Outgassing test methodology for contaminant emission model based on diffusion theory

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Abstract. Contamination is always troublesome in spacecraft development, but it has yet to be investigated because outgassing, transportation, deposition, and re-emission largely depend on spacecraft design. Designing spacecraft requires an accurate estimate of contaminant emission and deposition. Particularly for today's sophisticated spacecraft, analytical tools would be indispensable—but current simulations need to be improved. Our study addresses the first phase in the occurrence of contamination: improving the outgassing model. We focused on diffusion-limited phenomena because the diffusion rate of outgassing molecules in materials is thought to be much slower than their desorption rate at the surface. A new outgassing test method and analytical procedure was originally devised for extracting the parameters of the diffusion model. In comparing the desorption and diffusion models, we developed a model for the emission of outgassing molecules based on the diffusion theory and updated some functions of Japan's Spacecraft Induced Contamination Environment analysis software (J-SPICE). From this, we developed J-SPICE2 and installed the diffusion model to the software for calculating outgassing behavior. © *2021 Society of Photo-Optical Instrumentation Engineers (SPIE)* [DOI: 10.1117/1.JATIS.7.1 .018001]

1 Introduction

Molecular contaminants outgassed from organic materials are deposited on the solar arrays, thermal-control surfaces, and optical components of spacecraft. This can result in a severe degradation of the optical performance.[1–3] The selection of materials for spacecraft components and baking out of materials are important in avoiding such degradation. In addition, the amount of contaminant deposition and its influence on optical performance need to be estimated. It is important to estimate the amount of contaminant in ground tests and on orbit as accurately as possible. Several contamination analyses tools[4–8] for use in designing spacecraft have been developed toward that end, including Japan's Spacecraft Induced Contamination Environment analysis software (J-SPICE),[9–11] but these tools require considerable modification. A contamination analysis generally considers the effects of outgassing, transportation, and deposition, and uses several equations for modeling these phenomena. Current models still have room for improvement though. Consequently, we have tried to improve the modeling of outgassing phenomena that mark the first phase in solving a contamination problem.

It is still an open question as to whether outgassing is dominated by desorption or diffusion. The contamination sources considered in our study are such organic materials as cured adhesive, resin-coated wire, and thermal fillers. It has been reported that the theory of limitation by desorption could be a good model for explaining outgassing,[12] but because the diffusion rate of outgassing is much slower than the desorption rate at the material surface, we focused on

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diffusion-limited phenomena. For this paper, we therefore simulated the outgassing rate using both desorption and diffusion models, and then compared them. As is commonly known, diffusion phenomena follow Fick's laws of diffusion.[13] Outgassing behavior from the inside of materials was modeled by the diffusion equations (Fick's first and second laws).

In addition, the models must acquire the fitting parameters for each material that are necessary to simulate the outgassing. We devised a new test method for applying the diffusion equation to an analytical procedure for extracting those parameters. This done, we successfully modeled the emission behavior of outgassing molecules based on the diffusion theory.[14] The simulation results agreed well with the those of the experiment. In addition, we developed J-SPICE2, which applied the diffusion model for calculating outgassing, and we updated some of its functions. This paper briefly introduces J-SPICE2 and presents the emission model of outgassing molecules, how to extract the parameters for the calculations, the experimental method, and results.

2 Overview of J-SPICE and J-SPICE2

2.1 J-SPICE

Table 1 summarizes the specifications of J-SPICE as applied to contamination analysis. The input data include: the shape of the spacecraft, temperature of the emission and adhesion surfaces of contamination, type of material, trajectory of the spacecraft, and view factors between elements of contaminated surfaces and contamination sources. J-SPICE outputs the amount of contaminant deposition and the adhesion rate. The view factor is calculated by Thermal Desktop® (C&R Technologies, Inc.) from the shape of spacecraft. The amount of contaminant deposition and the adhesion rate of contamination, both output by J-SPICE, can be displayed graphically using Thermal Desktop®. Figure 1 shows the result[9] of contamination analysis for the Japanese Experiment Module (JEM) on the International Space Station.

2.2 J-SPICE2

J-SPICE had some issues that needed to be resolved. J-SPICE adopted the ASTM method as its emission model. The emission behavior is modeled by curve fitting the data exponentially and logarithmically as a function of a time, so the model has no temperature dependence on the outgassing rate. The simulation assumed that outgassing consists of one species from each material, although in actual practice, outgassing from a material consists of multiple species. We developed J-SPICE2 to solve these problems. Table 2 shows the differences between J-SPICE and J-SPICE2, the major modification being that the diffusion model described later has been incorporated as the emission model. In addition, it has functions such as calculating the bake-out effects and modeling the outgassing with multiple species.

