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Simulation Framework for Space Environment Ground Test Fidelity

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ABSTRACT

We present initial work to develop an extensible model for spacecraft environmental interactions. The starting point for model development is a rarefied gas dynamics model for hyperthermal atomic oxygen. The space environment produces a number of challenging stimuli, including atomic oxygen, but also charged particles, magnetic fields, spacecraft charging, ultraviolet radiation, micrometeoroids, and cryogenic temperatures. Moreover, the responses of spacecraft to combinations or sequences of these stimuli are different from their responses to single stimuli.

New multi-stimulus test facilities such as the Space Threat Assessment Testbed at the USAF Arnold Engineering Development Complex make understanding the similarities and differences between terrestrial test and on-orbit conditions increasingly relevant. The extensible model framework under development is intended to host the variety of models needed to describe the multiphysics environment, allowing them to interact to produce a consistent unified picture. The model framework will host modules that can be validated individually or in combination.

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

1. INTRODUCTION

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. Because of the significant resources involved in fielding spacecraft, ground testing against these effects is desirable.

Physics-based models can help test consumers knowledgeably interpret the responses of the spacecraft and the uncertainties in the measurements. Breakdown of approximations and synergies between effects can lead to nonlinear responses that without appropriate calibration or model-based guidance can cause inaccurate test readings. For example, Ref. 1 shows that accelerated atomic-oxygen tests can produce multicollision effects that decrease the average surface-impact energy of the atomic oxygen fluence. Although individual space effects models exist, we are not aware of a comprehensive model for space effects or for test chambers.

We present initial progress to fill this gap with an extensible multiphysics model network. The model network is designed to adapt to different levels of understanding and/or approximations, including several levels of physics from fundamental rates and parameters to space and test chamber simulations. The starting point for the effort is a rarefied gas dynamics model for atomic oxygen exposures. We present the status of the model, the roadmap for its development, data needs, and likely validation pathways.

The context of the model construction is support for the Space Threat Assessment Testbed (STAT) program.[2] The testbed is analogous to a wind tunnel for orbiting spacecraft, and is capable of testing spacecraft performance with simultaneous combinations of the aforementioned space environmental effects. The STAT system offers stimuli that are representative of all of the aforementioned space-environment challenges. Additionally, sets of

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stimuli may be combined and/or sequenced, so that a test article may be exposed to environmental stimuli in the same combinations and sequences as found in orbit. Perhaps equally important is the capability for the STAT system to provide for multi-factor analysis, as the responses to sequences and/or combinations of stimuli can be systematically surveyed for correlation, competition, and synergy.

2. APPROACH

The model framework is called the Space and Chamber Effects Simulator (SPACES). Shown conceptually in Figure 1, it 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. After the main phase of development, the SPACES model could see a second application in predicting environmental effects on spacecraft and interpreting stimuli received on-orbit, or forecasting how a satellite may behave under the influence of a stimulus.

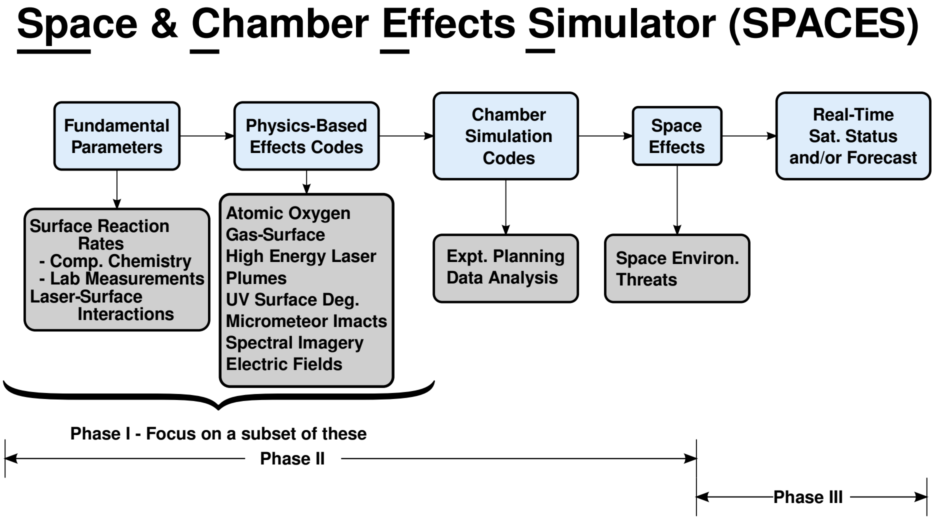

Figure 1. Overview of the SBIR program, showing the basic conceptual elements.

