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# OAK RIDGE NATIONAL LABORATORY



# Aerosol Release and Transport Program Semiannual Progress Report for April 1985–September 1985

R. E. Adams M. L. Tobias

Prepared for the U.S. Nuclear Regulatory Commission Office of Nuclear Regulatory Research Under Interagency Agreements DOE 40-551-75 and 40-552-75

OPERATED BY MARTIN MARIETTA ENERGY SYSTEMS, INC. FOR THE UNITED STATES DEPARTMENT OF ENERGY

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#### Engineering Technology Division

# AEROSOL RELEASE AND TRANSPORT PROGRAM SEMIANNUAL PROGRESS REPORT FOR APRIL 1985-SEPTEMBER 1985

R. E. Adams M. L. Tobias

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#### FOREWORD

This report summarizes progress under the Aerosol Release and Transport Program [sponsored by the Division of Accident Evaluation, Office of Nuclear Regulatory Research, Nuclear Regulatory Commission (NRC)] for the period April 1985-September 1985.

Work on this program was initially reported as Volume III of a fourvolume series entitled Quarterly Progress Report on Reactor Safety Programs Sponsored by the NRC Division of Reactor Safety Research. Prior reports of this series are

Report No.	Period covered
ORNL/TM-4655	April-June 1974
ORNL/TM-4729	July-September 1974
ORNL/TM-4805	October-December 1974
ORNL/TM-4914	January-March 1975
ORNL/TM-5021	April-June 1975

Beginning with the report covering the period July-September 1975 through the report for the period July-September 1981, work under this program was reported as LMFBR Aerosol Release and Transport Program Quarterly Progress Report. Prior reports under this title are

Period covered			
July-September 1975			
October-December 1975			
January-March 1976			
April-June 1976			
July-September 1976			
October-December 1976			
January-March 1977			
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January-March 1980			
April-June 1980			
July-September 1980			
October-December 1980			
January-March 1981			
April-June 1981			
July-September 1981			

Beginning with the report covering the period October-December 1981, work under the program was reported as Aerosol Release and Transport Program Quarterly Progress Report. Prior reports under this title are

Period covered
October-December 1981
January-March 1982
April-June 1982
July-September 1982
October-December 1982
January-March 1983
April-June 1983
July-September 1983

Beginning with the report covering the period October 1983-March 1984, work under the program is now being reported as Aerosol Release and Transport Program Semiannual Progress Report. Previous reports under this title are

Report No.	Period covered
ORNL/TM-9217/V1	October 1983-March 1984
ORNL/TM-9217/V2	April 1984-September 1984
ORNL/TM-9632/V1	October 1984-March 1985

#### SUMMARY

#### M. L. Tobias

The Aerosol Release and Transport (ART) Program at Oak Ridge National Laboratory (ORNL) is designed to investigate the behavior within containment of aerosols originating from severe accidents resulting in core melting. The program applies mainly to light-water reactors (LNMRs). The experimental programs are being conducted in the NSPP Face (20) and the Aerosol-Moisture Interaction Test (AMIT) Facility. The analytical efforts are designed to support the experiments and to provide comparisons between the experimental observations and the results of computer codes intended to simulate aerosol behavior.

During this period, test NSPP-059, the third in a series of simulations of steam conditions in aerosol tests, was conducted in the NSPP vessel. In this test, the steam heater and plasma torch were used (without aerosol generation) to provide data on heat and gas input. Following this run, a steam separator was installed in the supply line to the steam heater to improve the quality of the steam feed.

Test NSPP-DT-3 in the development test series in the  $0.35\text{-m}^3$  test vessel was performed to obtain thermal input data and determine Fe<sub>2</sub>O<sub>3</sub> aerosol-generation efficiency. The two-section aerosol delivery tube configuration was used. It proved effective in keeping aerosol and torch gas temperatures below 125°C (398 K). Preliminary examination of test results shows that generation efficiency was comparable to earlier tests where a one-section delivery tube was used and in which inlet temperatures up to 900°C (1173 K) had been observed.

The AMIT facility was completed during this period, and the first two tests, AMIT-5001 and AMIT-5002, were conducted. In addition to these, two development tests, AMIT-DT-1 and AMIT-DT-2, were conducted to study aerosol-generation efficiency and thermal input to the test vessel. A preliminary test, AMIT-PT-1, was run to determine the response of the humidity measurement system to plasma torch operation without generation.

Both AMIT-5001 and AMIT-5002 were  $Fe_2O_3$  aerosol tests. AMIT-5001 was at ~54% relative humidity (RH). The torch was operated for 60 s and was fed with 9.8 g of iron powder during the last 30 s of torch operation. Filter, cascade impactor, and electrostatic precipitator samples were taken during the 2 h following torch operation. Pressures, temperatures, RHs, and mass concentrations are reported as a function of time; aerodynamic mass median diameter (AMMD) values were measured at two times. Test AMIT-5002 was conducted at 79% RH, with 10.4 g of iron powder fed during the last 23 s of the 63-s torch operation period. In both tests, scanning electron microscopy showed that nearly all of the aerosol was in the chainlike agglomerate form.

