Final Technical Report for

FACETS (Framework Application for Core-Edge Transport Simulations)

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Abstract

The FACETS (Framework Application for Core-Edge Transport Simulations) project of Scientific Discovery through Advanced Computing (SciDAC) Program was aimed at providing a high-fidelity whole-tokamak modeling for the U.S. magnetic fusion energy program and ITER through coupling separate components for each of the core region, edge region, and wall, with realistic plasma particles and power sources and turbulent transport simulation. The project also aimed at developing advanced numerical algorithms, efficient implicit coupling methods, and software tools utilizing the leadership class computing facilities under Advanced Scientific Computing Research (ASCR). The FACETS project was conducted by a multi-discipline, multi-institutional teams, the Lead PI was J.R. Cary (Tech-X Corp.).

In the FACETS project, the Applied Plasma Theory Group at the MAE Department of UCSD developed the Wall and Plasma-Surface Interaction (WALLPSI) module, performed its validation against experimental data, and integrated it into the developed framework. WALLPSI is a one-dimensional, coarse grained, reaction/advection/diffusion code applied to each material boundary cell in the common modeling domain for a tokamak. It incorporates an advanced model for plasma particle transport and retention in the solid matter of plasma facing components, simulation of plasma heat power load handling, calculation of erosion/deposition, and simulation of synergistic effects in strong plasma-wall coupling.

1. Accomplishments

For the Grant period: February 15, 2007 through February 15, 2011, the work was conducted in the following four main areas: (i) development of an advanced transport model for hydrogen species in wall materials and the WALLPSI code; (ii) validation of WALLPSI against experimental data; (iii) testing the coupled plasma-wall modeling scheme; and (iv) implementation of WALLPSI into the FACETS framework.

The accomplishments in these areas are briefly discussed in the corresponding subsections. The results were reported in 21 oral and poster presentations (listed in Sect. 4) and 7 papers were published (listed in Sec.2). Two M.S. Thesis were defended by the UCSD graduate students (listed in Sec.3).

1.1 Development of WALLPSI code

WALLPSI considers transport of particles and heat in the material wall along coordinate x, the depth into the wall. Modeling wall segment (Fig.1) includes 1-D bulk and 0-D plasma facing surface (PFS) and coolant facing surface (CFS). The code distinguishes mobile, adsorbed, and trapped hydrogen on surfaces and in the bulk. Wall segment is covered with non-uniform mesh with ~1 A resolution near the surfaces. The code is multiscale, the shortest time is about a ns to describe collisions within continuum approach.

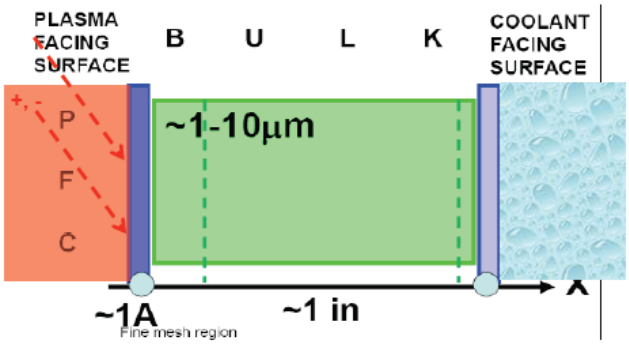

Fig. 1: Figure displays the modeling domain of WALLPSI code.

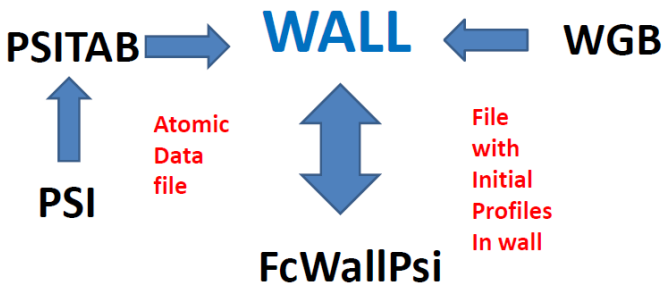

Fig. 2: Data flow in WALLPSI code.