Table 1 Specification overview of J-SPICE.

| Items	Brief specification
External software	Thermal Desktop®/AutoCAD
Input data	Shape, temperature, material, trajectory, atmospheric density, view factor, etc.
Configuration component	Rectangle/sphere/circle/ellipse/cylinder/conical surface/parabolic surface
Format of shape model	NEVADA
Analysis model	Emission model, transport model, and adhesion model
Output	Amount of adhesion (g/cm^2) and adhesion rate ($g/cm^2/s$)
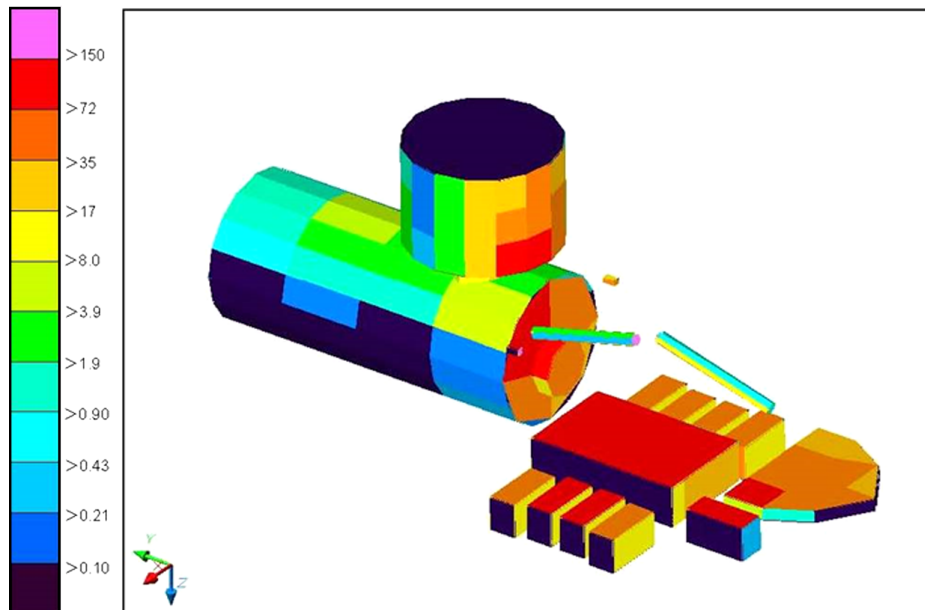
Fig. 1 Example result of contaminant analysis for JEM.[9]

Table 2 Differences between J-SPICE and J-SPICE2.

Items	J-SPICE	J-SPICE2
Maximum number of elements	5000	10,000
Parameter estimation tool	None	Available
Emission model	ASTM method	ASTM method Diffusion model (1D and 2D)
Temperature	Constant	Variable
Calculation of bake-out effect	None	Available
Sunshine/shade	None	Available
Number of outgassing species per one material	One	Multiple

3 Outgassing Model

Outgassing is usually described by a desorption model[12] or a diffusion model.[15] Of course, both models can be applied simultaneously. Figure 2 shows images of the desorption and diffusion models. In the desorption model, the outgassing molecules desorb at the surface of a material, with a uniform concentration distribution of outgassing molecules into the material. Conversely, the diffusion rate of outgassing molecules in the subject materials was considered slow, and the closer to the sample surface, the larger the reduction in the number of outgassing molecules in each material. Thus the concentration distribution of outgassing molecules is not uniform. We therefore address which model is better for simulating outgassing.

We will apply the terms "function" and "equation" to a model as follows: function is a solution of a differential equation of a model, and equation refers to the differential equation itself. Although equation is accurate, it is extremely time-consuming to numerically solve and difficult to estimate the probable fitting parameters described later without the appropriate initial values. Although function is limited in use, its calculation speed is faster than that of equation.
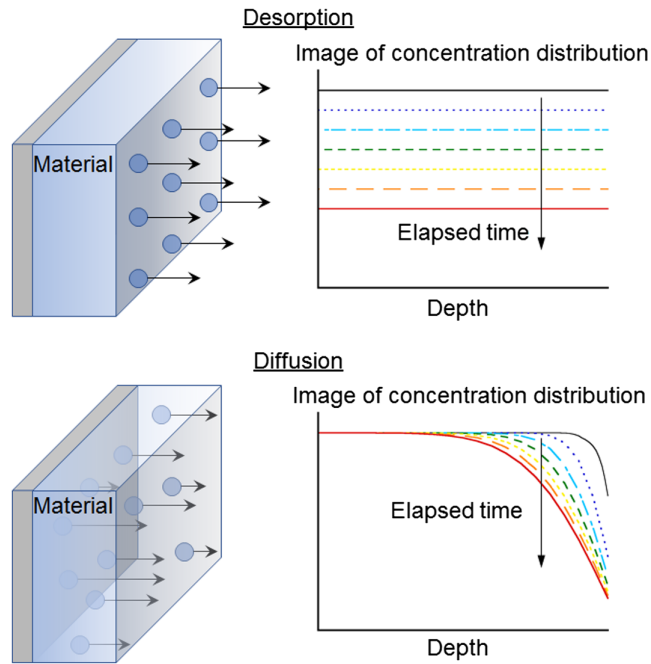
Fig. 2 Images of desorption and diffusion phenomena.

Thus we initially used function to estimate the initial fitting parameters and then employed equation to obtain the final fitting parameters and simulate the outgassing behavior.

3.1 Desorption Model

3.1.1 Function of desorption

This study assumes that heating a material causes outgassing, an emission phenomenon, and creates a contamination source. When the heating rate of a material is constant, the function of desorption for an arbitrary species is expressed by functions Eqs. (1) and (2).[16] The functions hold when the heating is started from absolute zero. The functions were fitted to the experimental outgassing data described later to estimate the fitting parameters M_0, τ_0, and E:

$$\dot{M}_i(T) = \frac{1}{\tau_{0i}} \exp\left(\frac{-E_i}{RT}\right) \cdot M_{0i} \exp\left\{ -\frac{RT^2}{\tau_{0i}\beta E_i} \exp\left(\frac{-E_i}{RT}\right) \Psi_i(T) \right\}, \tag{1}$$

$$\Psi_i(T) = \sum_{j=1}^{\infty} j! \left(-\frac{RT}{E_i}\right)^{j-1}, \tag{2}$$

where $\dot{M}$ is the outgassing rate (g/cm^2/s), M_0 is the initial amount of adsorption at the material surface (g/cm^2), τ_0 is the Arrhenius pre-exponential factor of surface residence time (s), E is the desorption energy (J/mol), R is the gas constant (J/K/mol), T is the temperature of the source of contamination (K), β is the heating rate of the contamination source (K/s), and i is the number of species.