In LWR Aerosol Containment Experiment (LACE) Program support work, a manganese oxide aerosol was generated in a steam-air atmosphere in the NSPP test vessel (NSPP-541). The aerosol was found to consist mainly of  $\gamma$ -Mn<sub>2</sub>O<sub>3</sub>. The plasma torch was fed with 679 g of manganese powder for 16 min. Low-level steam injection continued for the next 6 h. At the end of aerosol generation the vessel pressure was 0.178 MPa (abs), and

the temperature was 381 K. At the end of the subsequent 6-h period, the pressure and temperature had risen to 0.217 MPa and 386 K, respectively. Steam injection was stopped and the vessel was allowed to cool for another 18 h. Aerosol concentrations as a function of time are reported. The aerosol concentration at the time of torch cutoff was estimated at about 2.5 g/m<sup>3</sup>.

Results of AMMD values are also given, as measured by in-vessel and ex-vessel measuring systems. The in-vessel values are about twice as large as the ex-vessel values.

In analysis work, an impactor loading analysis has been performed to modify existing Andersen Mark III impactors for the AMIT sampling system. The analysis was based on AMIT-5001 experimental data. Recommendations are given for the number of plates in each of the modified impactors, as well as for other changes in design. In particular, it is proposed to blank off all but the innermost circles of holes in the impactor plates to reduce the flow of the aerosol-gas mixture to a level appropriate to the size of the AMIT vessel while maintaining an adequate linear velocity through the orifices.

The theory of a proposed capillary mechanism for condensation of water vapor on aerosol particles is presented. The presence of concave surfaces, where the vapor pressure would be significantly reduced below that for a plane surface, is suggested as offering the possibility of condensation even if the environment is unsaturated. The surface tension forces so induced could lead to aerosol agglomerate spheroidization.

Work in modifying data processing codes to accommodate changes in the data retrieval equipment is briefly discussed. The task of correcting the sample volume calculations for the 400-, 500-, and 600-series of experiments has been completed; the changes in the calculation procedure are outlined.

The CONTAIN code has been converted to double-precision operation as a load module on the IBM computers. This was done to deal with numerical difficulties encountered in using the single-precision version of the code. The code has been used to perform calculations for pretest predictions of the LA-1 LACE test. Additionally, calculations have been done to check analytical calculations of condensation rates on stagnant aerosols.

# GLOSSARY OF ACRONYMS

AMIT	Aerosol-Moisture Interaction Test
AMMD	aerodynamic mass median diameter
ART	aerosol release and transport
BCL	Battelle-Columbus Laboratories
CDA	core-disruptive accident
CDV	capacitor discharge vaporization
CNC	condensation nuclei counter
CRBR	Clinch River Breeder Reactor
CSTF	Containment Systems Test Facility
DEMONA	name of an aerosol experimental facility at Battelle-Frankfurt (Demonstration Nuklearen Aerosolverhaltens)
DMA	differential mobility analyzer
FAST	Fuel Aerosol Simulant Test
GSD	geometric standard deviation
HCDA	hypothetical core-disruptive accident
HEDL	Hanford Engineering Development Laboratory
ICP	inductively coupled plasma (spectrometric method)
IDCOR	Industry Degraded Core Rulemaking Program
IMSL	International Mathematical and Statistical Libraries
ITRI	Inhalation Toxicology Research Institute
KfK	Kernforschungszentrum Karlsruhe
LACE	LWR Aerosol Containment Experiments
LANL	Los Alamos National Laboratory
LMFBR	liquid-metal fast breeder reactor
LWR	light-water reactor
NRC	Nuclear Regulatory Commission
NSPP	name of a facility in which secondary containment aerosol experiments are conducted (originally, Nuclear Safety Pilot Plant)
ORNL	Oak Ridge National Laboratory
PSL	polystyrene latex
PWR	pressurized-water reactor
WROS	wall run-off sampler

AEROSOL RELEASE AND TRANSPORT PROGRAM SEMIANNUAL PROGRESS REPORT FOR APRIL 1985-SEPTEMBER 1985

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#### ABSTRACT

This report summarizes progress for the Aerosol Release and Transport Program sponsored by the Nuclear Regulatory Commission, Office of Nuclear Regulatory Research, Division of Accident Evaluation, for the period April 1985-September 1985.

Topics discussed include (1) a steam-only test performed in the NSPP vessel; (2) development tests to study thermal input and generation efficiency; (3) Aerosol-Moisture Interaction Test (AMIT) preliminary and development tests to check various features of the AMIT faci ity; (4) data from the first two tests in the AMIT program; (5, an analysis of changes necessary in Andersen Mark-III impactor design for AMIT experiments; (6) the theory of capillary condensation on aerosols at nominally undersaturated humidity levels; (7) work in modifying data processing codes to accommodate data retrieval equipment changes; (8) correction of sample volume calculations for NSPP experiments on aerosols in steam-air environments; and (9) implementation and application of the CONTAIN code.

#### 1. INTRODUCTION

The Aerosol Release and Transport (ART) Program at Oak Ridge National Laboratory (ORNL), sponsored by the Nuclear Regulatory Commission (NRC), Office of Nuclear Regulatory Research, Division of Accident Evaluation, is a safety program concerned with aerosol behavior within containment. The overall goal of the program is to provide the experimental data necessary to assess the validity of computer codes used to predict the behavior of radioactive aerosols released into containment as a result of postulated events of varying severity up to and including accidents resulting in core melting.

