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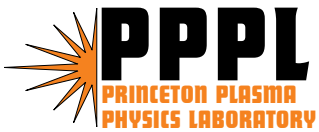
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Towards a Revised Monte Carlo Neutral Particle Surface Interaction Model

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Abstract

The components of the neutral- and plasma-surface interaction model used in the Monte Carlo neutral transport code DEGAS 2 are reviewed. The idealized surfaces and processes handled by that model are inadequate for accurately simulating neutral transport behavior in present day and future fusion devices. We identify some of the physical processes missing from the model, such as mixed materials and implanted hydrogen, and make some suggestions for improving the model.

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1   Introduction

The magnetic fusion community hopes to develop simulation codes with a predictive capability and use them to facilitate the design and operation of future devices, including burning plasma experiments. The principal embodiment of this desire is the Fusion Simulation Project [1], a $20 million per year undertaking to integrate existing models into a single entity. That many aspects of the component models will need substantial development is widely acknowledged. In particular, tokamak experiments have displayed a great sensitivity to the condition of the plasma facing surfaces [2] that is not directly reproduced by most simulation models.

Simulating the behavior noted in [2] with the DEGAS 2 [3] Monte Carlo neutral transport code would require empirical and even ad hoc modifications to the parameters it employs to control plasma-surface interactions. In fact, the models used to treat interactions of hydrogen atoms and molecules with material surfaces in DEGAS 2 are roughly twenty years old. During that period both theoretical and experimental advances have been made in our understanding of plasma-surface interactions. Moreover, the prodigious increases in computing power that have occurred simultaneously enable us to simulate plasma-surface interactions in great detail and to incorporate more complex models into codes such as DEGAS 2.

Present and envisioned computing resources are nonetheless finite; comprehensive, brute force approaches such as treating the entire vacuum vessel with a molecular dynamics model are far from practical. Instead, we need to develop reduced models that effectively bridge the gaps in time and length scales between those of the molecular dynamics codes and those of transport codes like DEGAS 2. An improved model would incorporate the additional parameters needed to specify the state of a particular piece of material surface in enough detail to yield a realistic, and perhaps even predictive capability. In this paper, we examine some of the pieces of physics to be built into such a model, making references to pertinent experimental results and to attempts at integrating those details into existing models. Since this is not a review paper, the literature citations are not intended to be comprehensive, but just illustrative.

2   Existing Model

Applications of the DEGAS 2 code to date have focused largely on hydrogen (e.g., see [4]). The plasma-material interaction processes used for such work are essentially as described in connection with the original DEGAS code [5], consisting of backscattering (also known as reflection), absorption, and desorption.

The backscattering process in which an ion or atom incident on a surface is reflected with most of its incoming energy is relatively well characterized [6]. The most general description is as a probability distribution $P(E_{in}, \theta_{in}; v, \alpha, \phi)$, where E_{in} and θ_{in} are the incident energy and polar angle respectively, and v, α, ϕ are the outgoing speed, polar angle, and azimuthal angle, respectively. Binary collision approximation (BCA) codes, such as

TRIM [6] can generate these distributions for almost arbitrary combinations of incident particle and target material. A compact representation of this probability distribution and an efficient method for sampling it have been developed for use in Monte Carlo simulations [5].

The absorption process is modeled in DEGAS 2 simply by a specified absorption probability. While this absorption fraction can vary in space and with species, its value must be specified directly by the user. The absorption characteristics of the material being considered must be somehow ascertained by the user and converted into a probability.

The fraction of the incident particle flux that is not reflected or permanently absorbed is assumed to be temporarily absorbed and subsequently desorbed, typically as a molecule [5]. In a time independent simulation, the interval between the absorption and desorption can be ignored. The outgoing particle has a thermal energy distribution at the wall temperature with a cosine angular or biased-Maxwellian [7] distribution.

The limitations of the existing reflection model are revealed by an apparent discrepancy in the expected trend of reflection coefficients at low incident energies. Eckstein [6] holds that the reflection coefficient should decrease as the incident energy drops below about three times the surface binding energy; these low energy particles will likely be trapped at the surface. In contrast, Vietzke [8] shows experimental data in which the reflection coefficient is increasing as the incident energy is reduced.

The missing variable that might resolve the discrepancy is the surface concentration of hydrogen [9]. Namely, the simulations referred to by [6] assume pristine surfaces with no implanted hydrogen. On the other hand, the surfaces used in the experiments cited by [8] likely contained significant amounts of near surface hydrogen. In this case, a high reflection coefficient at low incident energies is plausible. A realistic treatment of reflection of such surfaces thus needs to take into account, in some way, the near-surface concentration of hydrogen.

