MACHINE LEARNING MODELS FOR THE PREDICTION OF SPACECRAFT CONTAMINATION FROM MATERIALS OUTGASSING  S. A. Cofer 1,2, A. Dias-Ribeiro 2,3, J. M. Alred 2, W. A. Hoey 2, C. E. Soares 2, 1 Department of Mechanical Engineering, Rice University, Houston, TX 77005, USA, 2 NASA Jet Propulsion Laboratory, Pasadena, CA 91109, USA, 3 ESA European Space Research and Technology Centre, 2201 AZ Noordwijk, Netherlands.

Introduction: Molecular outgassing is defined as the spontaneous evolution of a gas from a solid or liquid, often through dissolved gas molecules that diffuse to the surface of a bulk material and are then released. Polymers, for instance, can dissolve particularly large quantities of water vapor due to their amorphous structures, resulting in high outgassing rates. These volatile molecular contaminants may condense and accumulate on spacecraft surfaces under certain environmental conditions [1]. In contrast to particulate contamination, which refers to the deposition of micrometer scale conglomerations, molecular contamination does not have a definite length, width, or thickness. In most aerospace applications, even minuscule quantities of contamination through outgassing have been demonstrated to degrade the performance of spacecraft hardware [2]. Since UV radiation can cause contaminants to darken, molecular films even just a few hundred monolayers thick can significantly degrade instrument performance [3]. Thus, it is important to understand and mitigate the potentially detrimental effects of molecular outgassing in any spacecraft design.

Classical reaction kinetics describe molecular outgassing primarily as a first order reaction, where the reacting weight solution has an exponential dependence on time. While this modeling solution has proven accurate in homogeneous reactions, it is lacking in heterogeneous reactions where reactants are geometrically constrained [4]. When surface chemistry models are insufficient for contamination prediction, experimental data can be used to support mathematical model generation. ASTM E1559 is the standard U.S. test method for characterizing outgassing rates of spacecraft materials and focuses on molecular contaminant generation, migration, and deposition. This test method also allows for customized specimen and collector temperatures, material and test geometry [5]. Predictive outgassing and deposition models for specific aerospace applications can then be developed based on experimental data collection from relevant materials.

Because the Mars 2020 Rover mission aims to collect core and regolith samples for potential return to Earth, there are more stringent contamination requirements on Mars 2020 than any previous NASA mission. In the highest cleanliness zone used for sample collection, total organic carbon (TOC) must be kept below 10 ppb in the sample collection, and inorganic compounds must have a concentration no greater than 0.1% to 1% of their average concentration measured previously in Martian meteorites [6]. In addition to sample collection purity, UV Raman spectroscopy and fluorescence instruments on the Mars 2020 Rover are highly sensitive to contamination [7]. The unique challenges posed by the Mars 2020 Rover mission invite potential innovation in the area of contamination control.

However, the need for a predictive material model is not limited to the Mars 2020 Rover. As future missions become more sensitive to contamination, it will become increasingly necessary to make predictions on materials which have not been extensively tested or cannot be tested in the environmental conditions that they will experience. For instance, the Europa Clipper mission will face low operational temperatures and an intense radiation environment, making established methods of testing inadequate. The combination of high sensitivity experimentation with extreme environments for the Mars 2020 Rover, Europa Clipper, and Psyche missions creates an increased need for accurate predictions regarding material outgassing behavior. Therefore, the objective of this project is to develop a multi-species, material based model to predict the time and temperature dependent behavior of molecular outgassing for spacecraft applications.

Experimental Test Methods: The outgassing rates of the Mars 2020 Adaptive Caching Assembly (ACA) were determined following the ASTM E1559 protocol. This standardized test method was used to determine time and temperature dependence of outgassing kinetics [5]. For a wide variety of spacecraft materials, the ASTM E1559 has been applied to the largest known outgassing surfaces of the Mars 2020 Rover. However, collecting a full 72 hour isothermal outgassing curve for the entire rover greatly exceeded time and cost limitations, necessitating development of a data-driven outgassing model. In the ASTM E1559 test method, a material sample is held in vacuum conditions in a temperature controlled effusion cell. The sample is in view of several quartz crystal microbalances (QCM) held at various temperatures, and the total outgassing rate is calculated based on the frequency change of the coldest 80K QCM. Next, in the QCM Thermogravimetric Analysis (QTGA) test, the coldest QCM is heated.
gradually as the frequency continues to be measured, indicating mass loss from the surface of the QCM as various species evaporate.

**Activation Energy Determination:** While single species Arrhenius law fitting has been the previously accepted method for predicting the Total Organic Carbon (TOC) generated for the Mars 2020 Rover, the method assumes a single activation energy and does not account for the multiple species present in most spacecraft materials. The first step in feature analysis is to determine the activation energy distribution for a multiple species sample to correlate this distribution with an outgassing rate. In order to determine the activation energy distribution of each tested sample, an evolutionary algorithm implemented through PyGMO (Python Global Multiobjective Optimizer) was applied to fit multiple single species curves to the full QTGA curve. After generating random populations of alkane lengths $N$ and concentrations $C$, the algorithm reduces the root mean square error with each iteration by selectively choosing the best set of $N$ and $C$. Activation energies are then calculated according to the mass of each alkane. This conversion was determined through density functional theory (DFT) simulation of $n$-alkanes on a titanium nitride (TiN) substrate.

**Modeling Approach:** Figure 1 illustrates the general process for constructing a predictive outgassing model. The raw data from each material sample was collected through the standard ASTM E 1559 test method. The high dimensionality of the as-collected data makes it difficult to establish a strong correlation between a material and its outgassing behavior. Feature extraction through QTGA curve decomposition and principle component analysis serves to simplify the data set into the most meaningful components. Based on these extracted features, machine learning algorithms can be applied and then verified for accuracy within the training data set. Based on the cross validation accuracy of each model, the most effective combination of feature extraction method and machine learning model can be used to create a prediction.

**Results:** The current needs for spacecraft contamination control reflect two objectives for predictions that would be immediately beneficial for mission-specific applications. First, it would be valuable to expand on a temperature dependent model, extrapolating an outgassing curve to low temperatures present on other planets but challenging to replicate on Earth. Second, it would be valuable to predict a time-dependent isothermal outgassing curve for the Mars 2020 mission based on QTGA data, since the full isothermal test is prohibitively long and expensive for such a large mission. To create the outgassing curve prediction for the Mars 2020 Rover, the activation energy distribution was calculated for 112 material samples and used as training data. After parameter tuning, a random forest model with 24 activation energy bins and 1000 estimators was selected. The initial outgassing rate of the Mars 2020 Rover is known, so the model required only a single variable output of the outgassing decay rate. The final isothermal prediction for Mars 2020 was found to have a power law coefficient of -0.92 and a cross-validation accuracy of 35%. On a practical level, this means that the decay is primarily desorption limited (closer to -1) rather than diffusion limited (closer to -0.5), which is preferential for limiting contamination.

**Acknowledgments:** This work was sponsored by the Caltech Education Office through the Caltech Summer Undergraduate Research Fellowship (SURF) program. We thank the NASA Jet Propulsion Lab Contamination Control group in Division 353 for supporting this work. Special thanks to JPL mentors John Alred, William Hoey, and Carlos Soares.


![Fig 1. Schematic for predictive model development used to predict the Mars 2020 outgassing curve.](image-url)