The program is divided into several related experimental and analytical activities:

- study of the characteristics and behavior of fuel-simulant aerosols in several small vessels;
- production and study of aerosols in the NSPP for the validation of models, with particular emphasis on the behavior of mixtures of nuclear aerosol species relevant to light-water reactor (LWR) systems;
- comparison of the results of experiments with calculations using existing aerosol computer codes or with specifically developed analytical procedures.

#### 2. EXPERIMENTAL PROGRAM

#### 2.1 Secondary Containment Aerosol Experiments

A.	W.	Longest	M.	Τ.	Hurst
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#### 2.1.1 Introduction

Studies are in progress to determine the behavior of aerosols assumed to be released into containment environments during LWR accident sequences. In general, the experimental program is comprised of the following three kinds of tests: (1) NSPP large-scale multicomponent (U308, Fe203, and concrete) aerosol behavior tests in dry air and condensing steam-air environments, (2) aerosol-moisture interaction tests (AMIT) to study the effect of humidity level on the shape of agglomerated aerosols, and (3) development tests to obtain specific information needed for various experimental and model development efforts.

As described in the last semiannual progress report,<sup>1</sup> the LWR ART Program at ORNL was redirected in response to several needs for additional experimental data identified at NRC aerosol experiment-code analyst meetings in Silver Spring, Maryland, June 12-13, 1984, and March 28-29, 1985. New studies designed to fulfill these needs in ved obtaining detailed information on (1) thermal-hydraulic conditions during NSPP aerosol tests in condensing steam-air environments, (2) thermal output and aerosol mass generation rates for the plasma torch aerosol generators, and (3) influence of humidity on aerosol particle shape factors. Progress in each of these areas continued into the current report period and is described in Sects. 2.1.2-2.1.4.

Several suggestions for improvements and for special tests were also made at the NRC aerosol experiment—code analyst meetings. Receiving greatest emphasis was the need to fully characterize the aerosol and plasma torch gases (heat content, particle size distribution, and flow rates) at the point of their entry into the test vessel and to minimize the input of large unvaporized particles of raw material and of heat by radiation from the aerosol generator tube. As a step toward this characterization, a modification was made to the existing plasma torch aerosol-generator delivery tube to lower the temperature of the entering aerosol and to provide a place in the delivery tube for fallout of large particles by the addition of a horizontal section to the tube. The effectiveness of this modification is being determined in NSPP and AMIT development tests.

In addition to this work, substantial support work for the LWR Aerosol Containment Experiments (LACE) Program at Hanford was completed to determine the suitability of plasma torch aerosol generators for the production of manganese aerosols. This development effort is described in Sect. 2.1.5. The last test of the LACE series was a large-scale Mn<sub>2</sub>O<sub>3</sub> aerosol behavior test in the NSPP vessel in a condensing steam-air environment. Detailed results from this experiment are given in Sect. 2.1.6.

#### 2.1.2 NSPP thermal-hydraulic conditions

Analysis of several earlier NSPP steam tests indicated a need for three more tests to obtain additional information on thermal-hydraulic conditions during NSPP tests in condensing steam-air environments. As mentioned in the last progress report,<sup>1</sup> the first test (NSPP-057) was conducted on March 25, 1985, under normal test conditions (Table 1), with the steam heater but not the plasma torch in operation. On March 28, a similar steam test (NSPP-058), without steam heater operation, was carried out to simulate steam conditions in aerosol tests conducted prior to the addition of the steam heater. The third test (NSPP-059) was conducted on April 3, 1985, under normal test procedures, with the steam heater and plasma torch in operation to simulate heat and gas input but without aerosol generation.

# Table 1. General procedure for performing NSPP aerosol behavior tests in a condensing steam-air environment

- NSPP vessel atmosphere [air at ~0.030 MPa (abs) and ambient temperature] preconditioned by steam injection; steam injection rate then reduced to maintain steady state conditions [air and steam at ~0.16 MPa (abs) and 378 K]
- 2. Test aerosol generated and introduced into vessel
- 3. Aerosol sampling procedures conducted for 9 h
- 4. Low-level steam injection rate terminated after 6 h
- Vessel and vessel atmosphere allowed to cool until 24 h elapsed from start of aerosol generation
- 6. Final sampling procedures conducted at 24 h

After these steam tests were completed, a steam separator was installed in the steam supply line immediately upstream of the steam heater. The separator will remove moisture particles and improve the quality of the steam entering the steam heater.

# 2.1.3 Plasma torch aerosol-generator characteristics under NSPP test conditions

Tests are being conducted in a small  $(0.35-m^3)$  development test vessel to obtain detailed information on the operating characteristics of the NSPP plasma torch aerosol generators. Two tests were completed and described in the last progress report<sup>1</sup> (NSPP-DT-1 and NSPP-DT-2); the third test (NSPP-DT-3) of this series was conducted during this report period.

