Summers, The ADAS User Manual, Version 2.6 (2004), <http://adas.phys.strath.ac.uk>.
- [9] D. Reiter, [www.eirene.de/eigen/](http://www.eirene.de/eigen/)





## **ACKNOWLEDGMENT**

This work was supported in part by the US Department of Energy under DE-FC02-04ER54698, DE-AC52-07NA27344, DE-FG02-07ER54917, and DE-AC04-94AL85000. The authors would like to acknowledge the DIII-D Team for their continued efforts in assisting our experiments and providing long time support, in particular, the DIII-D DiMES Group, including D.L. Rudakov, N.H. Brooks, C.P.C. Wong, and W.P. West. Support by the Natural Sciences and Engineering Research Council of Canada is acknowledged.