Status Report III
Grant No. NAG-5-865
December 1, 1987 - August 31, 1988

MICROGRAVITY NUCLEATION AND PARTICLE
COAGULATION EXPERIMENTS SUPPORT

Submitted to:
National Aeronautics and Space Administration
Goddard Space Flight Center
Greenbelt, MD 20771
Attention: Dr. Joseph A. Nuth
Code 690
Laboratory for Extraterrestrial Physics
Space and Earth Sciences Directorate

Submitted by:
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Associate Professor
F. T. Ferguson
Graduate Assistant
J. R. Stephens
Matrix, Inc.

Report No. UVA/528260/CHE89/103
October 1988

SCHOOL OF ENGINEERING AND
APPLIED SCIENCE

DEPARTMENT OF CHEMICAL ENGINEERING

UNIVERSITY OF VIRGINIA
CHARLOTTESVILLE, VIRGINIA 22901
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I - SUMMARY

A number of refinements have been incorporated in our finite difference model for the developing temperature and supersaturation profiles in the nucleation chamber. These include: conduction through the chamber walls, the effect of various thermal breaks such as joints and seals, and improved method of accounting for thermal radiation. In addition, the programs have been converted to using an alternating-direction implicit (ADI) method to make them more efficient to run (University of Virginia).

Major effort during the summer was devoted assembling the nucleation chamber and its accessories. Preliminary tests have shown that the heaters are capable of producing temperatures well above the necessary minimum. “Smoke” has been produced with zinc; however, attempts with magnesium vapors have not been successful in these initial trials, most probably due to oxide formation on the molten metal surface (Goddard Space Flight Center and the University of Virginia).

Work has continued on defining the experimental configuration and development of the software for the data acquisition system. Recommendations for additional hardware and software have been submitted to allow the development of a more robust and capable overall system (Matrix, Inc.).
II - INTRODUCTION

Researchers at NASA Goddard Space Flight Center have embarked on a program to study the formation and growth of cosmic grains. This includes experiments on the homogeneous nucleation of refractory vapors of materials such as magnesium, lead, tin and silicon oxides. As part of this program, the Chemical Engineering Department of the University of Virginia has undertaken to develop a mathematical model for these experiments, to assist in the design and construction of the apparatus, and to analyze the data once the experiments have begun.

Status Reports I and II addressed the design of the apparatus and the development of mathematical models for temperature and concentration fields. The bulk of this report discusses the continued refinement of these models, and the assembly and testing of the nucleation chamber along with its ancillary equipment, which began in the spring of 1988.
III - RESEARCH ACCOMPLISHMENTS

A. Model Development

Most of the early spring was spent on improving the programs for the temperature and supersaturation profiles. In Status Report II, plots were given for the temperature distribution and supersaturation ratios for several different operating conditions. The program which modeled the temperature distribution included the effects of conduction through the containing aluminum wall, conduction through the ambient gas, and radiation heat transfer. This early version of the program used an explicit finite difference method to solve the equation of energy for the temperature at various nodes. It took a significant amount of time to run, though, because it used an explicit method to solve the finite difference equations. The time step in this method had to be limited to rather small values because of problems with stability. The program for the supersaturation ratio used the same method, but since the transient data are only needed for a 20-second real time period, the small time step problem was not as critical in that program.

During the spring, these temperature distribution and supersaturation programs were converted to using an implicit finite difference method, namely the alternating-direction implicit or ADI method. Although the ADI method is computationally more difficult, and takes more time to sweep through a single iteration, it has the distinct advantage that it is stable for any size time step. Of course, the choice of the time step will affect the accuracy of the solution, but the implicit time step can usually be much larger than that required by the explicit method. In our case, we were able
to use a time step on the order of 125 times larger, thus making the program much more efficient to run.

Status Report II also mentioned the possibility of modeling convection within the nucleation apparatus. This would involve the simultaneous solution of the equations governing the velocity and temperature fields within the chamber. After completing the work on the temperature and supersaturation programs, we began to tackle these equations. We started with a relatively simple geometry so that our method of solution could be verified with published work. The results have been very close, but there are still some slight discrepancies that need to be worked out before we attempt to model the natural convection process in the nucleation apparatus, though.

