PROGRESS REPORT

DE-FG03-86ER52130

UCLA Program in Plasma Surface Interaction – Theory and Modeling

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I. Extended Summary of Proposed Work

The impurity control/particle exhaust system is one of the most critical components in any fusion device. On the one hand, the impurity control system determines the characteristics of the edge plasma and scrape-off layer (SOL) which in turn control core plasma confinement and impurity and particle transport. The impact of the impurity control system on global confinement has been delineated in many tokamak experiments, the most notable being the edge requirements in devices with divertors for achieving the regime of improved confinement known as the H-mode.

On the other hand, the impurity control/particle exhaust system as well as other plasma facing components are subjected to large fluxes of plasma particles and energy. Sputtering and erosion on the plasma facing components are causes for major concerns. First, the sputtered material represents a source impurity that can contaminate the core plasma and degrade the plasma performance. Furthermore, erosion of the plasma facing components can seriously limit their useful lifetime once the engineering requirements for cooling these components are taken into account. The impurity control/plasma exhaust system should therefore fulfill the physics requirements for clean and controlled edge plasma and adequate fusion ash exhaust as well as technological constraints imposed by the large particle and heat fluxes. With the advent of large and hot fusion experiments, the importance and the need for efficient and innovative impurity control system has been underlined and will become critical for next generation fusion experiments such as BPX and ITER [1].

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The PMI program at UCLA is directed towards understanding and modeling edge plasma phenomena and towards innovative solutions to design and operation of impurity control, particle exhaust, and plasma-facing components. On one hand, we have been striving to produce reliable and quantitative understanding of all the physical processes occurring in the edge plasma responsible for the experimental observations. In parallel, models developed for this purpose provide insight into the key issues of impurity and particle control and therefore, point towards areas where innovative solutions are needed.

One of the exciting new innovations is the application of RF ponderomotive forces to the scrape-off-layer in order to control plasma edge characteristics and affect the global particle and energy confinement. Initial experiments of this technique were successful on PISCES and experiments are planned on TEXTOR and PBX-M. We have developed, for the first time, an analytical and numerical transport model which includes both ponderomotive and electrostatic potentials. This model is designed to allow detailed comparison with experiments that have been performed on the PISCES linear edge simulator, and that are proposed for the PBX experiment, which include both biasing and RF ponderomotive divertor. Our initial estimates also show that for a device like ITER, application of RF ponderomotive forces can result in reducing the peak heat flux substantially with a small amount of RF power. Our modeling activity in this area is described in detail in Sec. III.

The first generation of two-dimensional edge-plasma simulation code, such as B2 [2] and EPIC [3,4] codes, demonstrated the value of edge-plasma simulations of the SOL and have been used extensively for simulation of the divertor tokamaks. It should be mentioned that EPIC, the first U. S. two-dimensional edge code, was developed at UCLA under our PMI grant at UCLA. Even though the first-generation two-dimensional edge-plasma codes have clearly established the need for this class of simulations, the experience with these codes have also exposed many shortcomings and the need for the second-generation edge-plasma simulation codes. During the last few months we have started work with advanced features. The aim is to develop a second-generation code which is more accurate and includes improved physics models but also flexible enough such that it can be used for

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a range of machines from small laboratory experiments to full-scale fusion devices. Our modeling goals for this are are described in detail in Sec. IV.

In summary, our activities in the next period will include development of model and simulation codes as well as application and refinement of these models in the following areas: (1) active control of scrape-off-layer plasma by ponderomotive and electrostatic forces, (2) development and application of second-generation, two-dimensional edge-plasma simulation codes, and (3) engineering design of the plasma-facing components and impact of disruptions (Sec. V). As always we will coordinate and relate our theoretical work with experimental programs especially in the PISCES facility. Cooperative programs with other experiments outside UCLA will be continued and expanded (Sec. VI). We will use our expertise to model and explain experimental measurements as well as propose innovative ideas and procedure to improve the efficiency of the impurity control system in these experiments. Interaction with other programs at UCLA especially those focused on ITER and ARIES tokamak fusion reactor study will be extremely beneficial and further enhance our leadership role in the PMI area.