The program is funded through a Small Business Innovative Research (SBIR) contract, that provides two funded phases and a third unfunded phase. The program is now in between the Phase I proof-of-principle effort and the Phase II main development effort. The Phase I program focused on establishing the framework design and showing capability for modeling a single influence: atomic oxygen. The majority of the Phase I work is devoted to applying the rarefied gas model to the internal flow of atomic oxygen in the test chamber. There was also significant emphasis on making an architecture that is easy to extend to include other models.

Phases II and III will incorporate additional physical models and will require more scientific investigation in the multiphysics synergies. With these additional models, SPACES will evolve into a mature predictive design tool as well as a testing analysis aid. The SPACES framework is designed to host, rather than usurp, the many validated models already in existence. As only a subset of the existing models are truly multiphysics, we anticipate that the work will be roughly equal measures of (a) incorporating and verifying individual models, and (b) validating multiphysics (sequential or simultaneous) effects. We anticipate using data from STAT as well as from space experiments and other experiments to validate the models.

3. FRAMEWORK DESIGN

The purpose of the framework is to support multi-physics interaction models. Figure 2 illustrates with a notional block diagram how stimuli might cause different physical phenomena in the multi-physics problem. There are many effects, and while the figure is very complex already, it is probably not complete. The software framework is designed for flexibility, and Figure 2 only serves as a guide to show the types and complexities of the interactions.

The responses to the environmental stimuli involve a wide variety of physical processes. Many or perhaps all of these processes, individually, have been the subject of scientific modeling at some level. Therefore a prerequisite for the framework is that it provide a way to communicate with the diversity of existing models. In our design, this prerequisite is addressed through the facilities available in the Python language. Although Python is not itself a high-performance computing language, it is both portable and a very efficient “glue” code. As we will describe later, Python will be used for top-level organization and data sharing, while we plan on performing the compute-intensive work in the existing C- and Fortran-based models.

In the Phase I work we reviewed several different designs: adaptations of large monolithic codes; designs based on Department of Energy libraries such as Cactus; usage of existing multiphysics codes. The considerations of ease of distribution, low per-user cost, and a desire to use the model from a desktop computer suggested a model that could be quickly and repeatedly used at low or medium fidelity, but that could incorporate large high-fidelity models and run on supercomputers when required.

3.1 Software Interfacing

There are several levels at which software can be interfaced to the SPACES framework. First we will describe the ideal situation then move toward how we handle decreasingly accommodative codes.

The ideal scientific-code *module* is a linkable code library with an application programmer’s interface (API) that supports programmatic setup, calculation, and breakdown, and allows for interrogation of the field values and boundary conditions. The ideal module also provides hooks for callback functions, so that external routines might contribute to the calculation of certain quantities. For example, the attenuation of UV light shining on