3.1.2 Differential equation of desorption

For a temperature rise beginning from an arbitrary temperature, the differential equation of desorption for an arbitrary species is expressed by the following equations:[16]

$$\dot{M}_i = \frac{dM_i}{dt} = -\frac{M_i}{\tau_i}, \tag{3}$$

$$\tau_i = \tau_{0i} \exp\left(-\frac{E_i}{RT}\right), \qquad (4)$$

where M is the amount of adsorption at the material surface (g/cm^2) and τ is the outgassing time constant (s).

3.2 One-Dimensional Diffusion Model

3.2.1 Function of 1D diffusion

When the heating rate of a material is constant with time and the material thickness is small compared to the surface area and the effect of the sample edge is negligible, the function for a one-dimensional (1D) diffusion model with one arbitrary species can be expressed by functions Eqs. (2) and (5).[16] These functions hold even if heating were started from absolute zero and are used to estimate the fitting parameters of C_0, D_0, and E needed for fitting to experimental data described later:

$$\dot{M}_i(T) = \frac{2C_{0i}D_{0i}}{d} \exp\left(\frac{-E_i}{RT}\right) \times \sum_{m=0}^{\infty} \exp\left[-\left\{\frac{(2\ m+1)\pi T}{2d}\right\}^2 \cdot \frac{RD_{0i}}{\beta E_i} \exp\left(\frac{-E_i}{RT}\right)\Psi_i(T)\right], \quad (5)$$

where C_0 is the initial outgassing concentration in the material (g/cm^3), d is the sample thickness (cm) when outgassing from one side surface is calculated, D_0 is the Arrhenius pre-exponential factor of the interdiffusion coefficient (cm^2/s), and E is interdiffusion energy (J/mol).

3.2.2 Differential equation of 1D diffusion

When the temperature starts to rise from an arbitrary temperature and the material has dimensions much larger in both directions than the thickness, the differential equation of diffusion for an arbitrary species is expressed by the following equations:[13]

$$\dot{M}_i = -\frac{d}{dt}\int C_i dx, \qquad (6)$$

$$\frac{\partial C_i}{\partial t} = D_i \cdot \frac{\partial^2 C_i}{\partial x^2}, \qquad (7)$$

$$D_i = D_{0i} \cdot \exp\left(-\frac{E_i}{RT}\right), \qquad (8)$$

where C is the outgassing concentration in the material (g/cm^3), x is the distance from the sample surface (cm), D is the interdiffusion coefficient (cm^2/s) and t is the elapsed time (s).

3.2.3 Differential equation of 1D diffusion (constant temperature)

When a sample is much larger in two-dimensions (2D) than the thickness and the temperature is constant, the 1D diffusion model of an arbitrary species is expressed by Eq. (9).[13] Equation (9) calculates the amount of emission outgassed from one side of the plate sample. In addition, since the amount of outgassing is calculated when the temperature is constant, the equations can be used for evaluating the effects of bake-out.

$$M_i(t) = M_{\infty i}\left\{1 - \sum_{n=0}^{\infty} \frac{8}{(2n+1)^2\pi^2} \exp\left[\frac{-D_i \cdot (2n+1)^2\pi^2 t}{4l^2}\right]\right\} + c, \qquad (9)$$

where $M(t)$ is the amount of outgassing at elapsed time t (for emission from one side) (g/cm^2/s), and M_∞ is the initial amount of outgassing concentration in the material (for emission from one side) (g/cm^2). When outgassing from one side surface is calculated, l is the

thickness of the sample (cm). If the outgassing from two surfaces is calculated, l is the half thickness and double the calculation result $M(t)$. Here $M_\infty = C_0 \times l$. C_0 is defined in Eq. (5).

3.3 Outgassing Rate Experiment with Constant Heating Rate

To apply these equations, it is first necessary to obtain the unknown fitting parameters. Those parameters are obtained by fitting the functions or equations to the outgassing rate data. Figure 3 shows the apparatus used for outgassing rate tests. This apparatus is compliant with ASTM E1559.[17] A shroud cooled by liquid nitrogen is installed in the chamber, and an effusion cell containing a contamination source is installed in the shroud. By heating the effusion cell, outgassing molecules are effused from the open orifice on the top of the cell and adhere to a quartz crystal microbalance (QCM) set at a height of 150 mm. The QCMs are cooled to about $-193°$C (see Fig. 4). The outgassing rate is calculated from the adhesion rate of outgassed molecules on the QCM surface. As mentioned earlier, the desorption and diffusion functions hold when the

Fig. 3 The outgassing rate measurement apparatus.
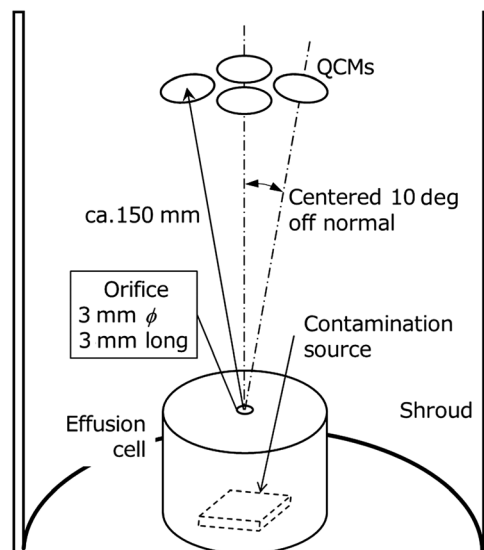

Fig. 4 Effusion cell and QCM locations.

heating rate of the contamination source is constant. A lower heating rate is desirable in order to distinctively separate the outgassed species due to differences in the needed temperatures. Considering the apparatus restriction and experiment time, a heating rate of 1°C/h was decided.

