

# **"Plasma Edge and Plasma/ Material Interaction Modeling Group Progress/Overview"**

J. N. Brooks  
Argonne National Laboratory  
Argonne IL, USA

ALPS/APEX Meeting  
Scottsdale AZ, Nov. 7, 2001

# Plasma Edge and Plasma/Material Interaction Modeling Group

## **Purpose**

**Undertake model integration and studies of the plasma edge and plasma/material interactions (PMI) that lead to:**

- 1) fundamental understanding of the influences of plasma facing surfaces on fusion plasma performance**
- 2) identifying performance limits and optimization strategies for advanced liquid and solid, first wall and PFC concepts.**

## **Near Term Goal**

**Support the ALPS and APEX programs to help determine the feasibility of and optimization strategies for advanced first wall and PFC concepts.**

## **Group Members**

J. Brooks (ANL) – Chairman  
T. Evans (GA)  
A. Hassanein (ANL)  
L. Owen (ORNL)  
M. Rensink (LLNL)  
T. Rognlien (LLNL)  
D. Ruzic (UIUC)  
C. Skinner (PPPL)  
D. Stotler (PPPL)  
R. Maingi (ORNL)  
D. Whyte (UCSD)  
C. Wong (GA)

## Current Tasks

**Task 1. Support NSTX and CMOD liquid surface module proposals via analysis of scrape off layer (sol) plasma with hydrogen-absorbing surface, lithium sputtering and transport, hydrogen, helium recycling characteristics, and related issues. (LLNL, ANL, GA, ORNL, UCSD, UIUC)**

**Task 2: Conduct plasma fluid code analysis (UEDGE code) of tokamak fusion reactor and FRC reactor sol with liquid wall (APEX designs). Estimate maximum permissible wall-temperature/wall-impurity-flux based on global plasma core plasma impurity limits and sol radiation limits. For tin, tin-lithium (tokamak), lithium etc. (FRC). (LLNL)**

**Task 3: Conduct plasma fluid code analysis (UEDGE code) of tokamak fusion reactor scrape off layer (SOL) with liquid divertor. (ALPS-ARIES design). Obtain initial hydrogen edge plasmas and later couple to the divertor impurity source from Task 3. Using combined UEDGE/REDEP analysis estimate sputtered impurity concentration in SOL. For lithium, tin (gallium). (LLNL, ANL)**

**Task 4: Conduct erosion/redeposition analysis (REDEP code package) of liquid surface fusion reactor divertor (ALPS-ARIES design). Via coordination with Task 2 analysis, estimate maximum allowable near-surface plasma temperature based on self-sputtering limits. Estimate core plasma contamination from sputtering. Use ALPS/APEX developed data and code estimates of sputtering yields. For lithium, tin, gallium. (ANL, LLNL, UIUC, SNL,GA)**

**Task 5. Support CDX-U (lithium) and DIII-D/DiMES (lithium, tin, etc.) experiments:**

- a) Conduct b2.5 and/or UEDGE analysis of DiMES background/SOL plasma parameters (ORNL, LLNL, GA).
- b) Estimate—to the extent possible from data and parametric modeling—near-surface plasma parameters for CDX-U (PPPL, ORNL, UCSD)
- c) Using above plasma parameter estimates (and DIII-D near-surface data) conduct REDEP and related code analysis of impurity sputtering and transport in DIII-D and CDX-U (ANL, UIUC, GA)
- d) Compare code predictions to data, and benchmark codes. (all)

**Task 6. Model particle fluxes (D-T, He) to and entrainment in liquid surfaces. Compare predictions with available test data. (ANL, LLNL, UCSD, SNL)**

**Task 7. Model the effects of ELMs on loss of material from liquid surfaces. Compare predictions with available test data. (ANL, GA, UCSD, SNL)**

**Task 8. Compute evaporation-limited surface temperature limits for divertor liquid surfaces based on BPHI-3D sheath kinetic code analysis. For lithium, tin, gallium (ANL)**

**Task 9. Coordinate and provide up-date on atomic physics data/models. (GA)**

# Plasma heat fluxes and impurity intrusion to the core plasma

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T.D. Rognlien and M.E. Rensink, LLNL

**Analysis of wall evaporation for Sn in ARIES (CLiFF) shows temperature limit increases with more detailed geometry and evaporation profiles -- 1100 K max.**

**Modeling of possible liquid modules for NSTX and C-MOD shows that substantial particle pumping could result without excessive heat loads**

**Simulation of lithium large-scale lithium influx for the disruptive DiMES shot on DIII-D shows lithium radiation can be much larger than the coronal equilibrium values**

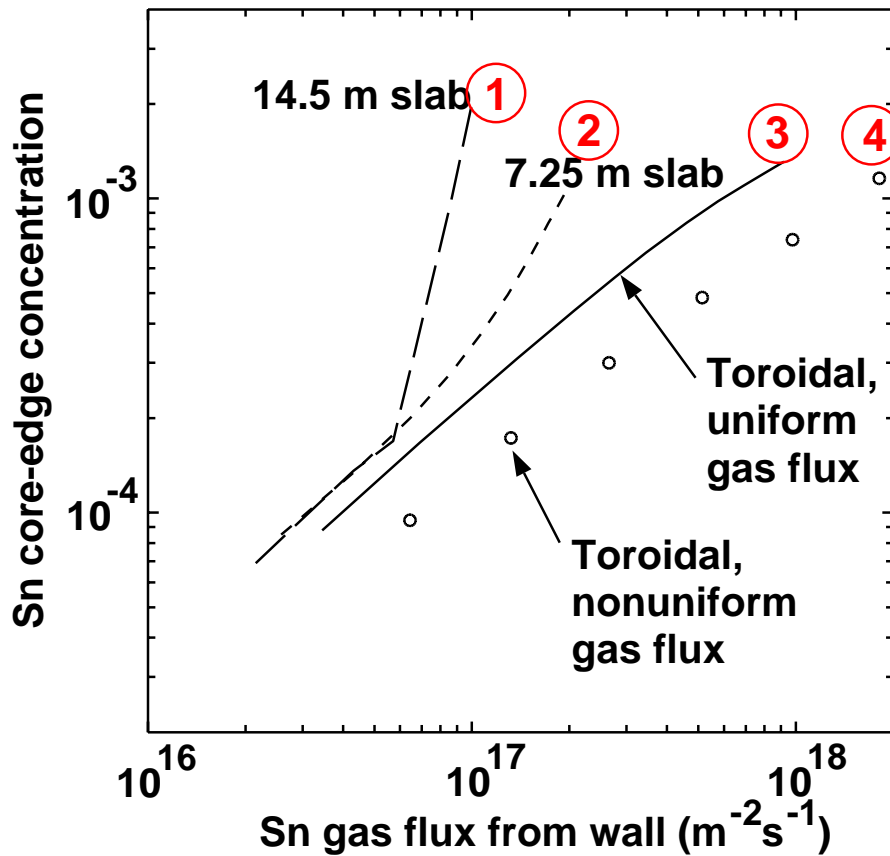
**Studies of divertor plate orientation for liquid wall / divertor integration shows ~50% heat flux reduction by moderate tilting (~50 deg), and that flux compression via divertor-leg length can be balanced by tilting**

**Scaling studies help clarify roles of high/low recycling, anomalous transport, core power density, and magnetic geometry**

# Sn tokamak impurity-based wall-temperature limits show substantial model sensitivity



## Core Sn concentration for 4 case



## Corresponding wall temperature limits

Case	1	2	3	4
$T_w$ [K]	1010	1030	1070	1100

# “Erosion/redeposition modeling for ALPS, ALIST, Misc.”

J.N. Brooks  
Argonne National Laboratory

- **Liquid tin divertor for ARIES-AT**

REDEP/WBC code sputtering erosion analysis using UEDGE (Ronglien, Rensink) high-recycle plasma parameters, TRIM-SP (Bastasz), VFTRIM (Ruzic, Allain) sputtering yields. Very low plasma contamination predicted.

- **Tin and gallium divertors for ARIES-AT**

Surface temperature limit analysis based on evaporation and superheat sheath theory. High limits appear possible ( $T_s \sim 1500$  °C)

- **Lithium module for NSTX and CMOD**

WBC code analysis using UEDGE plasma parameters. Plasma contamination negligible for CMOD, possible concern for NSTX.

- **DIH-D**

DiMES Li 99 solid-phase experiment analyzed via WBC code, IAX/VFTRIM sputter yields. Good match with data. Integrated SOL analysis underway via coupling to MCI. (with D. Whyte, T. Evans, D. Ruzic, et al.).

- **DIID-D**

DiMES neon-detached plasma carbon experiment being analyzed. (with D. Whyte et al.)

- **JET**

MK-II carbon divertor erosion, tritium codeposition in inner louver region being analyzed with rigorous coupling of impurity transport codes (REDEP/CARJET, ERO), carbon molecular dynamics (MolDyn), and carbon recombination (ADAS etc.). ITER FEAT implications. (with A. Kirschner, D. Alman, D. Ruzic, D. Whyte).

