HARMONIC CONTENT OF ELECTRON IMPACT SOURCE FUNCTIONS IN INDUCTIVELY COUPLED PLASMAS USING AN "On-the-Fly" MONTE-CARLO TECHNIQUE *

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October 2000

* Work supported by NSF, SRC & DARPA/AFOSR

AGENDA

- Introduction
- Description of 2D HPEM model
- Description of the conventional MCS technique
- On-the-Fly method
- Typical plasma parameters
- Results and Discussion
  - Variation with threshold energies
  - Variation with frequencies
  - Variation with pressure
- Conclusions

INTRODUCTION

- **Electron temperatures in low temperature inductively coupled plasmas do not significantly vary during the rf cycle.**
- **However the time dependence of the electron impact source functions has been observed to vary.**
- **As a result, the harmonic content of the source functions is significant.**
- **Most models for plasma processing reactor use time averaged values for obtaining these coefficients and sources.**
- **The use of harmonics better represent these rates and hence can provide a more accurate model of these plasmas.**
- **Including harmonic content of the source functions normally involves storing the spatial and time dependent electron energy distribution functions (EED), which are used later to compute moments.**

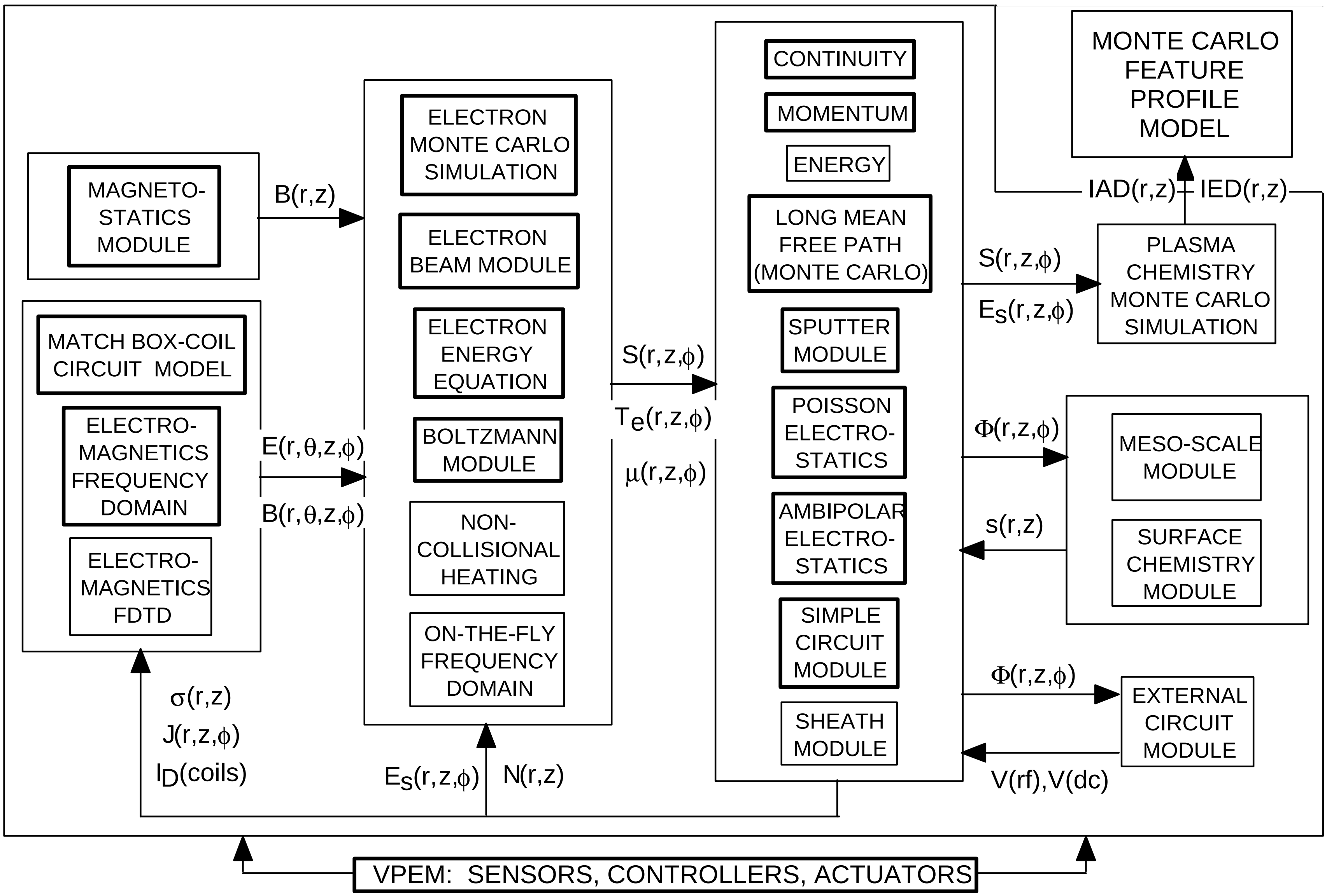
INTRODUCTION

- This approach presents computational problems in the form of more data storage space and large computer times

- To avoid this computational complexity a new “On-the-fly” method for calculating the moments of the EED’s is implemented in which the Fourier components are evaluated to calculate the harmonics of the source functions.

- The simulations are performed on the 2-D Hybrid Plasma Equipment Model (HPEM) for Ar/molecular gas mixtures.