The sample used as a contamination source was a two-part silicone adhesive (RTV-S 691: Wacker Chemie AG). The mixing ratio was part A:part B = 9:1 by weight. The mixed material was cured at room temperature more than 24 h. The sample was 40×40 mm^2 and 2.0-mm thick. The sample was installed in the effusion cell so that is could outgas from both surfaces.

4 Experimental and Model Fitting Results

The shape and configuration of the orifice and QCMs were modeled for calculating the outgassing rate. We simulated the rate of outgassing effused from the orifice and deposited on a QCM.

4.1 Determination of Fitting Parameters

4.1.1 Desorption model

Curve fitting was performed using functions Eqs. (1) and (2) on the measured outgassing rate data to obtain the initial values M_0, τ_0, and E. Figure 5 shows the measured results. The measured outgassing rate decreased rapidly right after the experiment started, but later increased to 60°C. The outgassing rate was reduced again around 80°C then continued to rise with the temperature. The curve showed two peaks, each corresponding to an outgassed species. We see that peak 1 was assumed to exist above 125°C, whereas peak 2 was at around 60°C.

In the next step, the final M_0, τ_0, and E of all peaks (i.e., all species) were determined by the nonlinear least squares method while numerically solving Eqs. (3) and (4) using M_0, τ_0, and E previously obtained as initial values. The fitting result is shown in Fig. 5 and Table 3 lists the final fitting parameters obtained. As can be seen in Fig. 5, the fitting result and measurement result agreed well above 50°C although curve fitting was done on the data above 50°C to improve the fitting accuracy in that region. The fitted results deviated considerably from measured values below 50°C. In addition, the fitted initial value of adsorption (M_0) was ~0.1 g/cm^2, which corresponds to a thickness of about 1 mm—a physically impossible value. This indicates that the desorption model did not to correctly express the outgassing behavior.

4.1.2 1D diffusion model

The curve was fitted to the measured outgassing rate data using functions Eqs. (2) and (5) to obtain the initial values C_0, D_0, and E. Two peaks were assumed in this calculation, each corresponding to an outgassed species. Peak 1 was assumed to exist above 125°C, whereas peak 2 was at around 60°C.
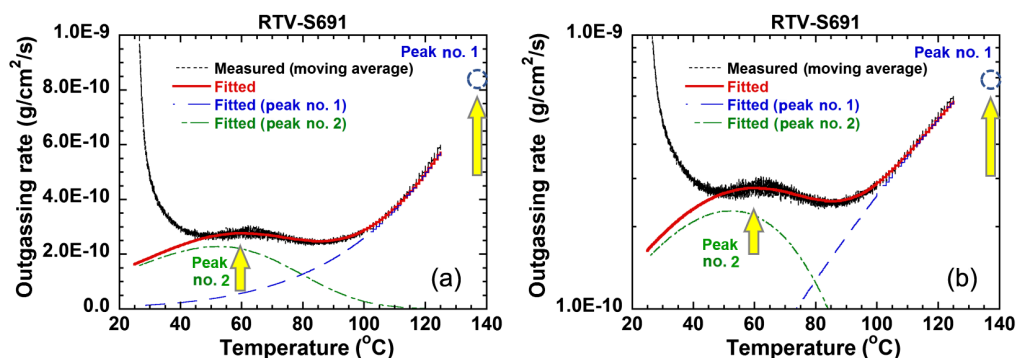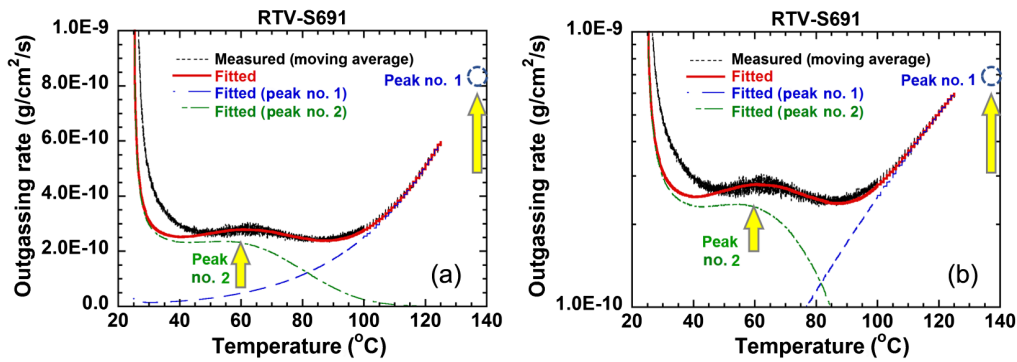

Fig. 5 Fitting desorption differential equations to measurements: (a) a linear scale and (b) a semi-logarithmic scale. The blue dot circle indicates peak 1 (RTV S-691).