3   Directions for Model Improvement

Plasma facing surfaces in present day fusion devices are "conditioned" via a variety of empirically developed techniques to optimize core plasma confinement and performance. Among those techniques are "discharge cleaning" and high temperature "baking". Both remove hydrogen and impurities from the near-surface region of the wall [10]. Particularly in the case of graphite surfaces, the resulting "clean" wall acts as a pump during subsequent tokamak operation, allowing greater control of the discharge density and, usually, improved plasma confinement. Wall coatings of low Z materials such as boron, beryllium, and lithium provide similar pumping capability, as well as acting as getters for troublesome impurities, like oxygen [10].

Being able to to simulate the wall conditioning processes themselves is not essential. But, we do need a plasma-surface interaction model that can reproduce the full range of wall behaviors, from treated to untreated. An even more capable model would allow the wall state to evolve from conditioned ("clean") to unconditioned ("dirty") as the implanted

hydrogen concentration builds up.

Erosion and redeposition need to be accounted for in an improved model. Physical and chemical sputtering by the plasma erode atoms from the material surfaces; those atoms are redeposited elsewhere, usually in films having structures and properties different from those of the substrate [10]. In the case of graphite, redeposition results in soft, amorphous carbon layers in low heat flux regions. Metal surfaces can also experience localized melting and re-solidification.

A realistic model of the plasma facing components thus needs to track, in eroded areas, the extent of the erosion and the resulting changes in surface structure. In areas of net redeposition, deposited layers should be characterized well enough to allow the plasma-material interaction processes occurring on them to be accurately represented (see, for example, [11, 12]).

Safety considerations place limits of the total amount of tritium retained in the vessel walls [10]. Being able to simulate the entrainment of tritium during redeposition would be very useful for estimating this tritium inventory. The presence of mixed materials, such as the use of beryllium, tungsten, and carbon in ITER, provides an additional degree of complexity [10, 11].

The relatively recent realization that plasma heat and particle transport to tokamak main chamber walls is intermittent or "bursty" rather than steady (see, for example, [13]) are additional complicating factors. Since the erosion process is nonlinear, the net erosion over a period of time may differ substantially from that predicted by a steady-state simulation based on the same time-averaged heat and particle flux [14].

Irradiation of plasma facing surfaces by fusion neutrons and fast alpha particles will lead to changes in structure and, thus, impact the hydrogen retention and diffusion characteristics of the materials (e.g., [15, 16]). Investigations utilizing fast ions from accelerators or fission neutrons, provide some insight into the nature of the changes brought on by irradiation. However, the combination of reactor relevant fluxes, energy levels, and realistic material compositions may only be achieved in a burning plasma experiment.

A qualitatively different model may be needed for simulating liquid surfaces, such as molten lithium, tin-lithium, or Flibe [17]. First, a variety of liquid configurations have been proposed. The simplest are stationary, thin (< 1000 Å) or thick [18] films. Flowing liquid surfaces, both thin [19] and thick, are currently being investigated for possible reactor configurations. Second, density stratification [17] can result in surface structures that are unlike those of the solid material, leading to corresponding changes in plasma-material interactions. Third, the process of evaporation [17] of the surface material must be considered. Finally, the presence of eddies and other motions generated in a flowing liquid will complicate modeling of the trapping and diffusion helium and hydrogen isotopes [17, 20].

Developing a model incorporating all of the above effects will undoubtedly take a very long time, if it is possible at all. The fundamental processes involved occur on femto-second time scales and angstrom length scales, both separated by many orders of magnitude from what is needed in a neutral transport model capable of simulating an entire fusion device for, say, an energy confinement time. Others have described the phenomena arising at each range of scales (micro-scales, meso-scales, and macro-scales) and the corresponding

hierarchy of tools available [21]. The model needed for use in a transport code like DEGAS 2 does not have to resolve the finest time scales and structures. Rather, the net effect of the processes occurring on those shorter scales should be incorporated into a reduced model that can be explicitly coupled into the transport code. For example, adjustable parameters in the reduced model could be calibrated to fit the results of more detailed simulations [21]. Of course, such parameters can also be chosen empirically to best match experimental results.

A key component of a reduced model would be a representation of the material state consisting of a manageable number of parameters; examples would be the substrate material, fraction of intermixed species, surface temperature, and trapped hydrogen concentration. While we might be able to compose such a (lengthy) list describing the effects noted in this paper, the more difficult task would be to isolate a subset of those parameters that permits the construction of a tractable, but realistic plasma-surface interaction model. For example, a simple approach to describing mixed material effects with a few adjustable parameters is already being pursued with the SOLPS code [22].

