Analysis and implementation of nonlinear radio-frequency sheaths

Matthew J. Poulos

Special thanks to N. Bertelli, S. Shiraiwa, E. H. Kim, and M. Ono





Motivations

- including ITER and SPARC
- It has been observed that ICRF power leads to the generation of impurities via RF sheath rectification; data is available from previous and ongoing experiments: C-Mod and WEST

• Goal of this talk: to elucidate the basic physics underlying RF sheath—plasma interactions and to develop the tools necessary to predict and model RF sheath rectification and the generation of impurities due to ICRF antennas

• Ion Cyclotron Radio Frequency (ICRF) antennas are planned to play roles in future fusion experiments

• First principle understanding of RF sheath rectification and its implications are topics of active research

Motivations

Measured sheath voltage rectification due to ICRF antenna in C-Mod



ICRF power leads to sheath rectification

S. J. Wukitch, M. L. Garrett, R. Ochoukov, et al. Phys. Plasmas 20, 056117 (2013); https://doi.org/10.1063/1.4803882

Molybdenum sputtering yield



Rectified sheath voltages lead to sputtering

RF actuator modeling should include

• High-fidelity modeling of realistic antenna/wall geometry

- Local FEM elements
- CAD antenna geometry
- Assumes cold plasma in SOL

• Nonlocal kinetic response in core plasma

- Flux surface geometry
- Toroidal/poloidal Fourier decomposition
- Nonlocal Landau/Cyclotron damping

Incorporation of nonlinear RF sheath boundary physics

- Motivations
- **RF** sheath physics and boundary conditions
- Three-dimensional implementation in plane-stratified geometry and emergent problems with fixed point iteration schemes
- Analytic results and nonlinear features
 - Unbounded half-space: multivaluedness, stability, and hysteresis
 - **Bounded domain: spontaneous symmetry breaking**
- Conclusions

Outline

RF sheath rectification

1D schematic of RF sheath

The total current normal to the sheath takes the form

$$\begin{split} & J_n = j_i + j_e + \frac{1}{4\pi} \frac{\partial E_n}{\partial t} \\ & \approx enc_s \left(1 - \exp\left(\Lambda - e(V_0 + V_{rf}(t))/T_e\right) \right) + \frac{1}{4\pi} \frac{\partial E_n}{\partial t} \end{split}$$

Requiring the DC current to vanish yields the rectified voltage

$$\langle J_n \rangle = 0 \quad \Rightarrow \quad V_0 = \frac{T_e}{e} \left\{ \Lambda + \ln \left[I_0 \left(e \,|\, \tilde{V}_{rf} \,|\, / T_e \right) \right] \right\} \approx \Lambda T_e / e + |\, \tilde{V}_{rf}$$

The Fourier component of the current density corresponding with the RF frequency is approximately given by

$$\tilde{J}_n = y_{sh} \tilde{V}_{rf}$$

where y_{sh} is a nonlinear complex RF sheath admittance.

Nonlinear RF sheath admittance

RF sheath admittance relates the local values of the oscillating total current J_n (particle + displacement) normal to the boundary and the RF sheath potential V_{sh}

$$J_n = y_{sh} V_{sh}$$

$$B_x = 0.3 T$$
 $B_y = 0 T$ $B_z = 2 T$
 $n_e = 1 \times 10^{18} m^{-3}$ $T_e = 15 eV$ $f = 80 MHz$

JR Myra, Phys. Plasmas 24, 072507 (2017)

Real and imaginary parts of nonlinear sheath admittance for varying sheath potential

RF sheath boundary conditions

In frequency space, Maxwell's equation (c.g.s. units) imply the wave equation

$$\nabla \times \nabla \times \overrightarrow{E} - k_0^2 \overleftrightarrow{\epsilon} \cdot \overrightarrow{E} = i k_0 \frac{4\pi}{c} \overrightarrow{j}_{ext}$$

On the sheath boundaries, the tangential components of the electric field satisfy

$$\overrightarrow{E}_t = -\nabla_t V_{sh}$$

The complex sheath potential V_{sh} is locally constrained by the <u>RF sheath boundary condition</u>

$$y_{sh}V_{sh} = J_n = \frac{\omega}{4\pi i}\hat{n}\cdot\overleftrightarrow{\epsilon}$$

- J_n : the total RF current density (particle + displacement) normal to the boundary
- y_{sh} : the sheath admittance, a nonlinear function of the absolute value of the local sheath potential $|V_{sh}|$, the RF frequency ω , and the local boundary plasma parameters (i.e., $y_{sh} = y_{sh}(|V_{sh}|, \omega, \overline{B}_0, n_e, T_e))$.