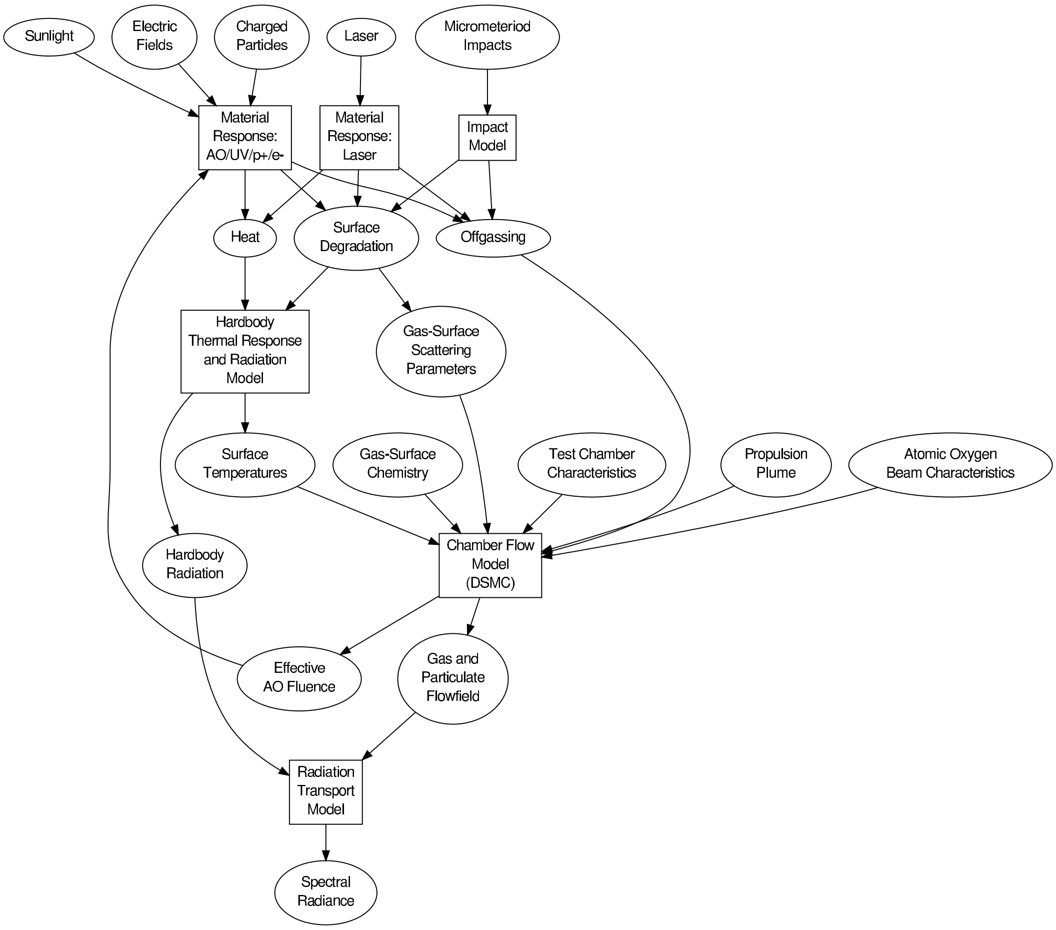

Figure 2. Notional block diagram of physical models.

a surface might depend on a far-field model of gases surrounding the test article plus a near-field model of gas-surface chemistry. The module would also generate its own spatial grid, or use and diagnose an externally-generated spatial grid. Truly ideal modules, if they incorporate multiple scientific concepts or correlations, would also provide separate interfaces for each. For example, a model for solar heating may include components having to do with solar illumination, surface reflectance, and internal heat conduction. It would be beneficial for SPACES to be able to access illumination, reflectance, and conduction individually.

However, we expect to find most models as being self-contained with source code available but not as a software library. The availability of source code allows many of these codes to be adapted into a library in a crude sense with minimal effort. A simplistic API, such as to facilitate setup, calculation, and breakdown, and something to transfer data into and out of the program, would be included. The level of effort to which the model is modified can be expanded as the importance of the model to the results warrants.

At the next level is a code that comes precompiled—one that is fast-running and serial, and can be repeatedly run in a subshell where its outputs are quickly parsed. A parallel code that is completely opaque may need special handling, or may not be compatible with SPACES. Some precompiled codes have controllable execution through files or POSIX signals, which could be beneficial. Depending on the specifics of the situation, some harder-to-handle codes might be run as a preprocessing step, to populate a lookup table.

3.2 Framework and Multi-Physics

A key objective of the framework is to access the information within each model, and communicate it between models in a physically consistent manner, such that synergistic effects among multiple stimuli on the test article can be simulated and understood. Additionally, the framework must be flexible enough to support models that are neither available nor known at the time of the framework design.

To accommodate this objective, we place a differential and algebraic equation (DAE) solver at the heart of the SPACES model. DAE solvers such as IDA in the SUNDIALS library[3] are robust and well-supported. Additionally, IDA is callable from C/C++ and Fortran, and has been bound to Python through programs such as PySUNDIALS[4] and PyDAE in DAE Tools.[5] The DAE solver allows us to bind the models together where they overlap: through shared fields, boundary conditions, and constitutive equations. Addition of a model to the network will require modification of the governing system equations, but this is primarily a scientific or engineering task in which a high-level equation set file is modified. Adding new models will require very limited changes in the SPACES framework itself.