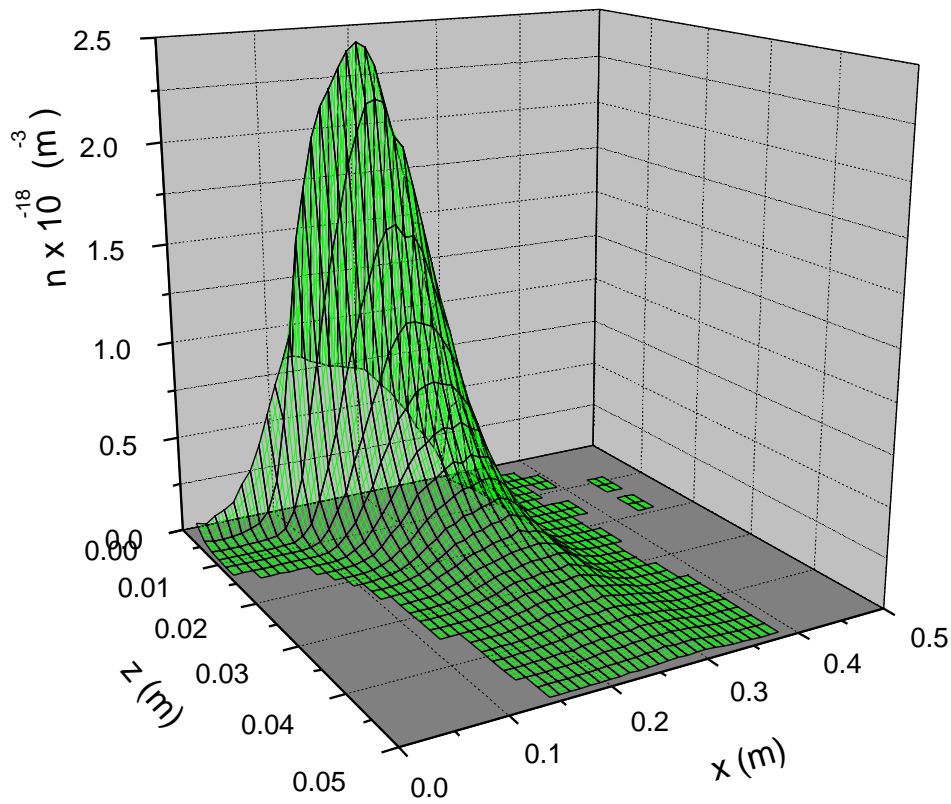
- **FIRE**

Integrated beryllium/tungsten sputtering, transport, surface mixing, tritium codeposition analysis underway. Using UEDGE plasma solution (Ronglien et al.), DEGAS CX analysis, WBC+ SOL transport, VFTRIM mixing model, WBC divertor erosion. (with D. Ruzic, M. Nieto, et al.)



## WBC Monte Carlo code analysis of liquid tin divertor for ARIES-AT

Sputtered tin ion density in the near-surface region.



(Divertor surface at  $z = 0$  along poloidal direction “x”). Analysis uses UEDGE near-surface, high-recycle plasma conditions (T. Ronglien et al.) for ARIES-AT tokamak design. Sputtering coefficients from VFTRIM (self-sputt., Ruzic et al.), TRIMSP (D-T sputtering, Bastasz).  $10^6$  particle histories.

- **Low plasma contamination: Peak Sn density is  $\sim 2.5 \times 10^{18} \text{ m}^{-3}$ . (Peak D-T density  $\sim 2.5 \times 10^{21} \text{ m}^{-3}$ )**
- **Sn density falls to  $\sim 0$  within 5 cm of the plate**

## Liquid tin and gallium divertor surface temperature limits

- **Surface temperature limit as set by evaporation.** (Limit, if any, due to enhanced *sputtering and/or “sputter-evaporation”* at high temperature not evaluated).
- **Rough estimate** based on BPHI-3D Sheath Superheat Analysis studies and extrapolation from flowing lithium system [1,2], and using UEDGE plasma parameters from ARIES-AT tilted divertor plate study [3].
- Roughly tolerable ratio of evaporated atom flux from surface, to D-T ion flux to surface,  $G = 1$ , for  $\sim 1$  cm overheated dimension. This defines a *rough estimate* of tolerable maximum surface temperature,  $T_s$ , *for these plasma conditions.*

$$T_s = \left\{ \begin{array}{l} 1630^\circ\text{C, Sn} \\ 1480^\circ\text{C, Ga} \end{array} \right\}$$

- [1] J.N. Brooks, D. Naujoks Physics of Plasmas 7(2000)2565.  
[2] D. Naujoks, J.N. Brooks, Journal of Nuclear Materials 290-293(2001)1123  
[3] T.D. Rognlien, M. Rensink, “Edge-plasma models and characteristics for magnetic fusion energy devices”, Fusion Engineering Design, to be published.

**Plasma-Liquid Interactions: Status and  
Future Modeling Efforts**

**Ahmed Hassanein**

**Argonne National Laboratory**

**Presented at the ALPS/APEX Meeting  
Scottsdale, AZ, November 5-8, 2001**

# Status of Plasma-Liquid Interactions

## I. Effects of Plasma Instabilities

### VDEs:

- Similar energy density about 50-100 MJ/m<sup>2</sup>
- Deposition time is very long 100-300 ms.
- Related physics:
  - Little or no vapor shielding
  - Strong erosion
  - Structural effects
- For reactor conditions VDEs can be very serious surface erosion mechanism of coating materials. But may be in situ repair is possible.
- However, structural damage due to the long deposition can be a limiting factor in tolerating VDEs. Even one VDE will have serious implications on the structural integrity! Liquid surfaces are excellent SOLUTION!

# Status of Plasma-Liquid Interactions

## I. Effects of Plasma Instabilities

### ELMs:

- Much lower energy density about 1-2 MJ/m<sup>2</sup>
- Deposition time is about 1 ms.
- Complicated physics:
  - Lower density vapor cloud
  - Higher cloud temperature
  - Mixing effects of vapor and plasma
  - Higher velocity of vapor expansion
- For reactor conditions ELMS can be very serious and need to be studied in detail.
- Disruptions in current Tokamak machines (DiMES) may simulate ELMs in future large Tokamaks. Joint work on DIII-D disruptions may be relevant to simulate reactor ELMs!

# Sputtering of Liquid Metals

- Previous data (Russian) on He & D-T sputtering of liquid metals (Ga) clearly demonstrated that enhanced sputtering is due to gas-bubble formation/explosion.
- Enhanced sputtering erosion of liquids in US facilities (PISCES + UIUC) may indicate formation of bubbles and splashing! This makes the most sense.
- Need more data on He & D-T sputtering of Liquids ← work done in PISCES & UIUC is important. However, TIME DEPENDENT data is needed!
- Macroscopic sputtering due to bubbles bursting & Splashing ← can be very serious issue of using liquid metals. Need to study macroscopic particles in SOL.

# Helium Pumping by Liquid Metals

- **Need He diffusion coefficient  $\ll 10^{-4}$  cm<sup>2</sup>/s for reasonable liquid velocities  $\approx 10$ -50 m/s. More diffusion data is needed.**
- **Helium self-pumping can only be enhanced due to bubble formation and trapping. NO Enhancement expected due to internal flows.**
- **However, He bubble bursting/explosion before removal will likely to de-trap He!**
- **D-T are completely pumped by flowing lithium!**
- **Need to study synergistic effects in moving liquids?**

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# Measurements and Modeling of Liquid Metal Sputtering in IIAX at UIUC

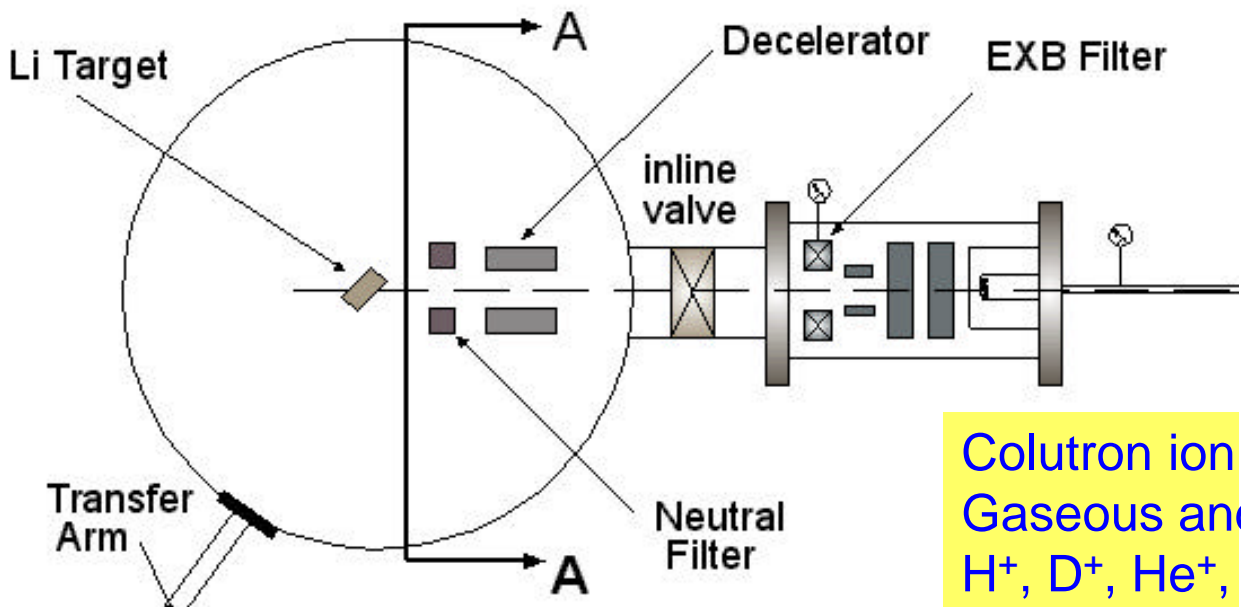
J.P. Allain and D.N. Ruzic

*University of Illinois, Urbana-Champaign  
Department of Nuclear, Plasma and Radiological  
Engineering*