 $\cdot \overrightarrow{E}$ (\hat{n} is the unit vector pointing out of the plasma)

Consequences of linearity

Maxwell's equations provide a linear relationship between the boundary values of the RF sheath potential and the total RF current density normal to the boundary

$$J_n(\vec{r}_t) = \int_{\partial \mathcal{D}} d^2 r'_t y_p(\vec{r}_t, \vec{r}_t)$$

- - scales linearly with the external antenna current
- the integral kernel $y_p(\vec{r}_t, \vec{r}_t')$ is termed the plasma wave admittance
 - depends only on zeroth-order plasma and geometry

Both $y_p(\vec{r}_t, \vec{r}_t')$ and $J_n^{ext}(\vec{r}_t)$ can be obtained in arbitrary geometry using a FEM code. Analytic solutions exist in special cases.

 $V_{sh}(\vec{r}_t) + J_n^{ext}(\vec{r}_t)$

• the source $J_n^{ext}(\vec{r}_t)$ is the total RF current density normal to the boundary when conducting walls are imposed

Self-consistent equation for the sheath potential

• The RF sheath boundary condition gives nonlinear, local condition

$$J_n(\vec{r}_t) = y_{sh}(|V_{sh}(\vec{r}_t)|)V_{sh}(\vec{r}_t)$$

• Maxwell's equations yield the linear, nonlocal condition

$$J_n(\vec{r}_t) = \int_{\partial \mathcal{D}} d^2 r'_t y_p(\vec{r}_t, \vec{r}'_t) V_{sh}$$

• Eliminating the total current J_n gives a nonlinear integral equation for V_{sh} on the boundary

$$y_{sh}(|V_{sh}(\vec{r}_t)|)V_{sh}(\vec{r}_t) - \int_{\partial \mathcal{D}} d^2r'_t y_p$$

.). (1)

(2) $J_n(\vec{r}_t) + J_n^{ext}(\vec{r}_t)$.

 $V_{n}(\vec{r}_{t},\vec{r}_{t}')V_{sh}(\vec{r}_{t}') = J_{n}^{ext}(\vec{r}_{t}).$

- Motivations
- **RF** sheath physics and boundary conditions
- Three-dimensional implementation in plane-stratified geometry and emergent problems with fixed point iteration schemes
- Analytic results and nonlinear features
 - Unbounded half-space: multivaluedness, stability, and hysteresis
 - Bounded domain: spontaneous symmetry breaking
- Conclusions

Outline

In planar geometry, the integral kernel simplifies to a convolution

$$y_{sh}(|V_{sh}(\vec{r}_t)|)V_{sh}(\vec{r}_t) - \int_{\partial \mathcal{D}} d^2r'_t y_p(\vec{r}_t - \vec{r}'_t)V_{sh}(\vec{r}'_t) =$$

which yields a straight-forward fixed point iteration scheme leveraging fast Fourier transforms.

The Fourier transformed plasma wave admittance $\tilde{y}_p(k_t)$ is obtained analytically from Maxwell's equations.

$$B_x = 0.3 T$$
 $B_y = 0 T$ $B_z = 2 T$
 $n_e = 1 \times 10^{18} m^{-3}$ $T_e = 15 eV$ $f = 80 MHz$

Sheath potential magnitudes for varying antenna current

Fixed point iteration does not converge for $K_{max} > 1.1 \ kA/m$

Solutions exhibit oscillatory behavior before going numerically unstable

1.5

Maximum sheath potential for varying antenna surface current

Fixed point iteration convergence is very slow when entering the nonlinear regime and exhibits clear converge issues for large antenna currents

Newton-Ralphson method is prohibitively expensive, as each iteration requires the inversion of a large, dense Jacobian matrix with ~ $O(N^4)$ elements

Are converged solutions unique? Bounded? Stable?

Analytic results lead to insight regarding these questions

- Motivations
- **RF** sheath physics and boundary conditions
- Three-dimensional implementation in plane-stratified geometry and emergent problems with fixed point iteration schemes
- Analytic results and nonlinear features
 - Unbounded half-space: multivaluedness, stability, and hysteresis
 - Bounded domain: spontaneous symmetry breaking
- Conclusions

Outline

Analytic solution for plane wave sourcing

For a plane wave surface current imposed at $x = x_a$ $\vec{j}_{ext}(x, y, z) = \hat{y}\delta(x - x_a)K_{ext}e^{ik_z z}$

Linearity and symmetry imply at x = 0

 $J_n^{ext}(y,z) = \tilde{J}_n^{ext} e^{ik_z z} \qquad V_{sh}(y,z) = \tilde{V}_{sh} e^{ik_z z}$

where \tilde{J}_{n}^{ext} and \tilde{V}_{sh} are complex constants.