This development test series was originally designed to determine thermal output and aerosol mass generation rates under the plasma torch aerosol-generator operating parameters and configuration used in previous NSPP tests. The test objectives were expanded (at the request of aerosol code developers) to include (1) a full characterization of the aerosolplasma torch gas mixture (heat content, aerosol particle size distribution, gas velocities, etc.) at the point of entry into the test vessel; (2) system modification to reduce heat transfer into the test vessel by radiation from the aerosol delivery tube; and (3) system modification to minimize the introduction of large particles of unvaporized aerosol raw material. The existing aerosol delivery tube was extended to twice its former length (two sections instead of one) to provide means for reducing the temperature of the input aerosol and torch gases, as well as to provide a horizontal section for fallout of large particles of unvaporized aerosol material. The effectiveness of this modification was tested in the NSPP-DT-3 test.

The NSPP-DT-3 development test was conducted during the period July 18-19, 1985, to obtain data on thermal input to the test vessel and  $Fe_2O_3$  aerosol-generation efficiency under the plasma torch operating parameters used in previous NSPP tests and with the two-section aerosol delivery tube configuration. The two-sec<sup>-1</sup> on tube was effective in reducing the temperature of the inlet aerosol and torch gases to <125°C during  $Fe_2O_3$  aerosol generation for the NSPP- 3 test. Temperatures up to 900°C had been measured previously using the one-section delivery tube. Also, preliminary examination of the test data indicated that the  $Fe_2O_3$  aerosol-generation efficiency was comparable to that obtained in the NSPP-DT-I and -2 tests (~25%) in which the one-section delivery tube was used.

Several more tests are planned to obtain data on thermal input and generation efficiency for  $U_3 O_8$  and concrete aerosol generation.

# 2.1.4 Aerosol-moisture interaction tests

The AMIT tests are designed to (1) investigate the effect of various levels of humidity on the physical characteristics of single-component and multicomponent aerosols of interest in LWR accident sequences, (2) determine the humidity levels at which agglomerated aerosols change from chainlike to spherical in shape, and (3) provide aerosol particle shape data to aid development of aerosol behavior codes.

Preparation of the AMIT facility was completed, and the first two tests, AMIT-5001 and AMIT-5002, of the planned AMIT series were conducted during this report period. The first of these tests was conducted in June 1985 as planned. Leading up to this initial test were development tests to determine suitable plasma torch operating parameters for use in AMIT tests and a preliminary test without aerosol generation. These development and preliminary tests and two AMIT tests are described in this section.

The AMIT test vessel  $(0.52 \text{ m}^3)$  features a humidity measurement and control system, as indicated in Fig. 1. This external loop system consists of an optical condensation hygrometer for humidity determination, components for water vapor injection and/or removal, and flow measurement and control devices. The normal mode of operation is to adjust the relative humidity (RH) to a desired initial value and then measure the RH

ORNL DWG 85-7828R



Fig. 1. Schematic of AMIT vessel.

(without further water vapor injection or removal) for the duration of the test.

2.1.4.1 <u>Plasma torch aerosol-generator operating parameters for</u> <u>AMIT tests</u>. A series of development tests is being conducted to determine suitable plasma torch aerosol-generator operating parameters for use in generating aerosols for the AMIT tests. Heat and gas input into the AMIT test vessel atmosphere during aerosol generation should be minimized to reduce perturbations in the humidity level specified for each test.

A small  $(0.35-m^3)$  vessel, prepared for earlier tests, was used to obtain detailed information on the operating characteristics of the plasma torch aerosol generator (e.g., thermal output and aerosol mass generation rates). A rack containing 24 thermocouples (6 at each of 4 axial locations) was provided for measurement of gas temperatures inside the test vessel. The temperature of the torch gases and aerosol was monitored by using a rig of five thermocouples (each shielded from other surfaces by three concentric shields to reduce radiation errors) placed across the diameter of the inlet tube to the test vessel. These thermocouples, along with outside-wall thermocouples and heat flux meters, were used to monitor the thermal input to the vessel by the aerosol generator, which is installed at one end of the cylindrical vessel. Generator power and cooling water heat losses were also measured. Information on aerosol mass generation rates was obtained by (1) filter sample measurements of aerosol mass concentration vs time and (2) posttest collection and sieve analysis of deposited material to determine the amount of the feed material that was converted to an aerosol.

A smaller  $(0.13-m^3)$  but similarly equipped vessel was prepared for future development tests to obtain detailed information on the operating characteristics of the plasma torch aerosol generator used for generation of U<sub>3</sub>O<sub>8</sub> aerosols. This test vessel is rated for pressures up to 1.03 MPa (gage) and temperatures up to 616 K.

As described in the last progress report,<sup>1</sup> the first development test (AMIT-DT-1) was conducted in several steps in the  $0.35-m^3$  vessel. The original one-section aerosol delivery tube was used. Data were obtained on thermal input to the test vessel at torch operating power levels of 5, 10, 20, 30, and 40 kW. The Fe<sub>2</sub>O<sub>3</sub> aerosol-generation efficiency was measured at the intermediate torch power of 20 kW. Results from the test indicated that a very good aerosol-generation efficiency (~40%) was obtained, but the heat input into the vessel was much higher than desired.