ALPS Annual Meeting  
November 5-7, 2001

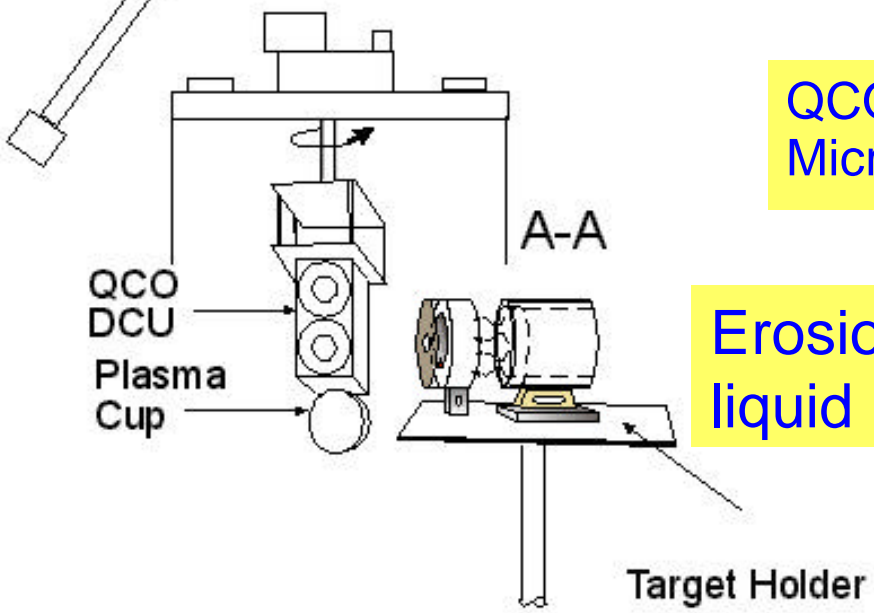
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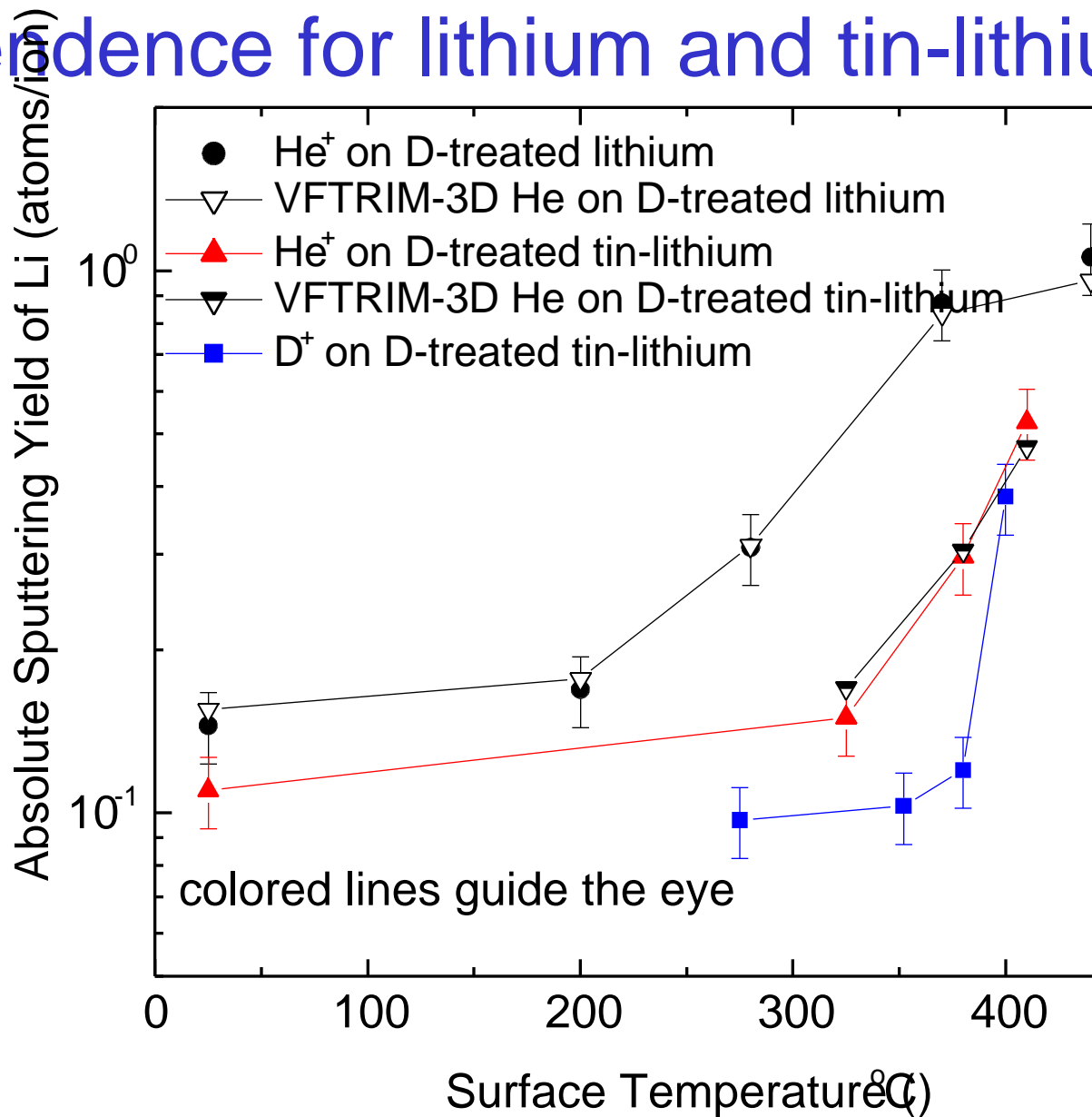
Colutron ion source for both  
 Gaseous and metal species  
 $H^+$ ,  $D^+$ ,  $He^+$ , and  $Li^+$

QCO (Quartz crystal oscillator  
 Microbalance dual unit,  $\pm 0.1 \text{ \AA}$ )