Models to be integrated into the framework typically have their own time steps and spatial meshes. They are not necessarily constructed in a way that anticipates integration into a multiphysics framework. No matter the form, they all express a continuous function of position $\mathbf{x}$ and time t (generally, a time-dependent field function) at some sampled resolution. Therefore, the models that participate in the framework, if they have spatial or temporal resolution, will be interfaced such that appropriate information can be interrogated, shared between models, and potentially, reassigned.

The framework must also impose the appropriate global conservation constraints. For example, if one model indicates an exothermic surface recombination reaction ($2\ \mathrm{O} \rightarrow \mathrm{O}_2$), the gas model should receive information about the chemical conversion and the new number of gas molecules, and the thermal response model should receive the heat information.

3.3 Future Modules

Another objective is that the framework easily incorporate additional models. Members of our team also develop models for offgassing, cryofilms, and directed energy. While offgassing and cryofilms might be considered *friendly* to incorporate alongside a rarefied gas model, the directed energy model presents a very different profile. The integration challenge will be to adopt the physics represented by the model without significant software engineering.

For example, the Integrated Simulation of Laser Effects (ISLE) code[6, 7] solves a coupled problem of laser energy deposition and heat conduction into a solid surface, plus surface vaporization, absorption of laser energy by the vaporized surface, and reradiation of that energy. It is already very much a multiphysics model with several components that may need to be considered individually. Another candidate is a three-dimensional thermal analysis code[8] that provides a first-principles time-dependent description of laser damage. Again the model may have different time and length scales than the rarefied gas model, but must be able to share boundary conditions, constitutive equations, and some field variables (such as solid surface temperatures).

Consideration of these "foreign" models showed that the rarefied gas model would be an inappropriate choice as a host program. Rather it spurred the neutral-ground approach described previously.

4. APPLICATION TO ATOMIC OXYGEN

In low earth orbit, spacecraft encounter an atmosphere which although dilute, is traversed at such high speeds that over time significant external damage can be realized. The energetic impingement of atomic oxygen (AO) upon external spacecraft materials causes erosion and degradation in some cases and contamination of neighboring surfaces in others.[9–11]

The first application of the SPACES model is for modeling propagation of atomic oxygen. In its simplest form it is a "single-physics" problem, and because of that, it could be considered without the general framework we are developing. The model is a rarefied gas dynamics model that uses the direct simulation Monte Carlo (DSMC) method.

DSMC is a statistical method for solving the Boltzmann equation for gas flows.[12] It is particularly applicable to high Knudsen-number systems which cannot be treated by continuum methods, including both molecular beam experiments and Earth's atmosphere above 110 km. Using DSMC we can track the time-dependent evolution of a beam pulse as it impacts, envelops, and rebounds from a sample. DSMC can also be used to compute how the atmosphere interacts with a spacecraft in orbit. Outputs of DSMC calculations include 2D or 3D spatially-resolved gas density, velocity, temperature, and composition flowfields, gas-mediated energy transfer to/from surfaces, and surface reaction forces (drag).

We have multiple options for applying DSMC to vacuum chambers, molecular beams, and space simulations.[1, 13–15] In our DSMC calculations, we use the variable hard-sphere (VHS) potential model[16] to compute collisional cross sections.

$$\sigma = \sigma_{\text{ref}} \left(\frac{v_{\text{ref}}}{v} \right)^{2\omega} \tag{1}$$

Subscript "ref" denotes a reference value. Table 1 lists the VHS parameters for the species involved in these computations. These are derived from viscosity data[14, 17] with the constraint that the VHS exponent ω be constant at 0.25. (Note: Our ω corresponds to the v in Ref. 12's Equation 2.34.)

Table 1. VHS cross-section parameters, as evaluated from tabulated viscosity data.[14, 17]

	σ_{ref} 10^{-19} m^2	v_{ref} 10^3 m·s^{-1}	ω
N_2	3.54	2.13	0.25
O_2	3.17	1.98	0.25
O	1.75	2.49	0.25

Below, we principally consider a 300 km notional altitude, for test conditions and for on-orbit conditions. The MSISE90 atmospheric model[18] 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·s^{-1} which, for AO, is a continuous 7.3×10^{18} m^{-2}·s^{-1} flux at about 5 eV.

4.1 On-Orbit Conditions

As an example we show a calculation involving the 300 km altitude environment described earlier. We neglect minor atmospheric species, and accordingly normalize the species mole fractions to 0.82 for O and 0.18 for N_2.

