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Sensitivity of Rarefied Gas Simulations of Ground Tests to Gas Surface Models

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ABSTRACT

The space environment produces a number of performance challenges to satellite and spacecraft manufacturers that require measurements, including effects from hyperthermal atomic oxygen, charged particles, magnetic fields, spacecraft charging, ultraviolet radiation, micrometeoroids, and cryogenic temperatures. Ground tests involving a simulated space environment help explore these challenges, but also benefit from simulations that predict the anticipated physical phenomna, or help reconcile the measured observations to physical parameters. We present an update and application of a flexible multi-physics software simulation framework intended for predicting space environment performance and ground-test simulations of spacecraft. In this specific application we show how the energy dependent erosion yield may be applied with a rarefied gas dynamics simluation to aid comparison of terrestrial erosion rate measurements and on-orbit materials degradation.

Keywords: atomic oxygen, AO, materials performance, fluence, simulation, rarefied gas dynamics

1. INTRODUCTION

The space environment has a number of challenging aspects, including effects from hyperthermal atomic oxygen, charged particles, magnetic fields, spacecraft charging, ultraviolet radiation, micrometeoroids, and cryogenic temperatures.[1] Because of the significant resources involved in fielding spacecraft, satellite and spacecraft manufacturers and operators perform ground testing to ensure reliable performance in space.

Physics-based models can help testers knowledgeably interpret the responses of the spacecraft and the uncertainties in the measurements. Such models are important for several reasons. They can show the differences between chamber tests and true orbital conditions. Space environmental effects can be complex, involving multiple disciplines. And, the combined-effects of space environment stimuli may have synergies between effects that lead to nonlinear responses. Model-assisted experiment design and data reconciliation can improve interpretation and predictive capability.

To assist with these interpretations, we are producing a multi-physics software simulation framework that aids ground-test planning, interpretation, and reconciliation of measured data. Last year we reported initial progress[2] on the model framework that we call the Space and Chamber Effects Simulator (SPACES). Shown conceptually in Figure 1, SPACES is designed to take fundamental knowledge and a heuristic knowledgebase and build into higher levels of complexity, such as physics-based material response codes and full chamber simulation codes. A design goal for SPACES are that it be able to adapt to our evolving understanding of the system under test and to accommodate appropriate approximations, including several levels of physics from fundamental rates and parameters to space and test chamber simulations. The starting point for the effort has been a rarefied gas dynamics model for atomic oxygen exposures, which will be incrementally broadened with modules to address specific "multi-physics" phenomena.

In this paper we present an analysis that applies our research-grade SPACES code and still-disconnected code modules to a small problem for verification and testing. We consider the specific example of atomic oxygen erosion. Measurements[3] show that there is an energy-dependence of atomic oxygen erosion rates, and we specifically consider the fluoropolymers of Ref. 3. Through combining materials response characteristics with the rarefied gas dynamics modeling of space and chamber flows, we will elucidate some aspects of the relationship between the ground tests and on-orbit tests.

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Figure 2 shows our development roadmap. We are very early in the process. After initial Government-funded development, we are now leveraging a small internal research and development task.

2. UPDATES AND APPROACH

It is useful during development to apply the model to problems and analysis throughout development. Practical experience guides the interface development and keeps the software development and the scientific development in a tight feedback loop.

The application we consider in this paper is an atomic oxygen materials performance measurement. Tagawa *et al.*[3] measured an energy dependence in the erosion of certain polymers by atomic oxygen. This energy dependence suggests that erosion rate measurements and materials lifetime predictions will in general benefit from knowing the energy spectrum of the atomic oxygen impinging upon the sample. Additionally, consideration must be given to the potential for multicollision effects, because a build up of gases around the sample can alter the energy spectrum.[4]

We can apply the findings of Tagawa *et al.* through SPACES. This heavily employs our rarefied gas dynamics simulator. Described in previous work,[2] our rarefied gas dynamics model uses the direct simulation Monte Carlo (DSMC) approach.[5] In particular, we examine the gas collision environment around a 75-cm cube in LEO and make comparisons with a test chamber.