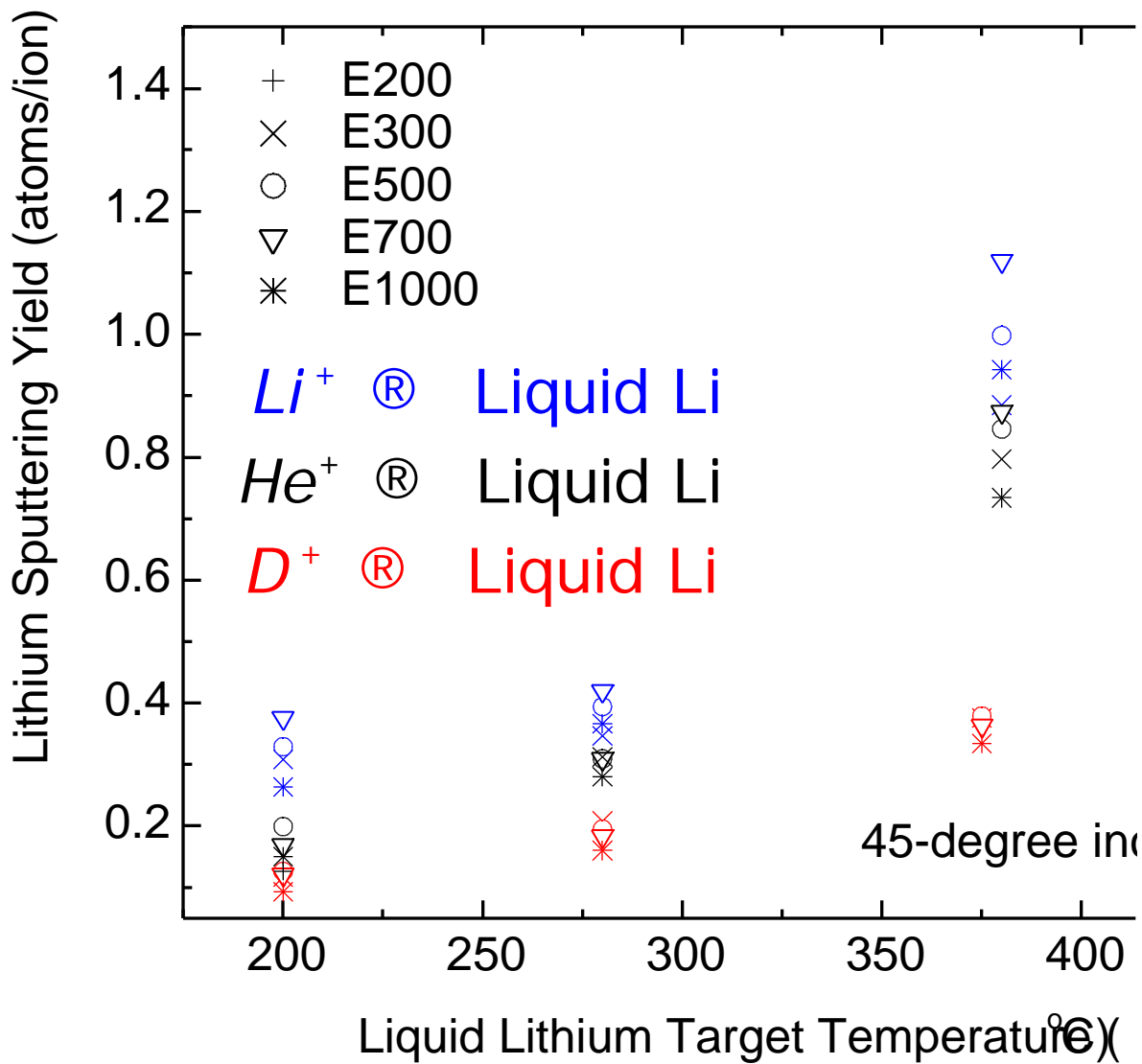


Erosion measurements on stable  
 liquid metals

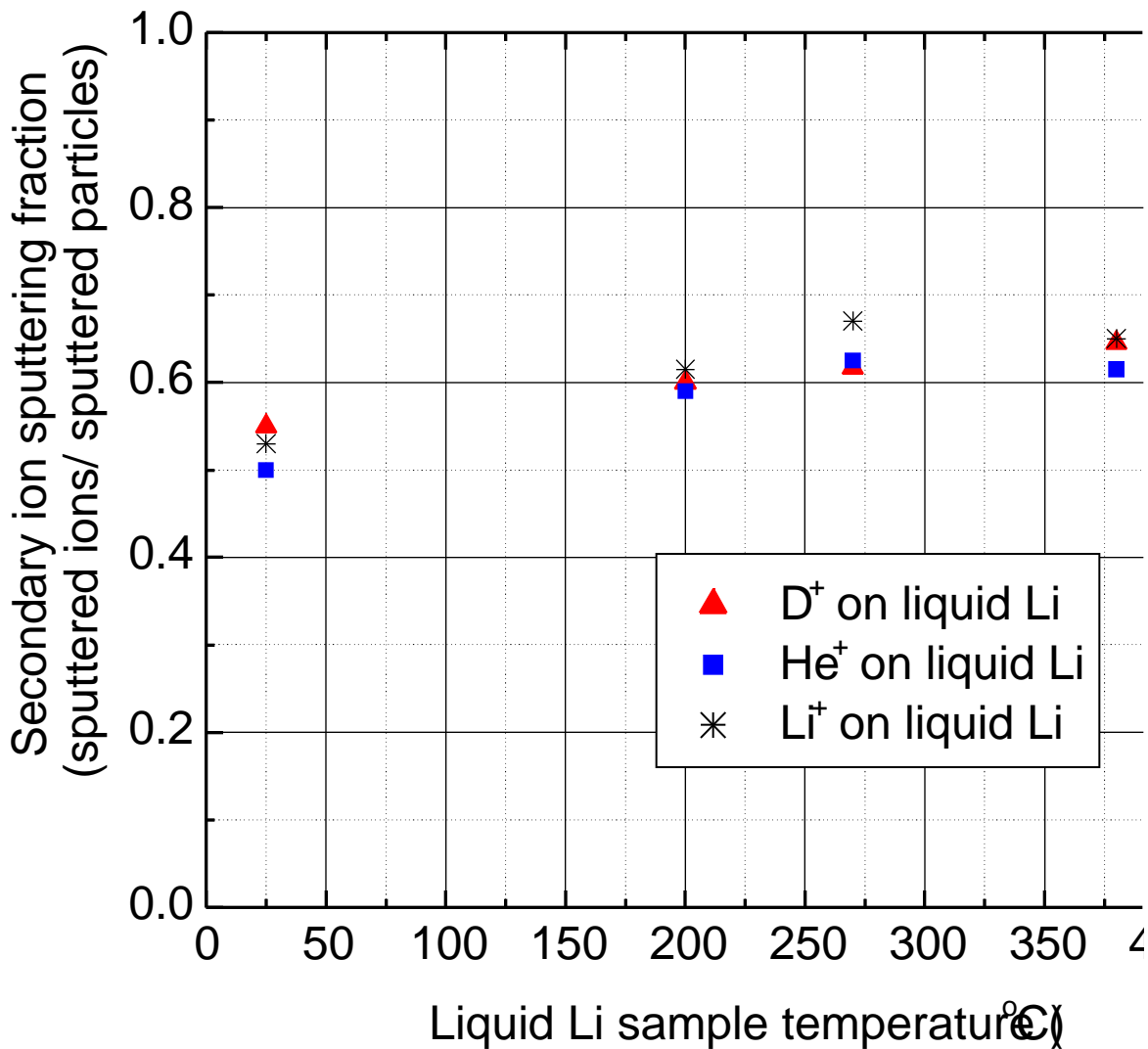
# Lithium sputtering yield temperature dependence for lithium and tin-lithium targets



# IIAX temperature-dependent yields for various incident particle energies



# Secondary ion sputtering fraction ( $Y_{sp}^+$ ) dependence on target temperature for Liquid Lithium



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## Baseline Experiments with solid Li in tray nearing completion in CDX-U

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- Baseline after Argon glow discharge cleaning:  
 $I_p \leq 70 \text{ kA}$ ,  $n_e \leq 10^{19} \text{ m}^{-3}$
- Fast camera images with Li-I filter show strong emission from tray, including "hot spots" and "droplets"
  - ➡ Maybe some melting occurring?
  - ➡ Initiating a plan to determine surface composition
- $D_\alpha$  emission goes down during discharge
- Oxygen and carbon levels appear to be much lower later in the week
  - ➡ Li effect or wall condition improvement?
- Will do molten Li comparison by APS

# Lithium modeling in quiescent and disruptive DIII-D plasmas

T. E. Evans, GA with input from: D. Whyte UCSD, R. Maingi ORNL, L. Owen ORNL, J. Brooks ANL, C. Wong GA and P. West GA

## Objectives

- Validate physics models used to calculate the release of solid or liquid Li and its transport through the divertor, SOL, and pedestal plasma into the core.
- Understand mechanisms leading to massive Li injection events and the effects of Li on MHD stability of the core.
- Identify innovative new approaches to prevent Li or other liquid materials from disrupting the plasma or degrading the core plasma performance.

## Approach

- Analyze DIII-D experimental data and compare to modeling results.
- Use kinetic sputtering (WBC) and transport (MCI) models running in fluid background plasmas (UEDGE and b2.5) to interpret experimental results, assess reactor scalability and identify plausible operating scenarios.

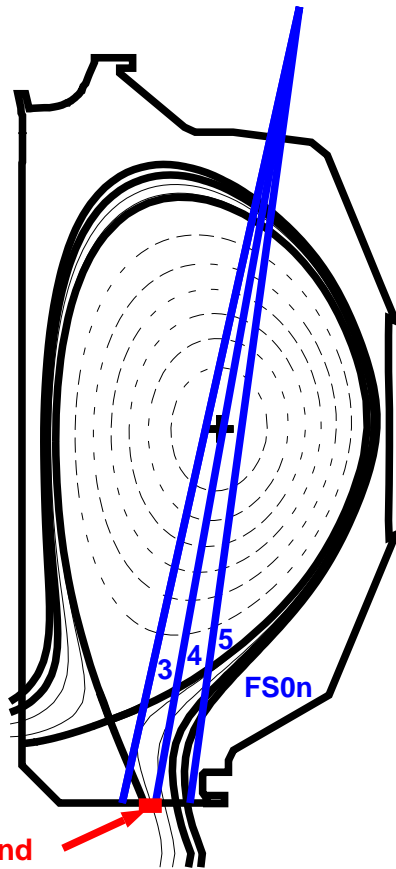
## Status

- Li induced disruption data analyzed and results reported. MHD modeling of plasma-liquid interface underway (UCLA).
- Background solution (ORNL) and sputtering simulation results (ANL) are being integrated into the MCI code. Initial Li kinetic transport runs in quiescent plasma are in progress.

# A liquid Li droplet disrupted DIII-D when it was ejected from the DiMES probe

## DIII-D shot 105511

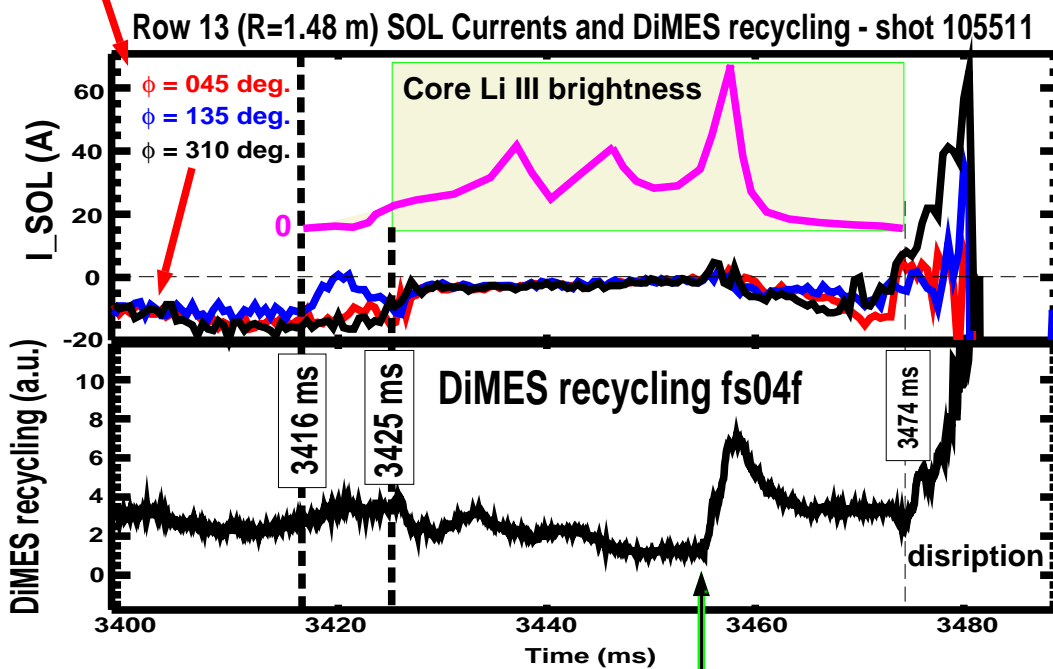
time	3425.00
chi**2	22.731
Rout(m)	1.706
a(m)	0.567
elong	1.678
V (m**3)	16.409
A (m**2)	1.579
q1	8.085
q95	3.769
dsep(m)	0.081
BT(0)(T)	-2.005
gapin(m)	0.123
gapout(m)	0.081
dRsep	-0.400



- As the Li sample in the DiMES probe melted part of it was ejected into the core plasma.
- The Li radiation in the core caused a change in  $j(r)$  and initiated a locked mode.
- The locked mode triggered a VDE type disruption, which removed the remaining Li.