HYBRID PLASMA EQUIPMENT MODEL (HPEM)



DESCRIPTION OF CONVENTIONAL MCS

- **In the 2-D HPEM, Monte-Carlo simulations are used to calculate the EED's.**
- **In the conventional technique, statistics are gathered whereby actual EED's are calculated.**

$$f_i = \frac{\sum_j w_j d\left(\left(e_i \pm 1/2\ \Delta e_i\right) - e_j\right)}{\sum_j w_j}$$

- **When sufficient statistics are obtained, these EED's are used to calculate the rate coefficients.**
- **Because of the intermediate step of calculating the EED's the conventional method involves large computer times and huge data storage arrays.**

ON-THE-FLY METHOD

- **To avoid this computational burden a new method "On-the-fly" was developed and used for our simulations.**

$$k_m(\vec{r}) = \frac{\sum_j w_j d(\vec{r}_j - \vec{r}) s_m(e_j) v_j \Delta t_j}{\sum_j w_j \Delta t_j}$$

v_j = **particle speed**
Δt_j = **time interval over which particle trajectory sampled**

- **In this method the moments of the EED's are calculated in real time as opposed to the EED's themselves.**

- **By storing the denominator and the numerator separately in the rate equation formula, the source functions can be obtained in real time and the intermediate step of calculating the f_i's is not required.**

- **To obtain the Fourier components, when collecting statistics we include the corresponding frequency terms.**

ON-THE-FLY METHOD

$$k_h(\vec{r}) = \frac{\sum_j w_j d(\vec{r}_j - \vec{r})\, s_m(e_j) v_j \Delta t_j \exp(\mathrm{i}\,(\mathrm{t} - \mathrm{t_h})\,\mathrm{h}w)}{\sum_j w_j \Delta t_j}$$

- **These rate constants are then used to obtain the different Fourier components of the source functions in real time.**
- **Since only the moments of the EED's are stored, the additional space requirements are less and so are the computer times required to generate the harmonics of the source functions.**
- **The source functions are then updated by adding the harmonic components to the D.C value of the source function and the rates are updated using the new source values to get more correct rate values.**

$$\mathrm{S} = \mathrm{Max}\ (0, (\mathrm{S_{D.C}} + \sum_{h=1}^{\infty} S_h \sin(w_h t + f)))$$

SUMMARY OF EQUATIONS USED

- **Electron Energy Distribution**

$$f_i = \frac{\sum_j w_j d\left((e_i \pm 1/2\ \Delta e_i) - e_j\right)}{\sum_j w_j}$$

- **Calculating rte coefficients in the On-the-fly technique**

$$k_m(\vec{r}) = \frac{\sum_j w_j d(\vec{r}_j - \vec{r})\, s_m(e_j) v_j \Delta t_j}{\sum_j w_j \Delta t_j}$$

- **Using the On-the-fly technique to calculate the harmonic content of the source functions**

$$k_h(\vec{r}) = \frac{\sum_j w_j d(\vec{r}_j - \vec{r})\, s_m(e_j) v_j \Delta t_j \exp(\mathrm{i}\ (\mathrm{t} - \mathrm{t_h})\ \mathrm{h}w)}{\sum_j w_j \Delta t_j}$$

- **Effective Source function**

$$\mathrm{S} = \mathrm{Max}\ (0, (\mathrm{S_{D.C}} + \sum_{h=1}^{\infty} S_h \sin(w_h t + f))$$

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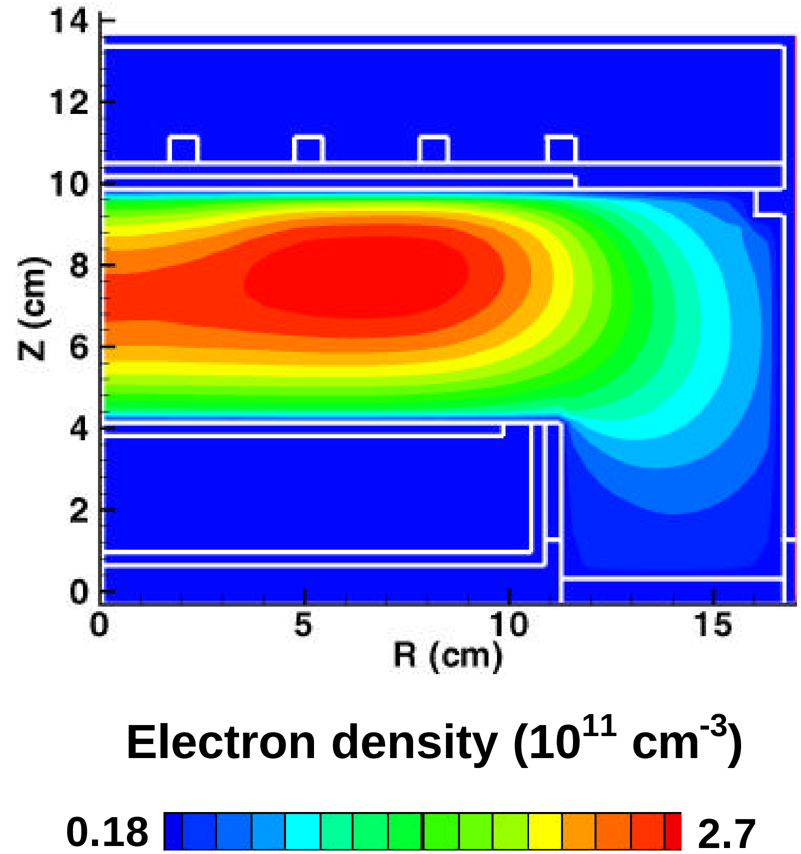
TYPICAL PLASMA PARAMETERS

