

S7-72

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N88-10836

AN INVESTIGATION OF THE BEHAVIOR OF OUTGASSED MOLECULES IN THERMAL VACUUMS

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NC 452981

ABSTRACT

Personnel at the White Sands Test Facility (WSTF) are currently developing a method to evaluate the amount of outgassing from active surfaces in individual Shuttle payload items that may condense on functional surfaces. To develop a viable method of assessing the extent to which materials can contaminate surfaces in space vehicles, an experimental apparatus has been designed in which space-simulation studies are being conducted. The objective of these studies is to understand how surfaces outgas and how the outgassed substances subsequently condense on other surfaces.

There are two techniques for evaluating the mass flux from a surface. The Langmuir technique measures directly the mass flux from a surface (Langmuir 1913). The Knudsen technique (Knudsen 1909), on the other hand, measures the mass flux through an orifice. This method measures the mass flux from the surface indirectly since it will be equal to the mass flux through the orifice at equilibrium.

A device used to measure partial pressure is necessary to evaluate experimentally the mass flux through the orifice. Two instruments have been incorporated into the design of the experimental apparatus that will not only allow the determination of the partial pressure in the inner chamber, but will also provide direct information about the relationship between outgassing and condensation for various materials. One of these instruments, a mass spectrometer, measure the partial pressure directly. The other instrument, a thermally controlled quartz crystal microbalance (TQCM), evaluates the partial pressure of condensable materials by measuring the condensation rate.

The advantage of the Knudsen technique becomes obvious when the following expression for the rate of mass flux through the orifice is considered:

$$dm/dt = A_p (V_u * D_u - V_1 * D_1) / 4 \tag{1}$$

Here A_p is the area of the exit orifice; V_u is the average molecular velocity of the gas in the inner chamber (where the sample is located); V_1 is the average molecular velocity in the outer chamber; D_u and D_1 are the gas densities in the inner and outer chambers, respectively. When ideal gas conditions are satisfied, the density of the i th gaseous species D_i is related to the partial pressure by the following equation:

$$D_i = P_i * M_i / R * T \tag{2}$$

where M_i is the molecular weight of the i th species; R is the universal gas constant; and T is the absolute temperature of the gas. These equations show that by monitoring the equilibrium partial pressure of an outgassed species in an inner chamber, the rate at which outgassing is occurring for all the surfaces in the chamber can be determined.

If it is assumed that every outgassed molecule that strikes a surface, such as a TQCM crystal, becomes an adsorbed molecule, the following relationship between the condensation rate and the partial pressure will hold:

$$P_i = B \cdot (R \cdot T / M_i) \cdot r_i \quad (3)$$

where r_i is the condensation rate of the i th gaseous species on a surface and B is a constant. Partial pressures can be calculated from TQCM condensation rates using equation (3). The partial pressures can then be substituted into equation (2) to calculate densities. Those densities can then be substituted into equation (1) to calculate semi-empirical outgassing rates for single-component samples (sublimation rates). These outgassing rates can be integrated over the test time to generate calculated total mass losses.

Preliminary tests conducted at WSTF produced calculated mass losses that were found to be in reasonable agreement with mass losses determined by weighing the sample before and after testing on analytical balances. However, tests using materials with various molecular properties showed characteristic variations in the ratios of calculated total mass loss to experimental loss. These variations indicate that for some molecules energetic barriers to adsorption and desorption can exist between outgassed molecules and the surfaces on which they condense.