The figure below shows the sequence of events leading to the disruption. The Li melts ( $t < 3416$  ms), JXB force ejects Li droplet ( $t = 3425$  ms), Li III core radiation increases, locked mode ( $t = 3455$  ms) followed by the disruption ( $t = 3474$  ms).

DiMES Probe and row 13 TCA monitors



# Progress on lithium sputtering and transport modeling in quiescent DIII-D plasmas

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## Progress to date

- A fluid background plasma solution was completed by L. Owen (ORNL) for DIII-D shot 105508 and is available for MCI runs.
- A complete set of metastable state resolved Li ionization data was created using the ADAS collisional radiative model and has been imported into MCI for the transport simulations.
- WBC data with the 3D position/velocity and the charge state of 654 Li particles that escaped the DiMES sample into a 5 cm region above the probe, from J. Brooks (ANL), is being used in MCI to specify the initial conditions for the transport runs.
- Initial MCI simulations of shot 150508 with the outer strike point on the center of the Li DiMES sample are in progress using the data and results from the fluid code, ADAS and WBC.

## Future plans

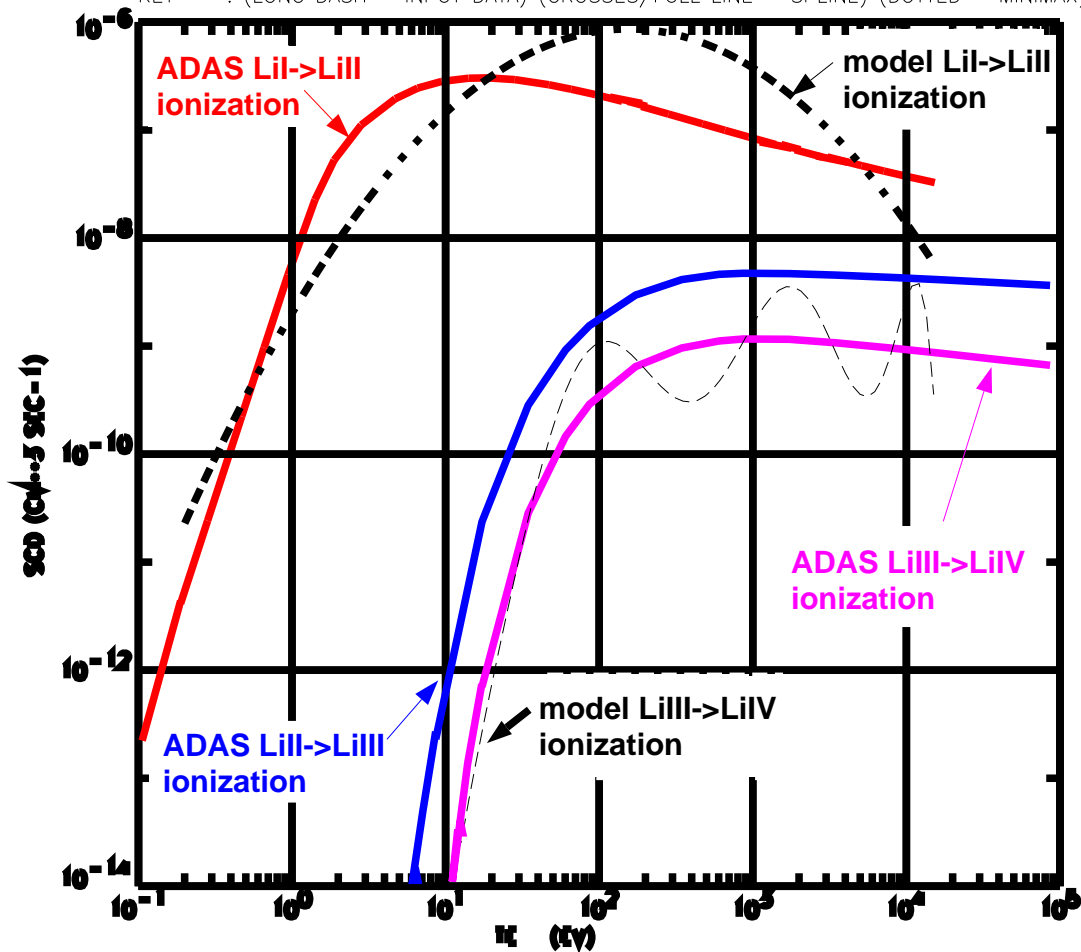
- A dedicated Li sputtering and transport experimental day was proposed for DIII-D (FY 2002) to obtain density and power scaling data that can be used to further validate the kinetic sputtering and transport models.



# High quality lithium ionization data, created with the ADAS collisional radiative model, is being used for ALPS modeling

COLLISIONAL-DIELECTRONIC COEFF. VS TEMPERATURE:

ADAS : ADAS RELEASE: ADAS98 V2.4 PROGRAM: ADAS402 V1.4 DATE: 07/06/00 TIME: 11:18  
 TITLE : LITHIUM IONIZATION RATE (96SCD DENSITY : 1.00e+13  
 FILE : /u/evans/adas/adf11/scd96/scd96\_li.dat  
 MINIMAX : LOGFIT - DEGREE= 2 ACCURACY=452.67% END GRADIENT: LOWER= 3.17 UPPER= -2.18  
 KEY : (LONG DASH - INPUT DATA) (CROSSES/FULL LINE - SPLINE) (DOTTED - MINIMAX)



- Li ionization and recombination rates were added to ADAS by M. O'Mullane and T. Evans specifically for ALPS modeling.
- This new ADAS Li data is being used for ALPS modeling and experimental analysis.
- Results using this data will be discussed during an IAEA Atomic Data Coordinating Meeting in Vienna on Nov. 12-13 by T. Evans.

# DEGAS 2 Status & Plans

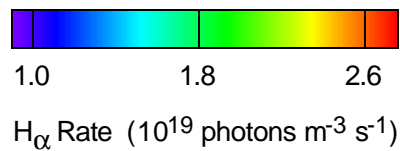
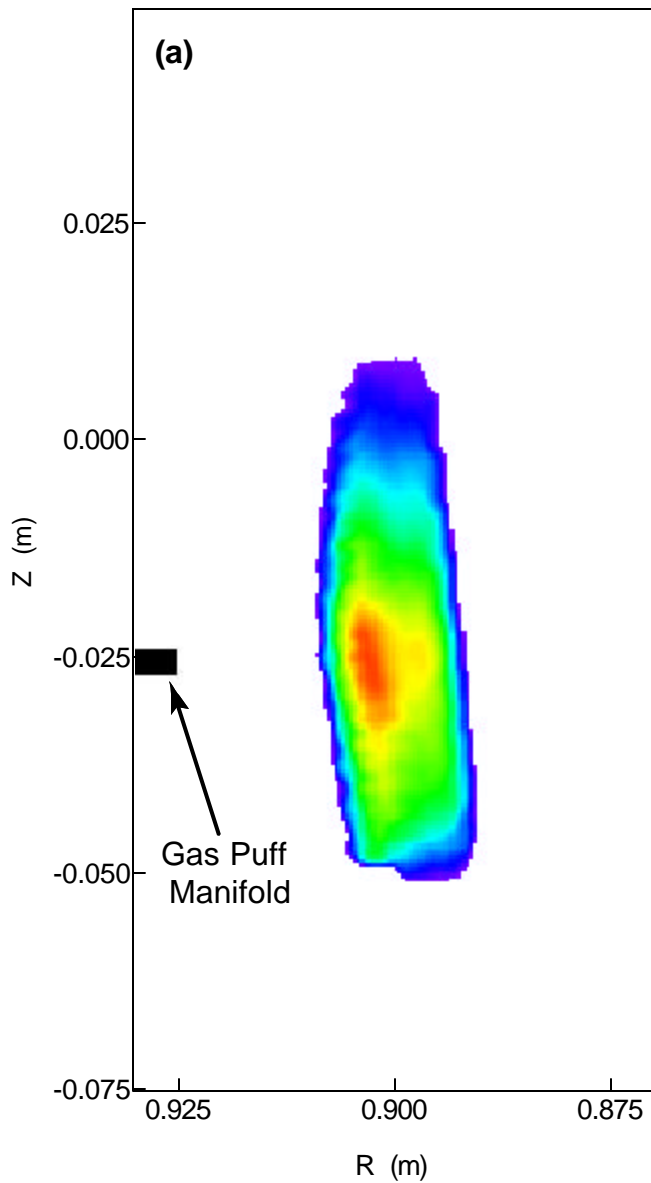
*Daren Stotler, PPPL*