II. Active Edge Plasma and Impurity Control

The impurity control/plasma exhaust system should fulfill the physics requirements for clean and controlled edge plasma and adequate fusion ash exhaust as well as technological constraints imposed by the large particle and heat fluxes. The effects of this plasma bombardment and high heat flux on these surfaces can alter the nature of the boundary in ways that are detrimental to the core plasma confinement. The peak power load and erosion of a divertor plate is governed by the area on the divertor plate over which power is deposited. That area is in turn governed by the scrape-off layer length which expresses the balance between cross-field transport and flow of plasma parallel to magnetic field lines to the divertor or limiter. To reduce the peak power load and erosion, it is beneficial to alter this transport balance.

Experiments have shown that the particle transport in a tokamak can be significantly altered by externally imposing an electrical potential to limiter and/or wall surfaces, or by imposing a ponderomotive potential within the plasma from an RF source. These experiments are not completely accounted for by present theoretical analyses. Even without these externally imposed potentials, there exists no universal picture of the scrape-off layer transport. For a scrape-off layer subject to an electrostatic bias, there are still fewer models [5] available for comparison with experiment, and still fewer transport models for the scrape-off layer with ponderomotive forces [6].

We have recently developed, for the first time, an analytic and numeric transport model which includes both ponderomotive and electrostatic potentials. This model helps us understand mechanisms responsible for the transport physics properties of the plasma in an ordinary scrape-off layer, as well as a scrape-off layer having ponderomotive potentials and biased surfaces. Moreover, in most of the experiments, the confinement properties of the core plasma also change, leading to the conclusion that not only does the potential influence transport in the SOL, but also on the closed magnetic flux surfaces near the plasma velocity. To understand this effect, a fully ionized transport model, appropriate for the core has been developed in parallel with the SOL model, we anticipate combining the two models in the near future. A separate, but related issue is the degree to which non-ambipolar transport can be supported by the the SOL plasma. Unlike the core, cross-field electron and ion fluxes are not constrained to be ambipolar within the SOL. Currents may flow along field lines through the limiter, an effect which is enhanced by limiter biasing.

Even in the absence of an externally applied bias, currents can arise in the SOL from such diverse mechanisms as differences in electron temperature, differences in potential due to drift effects and magnetically induced electric fields. In turbulence-free plasmas, these non-ambipolar boundary conditions can modify the density profiles that would ordinarily occur in an ambipolar plasma. In the presence of turbulence, this effect is not so clear, and to investigate it further, we have included such nonambipolar effects within the framework of a phenomenological model of edge density and potential fluctuation effects.

Since neutral-plasma interaction can play an important role, particularly in cases where the local ionization is important, such as high recycling or gas divertor plasmas, we have included within the model particle sources, including atomic and ionization cross-section calculations.

Our goal has been to develop a model which would apply equally well to tokamak geometry as well as simple cylindrical geometry, such as encountered in the PISCES linear edge simulator, so while a basic cylindrical coordinate system is utilized, we retain terms which arise from taking the gradient of the magnetic field, including curvature and radial inhomogeneity. The model is sufficiently general, that any of these mechanisms can be "turned off" and used to understand transport due to the remaining mechanisms. Thus the calculation can be used to design an "RF ponderomotive divertor", a "biased divertor/limiter" or an ordinary scrape-off layer plasma without any biasing or ponderomotive potentials. The analytic model is one dimensional, allows for biasing and ponderomotive potentials, uniform neutral sources, and provides a simple ordinary differential equation for the transverse density and electric potential profile in the plasma. These ordinary differential equations are solved for the density and potential profile and the conditions under which the density profile is a simple exponential described by a characteristic scrape-off layer length are found. The model clearly demonstrates how either an electrostatic bias or a ponderomotive potential can be used to change this scrape-off layer length.

To treat the more general two-dimensional geometry, including toroidal effects and drifts, a set of coupled partial differential equations are derived which describe density and electrostatic potential. Fluctuation driven transport is included by assuming the density and potentials have an average and a fluctuating term and resulting equations are averaged so that only correlations produce transport which are folded into a phenomenological anomalous diffusion coefficient. Terms coming from taking the gradient of the magnetic field are retained, so that the model can be used to describe tokamak transport. These magnetic field terms arise from the $\vec{E} \times \vec{B}$, diamagnetic, and ponderomotive force $\times \vec{B}$ drifts, and are fully retained in the model. The equations are finite differenced on a two dimensional grid and solved numerically for the density and potential distributions everywhere in the plasma, using standard matrix LU decomposition techniques. Boundary conditions include either the specification of density and potential (Dirichlet) or their derivatives (Neumann) or any combination at the boundary. Nonlinearities in the potential calculation are treated by standard Newtonian iteration techniques. At every iteration, a plasma potential is calculated, from which is obtained a floating potential at each node. Depending on the value of this floating potential relative to the biased surface, there will be a current flowing between plasma and the wall. With an additional iteration loop, we impose the condition of global ambipolarity which requires that overall this current be zero, so that even thought locally there may be currents floating, overall the net current is zero. This model is designed to allow detailed comparison with experiments that have been performed on the PISCES linear edge simulator, and that are proposed for the PBX experiment, which include both biasing and RF ponderomotive divertor.