The nonlinear integral equation

$$y_{sh}(|V_{sh}(\vec{r}_t)|)V_{sh}(\vec{r}_t) - \int_{\partial \mathcal{D}} d^2 r'_t y_p(\vec{r}_t - \vec{r}'_t)V_{sh}(\vec{r}'_t) = J_n^{ext}(\vec{r}_t)$$

Reduces to a nonlinear algebraic equation for \tilde{V}_{sh}

$$(y_{sh}(|\tilde{V}_{sh}|) - \tilde{y}_p(k_z))\tilde{V}_{sh} = \tilde{J}_n^{ext}$$

x = 0

Analytic result reveals all solutions for varying antenna current

Three solutions for a fixed antenna current

$$K_{y} = 2 \ kA/m$$

 $B_x = 0.3 T \qquad B_y = 0 T \qquad B_z = 2 T$ $n_e = 1 \times 10^{18} m^{-3}$ $T_e = 15 eV$ $f = 80 \ MHz$ $k_z = 10.8 \ m^{-1}$

 $e |V_{sh}|/T_e$ Root # 3.3 66.1 2 3 118.1

For these parameters and geometry, three solutions exist that are consistent with Maxwell's equations and the RF sheath boundary condition

RF sheath instability in multi-valued cases

For slow time variation of the external sourcing, a nonlinear equation describing the evolution of the sheath potential is obtained as

$$\frac{d}{dt_s}V_{sh} = \frac{J_n^{ext} - (y_{sh}(|V_{sh}|) - \tilde{y}_p(k_z))V_{sh}}{i\frac{\partial}{\partial\omega}(y_{sh}(|V_{sh}|) - \tilde{y}_p(k_z))},$$

The equilibrium solutions to this equation are the self-consistent solutions to the RF sheath-plasma problem.

Not all equilibrium solutions are stable to small perturbations.

Instability criterion:

$$\frac{\partial K_{ext}}{\partial \psi} < 0$$

Hysteresis formation for slow time variation

The nonlinear equation

$$\frac{d}{dt_s}V_{sh} = \frac{J_n^{ext} - (y_{sh}(|V_{sh}|) - \tilde{y}_p(k_z))V_{sh}}{i\frac{\partial}{\partial\omega}(y_{sh}(|V_{sh}|) - \tilde{y}_p(k_z))},$$

is evolved with an external current that is slowly ramped up and down in time.

Behavior of the system is different for increasing current vs. decreasing current.

RF sheath instability leads to jumping from branch to branch.

Lessons from the analysis of an unbounded half-space

- Multiple solutions can exist to the self-consistent RF sheath plasma problem
- An instability is always associated with the occurrence of multiple solutions
- Hysteresis behavior in the time domain is a generic consequence of the RF sheath instability
- Complicated function topology is the culprit behind non-convergence of fixed-point iterations in three-dimensional sheath implementation

- Motivations
- **RF** sheath physics and boundary conditions
- Three-dimensional implementation in plane-stratified geometry and emergent problems with fixed point iteration schemes
- Analytic results and nonlinear features
 - Unbounded half-space: multivaluedness, stability, and hysteresis
 - Bounded domain: spontaneous symmetry breaking
- Conclusions

Outline

Analytic solution in a bounded domain

Maxwell's equations imply the nonlocal linear relation

$$\begin{bmatrix} J_n^0 \\ J_n^L \\ J_n^L \end{bmatrix} = \begin{bmatrix} y_p^{00} & y_p^{0L} \\ y_p^{L0} & y_p^{LL} \end{bmatrix} \begin{bmatrix} V_{sh}^0 \\ V_{sh}^L \\ V_{sh}^L \end{bmatrix} + \begin{bmatrix} J_n^{cw,0} \\ J_n^{cw,L} \end{bmatrix}$$

The RF sheath boundary condition gives the local nonlinear relation

$$\begin{bmatrix} J_n^0 \\ J_n^L \\ J_n^L \end{bmatrix} = \begin{bmatrix} y_{sh}(|V_{sh}^0|) & 0 \\ 0 & y_{sh}(|V_{sh}^L|) \end{bmatrix} \begin{bmatrix} V_{sh}^0 \\ V_{sh}^L \\ V_{sh}^L \end{bmatrix}$$

Eliminating J_n^0 and J_n^L leads to the nonlinear matrix equation

$$\begin{bmatrix} y_{sh}(|V_{sh}^{0}|) - y_{p}^{00} & -y_{p}^{0L} \\ -y_{p}^{L0} & y_{sh}(|V_{sh}^{L}|) - y_{p}^{LL} \end{bmatrix} \begin{bmatrix} V_{sh}^{0} \\ V_{sh}^{L} \end{bmatrix} = \begin{bmatrix} J_{n}^{cw,0}/K_{ex} \\ J_{n}^{cw,L}/K_{ex} \end{bmatrix}$$