Table 3 Fitted parameters by desorption model (RTV S-691).

Peak number i	M_{0i} (g/cm^2)	t_{0i} (s)	E_i (J/mol)
1	1.46×10^{-1}	1.95×10^3	3.90×10^4
2	4.46×10^{-5}	2.37	2.91×10^4

Fig. 6 Fitting diffusion differential equations to measurements: (a) a linear scale and (b) a semi-logarithmic scale. The blue dot circle indicates peak 1 (RTV S-691).

Table 4 Fitted parameters by diffusion model (RTV S-691).

Peak number i	C_{0i} (g/cm^3)	D_{0i} (cm^2/s)	E_i (J/mol)
1	3.21×10^{-2}	5.91×10^1	9.19×10^4
2	7.88×10^{-5}	5.27×10^{-3}	3.24×10^4

In the next step, the final C_0, D_0, and E for each peak (that is, for all species) were determined by the nonlinear least squares method while numerically solving Eqs. (6)–(8) using the previously obtained initial values C_0, D_0, and E.

Figure 6 shows the fitting results, and Table 4 lists the final fitting parameters. Although the fitting was performed on data above 50°C, each fitting result and measurement agreed well except for data below 20°C. Unlike for the desorption model, the temperature dependence of an outgassing rate <50°C shows behavior similar to that indicated by the measurements. This point is explicitly different from the desorption model result.

4.2 Simulating Outgassing Behavior

To investigate the validity of the model and the obtained fitting parameters, it was examined whether the outgassing behavior by multi-stepwise method[18] can be simulated. Using the apparatus shown in Fig. 3, the outgassing rate was obtained by heating the contamination source (RTV S-691) in the temperature steps shown in Fig. 7. The sample measured was 40×40 mm^2 and 1.5-mm thick. The sample was installed in the effusion cell to outgas from both surfaces.

4.2.1 Desorption model

Equations (3) and (4) were numerically solved using the obtained fitting parameters listed in Table 3 and compared with the measured outgassing rate. Figure 7 shows the results. At 25°C, the simulated results deviated considerably from the measured ones. Between 50°C and 125°C,
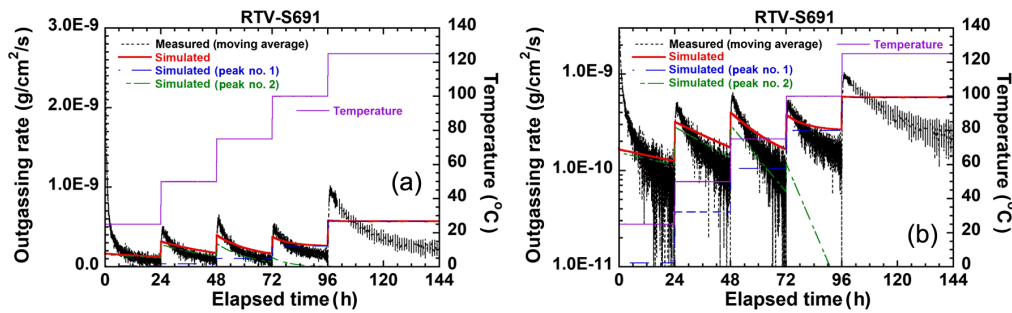
Fig. 7 Simulated results by desorption model versus outgassing rate data obtained by multi-stepwise method (RTV S-691): (a) a linear scale and (b) a semilogarithmic scale.
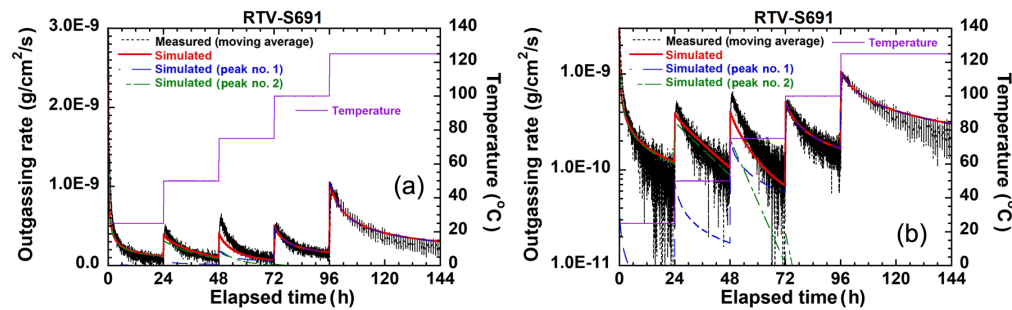

Fig. 8 Simulated results by diffusion model versus outgassing rate data obtained by multi-stepwise method (RTV S-691): (a) a linear scale and (b) a semilogarithmic scale.

the simulated results were less than half of the measured ones. And at a constant temperature of 125°C, the simulated rate was constant though the measured rate continued to decrease. This is attributed to the considerably large initial amount of adsorption (M_0) of peak 1. The initial amount of adsorption (M_0) was ~0.1 g/cm^2 (see Table 3), which corresponds to a thickness of about 1 mm. This finding suggests that the desorption model does not properly simulate outgassing behavior according to the multi-stepwise method.

4.2.2 *1D diffusion model*

Equations (6)–(8) were numerically solved using the obtained fitting parameters listed in Table 4 and compared with the measured outgassing rates. Figure 8 shows the results.