All of this computational machinery is already set up and tested to ensure that it can model real experimental situations. In the coming period, we will apply this model to planned experiments on TEXTOR and PBX-M. We will also investigate the use of RF ponderomotive forces to reduce peak heat fluxes on the ITER divertor plate. Our initial calculations have indicated that the peak heat flux can be reduced substantially with a small amount of RF power. In addition, we propose to develop the model further in order to provide a more extensive analysis of the edge plasma and its effects on the core. We propose to use this code as tool to understand some of the recent observations of how the edge influences the core, as well as a spring board for proposing additional novel techniques to be tried on the present generation of machines. The steady state model will be developed into a time evolution-to-steady-state model, which will include the following features:

1. Active means to influence plasma-wall interactions, particularly limiter biasing, ponderomotive forces and boundary magnetic field line ergodization.
2. Development of an impurity transport model including realistic impurity sources and

impurity generation models to understand and control impurity flow in the edge.

3. Development of combined edge and core plasma models in which MHD effects at the core are included, as well as coupling to the impurity transport model.
4. Development of time evolution models of the neutral particle distribution and related atomic physics processes, as well as coupling with the impurity and plasma transport models. We will use the ALADDIN system for the retrieving atomic data for these simulations.

Our ultimate goal is twofold: first the development of novel techniques for edge plasma control which include a combination of applied ponderomotive potentials, applied electrostatic potentials, ergodic limiters and gas target divertors and secondly, to understand how the edge plasma can be controlled to improve core plasma confinement.

III. Coupled Edge Plasma and Neutral Particle Transport

Fluid descriptions of Edge-plasma transport has been used to study the edge-plasma properties and the conditions at the surfaces in contact with plasma such as divertor plate, limiter, and the first wall/vacuum vessel. One-dimensional radial and axial plasma transport models have been the subject of much early research [7]. A quasi-two dimensional model [8] which took advantage of the localized nature of recycling to couple the axial and radial models into an axially averaged two zone model was developed under our PMI grant at UCLA a few years ago and used to successfully explain a number of features observed in the scrape-off layer of the TEXTOR ALT-I experiment. These early models clearly demonstrated that one dimensional models of edge-plasma do not produce an accurate description of the edge-plasma. This is not surprising because the parameters of the SOL are determined through the balance between axial and radial transports.

The first generation of two-dimensional edge-plasma simulation code, such as B2 [2] and EPIC [3,4] codes, demonstrated the value of edge-plasma simulations of the SOL and have been used extensively for simulation of the divertor tokamaks. It should be mentioned that EPIC, the first U. S. two-dimensional edge code, was developed at UCLA under our PMI grant. Even though the first-generation two-dimensional edge-plasma codes have clearly established the need for this class of simulations, the experience with these codes have also exposed many shortcoming and the need for the second-generation edge-plasma simulation codes. During the last few months, we have started development of a second-generation edge-plasma simulation code. The aim is to develop a code which is more accurate and include improved physics models but also flexible enough such that can be used for range of machines from small laboratory experiments to full-scale fusion devices. The advanced features we have targeted are the most important for a design and analysis code. The key features are:

1. **Computational efficiency and robustness** using state-of-the-art high speed and low-memory requirements algorithms while ensuring that calculations achieve converged solution to the transport equations. The aim is to have the code run on a modest desktop workstation rather than a supercomputer.
2. **Flexible geometry** through arbitrary meshing, flexible element connectivity, and strict local property conservation in order to handle realistic tokamak edge geometries.
3. **Ease of use** by using the X windows graphical interface with menu-driven input and output from mesh generation up to visualization tools for output presentation.
4. **Improved physics** by including multi-energy group neutral transport equation, non-ambipolar flows, and drifts.

The above-mentioned target features are set based on the experience with the first generation codes as described in detail below.