## CURRENT ACTIVITIES

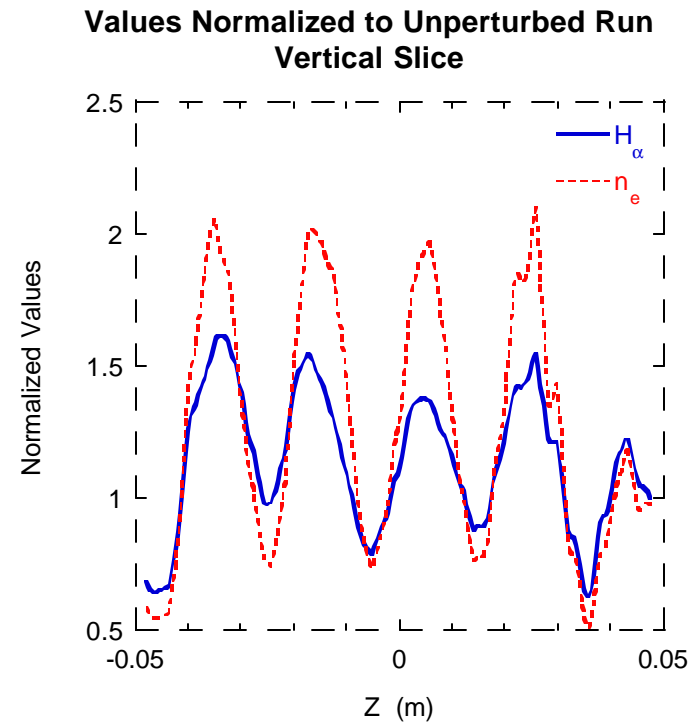
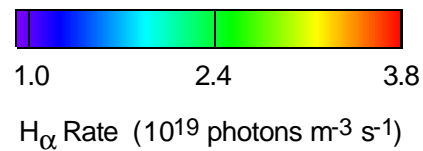
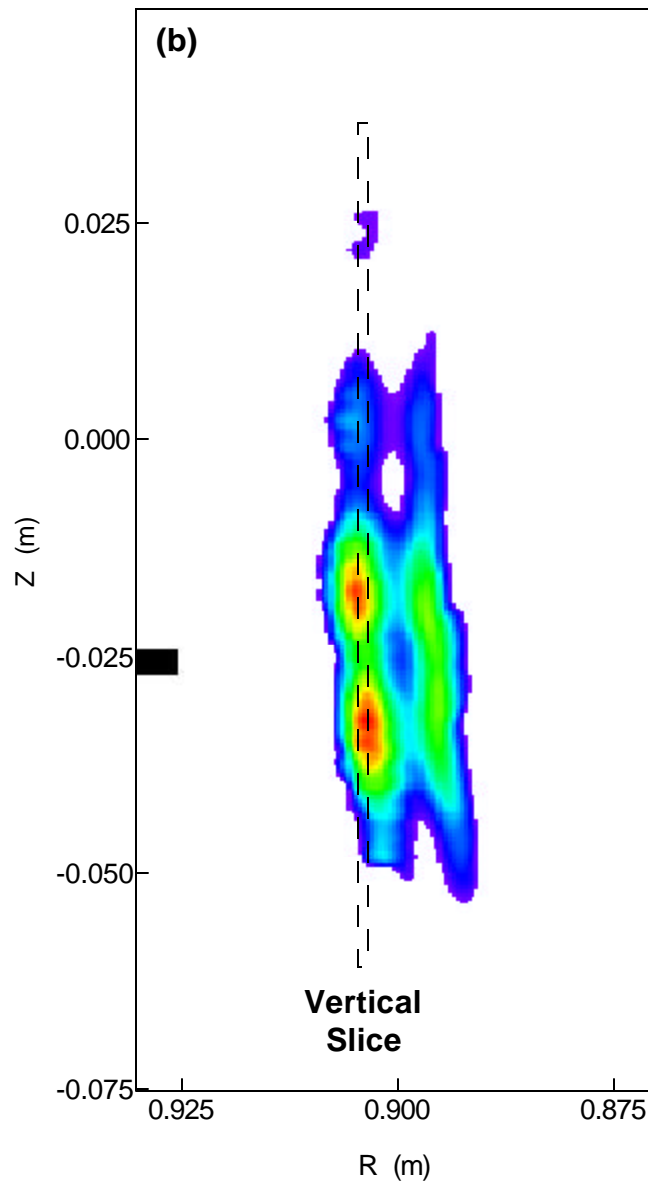
- Neutral Transport Modeling of Gas Puff Imaging (GPI) Experiments,
  - Experiments on NSTX & Alcator C-Mod (Zweben & Maqueda),
    - \* View light emitted by gas puff near outer midplane,
    - \* Infer nature of plasma fluctuations from visible emissions.
    - \* Use DEGAS 2 to understand relationship between the two.
  - Radial  $n, T$  profiles taken from probe data.
  - Axisymmetric simulation for now.
  - Figure (a) shows poloidal plot of  $D_\alpha$  emission with measured plasma,
  - For Fig. (b), apply 2-D perturbation to plasma density.
  - Figure (c) shows correspondence between density &  $D_\alpha$  modulations in a vertical slice through data.

# DEGAS 2 Simulations of Gas Puff Imaging Experiments

## Unperturbed Plasma



## 2-D Plasma Perturbation Imposed



## OTHER RECENT WORK

- Axisymmetric Simulations of National Compact Stellarator Design
  - Evaluate neutral penetration in narrowest poloidal cross section,
    - \* Too much could lead to beam ion loss or poor plasma transport.
  - Use assumed plasma parameters,
  - Compared simple divertor and limiter configurations.
  - Results presented at NCSX Physics Validation Review (3/2001),
    - \* <http://www.pppl.gov/ncsx/pvr/pvr.HTML>
  - Neutral penetration remains a design concern.
- Simulations of Magnetic Reconnection Experiment (MRX)
  - Need estimate of neutral density in reconnection zone,
  - Initial steady-state simulations carried out.
  - Will need to include time-dependence.

## FUTURE PLANS

- **Begin Using DEGAS 2's 3-D Capability**
  - Add toroidal resolution to gas puff imaging simulations,
    - \* Permit quantitative comparison of emission rates,
    - \* Allow direct simulation of camera view.
  - Simulation of discrete limiter structures,
    - \* E.g., to study main chamber recycling problem in C-Mod.
  - Analysis of toroidally resolved neutral pressure data,
    - \* NSTX installing large number of neutral pressure gauges.
  - Simple 3-D geometries
    - \* Plasma processing devices,
    - \* Gas injector used for NSTX Coaxial Helicity Injection (Raman),
    - \* Gas transport in ICF beam lines.
  - Complex 3-D geometries
    - \* E.g., NCSX.

## Modeling of JET erosion/redeposition & tritium retention

J.N. Brooks (ANL), A. Kirschner (KFA/Julich), D.G. Whyte (UCSD), D.N. Ruzic (UIUC), D. Alman (UIUC)

- Key issue: Carbon divertor chemical sputtering and tritium codeposition for low-temperature plasmas. Explain high tritium codeposition in JET. Do JET results extrapolate to DIII-D, future devices?

We are using a major model upgrade with:

- Wall and outer divertor sputtered carbon ions entering inner divertor region, and recombining to carbon atoms, including highly enhanced rates over “classical”.
- Carbon/hydrocarbon sticking/reflection coefficients at hydrogen-saturated carbon surfaces, from MolDyn molecular dynamics code.
- ERO code calculations of wall and adjacent-tile carbon erosion, transport to inner divertor region.
- REDEP/CARJET Monte Carlo code calculations of carbon transport in inner MK-2 JET divertor region.