2.1 Energy-Dependence of Erosion Yield

We insert the erosion yield of a proposed fluoropolymer into our model network. We review the source of the data and how we adapted it to our model.

In Ref. 3 a quartz crystal microbalance (QCM) coated with a test polymer is exposed to atomic oxygen. A frequency increase of the QCM is proportional to the mass loss; the frequency is measured directly as a function of exposure time. The AO beam is a pulsed source that is specially equipped with a synchronous chopper. Through time-of-flight separation, the chopper passes AO with a very narrow energy distribution. The total fluence per pulse varies depending on the selected energy, so that time-changes in mass must be normalized to a constant fluence.

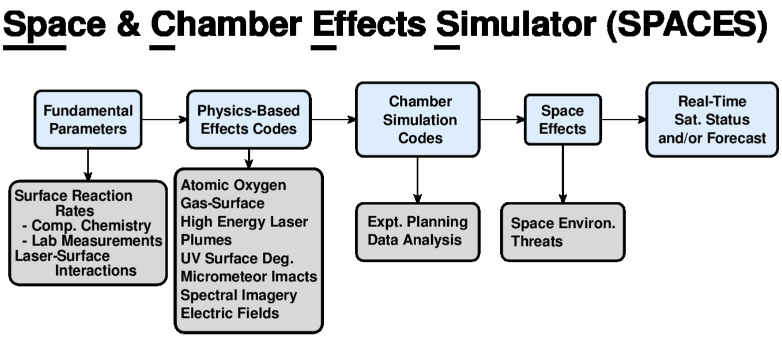

Figure 1. Overview of the SPACES development program, showing the evolution of scope as capability increases. From Ref. 2.

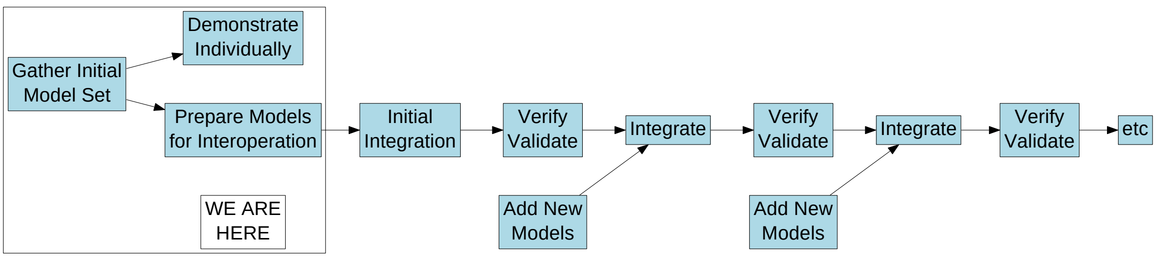

Figure 2. Overview of the SPACES development roadmap.

Figure 3 shows this normalized erosion rate of a fluorocarbon polymer as measured with a quartz crystal microbalance while the sample was exposed to the pulsed atomic oxygen beam at Kobe University. These data are in units of frequency change per fluence, and are proportional to mass change per fluence. Above 5 eV the data show a significant enhancement in the erosion yield of the atomic oxygen. The generally accepted Kapton H erosion yield is 3.00×10^{-24} cm^3/atom and is based on 4.5 eV of translational energy.

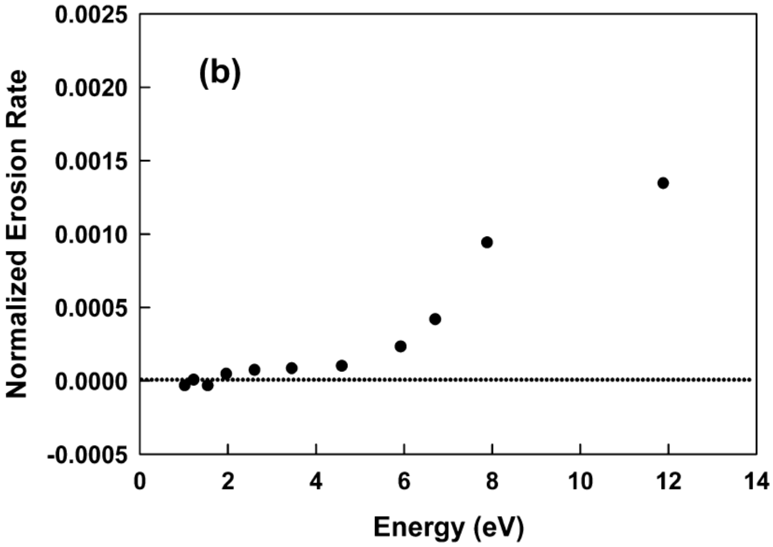

Figure 3. Normalized atomic-oxygen erosion rate of fluoropolymer as a function of atomic oxygen impingement energy. From Ref. 3.