Computational Efficiency and Robustness

The fluid-based edge-plasma transport codes solve a set of equations for the density, flow velocity, and temperature of each plasma species. These fluid equations are highly nonlinear because the transport coefficients and ionization reaction rates depend on the density and temperature. Furthermore, the system contains thousands of unknowns (density, velocity, and temperature of each plasma species at each of the thousands of the grid points). Solving such a large system of nonlinear equations is challenging, since unlike the linear systems, there is no algorithm that is guaranteed to yield a solution in a predictable number of steps. Among possible solution techniques, there is much variation in their ability to locate a solution, and the time required to do so. Methods that usually find a solution are called "robust," and those that require minimal time and memory are called "efficient."

Both B2 and EPIC use similar fully implicit techniques which are efficient. Unfortunately both algorithms are not robust (do not converge all of the time). In fact, attempts to improve the physics in these code has usually resulted in the code not being able to converge at all. Both codes are also extremely sensitive to the mesh used for computation, *i.e.*, they converge on certain meshes and do not converge on slightly different mesh.

One popular solution technique for nonlinear systems is the "Newton's Method" in which for a given guess for the steady state, an improved guess is found by linearizing the equations about the guess and solving the linearized problem. This process is repeated until it converges to the solution of the nonlinear problem. Prior work in general computational fluid dynamics, as well as recent work in edge-plasma modeling by Knoll and by Ronglien, has shown that the Newton's Method is robust for solving nonlinear equations of the type encountered in edge-plasma modeling. Typically about 20 iterations of Newton's method will usually yield a solution, compared to 2000 iterations in EPIC or B2 codes (which do not always reach a solution). Unfortunately, even though the Newton Method is robust and requires only 20 iteration to converge, existing implementations of Newton's Method are not "efficient," because they do not efficiently solve the linear problem arising in each iteration step. The existing codes solve the linear problem by direct elimination methods which consume much computer time and memory, restricting them to run only on supercomputers.

Given the previous difficulties with the numerical algorithm of the edge-plasma simulation codes, our aim is to develop two distinct algorithms. The first approach is improve the "efficiency" of the robust Newton's Method by using an state-of-the-art solver for linear systems instead of Gauss's direct elimination method. In this area, we are developing a fast linear solver for edge-plasma problems based on the so-called "preconditioned conjugate gradient" method which is a recently developed method by the computational fluid dynamics community. Our effort in this area is in very close consultation with the Fluid Dynamics Group in the UCLA Applied Mathematics Department in order to take full advantage of the their extensive experience and latest techniques.

Since the Newton's Method can only find steady state solution, we are also developing a fully implicit numerical algorithm for time dependent problems. The Fluid Dynamics Group at UCLA has also identified several state-of-the-art fully implicit package that we will modify and use in our new code.

Flexible geometry

All previous edge-plasma code divide the computational space into the orthogonal coordinates of the fluid equations. The B2 code, for example, uses a simple mapping function to project the angled coordinates corresponding to flux surfaces onto a flat poloidal plane of physical device symmetry. Because the mapping function is simple and analytical, this method use an approximation to the "real" flux surfaces. The EPIC code, on the other hand, uses the "real" flux surfaces from an equilibrium code. However, the mapping to the orthogonal coordinates is only approximate. Because the the code algorithm demands that the grid directions be orthogonal: (1) the final solution mesh is only an approximation, (2) local grid refinements are inefficient, and (3) it is impossible to model nonorthogonal field line intersections with the vessel walls.

We have solved this problem by formulated the discretization in the finite volume context which is independent of the orthogonal conservation coordinates. As a result, there is complete flexibility in the positions and sizes of the small volume elements that make up the computational domain. This allows arbitrary packing of cells only around the regions near walls and target plates that need to be resolved. The new scheme can now also properly "wrap" the domain where necessary for the circulating flow inside the separatrix, that is, in the same simulation, one can allow for the inboard, outboard, and private flux regions. Earlier codes do not have this dual functionality, and couldn't, for example, accurately simulate the "shear" region near the separatrix. Since the field strength and orientation is specified individually for each of the volumes, there is no need to align the grid exactly along the magnetic flux surfaces. This becomes important where there are poloidal field nulls or steeply angled flux surface interfaces. That is, the new code can solve for plasma conditions near the × point. Here, the older "orthogonal" codes cannot predict plasma behavior with sufficient confidence because they usually have to extrapolate from a position far upstream where the grid can terminate orthogonally. The oblique geometry presents no exception in our method, and is handled quite naturally. With the generalized system, automated accuracy improvements are easily obtained with the use of modern adaptive meshing algorithms that are based on solution gradients. These can be employed without explicit regard for the specified magnetic field orientation.