WALLPSI code consists of five modules: PSI, PSITAB, WALL, WGB, and FcWallPSI. The data flow chart between modules is shown in Fig. 2. PSI module is the library of functions which compute thermo-chemical and radiative properties of different materials as well as rate coefficients for various thermal and collision elementary processes occurring in the wall. These functions are used in the PSITAB module which prepares the internal data correspondent to the user specified set of incident particles and wall materials. This module also performs averaging of collision cross-sections over the distribution functions of incident plasma particles. The data are then used in the WALL module, which solves the system of coupled nonlinear reaction/diffusion/advection equations. The WGB module stands to predict the initial hydrogen inventory based on discharge history. The FcWallPSI module is the interface developed according to FACETS standards. WALLPSI code is written in C language, except for FcWallPSI which is in C++ according the FACETS framework requirement.

For WALL module, an advanced set of coupled equations was derived for dynamical calculation of wall temperature, hydrogen wall inventory, and erosion/deposition rates [2.1]. It includes:

(i) 1-D conduction heat transfer equation;

(ii) 1-D diffusion-convection-reaction equation to calculate the profile of concentration of mobile hydrogen in the bulk of the wall;

(iii) 0-D reaction equations for concentration of hydrogen retained at the plasma-facing surface (PFS) and coolant-facing surface (CFS);

(iv) 1-D reaction equations for concentrations of hydrogen in the stationary intrinsic traps in the bulk of solid material (simultaneously up to 3 traps are included whose density profile, capacity and binding energy are prescribed);

(v) 1-D reaction-advection equation for density of broken bond traps produced by incident plasma particles in the bulk;

(vi) 1-D diffusion-convection-reaction equation for hydrogen concentration in the broken bond traps;

(vii) 1-D diffusion-convection-reaction equation for concentration of recoil atoms;

(viii) volumetric source of implanted particles and distributed collisional rate coefficients of various processes in the bulk, which vary with plasma parameters; and

(ix) 0-D equation for velocity of plasma facing surface movement which describes the material balance (net erosion or deposition).

WALLPSI model incorporates new approaches [2.1]: (i) modeling of dynamics and transport of specific traps produced due to chemical bond breaking and of hydrogen inventory in-there, (ii) non-diffusive transport of hydrogen species via convection directed toward the entry surface (PFS) in the implantation region due to nano-voids created by the incident particles for a ns or longer timescales, (iii) moving PFS interface, (iv) dependence of diffusion coefficient on hydrogen concentration and on degree of material amorphization, and (v) interface and infrastructure necessary for WALLPSI coupling to plasma transport codes. These approaches allow WALLPSI to simulate more confidently: highly non-equilibrium kinetics of hydrogen, retention and release of hydrogen species from room up to sublimation temperatures, rates for chemical erosion and radiation enhance sublimation (RES), wall pumping via co-deposition, and hydrogen saturated wall condition.

The Plasma Surface Interaction (PSI) module incorporates data on projectile particle interaction with different materials, e.g. back-scattering and sputtering coefficients, distributions of projectile particle flux, implanted particle source and recoil atom flux over the depth which are functions of incident particle energy and angle. The data (at present, the set involves H, D, T, He and impurities impinging on Li, B, Be, C, and W targets) were calculated for WALLPSI using the latest version of TRIDYN code, fitted, and tabulated. Interaction data were numerically averaged over distribution function of incident particles. This work was done by N. Moshman for his M.S. degree project [3.2] at UCSD.

We made use for FACETS of our newly developed code, the Wall Gas Balance (WGB) code [4.7]. This is multi-region multi-species 0-D transport code which calculates evolution of average plasma/gas parameters in the different regions (core/edge/divertor plasma regions, NBI volume, tokamak ports, pressure gauges, etc) and particle inventory in the material surfaces (chamber wall and divertor plates) during and between discharges following realistic experimental scenario. Validation of WGB included modeling of featured gas balance experiments in NSTX. Initial modeling results with WGB were presented on APS DPP [4.3] and ITPA meetings. In FACETS, the WGB code can be a separate run process used to calculate the approximate initial conditions in the wall according to particle/heat loading which then used in dynamic calculations by WALL module.