Incremental progress towards a more comprehensive transport-scale particle-surface interaction model, like that of [22], is entirely acceptable. Three other recent publications provide examples of this sort of development. First, Hillis [23] combined the EIRENE Monte Carlo neutral transport code with the WDIFFUSE model of hydrogen diffusion and trapping in a material to analyze deuterium - hydrogen exchange experiments performed on JET. Incident neutral fluxes and energies from EIRENE were input to WDIFFUSE, allowing the temporal and spatial evolution of the wall hydrogen isotope inventory to be modeled. The effects of possible soft, a-C:H deposited films were also included.

Mioduszewski and Owen [24] used a model equation and TRIM computed deuterium trapping rates to tabulate a recycling coefficient that was a function of particle fluence and plasma temperature. Spatially varying particle fluxes computed by the DEGAS Monte Carlo neutral transport code were then used to determine the evolution of the recycling coefficient with time. As expected, segments of the vacuum vessel became saturated (recycling coefficient going to unity) within a fraction of a second, while locations near the top of the vacuum vessel were essentially unchanged.

Third, Warrier et al. [25] have published subroutines implementing existing models for sputtering, chemical erosion, radiation-enhanced sublimation, backscattering and evaporation. The intriguing aspect of their package is that it includes a routine for solving a 1-D heat diffusion equation so that the surface temperature can be estimated; the surface temperature is needed to evaluate the rates for chemical erosion, radiation-enhanced sublimation, and evaporation. The models used in these subroutines would need continued development to provide the level of realism that we would like to have. For example, quantitatively estimating the surface temperature requires additional detail, such as 2-D heat diffusion, variations in thermal conductivity, and the effects of active cooling.

4 Improvements of Kinetic Details

Recent articles suggest improvements in the kinetic details of the plasma-surface interaction models employed in DEGAS 2. The fact that these are "details" implies that they may not have a significant impact on a given simulation. But, there may be situations in which they do affect the results. Moreover, the Monte Carlo algorithm permits these details and refinements to be included at little expense.

The sheath model used in DEGAS 2 is based on standard theoretical analyses of the sheath behavior [26, 27]. Presently, the principal output of the sheath model is an estimate of the sheath potential. When simulating recycling at a divertor target, an ion is sampled from a Maxwellian distribution at local ion temperature. The computed sheath potential is added to the sampled ion's energy to determine the energy with which the particle, assumed to be neutralized near the surface, strikes the surface. The angle of incidence is taken to be 90°. A more realistic model would incorporate the structure of the sheath in a highly inclined magnetic field [27, 28] and estimate the ion's angle of incidence [29].

Secondary electrons are generally ignored in simulations of plasma material interactions. If the material's secondary electron emission coefficient is known, their impact on the sheath potential can be easily included [26]. Schou [30] examines in detail the mechanisms giving rise to electron emission and presents some specific examples of data for these processes.

Newly developed diagnostic capabilities permit the vibrational and rotational distributions of hydrogen molecules to be directly measured (e.g., [31]). Since the vibrational and rotational state of the molecule impacts its dissociation energy and the rate with which it will generate diagnostic photons, e.g., H_α, detailed modeling of regions dominated by molecules requires consideration of these vibrational and rotational effects.

Developing a similar capability within the simulations requires not only implementing the collisional processes that affect the rotational and vibrational state, but also incorporating the vibrational and rotational distributions of molecules coming off of surfaces. Vietzke [8] notes that the existing model for desorption should yield a Boltzmann distribution of rotational and vibrational populations. More interestingly, though, he describes two other potentially relevant desorption processes having significantly different kinetic distributions from those of the basic model. In particular, both processes are expected to result in enhanced vibrational and rotational excitation. Additional theoretical and / or experimental investigations appear necessary to characterize these processes sufficiently to permit their inclusion in a comprehensive model.

Other kinetic details that should be included in a more complete model are the increase in the atom / molecule fraction coming off of the surface at higher temperatures (e.g., > 1100 K [31]) and the possibility of charged products from plasma-surface interactions [32, 33].

5   Conclusions

The particle-surface interaction models employed in DEGAS 2 should be updated. Incorporating the kinetic improvements noted in Sec. 4 will be straightforward. However, the variety of phenomena occurring in the walls of present and future fusion devices is dauntingly great. A tractable model capable of handling erosion, redeposition, mixed materials, hydrogen trapping, irradiation, etc. seems nearly inconceivable. Yet, incremental attempts [22, 23, 24, 25] at improving transport models should help to identify the most relevant phenomena and provide insight into how they can modeled efficiently. The alternative approach of "scaling up" fundamental Molecular Dynamics simulations to transport-relevant time and length scales [21] will provide additional insight. The model utilized in transport codes twenty years from now could very well contain elements from both approaches. Additional and higher resolution diagnostic data, from fusion devices as well as laboratory experiments, will be essential for this development effort [10].

Acknowledgments

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