The mean free path of species i passing through a mixture of species is:

$$\lambda_i = \frac{v_i}{z_i} \tag{2}$$

where the collision frequency of species i is

$$z_i = \sum_j n_j \langle \sigma_{ij} v_{ij} \rangle \tag{3}$$

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, the grid dimension is finer than the mean free path, and is shown in Figure 3.

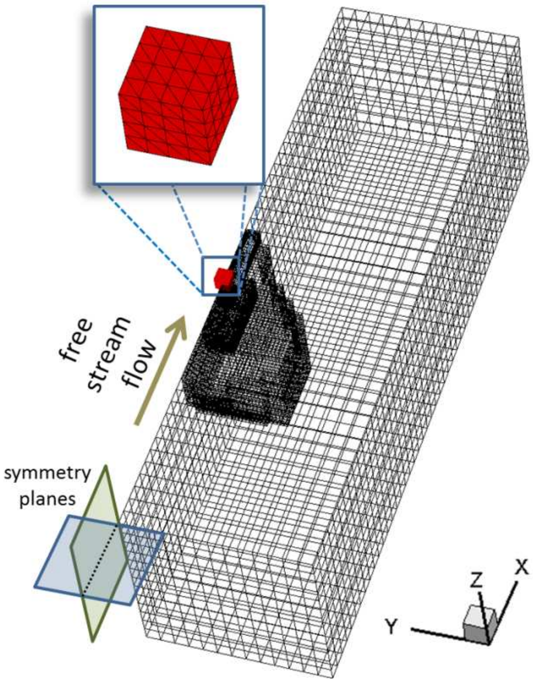

Figure 3. Simulation cell for orbit showing the DSMC grid (in black) and the solid cubic body (red).

The results are plotted in Figure 4. The flux to the surface is the same as the freestream AO flux: 7.3×10^{18} m$^{-2}\cdot$s^{-1}. Less than 1 in 1×10^4 molecules sees the surface more than once. The energy distribution of the molecules impacting the surface is Maxwellian at the expected 1124 K with a mean velocity (relative to the target body) of 7.8×10^3 m$\cdot$s^{-1}. Density at the forward-facing target surface is significantly enhanced (2.2×10^{16} m^{-3}, about a factor of 20) but the overall gas-gas collision frequency little more than doubles from the undisturbed LEO collision frequency of 5×10^{14} m^{-3}s^{-1}.

4.2 In-Chamber Calculations

Figure 5 shows the STAT Spiral 1 test chamber at Arnold Engineering Development Complex in Tennessee, as described in Ref. 19. STAT was designed with an atomic oxygen source that is typically pulsed up to order 0.1 Hz. The goals of this initial calculation are to apply SPACES to a faceted model of the chamber, show time-dependent propagation of the flow within the chamber, and compare to orbital conditions.RR

For our in-chamber calculations, we used a simplified solid model of the chamber. The DSMC modules of SPACES is capable of calculating flows around arbitrarily-shaped stationary and moving three-dimensional faceted hardbodies.