B. Chamber Assembly

The nucleation experiments will be conducted in a specifically designed cylindrical chamber. A set of resistive heaters centered at the top of the chamber will generate refractory vapors which will then be allowed to diffuse downward through the temperature gradient imposed by these heaters. The downward diffusion direction was chosen to reduce convection interference with the nucleation process. When the evolving vapor concentration profile exceeds the critical supersaturation ratio, nucleation and condensation will commence as evidenced by the formation of a particulate "smoke" cloud. A computer-based data acquisition system will monitor the nucleation conditions while a video camera records the location of the smoke front. After initial laboratory tests, the experiment will be prepared for runs aboard NASA's KC-135 research aircraft capable of flying a pattern with a sequence of 20-30 second
periods of microgravity conditions.

The resistive heaters for the nucleation apparatus arrived from the fabricator in January, 1988. During a one week period in January we were able to check these heaters at the Goddard Space Flight Center and observe their behavior as a function of the applied electrical power in a stainless steel bell jar. Some fabrication flaws were noted which required fabrication of new heaters. Although both heaters also had some local "hot spots", the measured temperatures seemed to be sufficiently high for producing vapors of the refractory metals.

Overall assembly of the apparatus began during summer, 1988 at Goddard. Since the equipment needs to be mobile for flights on the KC-135, we mounted the chamber and its accessories on a flat cart. These accessories included a vacuum pump, two transformers and variacs, a gas cylinder, and a portable computer and data acquisition system. We assembled the main components of the chamber itself and connected the heaters to the transformers and variacs. We also designed an attachment to the chamber for holding two lasers which will be used for experiments on scattering from the condensed smoke particles. This piece of equipment will probably be completed in October, 1988.

The second half of the summer was spent testing the heaters and attempting some initial nucleation runs. Thermocouples were placed within the chamber and connected to the data acquisition device, and a simple program was written to display the temperatures of the set of thermocouples. During the heater testing, we were able to get the crucible up to a maximum temperature of approximately 1100-1300°C. This was well above the necessary minimum temperature of approximately 750°C. After
mounting a shutter assembly to close and open the port to the crucible, we tried vaporizing magnesium to see if we could get smoke particles to form. Magnesium had been selected as one of the first test materials because it has a relatively low melting point and high vapor pressure. Attempts to produce magnesium vapors were unsuccessful, even after several trials and using hydrogen, rather than nitrogen, as the ambient (carrier) gas. Hydrogen was expected to eliminate the formation of oxide layer on the molten magnesium surface in the crucible. Finally we tried using zinc instead of magnesium. Zinc has a melting point somewhat lower than magnesium and a much higher vapor pressure at the temperatures we were using. We were able to produce smoke, but we believe that these smoke particles were actually from ZnO, rather than Zn metal. The motion of these smoke particles, whether they were Zn or ZnO, did confirm our suspicion that natural convection could still occur within the chamber, at least with the thermal operating and boundary conditions of these preliminary tests.

C. Data Acquisition System

The data acquisition system software package is being developed under a subcontract to J.R. Stephens of Matrix, Incorporated of Santa Fe, New Mexico.

During the above contract period, work continued on defining the experimental configuration and developing software to acquire data in the laboratory and in the flight. A configuration for a second computer system, which is to be used predominantly in the laboratory but could also serve as a backup for the flight has been recommended. Another Compaq Portable 1: was recommended with maximum on-
board memory and enhanced graphics adaptor. On a visit to Goddard, we attempted to load and test the Keithley software, but differences between the Keithley software and the Compaq Operating System prevented running the test programs developed during the last contract period. New Keithley software was ordered and now operates correctly.

Due to the complexity of new software development, it has been recommended that we plan to use Quick500, a compiled version of the Keithley Soft500, which makes use of the advanced capabilities of Microsoft’s QuickBASIC. This product will allow much more sophisticated software to be developed in a shorter time, at a lower cost, and still provide a more robust and capable data acquisition system.
IV - FUTURE WORK

The oxidation of the molten metal surface layer is probably due to small air leaks into the chamber. To fix these leaks, the chamber will have to be taken apart and rechecked to make sure all the seals are working properly. Once this is done, the la... mount and video camera can be attached to the chamber. These pieces of equipment will then be connected to the computer and the electrical wiring changed to make the chamber and the cart acceptable for flights on the KC-135.

If the oxide formation persists, we may be forced to use hydrogen in place of argon as the ambient gas. Consequently, the computer programs would need to be modified to reflect this change. This should not present any major difficulties, however. We also expect to continue modeling the natural convection within the nucleation chamber. Observations of smoke movements have shown that convective currents are likely to occur. Our modeling may be able to determine the significance of convection at gravities corresponding to, say, lunar or martian environments. Should convective effects at lunar or martian gravity levels be tolerable, then we could extend the length of the experimental runs aboard KC-135 since longer periods of reduced gravity at these levels are available on that aircraft.