The second development test (AMIT-DT-2) was conducted during the period May 15-21 in the  $0.35-m^3$  vessel to obtain data on thermal input to the test vessel at torch operating power levels of 24, 32, and 42 kW and to measure  $Fe_2O_3$  aerosol-generation efficiency at the highest torch power of 42 kW. The modified two-section aerosol-generator delivery tube, described in Sect. 2.1.3, was used in this test. It was effective in reducing the temperature of the inlet aerosol and torch gases to <100°C during  $Fe_2O_3$  aerosol generation for the AMIT-DT-2 test. Temperatures up to ~900°C have been measured previously using the one-section delivery tube. Examination of the AMIT-DT-2 test data indicated that the  $Fe_2O_3$  aerosol delivery rate to the test vessel was adequate under the AMIT-DT-2 conditions.

Similar development tests are planned to determine suitable conditions for generation of the other aerosols of interest in the AMIT tests (U<sub>3</sub>O<sub>8</sub>, concrete, and possibly  $Ag_2O/CdO$ ).

2.1.4.2 Preliminary AMIT test. A preliminary test without aerosol generation (AMIT-PT-1) was conducted to determine humidity level perturbations associated with plasma torch operation under the parameters selected for Fe2O3 aerosol generation. The AMIT-PT-1 test was conducted in two parts at initial RH levels of 45 and 75%, respectively. Examination of the test data indicated that the humidity measurement system performed satisfactorily. There was a net increase in the absolute humidity level associated with the plasma torch operation that was apparently due to the water vapor formed from the H2 and O2 components of the gas mixture used in the Fe2O3 aerosol generation. This increase was from 45 to 59% RH and from 75 to 84% RH in the two subtests, respectively. The new equilibrium humidity value was reached within ~10 min after termination

of the 60-s torch operation period. There was an initial depression in the indicated RH as a result of a 6°C increase in test vessel gas temperature; the gas temperature quickly returned to a value equivalent to the vessel wall temperature, and the indicated RH value rose quickly to the value reported.

2.1.4.3 <u>Aerosol-moisture interaction test AMIT-5001</u>. The AMIT-5001 test was the first of the planned aerosol tests at various humidity levels. As described in a previous progress report,<sup>2</sup> the AMIT test plan is designed to be a systematic study of the effect of moisture on the shape of agglomerated aerosols comprised of U<sub>3</sub>0<sub>8</sub>, Fe<sub>2</sub>O<sub>3</sub>, and either concrete or Ag<sub>2</sub>O/CdO in single-component and multicomponent tests (with equal masses of each component) at two aerosol mass concentration levels. Included in the statistical plan are four one-component, five twocomponent, and two three-component tests at each of two concentration levels, with tests at the low concentration (~1 to 5 g/m<sup>3</sup>) at four RH levels and tests at the high concentration (~20 to 30 g/m<sup>3</sup>) at dry conditions and 100% RH only.

The AMIT-5001 test was an Fe<sub>2</sub>O<sub>3</sub> aerosol test at ~54% RH. This test was conducted on June 21, 1985, starting from an initial steady state RH of 48%. Fe<sub>2</sub>O<sub>3</sub> aerosol was produced with the plasma torch aerosol generator with 9.8 g of iron powder passed through the torch over the last 30 s of a 60-s plasma torch operation period. As shown in Fig. 2, the RH increased from the initial value of 48 to 54% as a result of the torch operation; this increase was smaller than those noted in the preliminary test. This behavior could result from either a reduced production of



Fig. 2. Test vessel conditions during Fe<sub>2</sub>O<sub>3</sub> aerosol test at 54% RH (AMIT-5001).

water as a result of consumption of part of the available oxygen by oxidation of the iron vapor or by loss of water vapor from the gas space by adsorption onto the surfaces of the Fe<sub>2</sub>O<sub>3</sub> aerosol.

During the 2-h period following aerosol generation, nine filter samples, two cascade impactor samples, and five electrostatic precipitator samples were taken for determination of aerosol mass concentration as a function of time, particle size distribution, and physical characteristics of the aerosol, respectively. In this test, the filter sample gas was not returned to the vessel. This small sampling loss, combined with a leak in the electrostatic precipitator sampler, caused a pressure decrease of ~0.014 MPa (2 psi) and a corresponding RH decrease from 54 to 48% (see Fig. 2).

The mass concentration of Fe<sub>2</sub>O<sub>3</sub> aerosol as a function of time as measured by two different filter samplers and two cascade impactors is given in Fig. 3. Extrapolation of these data back to the time of aerosol generator cutoff (0.5 min) using the visual curve fit shown yields a value of  $\sim 2 \text{ g/m}^3$ .

The aerodynamic mass medium diameter (AMMD) of the aerosol was measured using cascade impactors (Andersen Mark III). Two samples as a function of elapsed time were taken for size analysis: one was taken inside the vessel with the impactor under existing vessel conditions of temperature and pressure; the other was taken outside the vessel, again with the impactor under approximately the existing vessel conditions of temperature and pressure. In taking each sample, vessel gas was pulled through the impactor and returned to the vessel. Table 2 contains the results from these samples.