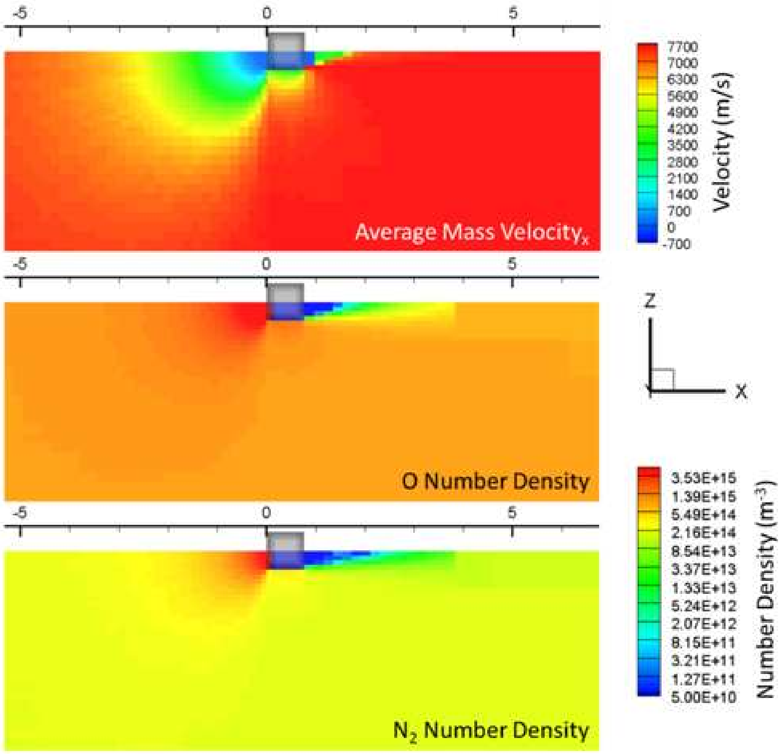

Figure 14. The steady-state flowfield for the 300 km case.

Figure 4. Simulation results for the on-orbit calculation.

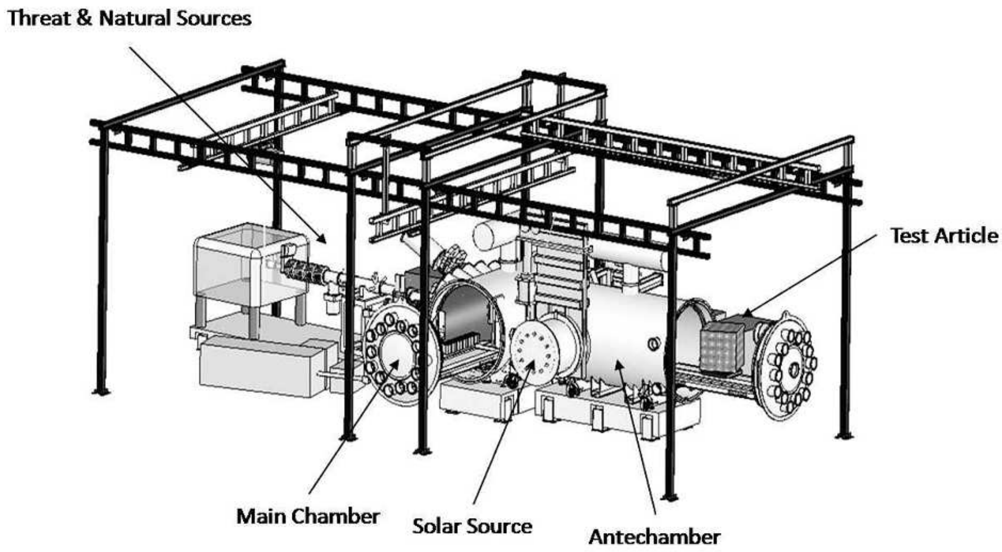

Figure 5. The STAT chamber, as depicted in Ref. 19.

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} $\mathrm{m{\cdot}s^{-1}}$, nozzle half angle of 12.5° and a 23.0 cm beam diameter at the nozzle exit. We also assumed a zero background pressure.

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 make three stops inside of the smallest cells. The walls were assigned a 300-K diffusely reflective boundary condition; this neglects potentially important features such as pumps and cryogenically cooled surfaces that may be present.

Figure 6 shows the propagation of a pulse of gas in the STAT chamber. The isocontour is drawn at a density of 1×10^{15} m^{-3} and is colored according to the gas translational temperature. The atomic oxygen source is a pulsed laser-detonation source of the type used in several facilities,[20–23] that operates by charging a nozzle with molecular oxygen and then detonating it with a fast laser pulse. In Figure 6a, the pulse front is first seen at the chamber inlet port that connects to the AO source. The beam is seen to expand in frames (b) and (c), perhaps being apertured somewhat in (c) by the main chamber, then finally striking the wall in frame (d).