- Using the "On-the-fly" method simulations of an ICP reactor were performed with the 2-D HPEM.
- The variation of the harmonic values with pressure, frequency and with the threshold value of the electron impact reaction is studied.
- Base case condition
  - Pressure : 5 mTorr
  - Frequency : 13.56 MHz
  - Tgas : 400 K
  - Ar / N2 : 90 / 10
  - Power : 650 W



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TYPICAL PLASMA PARAMETERS

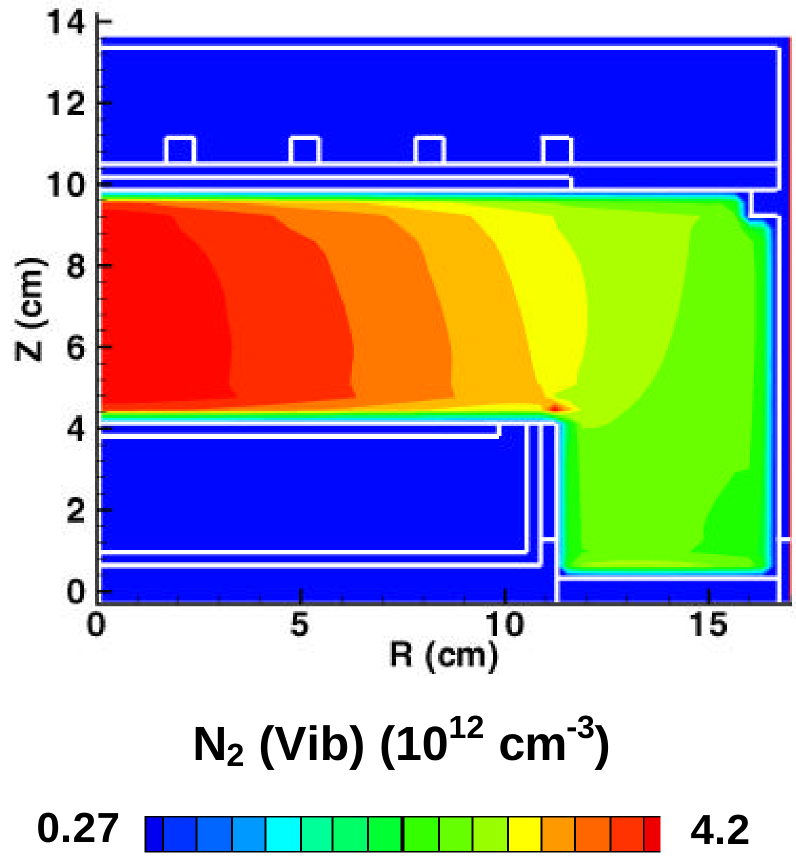
- For studying the variation of the harmonic content of the source functions with threshold energy of the reactions, the following reactions were considered.

- e^- + Ar ® Ar^+ + e^- + e- . De = 16.00 eV.

- Since the threshold is high this reaction captures the modulation of the tail of the EED with frequency.

- e^- + N_2 ® N_2 (vib) + e^- . De = 0.29 eV.

- The threshold is low and this reaction captures the modulation of the bulk of the EED with frequency.



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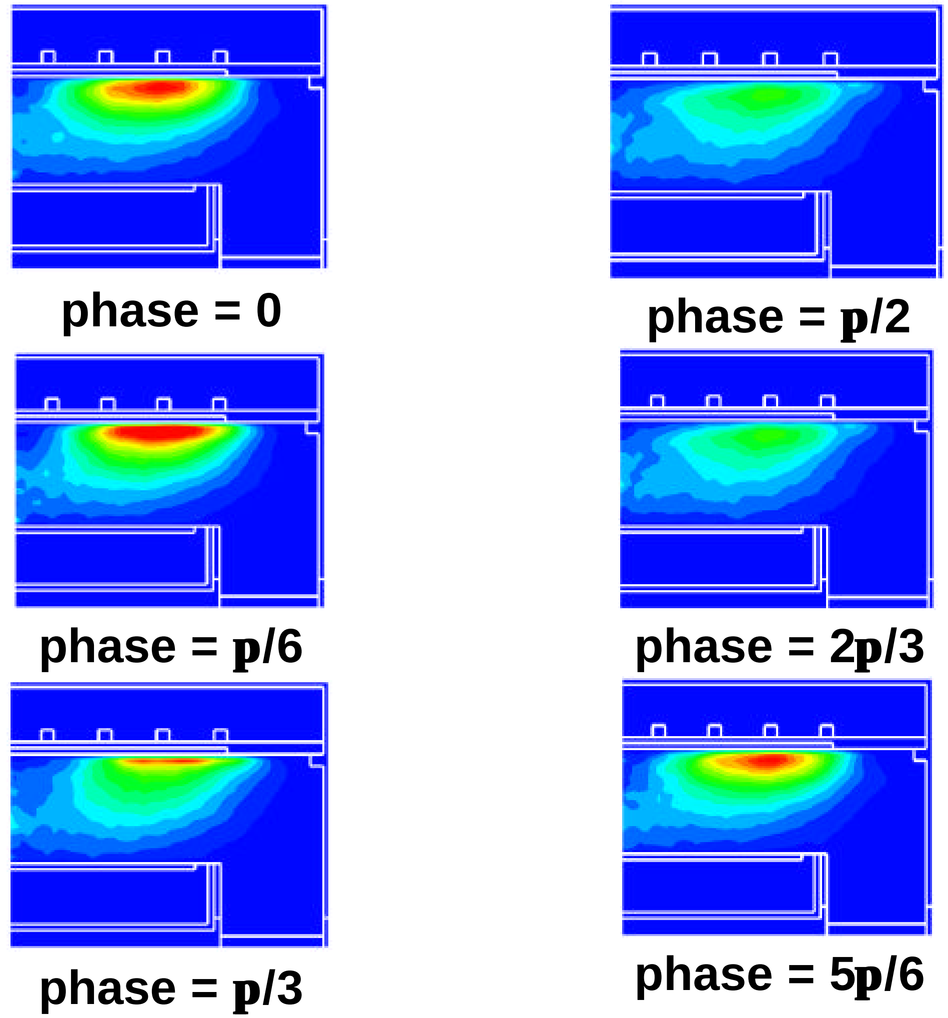
ELECTRON IMPACT IONIZATION OF Ar