Analytic solution in a bounded domain

To view the solution space of the nonlinear matrix equation

$$\begin{bmatrix} y_{sh}^{0} - y_{p}^{00} & -y_{p}^{0L} \\ -y_{p}^{L0} & y_{sh}^{L} - y_{p}^{LL} \end{bmatrix} \begin{bmatrix} V_{sh}^{0} \\ V_{sh}^{L} \end{bmatrix} = \begin{bmatrix} J_{n}^{cw,0}/K_{ext} \\ J_{n}^{cw,L}/K_{ext} \end{bmatrix}$$

define the two functions

$$K_{0}(|V_{sh}^{0}|, |V_{sh}^{L}|) = \left| \frac{(y_{sh}^{0} - y_{p}^{00})(y_{sh}^{L} - y_{p}^{LL}) - y_{p}^{0L}y_{p}^{L0}}{(y_{sh}^{L} - y_{p}^{LL})J_{n}^{cw,0}/K_{ext} + y_{p}^{0L}J_{n}^{cw,L}/K_{ext}} \right|$$
$$K_{L}(|V_{sh}^{0}|, |V_{sh}^{L}|) = \left| \frac{(y_{sh}^{0} - y_{p}^{00})(y_{sh}^{L} - y_{p}^{LL}) - y_{p}^{0L}y_{p}^{L0}}{(y_{sh}^{0} - y_{p}^{00})J_{n}^{cw,L}/K_{ext} + y_{p}^{L0}J_{n}^{cw,0}/K_{ext}} \right|$$

and note that solutions satisfy

$$K_0(|V_{sh}^0|, |V_{sh}^L|) = K_L(|V_{sh}^0|, |V_{sh}^L|) = K_{ext}$$

The functions K_0 and K_L are thought of as surfaces over the two-dimensional domain spanned by $|V_{sh}^0|$ and $|V_{sh}^L|$. The intersection of these two surfaces gives all the allowable values for the triplets $(|V_{sh}^0|, |V_{sh}^L|, K_{ext})$.

Analytic result shows all solutions for varying antenna current

RF sheath instability in multi-valued cases

For slow time variation of the external current

$$\frac{d}{dt_s} \begin{bmatrix} \psi_{sh}^0 \\ \psi_{sh}^L \end{bmatrix} = \left(i \frac{\partial}{\partial \omega} \begin{bmatrix} \hat{y}_{sh}^0 - \hat{y}_{p}^{00} & -\hat{y}_{p}^{0L} \\ -\hat{y}_{p}^{L0} & \hat{y}_{sh}^L - \hat{y}_{p}^{LL} \end{bmatrix} \right)^{-1} \cdot \left(\begin{bmatrix} J_n^{cw,0} \\ J_n^{cw,L} \end{bmatrix} - \begin{bmatrix} \hat{y}_{sh}^0 - \hat{y}_{p}^{00} & -\hat{y}_{p}^{0L} \\ -\hat{y}_{p}^{L0} & \hat{y}_{sh}^L - \hat{y}_{p}^{LL} \end{bmatrix} \begin{bmatrix} \psi_{sh}^0 \\ \psi_{sh}^L \end{bmatrix} \right)^{-1}$$

Analyzing the linear stability of equilibrium solutions leads to the instability criterion:

$$\frac{\partial K_0}{\partial \psi_0} \frac{\partial K_L}{\partial \psi_L} - \frac{\partial K_0}{\partial \psi_L} \frac{\partial K_L}{\partial \psi_0} < 0$$

Intermediate branch composed of symmetric solutions is unstable to any asymmetric perturbation

Implication: spontaneous symmetry breaking

Spontaneous symmetry breaking

Slowly increasing and decreasing the antenna current leads to the time evolution shown

Note that the symmetry of the problem is spontaneously broken by the RF sheath instability

Clear hysteresis behavior is observed

Directions for future research

- Incorporation of nonlinear RF sheath boundaries in high-fidelity 3D simulations (i.e., Petra-M)
- Development of 'smart' iterative solvers that anticipate nonlinear sheath effects
- Coupling to secondary emission model to evaluate impurity production due to RF sheath rectification
- Coupling to transport model to evaluate the transport of impurities

NSTX-U HHFW Antenna in Petra-M

Conclusions

- bounded domain). Precise conditions for the appearance of multiple roots are obtained.
- Non-intuitive spontaneous symmetry breaking is demonstrated in an otherwise completely plasma interactions.
- these nonlinearities and the exotic features they present.

• Analytical solutions exist for two classes of one-dimensional problems (unbounded domain/

• Multiple roots and sheath plasma resonance are linked to the presence of an instability that alleviates the ambiguity in the frequency domain and gives a physical mechanism for hysteresis.

symmetric problem, highlighting the nontrivial features of the physics underpinning RF sheath—

• Attempts to model and implement nonlinear RF sheaths in numerical codes should be aware of