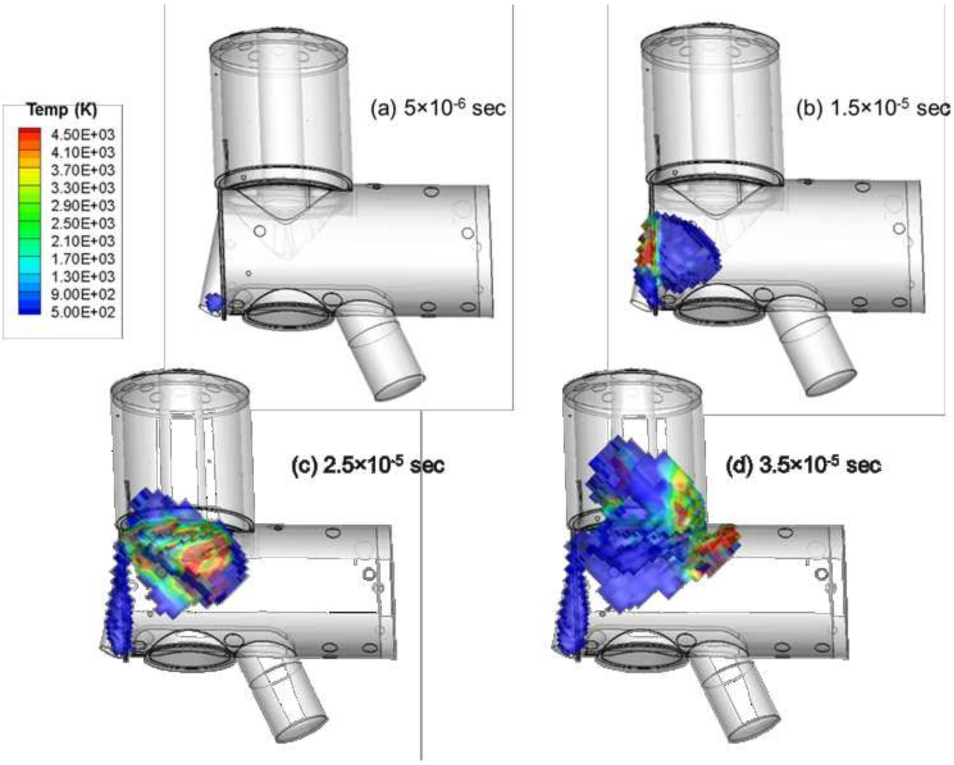

Figure 6. Time-dependent propagation of a gas pulse in STAT.

For the next phase of the demonstration, we insert a simple 30-inch cubic test article into the chamber. The article has its own 3D surface mesh (STL) file and can be placed in any arbitrary location and orientation in the chamber. The test article is positioned to protrude into the main chamber,[*] and is oriented to be approximately normal to the AO flux. We assigned the boundary condition to be a diffuse molecular reflector with thermal accommodation at a constant 300 K. Figure 7 shows the propagation of a pulse against the target. In this

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[*] We have since learned that test articles generally reside completely within the antechamber cylinder, which would be slightly farther from the AO source.

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.

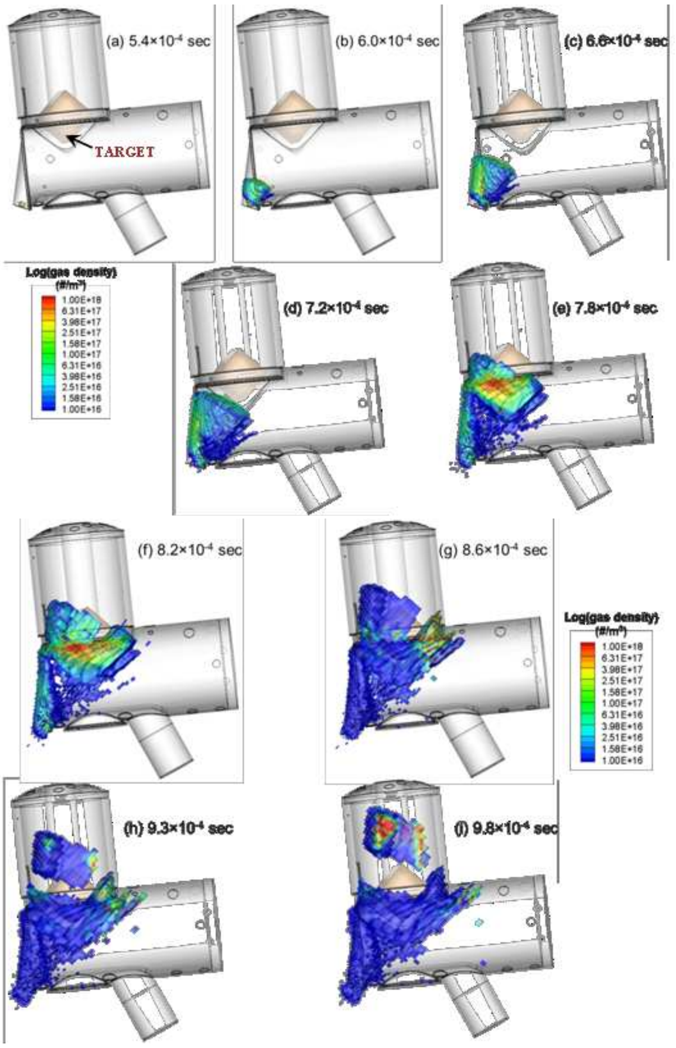

Figure 7. Time-dependent propagation of a gas pulse in STAT with a target present. The selections of time slices to display are arbitrary, for purposes of illustration.