Time from start of aerosol generation (min)	Sampler	Location	AMMD (µm)	Standard deviation, σ
18.2	Cascade impactor	Internal	3.7	2.3
44.4	Cascade impactor	External	2.4	2.3

## Table 2. Results from aerosol sizing samples (AMIT-5001)

Results from scanning electron microscopy (SEM) analysis of the five electrostatic precipitator samples indicated that essentially all of the Fe2O3 was in the form of chainlike agglomerates.

2.1.4.4 <u>Aerosol-moisture interaction test AMIT-5002</u>. AMIT-5002 was conducted on August 8, 1985, at an initial RH of 73%. Fe<sub>2</sub>O<sub>3</sub> aerosol was produced with the plasma torch aerosol generator with 10.4 g of iron powder passed through the torch over the last 23 s of a 63-s plasma torc operation period. As shown in Fig. 4, the RH increased from the initial





value of 73% to a final value of 79% after plasma torch operation. During the 2-h period following aerosol generation, nine filter samples, two cascade impactor samples, and five electrostatic precipitator samples were taken for determination of aerosol mass concentration as a function of time, particle size distribution, and physical characteristics of the aerosol, respectively. In this test all of the sample gas was returned to the vessel, and the vessel gas pressure and RH remained nearly constant (see Fig. 4).

As in the first test (AMIT-5001), results from SEM analysis of the five electrostatic precipitator samples indicated that essentially all of the  $Fe_2O_3$  aerosol was in the form of chainlike agglomerates. Analysis of the remaining test data is in progress.





The next test (AMIT-5003), an Fe<sub>2</sub>O<sub>3</sub> aerosol test at ~95% RH, will continue the search for the transition from chainlike to spherically shaped agglomerates. Beginning with this test, a measurement system will be applied, consisting of four parallel sampling trains, three of which contain a modified cascade impactor, a condensation nucleus counter (CNC), and an absolute filter. The fourth train will consist of only the CNC and filter. Data obtained with this system will be used for estimation of the aerosol dynamic shape factor  $\chi$ .

#### 2.1.5 LACE Program support work

As part of the NRC support of the LACE Program at Hanford, a development effort was carried out to determine the suitability of plasma torch aerosol generators for the production of manganese aerosols under the operating conditions of future LACE tests. Several preliminary tests (LACE-DT-1 through LACE-DT-5) in the 0.35-m<sup>3</sup> vessel without aerosol generation were first completed to determine the torch operating parameters necessary for operation against a vessel gage pressure of 0.276 MPa (40 psig).

The first manganese aerosol-generation test (LACE-DT-6) was conducted in the  $0.13-m^3$  development test vessel using an argon atmosphere under a pressure of 0.276 MPa. A second manganese aerosol-generation test (LACE-DT-7) was conducted in the AMIT vessel containing a 50/50 volume percent N<sub>2</sub> and steam mixture at 280°C and 0.276 MPa (40 psig). This test environment simulated the environment expected in the aerosol mixing vessel to be used in the first LACE test. Results from these aerosol tests were given in the last progress report.<sup>1</sup>

The next test of the LACE series was a reliability test (LACE-DT-8) conducted in the NSPP vessel ( $38.3 \text{ m}^3$ ) on March 13 to demonstrate operation of the plasma torch for an extended period (60 min) against a vessel pressure of 0.276 MPa gage (40 psig). This test was conducted with no aerosol generation, and there were no apparent problems resulting from this extended operation.

The last test of the LACE series was a  $Mn_2O_3$  aerosol behavior test in the NSPP vessel in a condensing steam-air environment. Detailed results from this experiment are given in Sect. 2.1.6.

The LACE test series demonstrated that the plasma torch method is feasible for manganese aerosol generation under LACE test conditions; however, suitable aerosol-generation rates remain to be demonstrated onsite using the actual LACE plasma torch aerosol-generation system.

#### 2.1.6 LWR aerosol experiment NSPP-541

The last test (NSPP-541) of the LACE series was a manganese oxide aerosol behavior test in the NSPP vessel in a condensing steam-air environment (~0.16 MPa absolute pressure and 378 K). This test was conducted on April 17, 1985, under normal NSPP test procedures (Table 1) and was intended to provide manganese oxide aerosol behavior data for comparison with the present NSPP data base (Fe<sub>2</sub>O<sub>3</sub>, U<sub>3</sub>O<sub>8</sub>, and concrete aerosols) and with data from future LACE tests.

The plasma gas for aerosol generation was argon plus helium (the same as was used in the other LACE tests described in Sect. 2.5), and the aerosol produced within the NSPP vessel atmosphere was shown by X-ray diffraction analysis to be primarily  $\gamma$ -Mn<sub>2</sub>O<sub>3</sub>. This is in contrast with the aerosol produced in the LACE-DT-7 test, which was conducted in the AMIT vessel containing a 50/50 volume percent N<sub>2</sub> and steam mixture at 553 K and 0.276 MPa gage pressure; in that test the aerosol was shown by X-ray diffraction to be ~50% MnO and 50%  $\beta$ -Mn metal.