The high flow regions in a tokamak are usually near the wall where there are steep gradients in the fluid properties. But these are also the most important regions to accurately resolve with an edge model. Purely explicit time stepping schemes might require as many as 10 million time steps for a reasonable time-dependent calculation. The computational fluid dynamics limit for numerical stability is most extreme in the smallest of the grid elements. Because our aim is to extend the plasma modeling capability to desktop workstations, we have constructed a discretization that is fully implicit. The time-stepping can be instead adjusted to capture only whatever physical coupling there is in the solution, and one doesn't need the high speed of a supercomputer.

Ease of use

A major difficulty with the present edge-plasma simulation code is that using them is an art by itself. It is very difficult to set up the proper mesh and because the numerical algorithms are not robust, parameters has to be fine tuned before a converged solution can be found. All of this has to be done on a supercomputer which is very slow in an interactive mode. As a result, each solution takes a long time to develop. Our plan is to implement the code on a desktop workstation which surpasses the supercomputers in the interactive mode. Furthermore, the X window graphical interface which is available on present workstations will drastically improve the efficiency of setting up the problem and analyzing the output results.

Improved physics

Introduction of improved physics models into the first generation codes have been hindered because the numerical algorithms used in these codes are not robust. Furthermore, the nature of the discretization in these code introduce errors which can be significant specially near the plasma facing components. With these issues addressed and resolved in our new code, we will be able to include improved physics models.

Our goal in this area include: (1) implementation of a multi-species, multi-energy group neutral transport package in order to address the recycling effects accurately, (2) addition of strong neutral/plasma interaction in the plasma transport equations in order to model gaseous divertors, (3) generalize the basic plasma transport equations to include active means to control the SOL utilizing our work in plasma biasing and RF ponderomotive forces, and (4) improving the basic fluid equation to include features like plasma pressure anisotropy.

IV. Engineering Design of In-Vessel Components

In collaboration with scientist of JAERI, we have started research activities in thermostructural design of plasma-facing components and analysis of the impact of hard disruptions. A study of the response of ARIES-I divertor plates to hard plasma disruptions were carried out by Dr. Hasan [9] using a code developed at JAERI. This analysis, although rigorous in terms of present-day understanding, underlined many approximations and limiting assumptions currently used. Developing a reliable engineering guideline/constraint in designing in-vessel components to withstand hard plasma disruption require further intensive research activity. In particular, lack of models and understanding of the formation and dynamics of the vapor shield and its interaction with the incident plasma particles, lack of models for the dynamic behavior of the melt layer with recoil and electromagnetic forces in addition to buoyancy and surface tension and the stability of this melt layer, and the absence of adequate experimental data base for verifying theoretical predictions are identified as critical areas that require further research.

We have also studied convective heat transfer in actively-cooled plasma facing components for various type of coolants (including MHD effects) [10,11]. Currently, thermostructural analysis of actively-cooled plasma facing material assumes a constant heat flux on the coolant channel. Our numerical analyses, however, shows that because the heat flux on a coolant channel of a plasma-facing component various circumferentially, the maximum structural temperature can be underestimated by 40% to 70% which can drastically alter the design of the plasma-facing components.

We propose to continue this activity for the coming period. Under an agreement between UCLA and JEARI on power reactor studies, each year, a JEARI scientist is stationed at UCLA for one year. Traditionally, the JEARI scientists stationed at UCLA have been expert in thermal hydraulic and heat transfer. As a result, our small activity in this area has been and will be highly leveraged.

V. Collaboration with Other Programs/Institutions

An important goal of the PMI theory/modeling effort at UCLA is to provide a sound theoretical framework which can explain the experimental observations. This framework can then be utilized to improve the effectiveness of impurity control system for future experiments and reactors. Our collaboration with other programs and institutes, therefore, is extremely crucial to achieving this goal.

At UCLA, we continue to relate and test our theoretical models and innovative ideas to simulations in PISCES plasma-surface interaction facility and to CCT tokamak. PISCES plasmas are very well diagnosed and are ideal to test certain models and ideas and our close interaction with PISCES experimental group facilitates the interaction substantially.

Outside UCLA, we will continue our modeling effort for TEXTOR tokamak with ALT-II toroidal belt limiters and coordinate this effort with the UCLA experimental program on TEXTOR. Lastly, we continue our involvement in modeling effort for PBX-M biasing and RF ponderomotive effects experiments.

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