- **Source functions for the electron impact ionization of Ar at different times of the rf cycle**
- **Since this reaction responds to the tail of the EED, the source functions are well modulated and so there is considerable harmonic content.**



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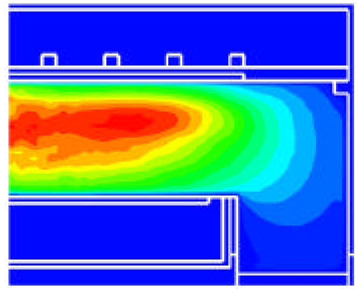
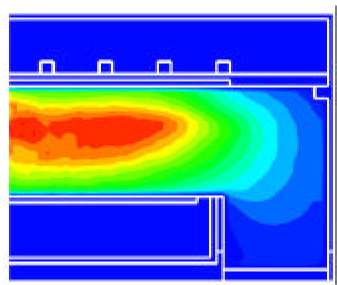
VIBRATIONAL EXCITATION OF N_2

- **The adjacent snap shots are the source functions for the vibration excitation of N_2 at different times of the rf cycle.**

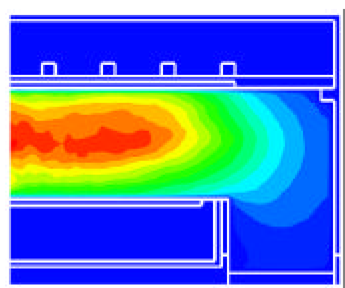
- **The threshold energy is low and this reaction responds to the bulk of the EED. Source functions aren't modulated and the harmonic content of the source functions is small.**