In contrast to the desorption model, the simulated outgassing rate agreed well with the measured results. At 25°C, the simulated results are close to the measurements, although the fitting was also performed on the data above 50°C. In addition, the outgassing behavior agreed well with the experiment at a constant temperature of 125°C. This suggests that the diffusion model is more accurate for simulating outgassing phenomena. Note that the diffusion model strongly depends on sample thickness. Moreover, it is possible to simulate the outgassing behavior of each species in this model. Figure 8 shows that species 1 (peak 1) is outgassed above 75°C, and species 2 (peak 2) is almost completely outgassed below 75°C.

5 Original Outgassing Rate Measurement to Improve Parameter Fitting

The diffusion model simulated outgassing behavior did better than the desorption model. However, the fitted total initial amount of outgassing concentration (ΣC_0) listed in Table 4 was one order of magnitude larger than the value estimated by ASTM E1559. ASTM E1559 is a simple alternative test method to roughly estimate ΣC_0. The ΣC_0 can be approximately estimated by *in situ* TML defined in ASTM E1559. The *in situ* TML is calculated using a view factor of QCM to the effusion cell orifice, sample surface area, and total mass density deposited on a

QCM cooled below $-183°C$. The sample volume is used in place of surface area for calculating ΣC_0 in this paper (see Ref. 17 for details). The ΣC_0 estimated by ASTM E1559 was 1.51×10^{-3}. This is why C_0 of peak 1, outgassed at a high temperature, was not estimated accurately. It is thus necessary to obtain a more precise initial concentration (C_0).

A new outgassing test method and analytical procedure was originally devised for extracting parameters. As previously mentioned, the adopted diffusion model holds when the heating rate of the contamination source is constant. A lower heating rate is desirable to separate the outgassed species due to differences in temperature. And to improve the accuracy of the estimated C_0 of the species outgassed at high temperature, after reaching 125°C, the contamination source was held at that temperature for a few days. In other words, the new outgassing test method is to heat a sample at a constant heating rate followed by an isothermal test.

The outgassing rate tests were carried out using the apparatus shown in Fig. 3 according to the above-mentioned conditions. The contamination source was RTV S-691 that was 40×40 mm^2 and 1.887-mm thick. The sample was installed in the effusion cell to outgas from both sides.

5.1 Determination of Fitting Parameters

Curve fitting was done by the procedure described in Sec. 4.1.2. The two peaks were assumed in this calculation to correspond to the two outgassed species. Peak 1 was assumed to exist above 125°C, whereas peak 2 was around 60°C. Curve fitting was performed on data above 50°C.

Figure 9 shows the fitting results, and Table 5 lists the fitting parameters obtained. The fitted total initial amount of outgassing concentration (ΣC_0) was 2.33×10^{-3}, close to the value estimated by ASTM E1559. Conversely, D_0 of peak 1 is one order of magnitude larger than the result in Table 4. The increase of D_0 might compensate for the decrease of C_0. Given the reasonable ΣC_0, however, this fitting result is better than the result in Table 4.

5.2 Simulating Outgassing Behavior

To check the validity of the obtained fitting parameters in Table 3, we simulated the outgassing behavior obtained using a multi-stepwise method. Figure 10 shows the results. The only difference is the parameters used. The simulated outgassing rate agreed well with the measured results.
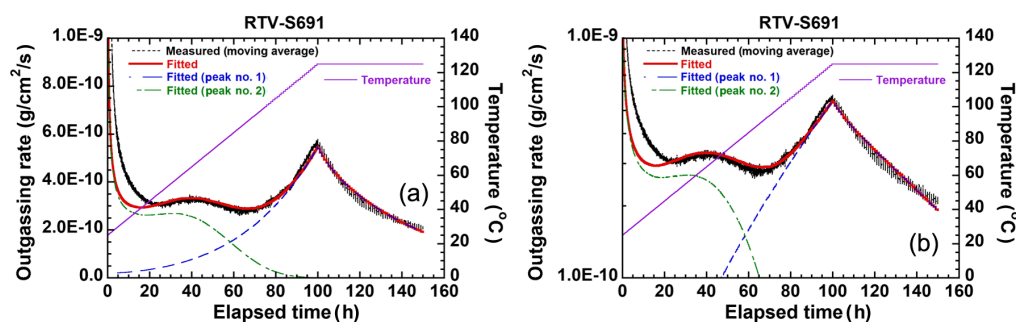

Fig. 9 Outgassing rate data versus fitted results using diffusion equations (RTV S-691): (a) a linear scale and (b) a semilogarithmic scale.

Table 5 Final fitted parameters by diffusion model (RTV S-691).

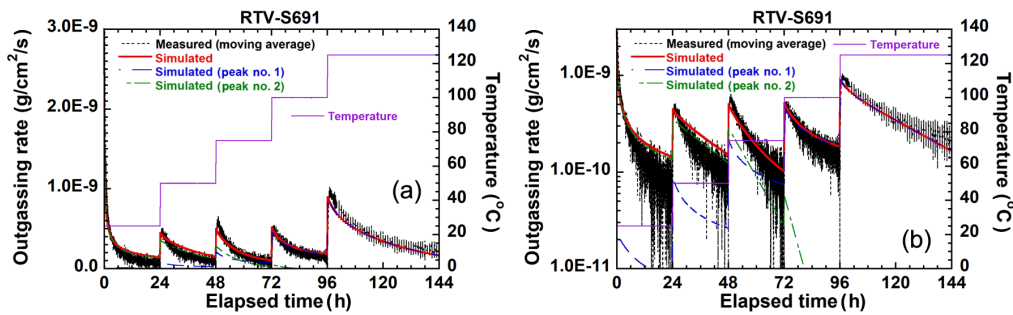| Peak number	C_0 (g/cm^3)	D_0 (cm^2/s)	E (J/mol)
1	1.64×10^{-3}	4.72×10^2	7.92×10^4
2	6.93×10^{-4}	3.22×10^{-3}	3.14×10^4

Fig. 10 Simulation results using fitted parameters and diffusion equations. Simulation and the experiment were performed according to a multi-stepwise method (RTV S-691): (a) a linear scale and (b) a semilogarithmic scale.