We implement this relative erosion yield as a weighting function that translates each AO impact into an erosion. For our purposes we neglect the negative-slope data, where in the experiment mass is gained (potentially through oxidation) instead of lost; we interpret that as zero erosion. Although the absolute erosion yield for this specific fluoropolymer was not reported, we equated it to Kapton H at 4.5 eV, which puts us in the right order of magnitude. Accordingly, the erosion yield function for this compound in SPACES has the shape of Figure 3 and is normalized to 3.00×10^{-24} cm^3/atom at 4.5 eV.

2.2 LEO (300 km) Environment Simulation

The MSISE90 atmospheric model[6] describes the LEO environment at 300 km altitude as principally (79%) neutral AO with some (17%) molecular nitrogen, with a total atmospheric density of 1.14×10^{15} m^{-3} and a neutral temperature of 1124 K. The relative velocity of the impinging gas centers around the orbital velocity of 7800 $m\cdot s^{-1}$ which, for AO, is a continuous 7.3×10^{18} $m^{-2}\cdot s^{-1}$ flux at about 5 eV. We neglect minor atmospheric species, and accordingly normalize the species mole fractions to 0.82 for O and 0.18 for N_2.

In the LEO environment at 300 km altitude, the mean free path of AO is about 2.4×10^3 m. However, because the spacecraft compresses the flow, and because we want to spatially resolve the flow surrounding it, the grid dimension is finer than the mean free path, and is shown in Figure 4.

Figure 5 shows the simulated energy distribution of particles impinging on the ram-facing side of a 75-cm cube at 300 km altitude. The model surfaces set for a diffuse reflective boundary condition with full thermal accommodation, and a surface temperature of 300 K. Figure 6 shows the centerline density profile of atomic oxygen for this system. There is a two order of magnitude enhancement in the AO density on the ram-facing side of the craft, followed by a rarefaction on the leeward side. The energy distribution is nearly perfectly Maxwellian, suggesting that despite the enhanced density, the multicollision effects are not important in this case. The energy distribution also has a width of 2 eV FWHM.

We can apply this normalized energy-probability distribution function to the energy-resolved atomic oxygen erosion yield to estimate the true erosion rate. We plot this in Figure 7 before integrating over all energies, to

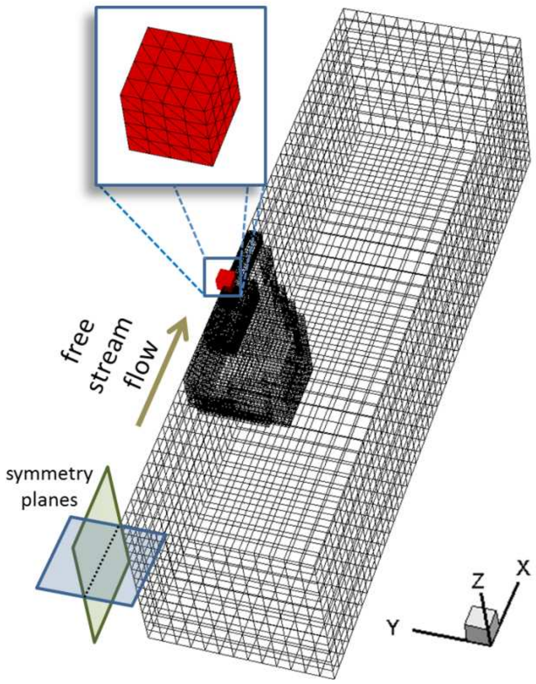

Figure 4. Simulation cell for orbit showing the DSMC grid (in black) and the solid cubic body (red).