WATER EROSION CALCULATIONS

258 26

P13 P

P8

2383

P9

247.1

P12

P11

PLANT BOUNDARY

P10

LAUNCH UNDERWAY

TILE #4

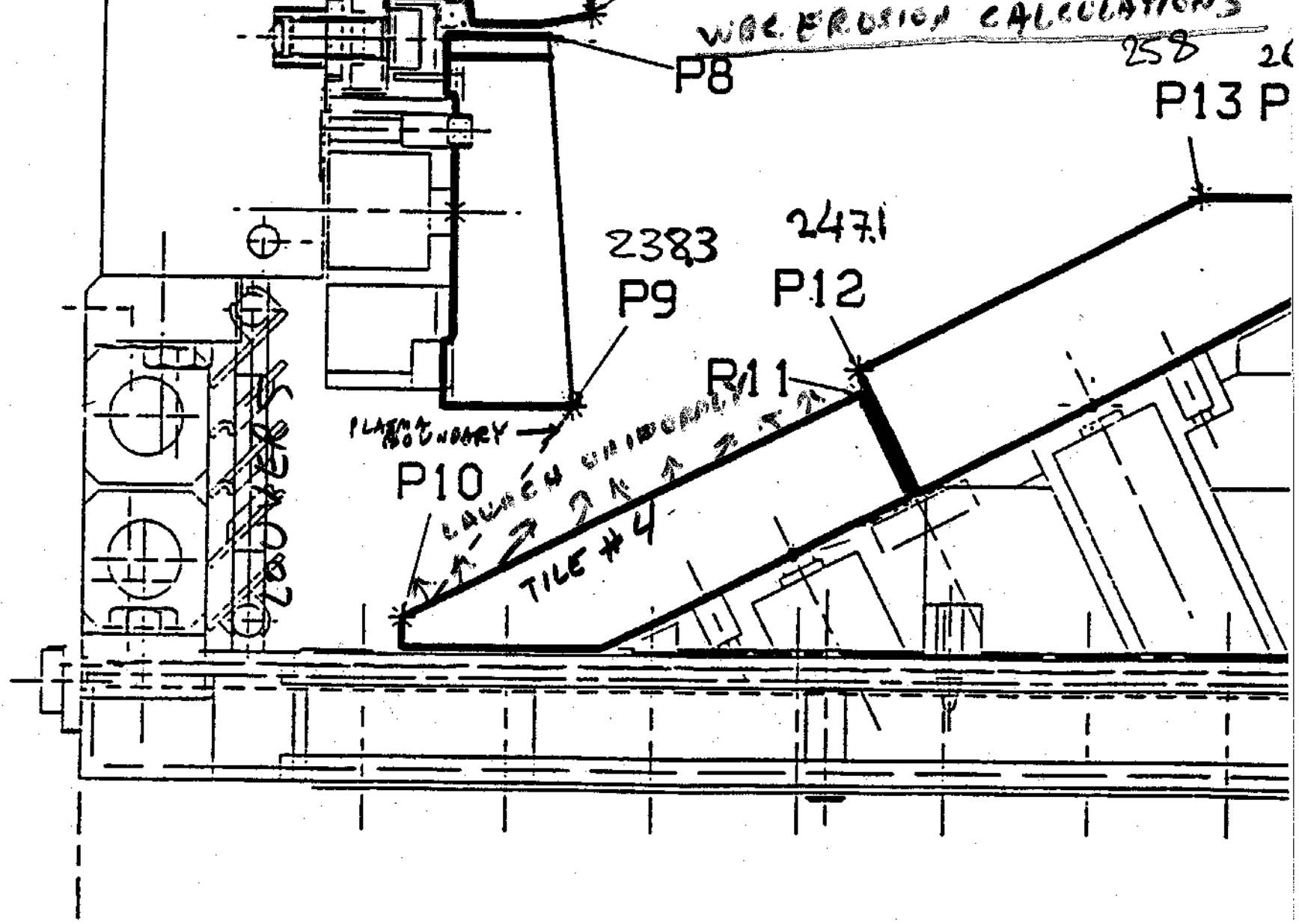
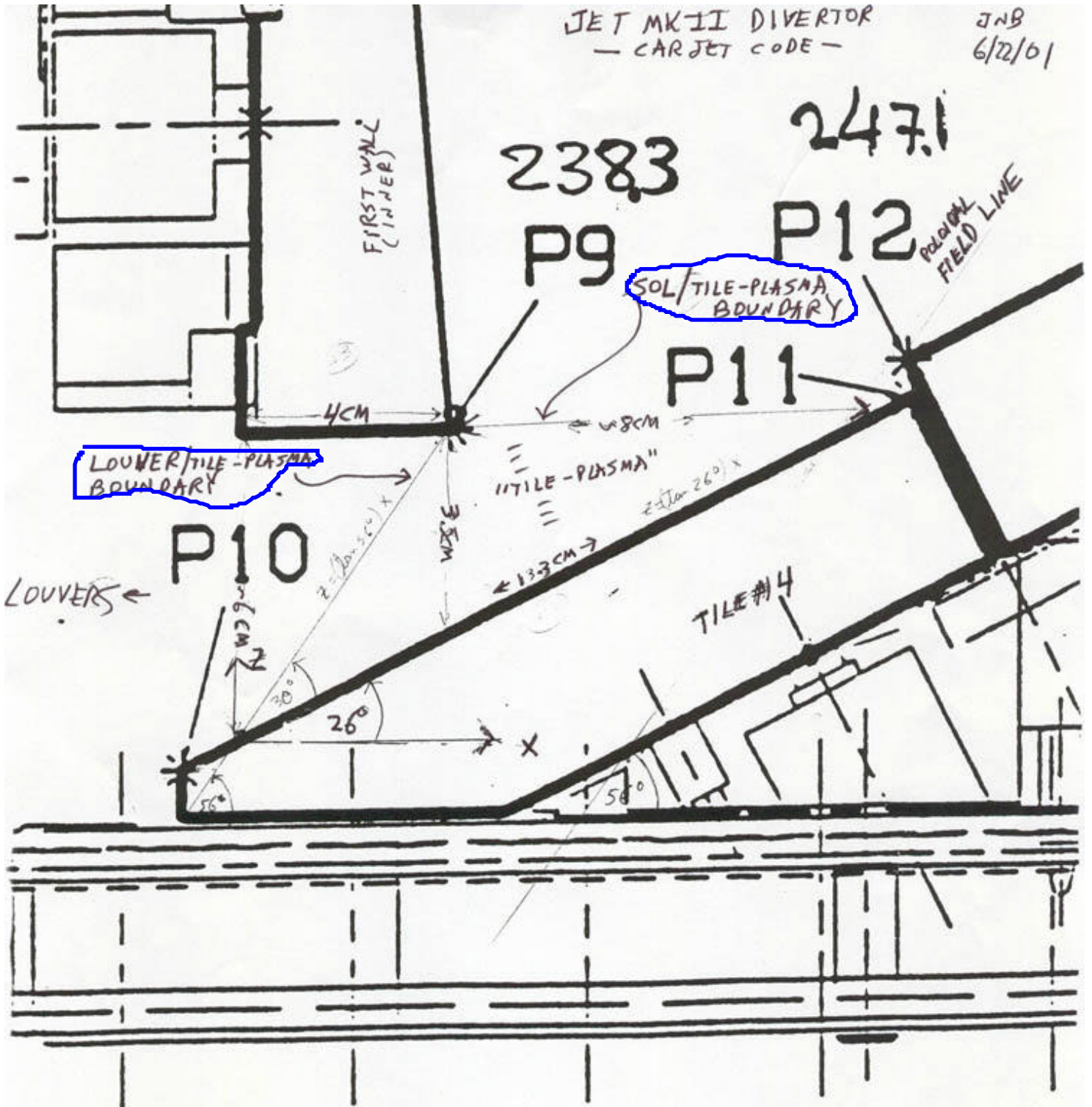


Figure 1 CARJET code JET analysis, geometry





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# Introduction

- Purpose – to calculate reflection coefficients of carbon and hydrocarbon molecules on a graphite surface
  - Molecular Dynamics modeling is used
  - Results will be used in codes for erosion/redeposition modeling
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# MolDyn Code

- Molecular dynamics code
  - Obtained from Robert Averback's group at the University of Illinois
  - Geared toward carbon/hydrogen systems
  - Uses Brenner hydrocarbon potential
  - Many modifications have been made
    - Graphical User Interface
    - Output, e.g. reflection info
    - Ability to run continually choosing random impact locations
    - Improvements to graphical output
    - Hydrocarbon molecules
    - H:C surfaces
-

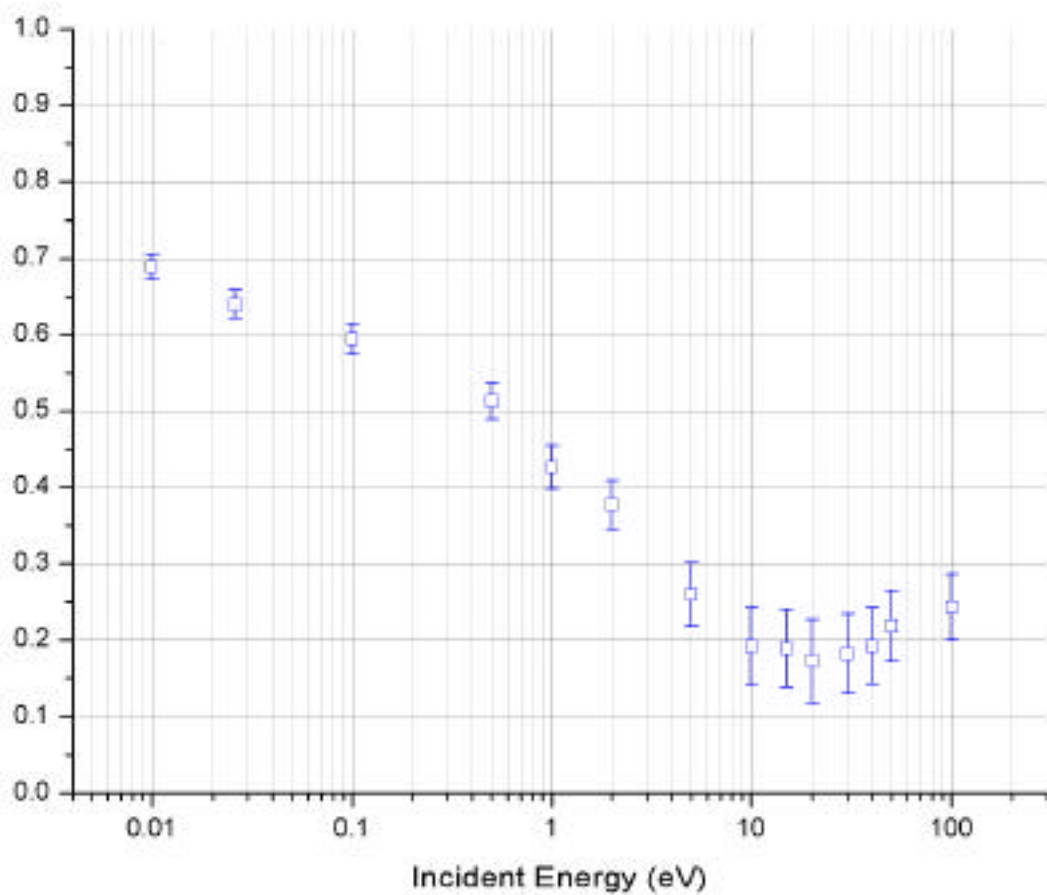
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# Use of Distributed Computing