The temperature dependence of each species on the outgassing rate was about equal to that shown in Fig. 8.

The results indicated that the fitting parameters determined by the new outgassing test method and diffusion model were a plausible analytical approach to simulating the emission behavior of outgassing molecules from inside a material.

6 Estimating the Bake-Out Effect

The bake-out effect was calculated using Eq. (9) and the fitted parameters in Table 5. Two species were assumed in this calculation. Figure 11 shows the calculated result of residual outgas volume in the sample when the sample is baked at arbitrary temperatures. The residual outgas volume was calculated by the following equation:

$$\text{residual outgas volume} = \frac{M_\infty - M(t)}{M_\infty} = \frac{C_0 \cdot l - M(t)}{C_0 \cdot l} = 1 - \frac{M(t)}{c_0 \cdot l}. \tag{10}$$

A residual outgas volume of zero means that all outgas species has been emitted from the material. The sample is assumed to be 2-mm thick and 40×40 mm^2 and outgassed from only one side. When baked at 60℃, it takes more than 100,000 h to release all outgas species. The inflection point is several hundred hours and is due to a change of outgas species released from the sample.

Changes in the residual outgas volume of each species baked-out at 60℃ as a function of time are shown in Fig. 12. The initial concentration of species 1 and 2 were 70% and 30% of the total initial concentration of M_∞, respectively. It can be clearly seen that species 2 is outgassed faster than species 1. After the outgassing of species 2, outgassing of species 1 continues for some time.
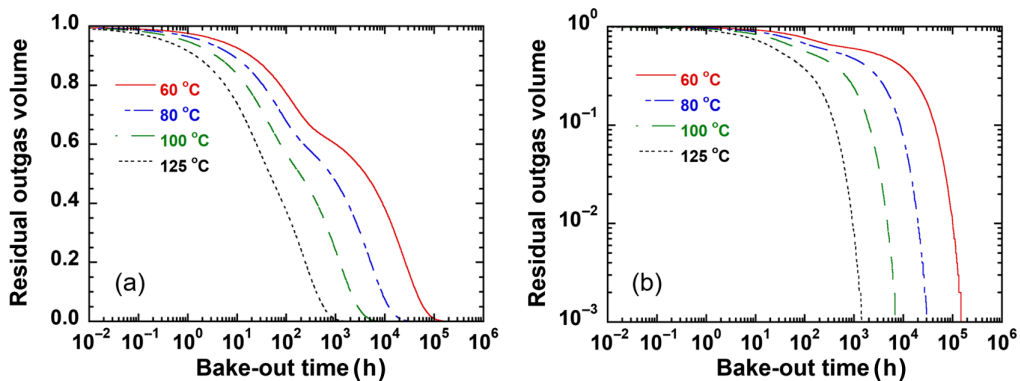

Fig. 11 Simulation results of bake-out temperature dependence of the residual outgas volume (RTV S-691): (a) a semilogarithmic scale and (b) a logarithmic scale.
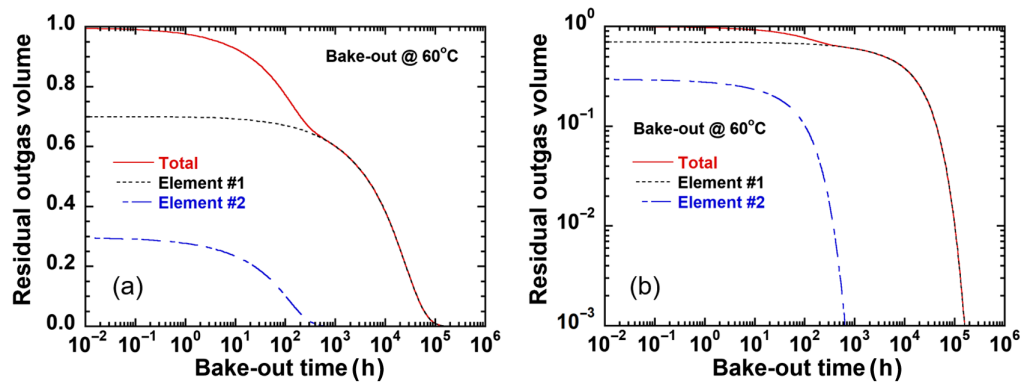
Fig. 12 Simulation results of changes in residual outgas volume in the material for each species baked-out at 60°C (RTV S-691): (a) a semilogarithmic scale and (b) a logarithmic scale.

In this way, it is possible to estimate the residual outgas volume of each species remaining in the material after bake-out. In addition, the final amount of outgassing and termination time of bake-out cannot be estimated from the initial outgassing rate because, as shown in this figure, the outgassing behavior depends on the species and because the total outgassing rate changes according to the behavior of each species. Therefore, it is very effective to estimate the final amount of outgassing and termination time of bake-out by this method.