The rarefied gas module in the SPACES framework provides potentially a wealth of information for general phenomenological understanding, performance prediction, and quantitative data reconciliation. Every spatial grid point include a time history of the composition, velocity, temperature, collision frequency, mean free path, molecular internal energy, and, if needed, chemical reaction rates. Every surface facet contains analogous information, also including collision rates and surface chemical reaction rates, plus heat and momentum transfer information. For example, in previous work involving similar modelling of 10 μs pulses in a system at Montana State University,[1] we were able to show how the impinging AO pulse density can affect the amount of energy transferred to the surface (Figure 8), and that this influences the fraction of the fluence that is actually erosive. This type of detail is typical in a DSMC calculation and can quickly be used to develop insights into the gas-dynamics aspects of chamber tests.

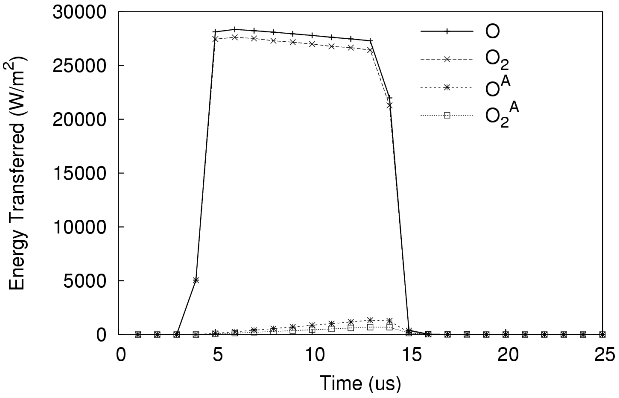

Figure 8. Translational energy deposited into the target. The nominal O fluence per pulse is 5.22×10^{17} m^{-2} in the left frame, and 5.22×10^{19} m^{-2} in the right frame. Superscript "A" denotes species that are returning to the surface after having struck it once once. From Ref. 1.

5. PATHWAY TO VALIDATION

A major effort in building such a model is continual and repeated validation. A multiphysics model such as SPACES will require not only validation of the individual single-physics models, but also compound validation of the combined effects. Even when each single-physics model itself has a rich validation history, the combined-effects possibilities are notably diverse.

The approach to validation will involve significant collaboration with the STAT chamber team, because this is one of the premier combined-effects systems. The predecessors to STAT, such as the Characterization of Combined Orbital Surface Effects (CCOSE) facility[24,25] may also have a role, as well as the community of facilities around the world. The validation of the models should also incorporate the knowledge gained from space experiments, such as MSX,[26,27] POSA,[28] LDEF,[29] and MISSE.

The development will be incremental and perhaps prioritized by the combination of the immediate data needs of the customers and the knowledgebase required to truly understand, interpret, and predict.

Because of the spatial aspect of the first module, there may already be a clear path to using the experiences of the MISSE experiment as a validation. The flight history and detailed geometry combined with the specific geometric features seen in the AO and UV damage may be a good starting point for validation of an AO damage or a combined AO/UV effects model.

6. SUMMARY

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.

As a first step, a rarefied gas model for atomic oxygen was applied. The pulsed hyperthermal oxygen beam was introduced into the 3D time-dependent model where the gases reflected off of the faceted chamber interior model surfaces. In addition to providing imagery of the propagating gas, the model provides other derived quantities such as energy transfer that will prove useful for understanding gas-mediated surface damage.

Model validation will be challenging and will proceed on an incremental basis, preferably on combinations as each model is added. There is already a wealth of validated models as well as true space-experiment data to draw from. The challenge is not only validation but usability and relevance. The initial priority will be on producing a framework, that by design is easily extended, but is initially deployed with limited capabilities that are useful and easy to exercise.

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