1.2.Validation of WALLPSI against experimental data

Several laboratory experiments had showed clear saturation of retained deuterium in beryllium and in graphite (e.g. pyrolitic graphite). In Ref. [2.1], we presented the results of simulations of static deuterium retention in graphite and beryllium with WALLPSI showing good agreement with experimental data (see Fig. 3). Here, deuterium is retained via collisional production of broken bond traps followed by population of these traps by deuterium atoms. The modeled saturated dose for deuterium in graphite is consistent with [D]/[C]=0.4, the measured concentration of statically retained deuterium averaged over the projectile range.

The work on validation of WALLPSI against experimental data from tokamaks and in-house divertor plasma simulator PISCES continues under another Grant [see A.Yu. Pigarov, P. Krstic, S.I. Krasheninnikov, R. Doerner, and T.D. Rognlien, Contributions Plasma Physics **52,** 465 (2012)].

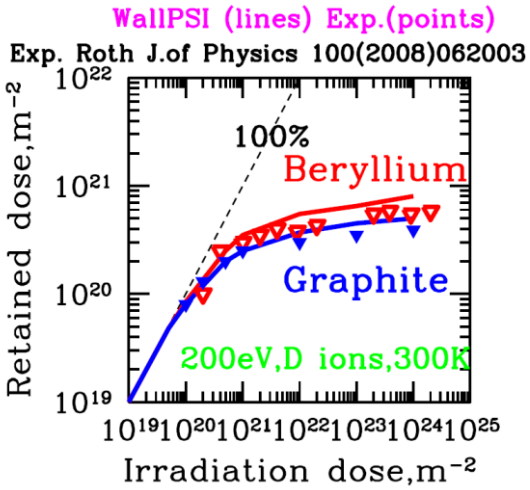

Fig. 3: Figure displays an example of WALLPSI code validation against experiments on room temperature retention of hydrogen isotopes in beryllium and graphite.

1.3. Testing the coupled plasma-wall modeling scheme

The coupled plasma-wall modeling scheme was first tested by calculating the inventory build-up of mobile, chemically bonded, adsorbed and trapped hydrogen in the wall as well as the nonlinear variation of hydrogen recycling coefficient in response to the incident plasma particle and energy fluxes [2.1].

In [2.1], we also calculated the mobile and trapped (covalently chemically bonded) deuterium inventories in graphite as functions of irradiation dose and surface temperature as shown on Fig. 4. As seen, at low wall temperatures and deuterium irradiation doses high enough for saturating the implantation region, the inventory of mobile deuterium is large and substantially larger than the inventory of trapped (chemically bonded) deuterium; that provides strong sensitivity of the deuterium output on the varying plasma conditions.

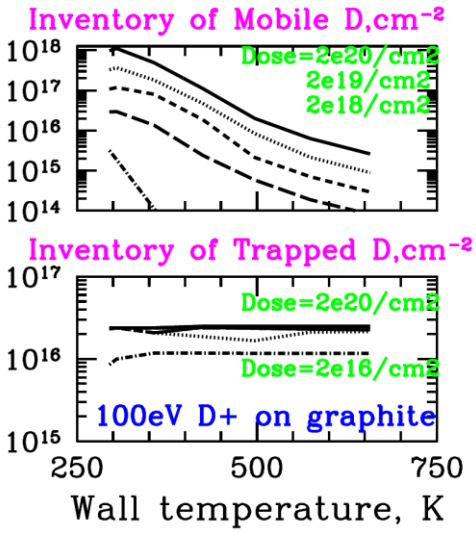

Fig. 4: Variation of mobile and trapped deuterium inventories in graphite with irradiation dose and wall temperature.