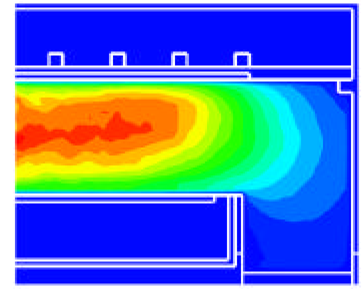
phase = 0



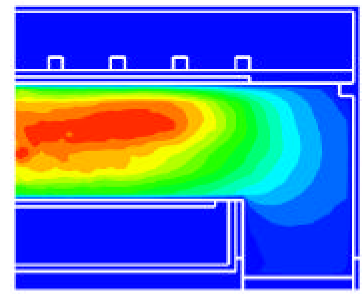
phase = p/6



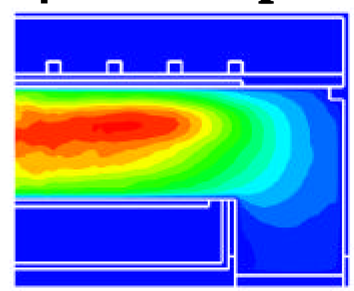
phase = p/3



phase = p/2

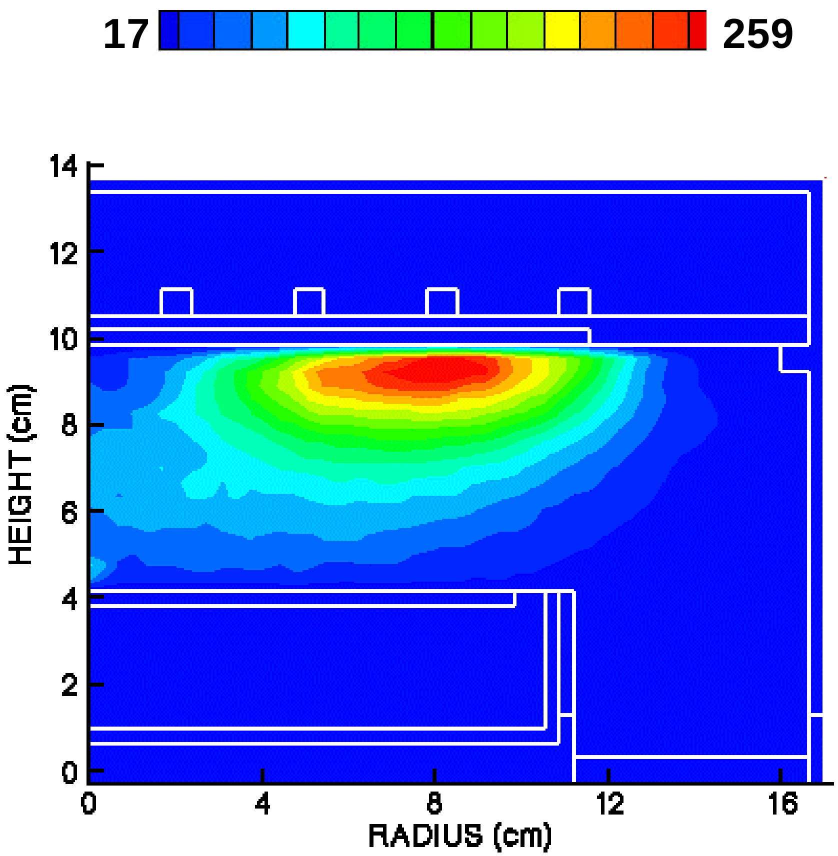


phase = 2p/3

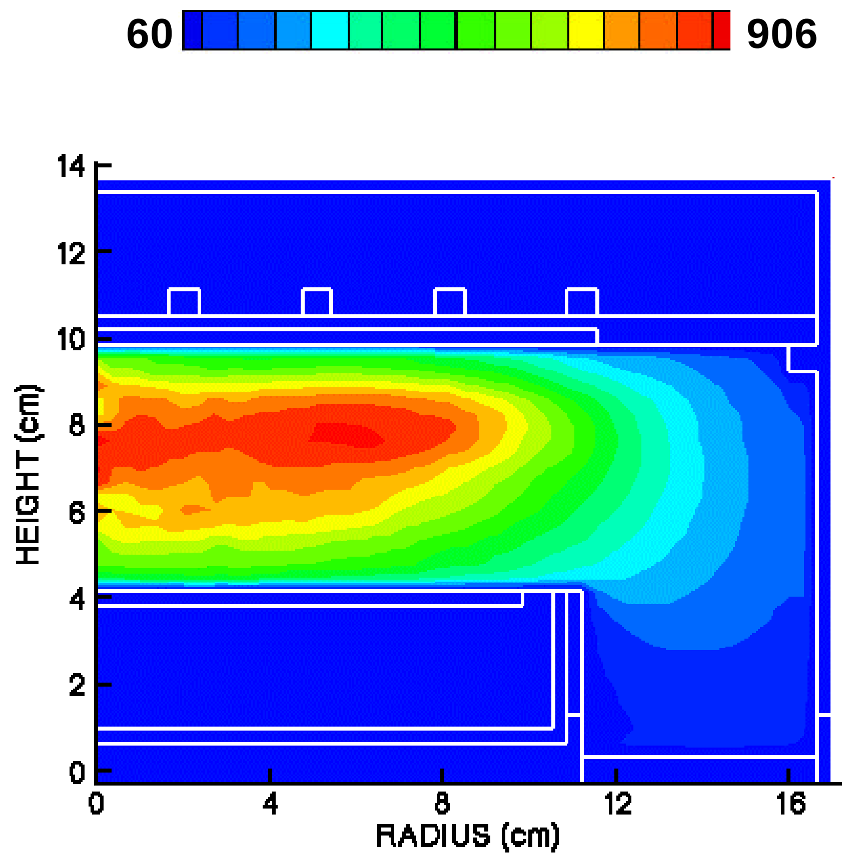


phase = 5p/6

Variation of source function with threshold



Electron excitation of Ar.
Threshold : 16 eV



Vibrational excitation of N_2.
Threshold : 0.29 eV

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VARIATION OF HARMONIC CONTENT WITH THRESHOLD

Ratio of harmonics wrt the DC value	Electron impact ionization of Ar	Vibrational excitation of N_2
Harmonic 1	0.019	0.007
Harmonic 2	0.222	0.041
Harmonic 3	0.017	0.005
Harmonic 4	0.049	0.008

- **As shown in the movies and snap shots, the harmonic content of the source function of the low threshold process is small and the time averaged value of the source function dominates for low threshold processes.**

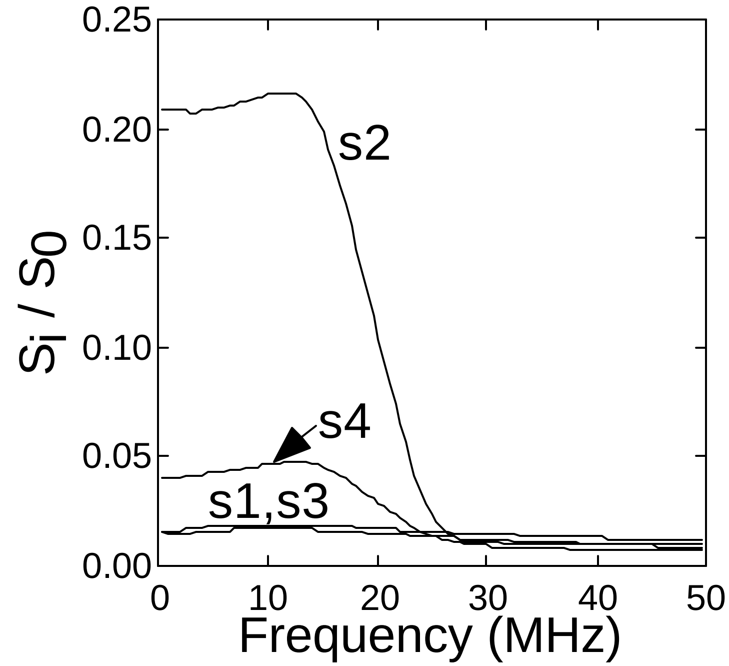
- **In each rf cycle the source functions have 2 positive peaks and hence the second harmonic is most prominent.**