To prepare the test atmosphere, the small fan-mixer inside the vessel was turned on, and steam was introduced into the vessel, which was initially at 0.033 MPa (abs) and ambient temperature of 297 K, to bring the vessel atmosphere (air and steam) to an absolute pressure of 0.168 MPa and an average temperature of 381 K. This heating step required about 1.1 h; at this point the rate of steam injection was reduced to the level required to offset heat losses through the walls of the insulated test vessel and maintain wall temperature nearly constant. Approximately 45 min later, the accumulated steam condensate in the NSPP vessel was removed to a holding tank, and Mn203 aerosol generation was started. The Mn203 aerosol was produced with the plasma torch aerosol generator with 679 g of manganese powder passed through the torch over a period of 16 min. The test environment was a mixture of air and steam at an absolute pressure of 0.178 MPa and a temperature of 381 K at the time of termination of aerosol generation. At the end of 6 h of low-level steam injection, the absolute pressure and temperature had increased to 0.217 MPa

and 386 K, respectively. At this point, steam injection was terminated, and the vessel was allowed to cool undisturbed for 18 h.

2.1.6.1 <u>Aerosol mass concentration</u>. The first set of aerosol mass concentration samples was taken 7 min after termination of aerosol generation. Subsequent samples were obtained over a 24-h period in accordance with the normal sampling procedures.

The mass concentration of Mn203 aerosol as a function of time as measured by the seven individual aerosol mass samplers is given in Fig. 5. It was expected that the small fan-mixer installed in the center of the vessel near the bottom would produce a homogeneous mixture of aerosol and steam. However, sampler 154, the lowest of the samplers (see Table 3), indicated that the aerosol mass concentration was higher near the bottom of the vessel than at the other sampler locations during the first hour following termination of aerosol generation. The fan-mixer was found to be still operable after the test.

Sampler	Radial direction	Distance from bottom [m (ft)]	Radial distance from centerline [m (ft)]
In-vessel 151	East	4.15 (13.6)	0.58 (1.90)
In-vessel 152	Southeast	4.15 (13.6)	1.06 (3.48)
In-vessel 153	East	2.80 (9.2)	1.09 (3.58)
In-vessel 154	Southeast	1.34 (4.4)	1.11 (3.64)
Wall 155	South	4.15 (13.6)	0.61 (2.0)
Wall 156	Southeast	2.80 (9.2)	0.025 (1 in.) from wall
Wall 157	Southwest	2.80 (9.2)	1.06 (3.48)

Table 3. Locations of NSPP aerosol mass concentration samplers

To facilitate comparison of the data with the results of other tests, each set of samples was averaged to produce the average aerosol mass concentration data plotted in Fig. 5. Extrapolation of these data back to the time of aerosol generator cutoff (16 min) yields a value of ~2.5 g/m<sup>3</sup>.

2.1.6.2 <u>Aerosol particle size</u>. The AMMD of the aerosol was measured using cascade impactors (Andersen Mark III). Four samples as a function of elapsed time were taken for size analysis: two were taken from an auxiliary sampling tank external to the NSPP vessel, and two were taken inside the vessel with the impactors under existing vessel conditions of temperature and pressure. In the external method, the sample was taken after the aerosol was diluted with dry instrument air, cooled, and brought to atmospheric pressure. Table 4 contains the results from these samples. These data for Mn203 in steam are essentially the same as those reported previously for Fe203 in steam (see Fig. 15 in Ref. 2) and









Time from start of aerosol generation (min)	Sampler	Location	AMMD (µm)	Standard deviation, σ
31.5	Cascade impactor	External	1.2	1.7
37 . 1	Cascade impactor	Internal	2.5	1.9
71.2	Cascade impactor	Internal	2.7	1.9
78.6	Cascade impactor	External	1.4	1.6

# Table 4. Results from aerosol sizing samples (NSPP-541)

again show the in-vessel values in steam to be a factor of about 2 larger than the ex-vessel values.

2.1.6.3 <u>Aerosol distribution</u>. At the termination of the test (24 h), the approximate aerosol distribution, as determined by the total fallout and total plateout samples and the final aerosol filter samples, was as follows: aerosol settled onto the floor of the vessel, 45%; aerosol plated onto internal surfaces, 55%; and aerosol still suspended in the vessel atmosphere, <0.1%.

#### 3. ANALYTICAL PROGRAM

#### N. C. J. Chen M. L. Tobias

# 3.1 Impactor Modification for AMIT Facility

# N. C. J. Chen

## 3.1.1 Introduction

An impactor loading analysis has been performed to modify existing impactors for the AMIT sampling system. The modification is necessary in characterizing aerosol dynamic shape factor  $(\chi)$  in humid environments, as part of the objectives of the AMIT experiment.

To obtain desirable impactor configurations, this study will (1) review the proposed sampling system, (2) evaluate impactor data from AMIT-5001, the first aerosol-moisture interaction test; and (3) recommend an optimal impactor configuration.

#### 3.1.2 Sampling system for x measurement

The proposed instrumentation for determining  $\chi$  requires a combination of a modified impactor, a CNC, and a filter. This combination will measure size ranges of aerodynamic diameter, particle number concentration, and fractionated volume mass concentration, respectively.