In order to study basic physics of plasma-wall interactions, WALLPSI was coupled to our newly developed EDGE1D code which is the 1-D edge-plasma transport code [2.1]. EDGE1D mimics the cross-field transport of plasma and neutrals in tokamaks with SOL by solving the system of 5 differential equations (for ion and neutral atom densities and for electron, ion and neutral temperatures). The code has been benchmarked against analytical solution derived in the case of one temperature, diffusion only, and plasma diffusivities are inversely dependent on the density.

The results of self-consistent plasma-neutrals-wall modeling were reported in Refs. [2.1,2.6] using WALLPSI/EDGE1D package and showing: (i) examples of strong plasma-wall coupling, (ii) nonlinear variation of wall hydrogen inventory and recycling coefficient with respect to incident plasma flux, and (iii) the featured plasma instabilities. For some wall materials (e.g. graphite) at low plasma heat fluxes (i.e. low surface temperatures), the hydrogen wall inventory built-up resulted in reaching the saturated hydrogen concentration in implantation region and in very high values of recycling coefficient and even >1 (the out-gassing case). Without external gas puff/pump stabilizing feedback, the out-gassing conditions resulted in formation of MARFE-like edge plasma.

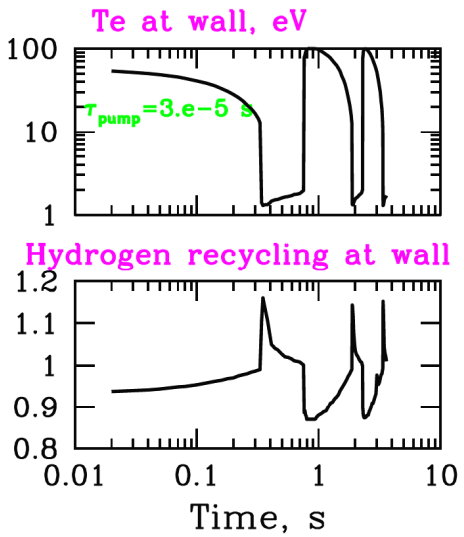

Fig. 5: Example of coupled WALLPSI - EDGE1D simulations showing the self-sustained oscillations of electron temperature near the wall (top) and deuterium recycling coefficient (bottom).

The modeled transitional effects include self-sustained oscillations in edge plasma due to switching from wall pumping to gas release as shown on Fig. 5. Here 15% variation in recycling coefficient corresponds to transitions between cold deeply-detached and hot sheath-limited edge plasmas.

We also continued theoretical analysis of thermal instability of plasma in contact with saturated wall initiated in our early work based on 0-D analytical model. This time, temperature perturbations of plasma and wall surface were analyzed based on a reduced 1D model showing conditions for features instabilities [3.1]. The case when the characteristic time for neutral atom release from wall is faster or comparable to the neutral transport time was considered. This work was a part of graduate degree project defended by I.V. Dobrovolskaia, the UCSD student supported from this Grant.

1.4. Implementation of WALLPSI into FACETS framework

In FACETS, the WALLPSI modules were auto-tooled, libraries were created, and internal plasma-surface interaction data files were generated for a number of test cases. WALLPSI component was added to the FACETS build system.

In 2009 FACETS formulated the requirements necessary for physics code to be the component (see https://www.facetsproject.org/wiki/InterfacesAndNamingScheme) and we

followed them with FcWallPSI module. This interface allows for component construction, initialization, and data dumping. It allows for communication of data between components. For time stepping the system, it allows for error, as in implicit advances a subsystem may not be able to take a step of requested size. It also allows for reverting to the previous state, as the failure to advance one component implies that all components must revert to the state at the start of the step prior to attempting a smaller step.