FREQUENCY VARIATION

- **Operating conditions**
  - **Pressure = 5 mTorr**
  - **Frequency is varied from a few MHz to 10’s MHz .**

- **At low frequencies, (w_{rf} << $u_{collision}$) So the electrons can follow the electric field and so there is a large harmonic content.**

- **When w_{rf} >>$u_{collision}$, electrons see the time averaged value of the electric field and hence there is small harmonic content.**



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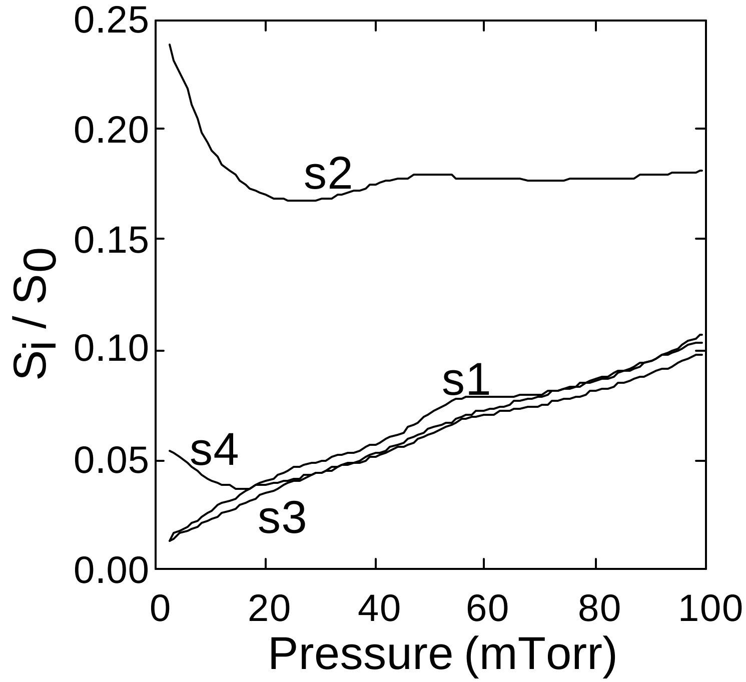
PRESSURE VARIATION

- **Operating conditions**
  - **Frequency : 13.56 MHz**
  - **Pressure varied from a few mTorrs to 10's mTorrs.**

- **As the pressure is increased the number densities and the rate constants of the electron impact reactions (at low pressures) increase.**

- **At higher pressures where the local field approximation is valid the harmonic content is expected to increase. This effect is seen in the less dominant harmonics.**

- **The dominant second harmonic remains nearly constant at higher pressures, which is yet to be resolved.**



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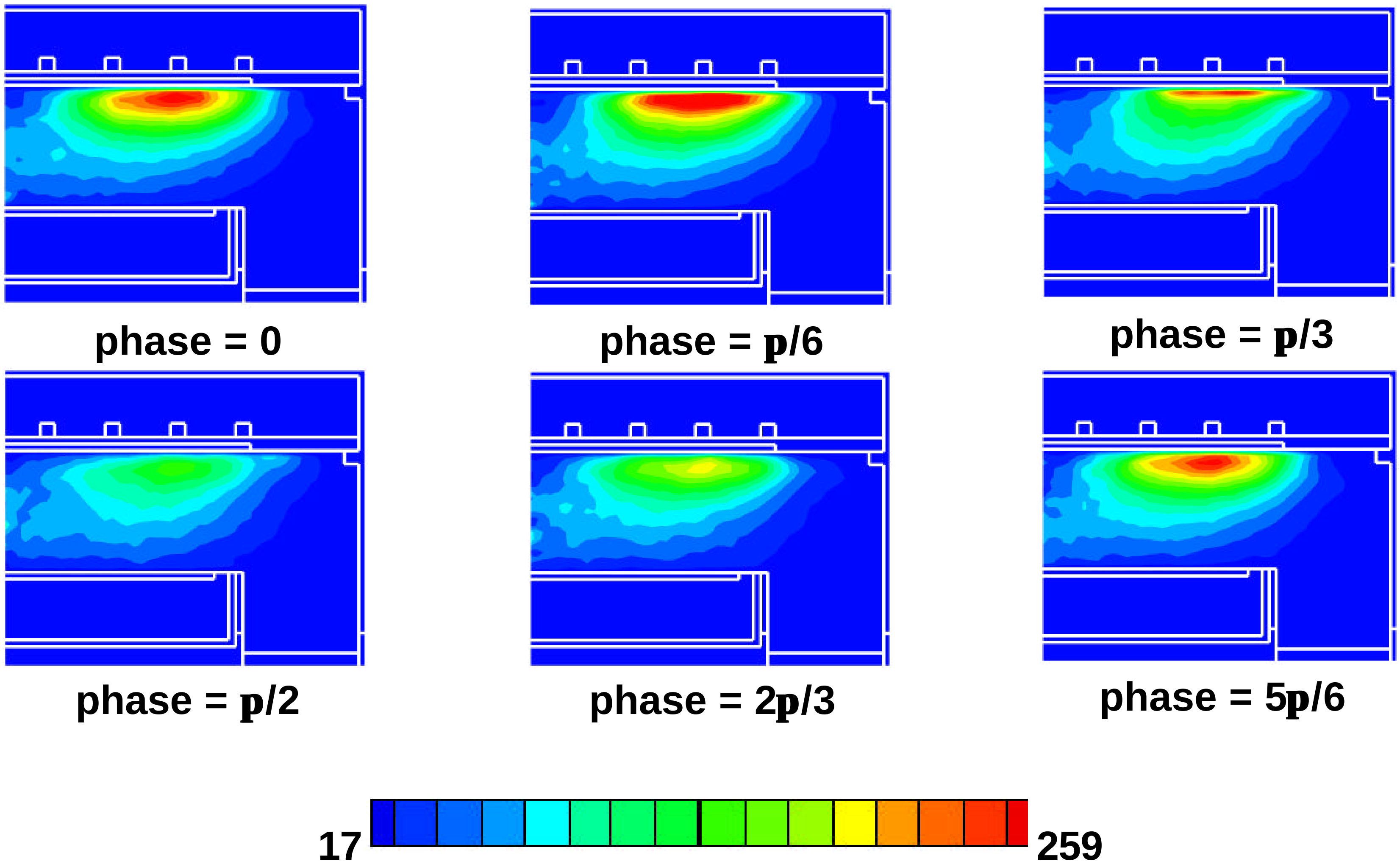
SOURCE FUNCTION WITH RF MAGNETIC FIELDS