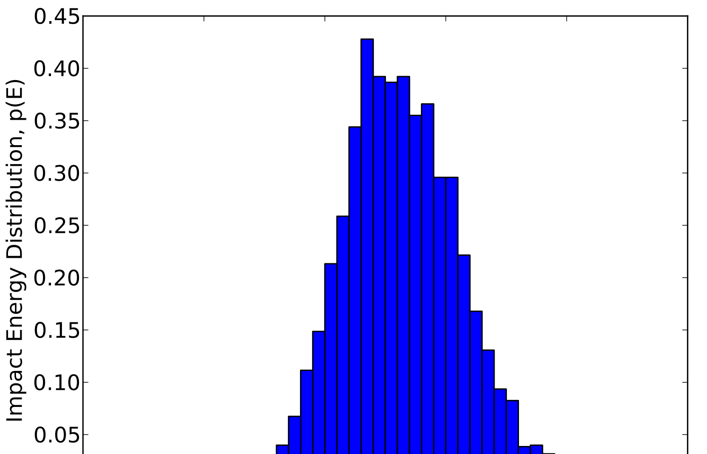

Figure 5. Energy distribution of the atomic oxygen impinging on a flat 75-cm square ram-facing satellite surface at 300 km altitude.

show the relative effect of AO fluence in each energy bin. The integrals show 2.9×10^{-30} m^3 erosion assuming a constant erosion yield, but 6.1×10^{-30} m^3—2.0 times as much—using the energy-dependent erosion yield.

2.3 Chamber Simulation

For comparison, we examine chamber conditions. We extracted the velocity distribution function at the test article surface from the calculations of Ref. 2. This is the STAT Spiral 1 test chamber (Figure 8) at Arnold Engineering Development Complex in Tennessee, as described in Ref. 7. We used the same physical model as before, except we changed the wall temperatures to 77 K. The test article remains at 300 K.

As presented previously,[2] for this calculation we took the atomic oxygen beam to be 90% atomic oxygen (AO) and 10% molecular oxygen, with an AO fluence of 7.10×10^{18} m^{-2} per 90 μs pulse at the nozzle exit. This produces a fluence at the target (60 cm distant) of 2.5×10^{18} m^{-2} per pulse. We used the nominal exit velocity of 7.3×10^3 m$\cdot$s^{-1}, nozzle half angle of 12.5° and a 23.0 cm beam diameter at the nozzle exit. The DSMC calculation was performed with a grid of 339200 cells, with a minimum cell dimension (near the AO source) of 0.024 m and a maximum of 0.17 m. The entire simulation fit inside a rectangular domain box of 6x4x6 m. The DSMC time step (resolution used to step molecules) was 1×10^{-6} s, which allows even the fastest atoms to have a residence time of three time steps inside of the smallest cells.

The atomic oxygen source is a pulsed laser-detonation source of the type used in several facilities.[8–11] It operates by charging a nozzle with molecular oxygen and then detonating it with a fast laser pulse. Figure 9 shows the propagation of a pulse against the target. In this case, much of the gas collides with the target, and some of it is able to bounce behind the target into the antechamber. Future enhancements to the model will include details regarding pumping and interior surface temperatures, so that we can realistically follow the gas from introduction to exit, and begin comparing the model to measurements.