Firstly, the automated interface incorporating adopted naming scheme for data exchange between components was developed. The 0-D accessors in WALLPSI input the specific heat fluxes and fluxes of incident particle species and pass the output fluxes back to FACETS (i.e., UEDGE). Secondly, the C++ driver employing specified interface methods was written. Thirdly, since there will be multiple WALLPSI instances in FACETS (running in parallel for wall segments of modeling domain) , the interface was optimized in a 1-D accessor way to reduce the number of MPI calls. Fourthly, for data storing, managing and exchange, the WALLPSI is using its own built-in package FC (File Channel) and recently WALLPSI was modified to include the HDF5 technology which is adopted in FACETS. The switch allowing a user to choose between FC and HDF5 was introduced. Software for conversion between FC and HDF5 stored data was also developed. Next, the WALLPSI/FACETS interface is complex since it requires to manipulate with input/output data (e.g. via re-absorption of thermal radiation and emitted electrons, via various emission sources, and via plasma sheath model). Specific recycling coefficients and standard electrostatic plasma sheath model were implemented. Finally, the test case using C++ interface driver to calculate the single wall segment response to ELM-like plasma pulse was tested and was employed for FACETS regression test system.

At present FACET has the infrastructure needed for coupling components either sequentially or in parallel. A component/coupler system allows coupled multi-physics simulations. Each component can be initialized on a separate set of processing elements (PE) and communication between nodes is handled by parent components using a client-server model as prescribed by an XML-like input file.

Then, the most efficient scheme of WALLPSI usage in the high-performance framework (Fig. 6) is the initialization of a number of WALLPSI instances covering each material segment of modeling domain, all running concurrently on separate PE (~200 PEs, in total).

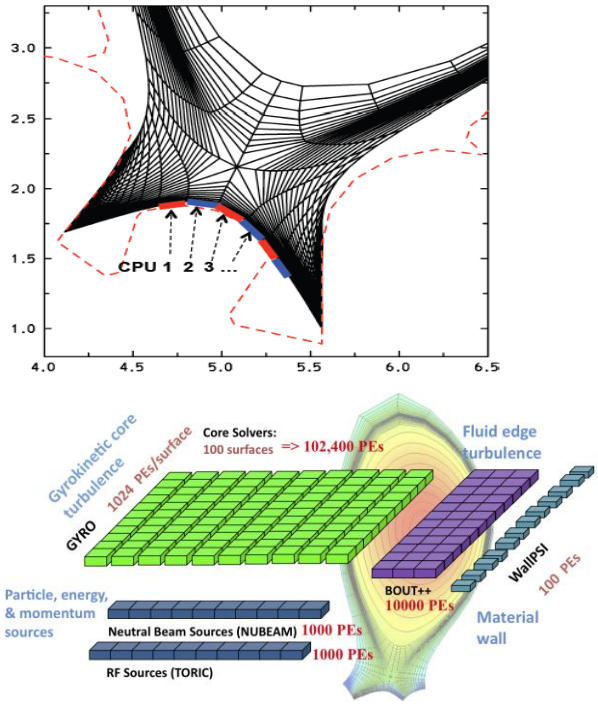

Fig.6: Scheme of WALLPSI application in FACETS. Each WALLPSI instance can run on different processors. Comparative PE load for FACETS components is shown in the bottom.

2. Publications.

[1] A.Yu. Pigarov, S.I. Krasheninnikov "Coupled plasma-wall modeling", Journal of Nuclear Materials **390-391**,597 (2009).

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4. Presentations

[1] S. Kruger, A. Pankin, J. Carlsson, J. Cary, A. Hakim, A. Pletzer, S. Shasharina, S. Vadlamani, R. Groebner, J. Callen, R. Cohen, T. Rognlien, T. Epperly, A.Yu. Pigarov, "Current and Future Computational Studies of Tokamak Transport Using the FACETS code", International Sherwood Fusion Theory Conference (May 2-4, 2011, Austin, TX) P3-13.

[2] A.Yu. Pigarov, "Modeling of hydrogen dynamics with coupled plasma-wall transport codes", 19th international Conference on Plasma-surface Interactions (May 24-28, 2010, San Diego, CA) P2-58.

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[14] S.I. Krasheninnikov, A.Yu. Pigarov, et al., "Theory and Modeling of Edge Plasma Transport, Plasma-Wall Interactions, and Dust Dynamics", poster (TH/P4-20) presented at the 22-nd IAEA Fusion Energy Conference, Geneva (October 2008).

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