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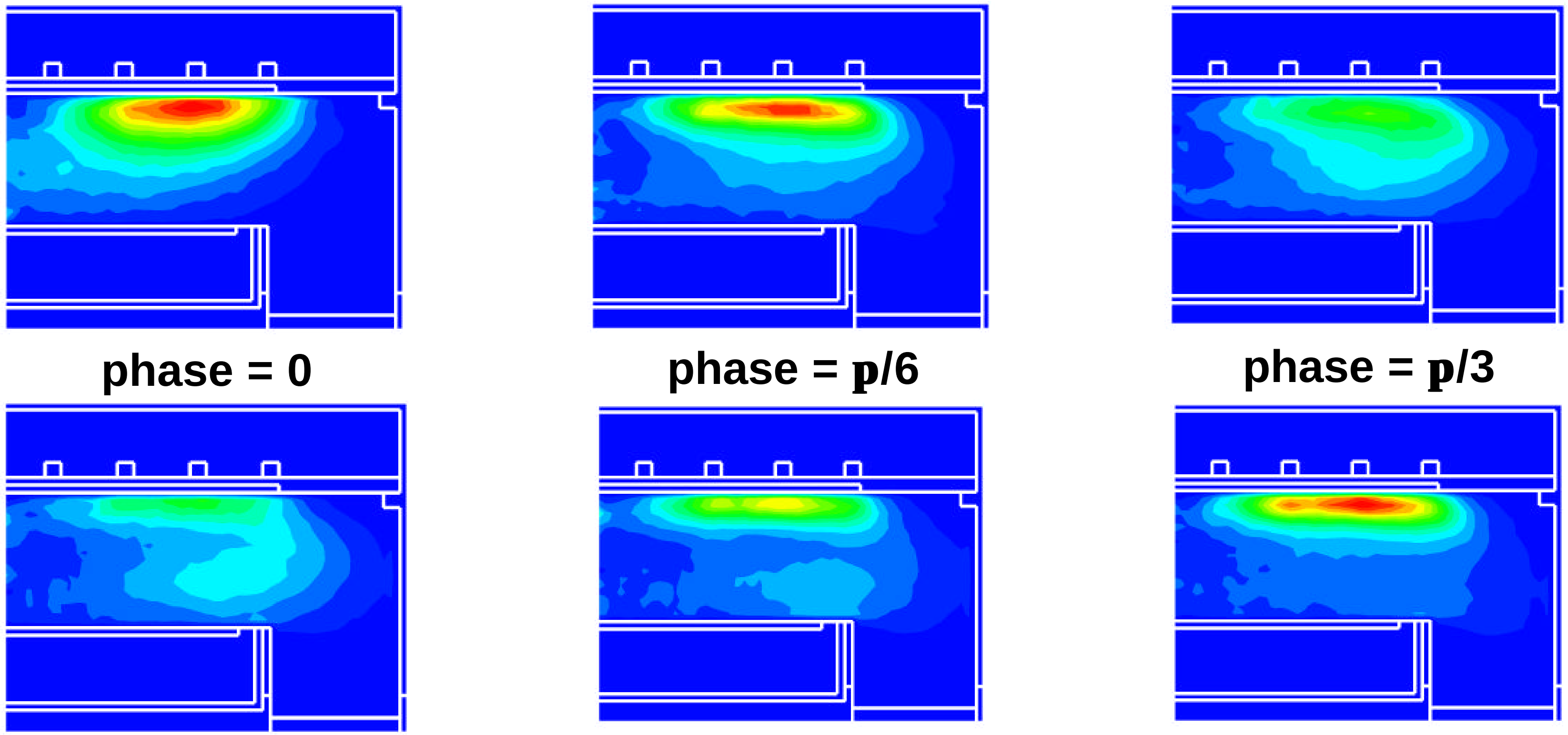
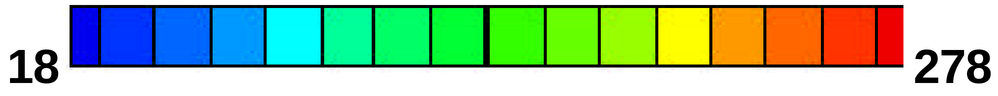
SOURCE FUCTION WITHOUT RF MAGNETIC FIELD