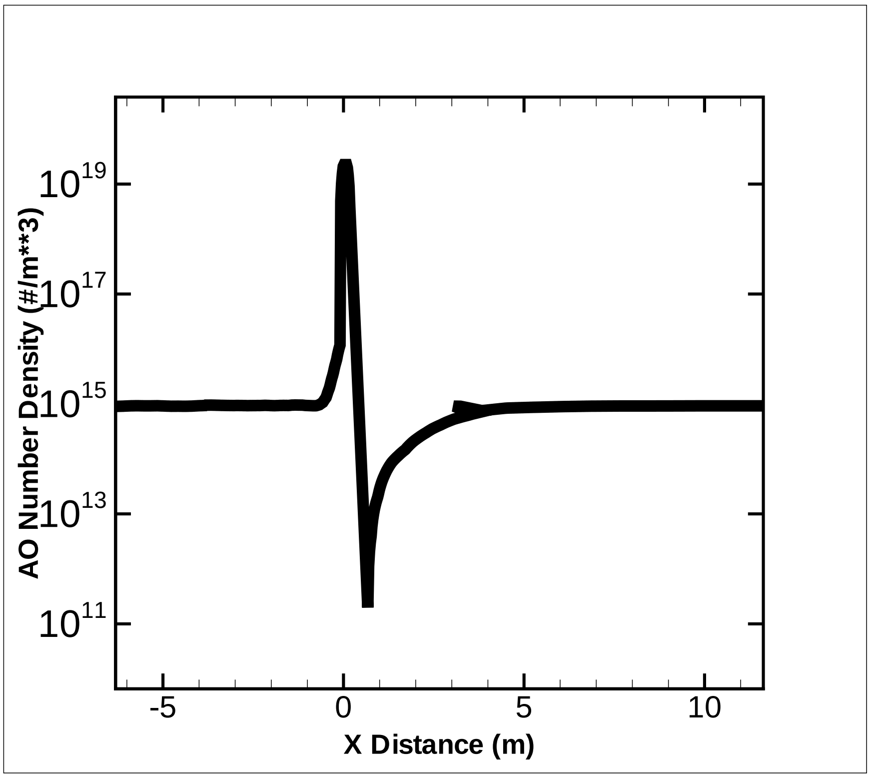

Figure 6. Density of atomic oxygen around a simulated 75-cm cubic satellite at 300 km altitude. We are moving with our 0.75 cm cubic satellite, so that in the graph the atmosphere would be moving left to right.

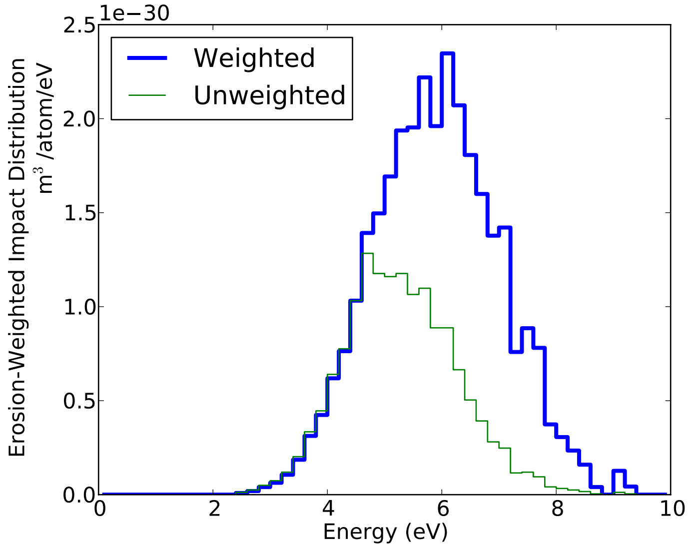

Figure 7. Computed erosion yields as a function of fluence in each energy bin, for atomic oxygen impinging on a flat 75-cm square ram-facing fluoropolymer satellite surface at 300 km altitude. The unweighted graph represents the outcome if the erosion yield were truly energy-independent. The absolute vertical scale is notional, tied to Kapton at 4.5 eV, and is suitable only for comparisons with the same scaling.