J-SPICE2 newly incorporates this calculation in estimating the bake-out effect, so it is possible to estimate the amount of outgas that may remain in the material after bake-out before launch. And the analysis of the ground-based bake-out can be used to calculate the amount of outgassing in orbit using the residual amount of outgassing as the initial value.

7 Summary

We discussed our improvement to the modeling of outgassing phenomena. The outgassing behavior was modeled based on desorption and diffusion theory. The desorption model did not properly simulate the outgassing behavior, but the diffusion model did, so the diffusion models is clearly preferable to the desorption model in simulating outgassing phenomena.

The new outgassing test method can be summarized as follows. The outgassing rate is measured using the original procedure for heating the contamination source as slowly as possible, and after reaching the maximum temperature, the source is held at that temperature for a specified period. The diffusion functions and equations are used to analyze the outgassing rate data and acquire the fitting parameters. Using these parameters, we can simulate the emission behavior of outgassing molecules using the diffusion equations. The new method is an innovative way to model outgassing phenomena and could significantly improve the accuracy in simulating outgassing behavior. We developed Japan's Spacecraft Induced Contamination Environment analysis software 2 (J-SPICE2), which incorporates a diffusion model. J-SPICE2 has a module for fitting and extracting the parameters of the diffusion model and simulating outgassing behavior based on the diffusion theory. Here 1D equations and solutions were introduced. However, 2D equations and solutions need to be used when an adhesive is sandwiched in the sample. J-SPICE2 can, therefore, perform calculations using a 2D diffusion equation. Additionally, the estimation of bake-out effects was included in J-SPICE2. The residual outgassing can be estimated from bake-out conditions before launch, and the analysis considering the bake-out effect in ground tests can be performed using residual outgassing.

In the future, we will apply the diffusion model to other contaminants and obtain the parameters for modeling the emission behavior of various outgassing molecules. Furthermore, it is necessary to experimentally verify the estimation of the effect of bake-out and compare the experimental data with those of the simulations. We will use J-SPICE2 for contamination analysis in the design of future spacecraft.

References

1. A. Tribble et al., "Contamination control engineering design guidelines for the aerospace community," NASA CR 4740 (1996).
2. D. Mossman et al., "Contamination induced degradation of optical solar reflectors in geosynchronous orbit," *Proc. SPIE* **0777**, 12–19 (1987).
3. V. Skurat et al., "Changes of solar array surfaces on orbital station Mir," *J. Spacecraft Rockets* **48**(1), 53–58 (2011).
4. H. W. Babel et al., "The effects of contamination from silicones and a modified-Tefzel® insulation on critical surfaces of the international space station," *Acta Astronaut.* **40**(2-8), 95–104 (1997).
5. J. Alred et al., "Modeling of thruster plume induced erosion," in *Proc. 9th ISMSE (ESA SP-540)*, Noordwijk (2003).
6. C. Theroude et al., "Overview of contamination modeling in EADS Astrium," in *Proc. 10th ISMSE and 8th ICPMSE*, Collioure (2006).
7. G. Chanteperdrix et al., "Recent advances in numerical simulation for outgassing at Airbus defense and space," in *Proc. 13th ISMSE*, Pau (2015).
8. J.-F. Roussel et al., "Contamination modeling: underlying principles and first examples for a new software," in *Proc. 8th ISMSE and 5th ICPMSE*, Arcachon (2000).
9. K. Yano and N. Baba, "Development of Japanese Spacecraft Induced Contamination Environment Analysis Software (J-SPICE)," in FY2004 Report of Joint Research Achievements of the Space Division of Institute of Aerospace Technology and Institute of Space and Astronautical Science: Basic Technologies of Satellite Systems, pp. 163–166 (2006) (in Japanese).
10. H. Ogawa et al., "Assessment of molecular contamination on the BepiColombo MMO spacecraft," in *Proc. 44th ICES*, Tuscon, Arizona (2014).
11. F. Urayama et al., "Molecular contamination analysis on SUZAKU X-ray imaging spectrometer," in *Protection of Materials and Structures from the Space Environment*. Astrophysics and Space Science Proceedings, J. Kleiman, M. Tagawa, and Y. Kimoto, Eds., Vol. **32**, Springer, Berlin, Heidelberg (2013).
12. J.-F. Roussel et al., "Progress on the physical approach to molecular contamination modeling," *J. Spacecraft Rockets* **48**(2), 246–255 (2011).
13. J. Crank, *The Mathematics of Diffusion*, 2nd ed., Clarendon Press (1975).
14. K. Shimazaki et al., "Innovative methodology for emission model of contamination molecules based on diffusion theory," in *Proc. 14th ISMSE and 12th ICPMSE*, Biarritz (2018).
15. W. Fang et al., "A mathematical model for outgassing and contamination," *SIAM J. Appl. Math.* **51**(5), 1327–1355 (1991).
16. N. Miyabayashi et al., "Thermal desorption analysis method," ESCO Ltd., 2005, (in Japanese), https://www.escoltd.co.jp/technical/temperature-rising-desorption/analysis-method
17. ASTM Standard E1559, *Standard Test Method for Contamination Outgassing Characteristics of Spacecraft Materials*, ASTM International, West Conshohocken, Pennsylvania (2009).
18. "ECSS-Q-TM-70-52A: Space product assurance, Kinetic outgassing of materials for space," 25 Nov. (2011).

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