phase = 0 | phase = π/6 | phase = π/3

phase = π/2 | phase = 2π/3 | phase = 5π/6



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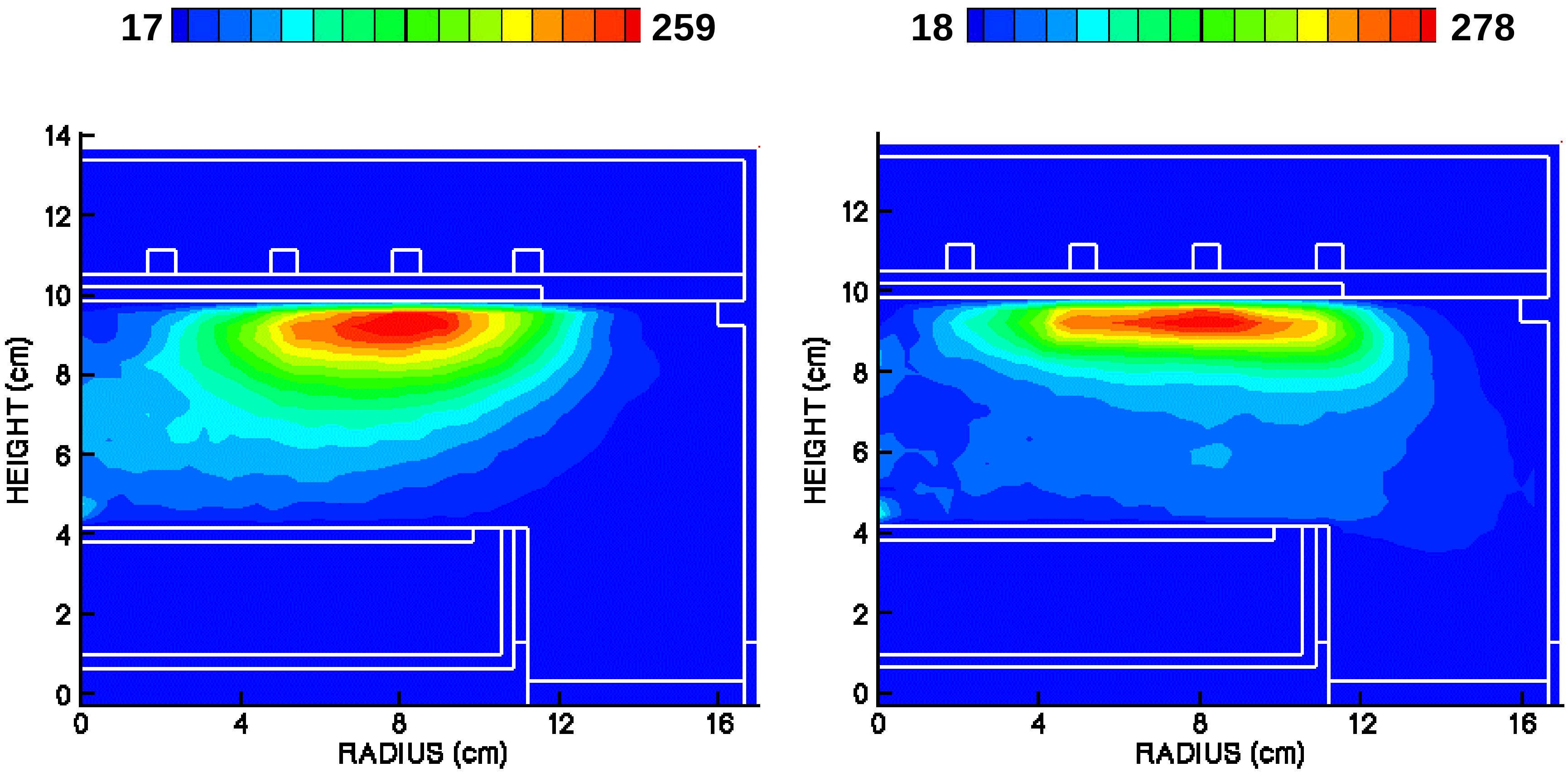
VARIATIONS OF SOURCE WITH RF MAGNETIC FIELD



Pr : 5mTorr, Freq : 13.56 MHz
rf magnetic field included

Pr : 5mTorr, Freq : 13.56 MHz
rf magnetic field excluded

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CONCLUSIONS

- The harmonic content of electron impact source functions was analysed using the On-the-Fly Monte-Carlo technique to determine the Fourier components.
- The second harmonic term had the maximum harmonic content.
- It was found that there is significant harmonic content in the high threshold electron impact reactions whereas the low threshold source functions were less modulated.
- As the pressure increases, the harmonic content as a fraction of the time averaged value increases. This value decreases with increasing frequency.
- The time variation of the source functions in the presence of rf magnetic fields were also studied and different spatial variations were observed.