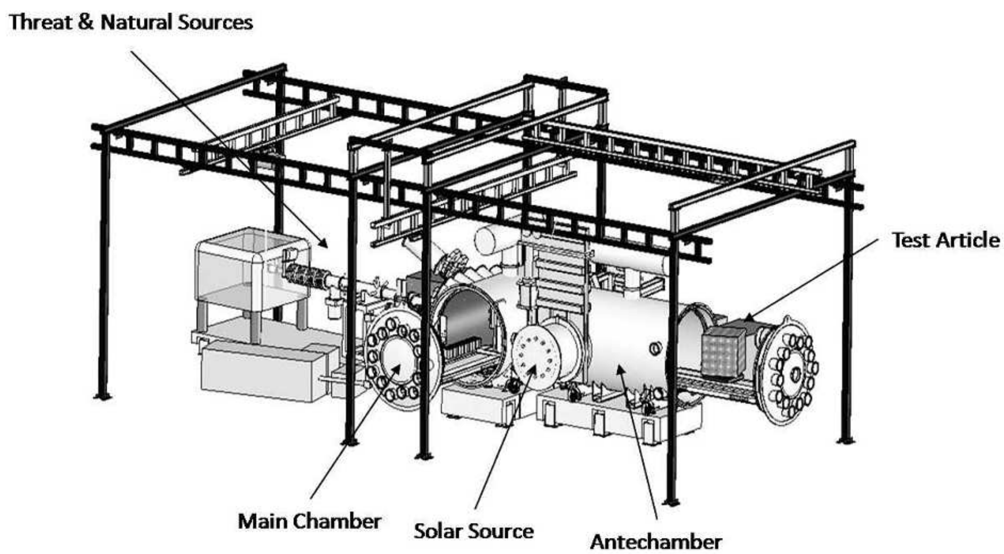

Figure 8. The STAT chamber, as depicted in Ref. 7.

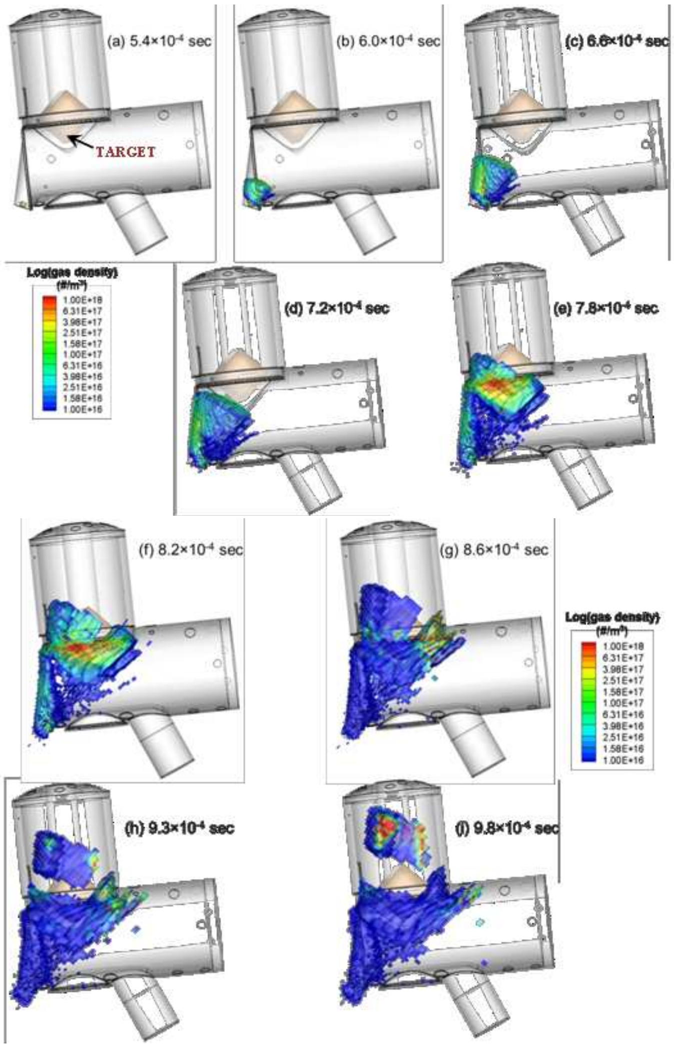

Figure 9. Time-dependent propagation of a gas pulse in STAT with a target present. The selections of time slices to display are arbitrary, for purposes of illustration. From Ref. 2.

Figure 10 shows the energy spectrum of gas reaching the test target surface. The main peak near 4.8 eV is orders of magnitude higher than any other contribution; i.e. the source is monochromatic in energy. Because of this, the enhancement due to energy-dependent erosion yield is just a multiplier. In this case, the yield-weighted erosion is 1.2 times the unweighted erosion. This has contrast to the on-orbit case where the weighted erosion was 2.0 times the the unweighted erosion.