- **Server**
    - On one central machine
    - Distributes work to clients
    - Compiles results
  - **Client**
    - Installed on all PCs at the laboratory (currently 10-15)
    - Contacts server to get next run to do
    - Runs the MolDyn code
    - Returns the results to the server
  - **Written in Java**
    - Platform independent
  - **Runs in background, uses otherwise idle CPU cycles**
  - **Multiprocessor-like speed-up at no additional cost**
-

# Results - Carbon

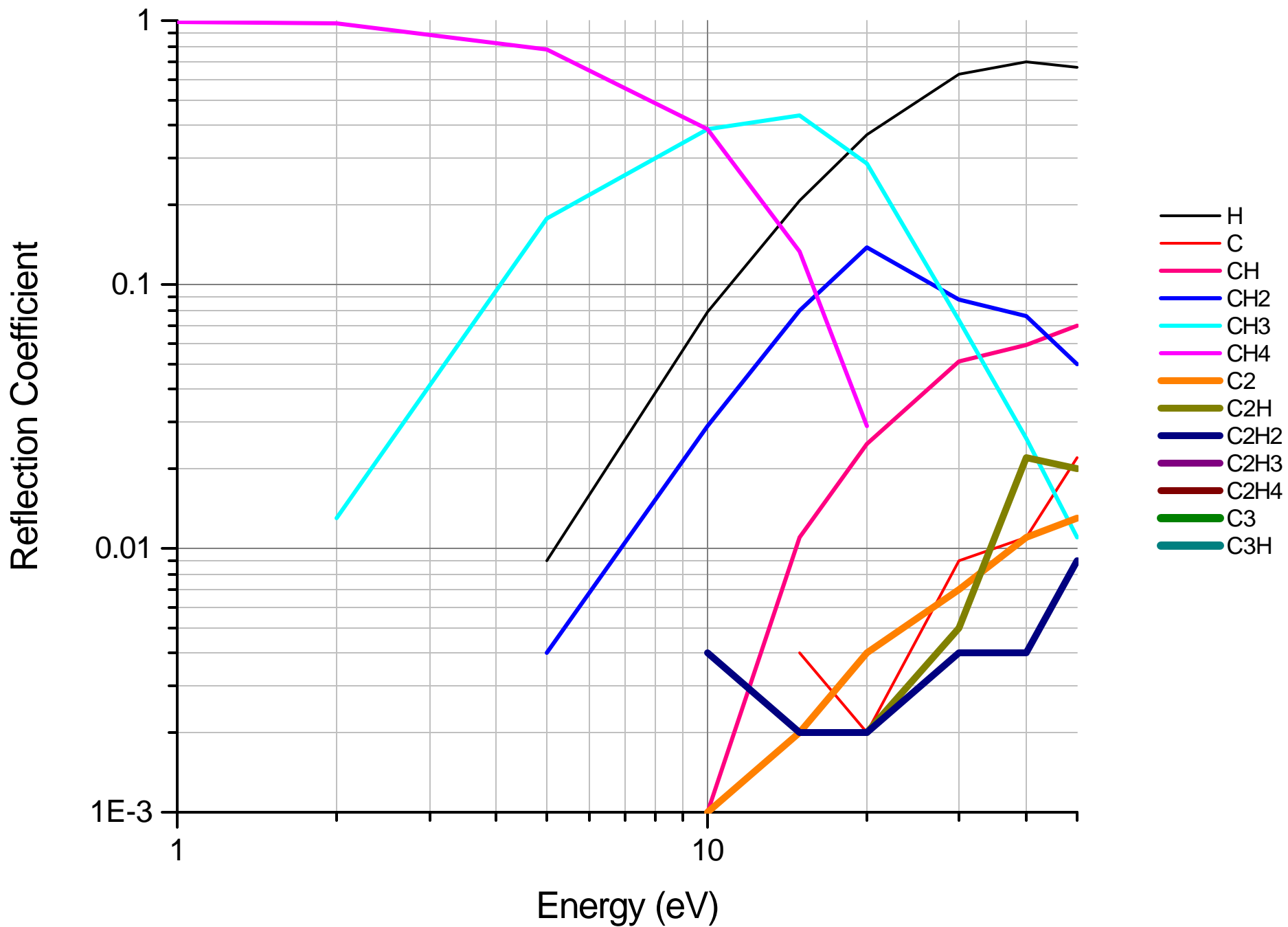
Carbon incident on ~0.4 H:C at 45 degrees



Next – look at entire spectrum of 16 hydrocarbons

CH-CH4  
C2H-C2H6  
C3H-C3H6

# CH<sub>4</sub> on 0.4 H:C Graphite at 45 degrees



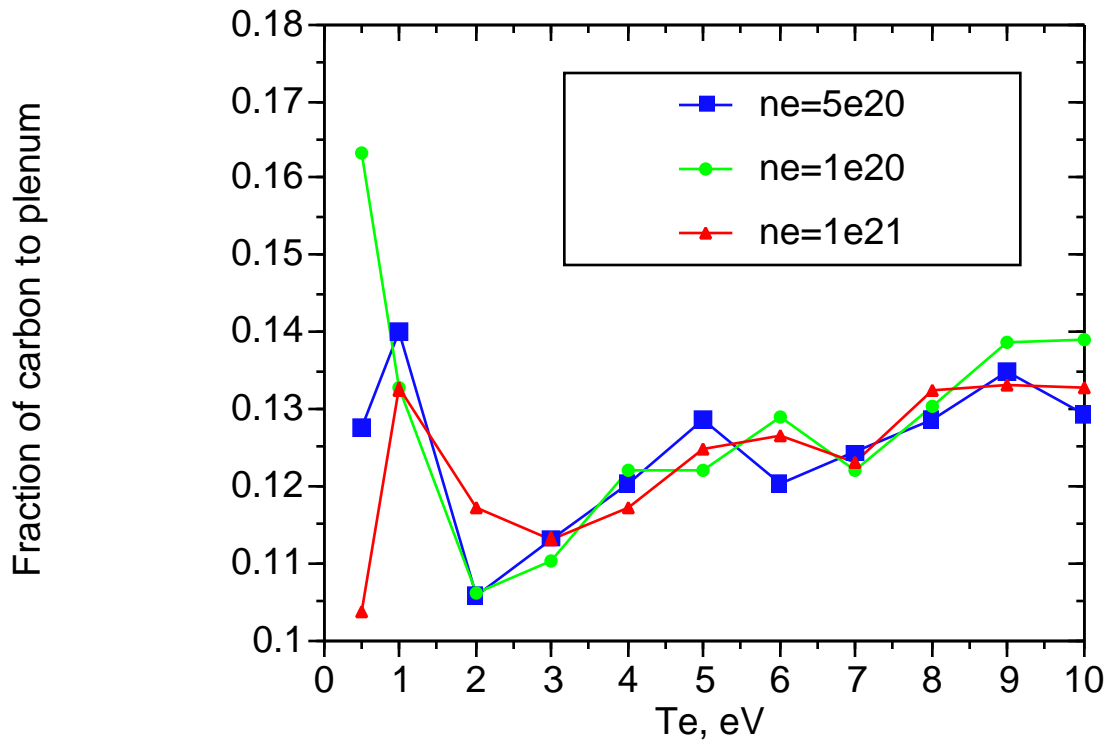


Figure 4. CARJET-JET Results: Plenum fraction vs. plasma electron temperature. For three values of electron density.

## Conclusions

Our group has an ambitious goal/charter; current progress is highly budget-constrained. We have made reasonable progress on our ALPS/APEX tasks:

- Temperature-dependent liquid material sputter yields and charge-fractions becoming available from data and modeling (IIAX, PISCES, SNL, VFTRIM, TRIM-SP) .
- DiMES lithium experiments under analysis with integrated plasma and impurity transport codes. Good understanding emerging of solid-phase exposure. MHD effects for liquid phase remains key issue.
- NSTX and CMOD lithium module analysis shows possibility of substantial deuterium pumping with zero-to-moderate lithium sputtering contamination.
- APEX-ARIES/CLiFF liquid tin wall analysis shows encouraging wall surface temperature limits ( $T_s > 800$  °C).
- ALPS-ARIES liquid tin divertor analysis shows negligible plasma contamination by sputtering. Analysis also shows high evaporation-limited surface temperature ( $T_s > 1500$  °C) for tin or gallium divertors with high-recycle plasma.

- Plasma-Liquid Interaction science/modeling under intense analysis. Highly sophisticated models being developed for plasma instability effects, D, T, He pumping, and thermally enhanced sputtering
- CDX-U lithium experiment/analysis—progressing well.
- Non-ALPS/APEX work—progressing well.

TFTR laser tritium removal

JET carbon erosion & tritium codeposition modeling

DEGAS code improvements/analysis