The narrowness of the energy spectrum in our model is somewhat artificial, because of limited fidelity of our AO source model. A similar source at Montana State University was modeled[4] with a 1 eV FWHM velocity distribution. Depending on operating point both the mean and the spread in energy in these laser-detonation sources can be altered. This further adds complications that should considered when reconciling data or planning a test.

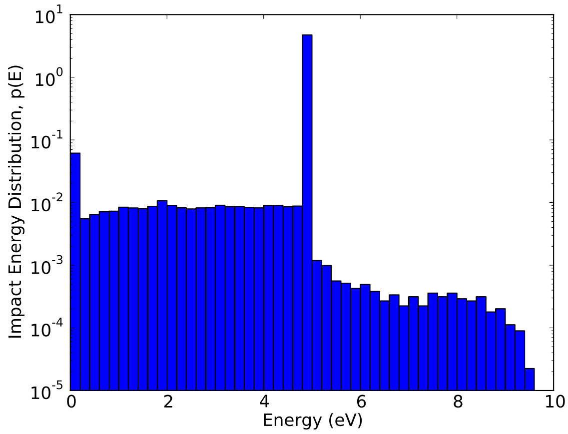

Figure 10. The energy spectrum of the fluence to the target, from a SPACES simulation, on a log scale. The log scale is used to show the the rarefied gas model does show a small multicollision effect.

Figure 11 shows the erosion yield for the chamber, for the hypothetically monodisperse model atomic oxygen source. Regardless of the energy spread, the peak of the function lies near an inflection where the erosion yield is beginning to increase. The erosion yield, whether forward-predicted, or reconciled data, will be sensitive to how the experiment is carried out.

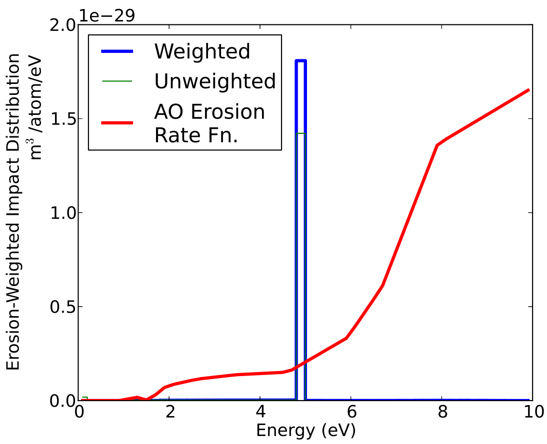

Figure 11. The erosion yield of the atomic oxygen on target, as a function of energy bin, from a SPACES simulation. The erosion yield of Ref. 3 is superimposed for reference.

These behaviors suggest several things. Knowledge of the energy dependent erosion yield for a material enhances understanding of the correspondence between orbit conditions and terrestrial tests. A beam source that is crafted to match the equilibrium energy distribution in orbit will have the highest fidelity erosion measurements, provided that multicollision behaviors do not degrade the energy spectrum. Finally, it may suggests a two-material QCM apparatus, where materials of different energy-dependent erosion behaviors are exposed simultaneously, may be useful for checking the AO source energy spectrum.

3. SUMMARY AND FUTURE WORK

A new multiphysics modeling framework is being developed specifically to support combined space environment effects tests and spacecraft development. The framework is designed to leverage existing scientific models as much as possible while facilitating communication between them, so that a physically consistent description of spacecraft–environment interactions may be developed. The model tool will allow for comparing test-chamber conditions with on-orbit conditions, and will enable development of an understanding of the limits of the approximations made in ground tests.

The fledgling model was applied to some baseline calculations to verify proper operation and to provide analysis. The application of the energy dependent erosion-yield to the DSMC-based rarefied gas model, for simulated systems both on-orbit and in-chamber, showed a sensitivities to the energy-dependent AO erosion yield of the material, and a conjugate sensitivity to the ground-based atomic oxygen source energy spectrum. Although we did detect multicollision effects in the chamber simulation, they were orders of magnitude lower than the main fluence energy peak. For this single-pulse and on-orbit calculation, the sensitivity to multicollision effects was negligible.

There are several plans for future work, including:

- user-selectable energy distribution in the AO source
- modularization of software units
- integration of modules through the DAE solver

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