Figure 7 shows the sampling system, which consists of four sampling lines that operate in parallel. Three of the sampling lines are composed



Fig. 7. Conceptual diagram of aerosol sampling system for AMIT facility.

of three components: a modified impactor, a CNC, and a filter. The fourth sampling line contains a CNC and a filter. In practice, all four lines would operate simultaneously.

The principle of  $\chi$  determination has been described in Ref. 1 and will not be repeated. We will concentrate only on the impactor modifications.

# 3.1.3 Impactor loading analysis

The impactor loading analysis was based on AMIT-5001 data. The data were acquired from an ex-vessel cascade impactor, an eight-stage Andersen Mark III stack sampler, upon which the modification will be made.

Table 5 shows the data reduction in a standard format. The last column has been added to present the mass fractions collected that are larger than the lower limit of each size range. For example, those particles larger than 4.0  $\mu$ m in diameter would make up ~26.46% of the total mass. This information will determine the number of plates to be used inside a modified impactor.

Stage No.	Mass collected (µg)	Mass fraction (%)	Effective cut diameter (µm)	Size range (µm)	Cumulative mass fraction (%)	Cumulative mass collected (%)
0	410	2.92	13.7	>13.7	100.00	2.92
1	510	3.63	8.5	8.5 to 13.7	97.08	6.55
2	1,100	7.82	5.8	5.8 to 8.5	93.45	14.37
3	1,700	12.09	4.0	4.0 to 5.8	85.63	26.46
4	3,200	22.76	2.5	2.5 to 4.0	73.54	49.22
5	4,000	28.45	1.3	1.3 to 2.5	50.78	77.67
6	2,000	14.23	0.78	0.78 to 1.3	22.33	91.90
7	970	6.90	0.53	0.53 to 0.78	8.1	98.80
Backup filter	169	1.20	0	0 to 0.53	1.2	100.00
Total	14,059	100,00				

Table 5. Ex-vessel impactor data reduction of test AMIT-5001

Particle size statistics can be obtained graphically if the cumulative mass fraction (next to last column) is plotted against the upper limit of each size range, as shown in Fig. 8; the bulk of the data follows a log-normal distribution with a mass median diameter of ~2.5 µm and a geometric standard deviation of 2.2.



Fig. 8. Iron oxide aerosol size distribution from AMIT-5001 exvessel impactor data.

# 3.1.4 Recommended impactor configuration

In a standard assembly, the Andersen Mark-III stack sampler should include the following: 10 plates numbered 0, 1, 2, 3, 4, 5, 6, 7, 8, and F; 11 Inconel spacers; 8 stainless steel crossbars; 8 glass fiber collection disks; 1 glass fiber filter; and 1 plate holder. Plate 0 is an orifice stage only. Plate 8 is a collection stage only. Plate F is a backup filter holder.

The configuration of modified impactors depends on the expected mass loading. Allocating the loading of impactors 1, 2, and 3, respectively, in the proposed sampling system (Fig. 7) by fractions of about 25, 50, and 75% of the total mass seems to be appropriate. Accordingly, it is recommended that the configuration of the modified impactors should consist of five plates (numbered 0 through 4), six plates (numbered 0 through 5), and seven plates (numbered 0 through 6), respectively.

#### Further modification should include

- 1. no backup filter in each impactor,
- 2. use of spacers for missing plates, and
- blank off of all but the innermost two circles of holes in each impactor plate (leaving about 20% open).

Partially blanking off orifices in each plate is important because it will prevent the flow of the aerosol/gas mixture within the vessel from falling off over the sampling period while at the same time maintaining an adequate linear velocity through the orifices. The recommended blank off of about 80% of the area was estimated from a flow reduction of 14.2 L/min as required by the manufacturer to 3 L/min as required by the AMIT sampling lines.

# 3.2 Data Processing Related to NSPP and AMIT Development and Preliminary Tests

## N. C. J. Chen

The AMIT facility is designed to study physical characteristics (shape factors) of aerosol spheroidization in humid environments. A series of development and preliminary tests was conducted to achieve this goal. In support of the experiments, data processing and analysis have been performed concurrently.

Nine development and preliminary tests have been completed (Table 6). The data compilation of the first two NSPP development tests was completed and analysis highlights were reported.<sup>1</sup> The processing of the two AMIT development tests has been fully completed and data were evaluated. Data processing for the two preliminary tests, AMIT-PT-1-1 and AMIT-PT-1-2, and for the first AMIT test, AMIT-5001, has been recently completed. Data processing for tests NSPP-DT-3 and AMIT-5002 is under way.

# 3.3 <u>A Capillary Mechanism for Condensation of</u> Water Vapor on Aerosol Particles

N. C. J. Chen

#### 3.3.1 Introduction

Transformation of aerosol agglomerate shapes has been observed in the NSPP tests. Some aerosols that exist as chain agglomerates in a dry air environment change into spheroids in a steam-air environment. This behavior has been attributed to the formation of a condensed water film on the aerosol surfaces as a consequence of supersaturation in the steamair environments. However, a similar behavior occurs in highly humid, but not supersaturated, environments; thus, the supersaturation theory does not seem to apply.

	Number of	D	ata process	ing cycle	12.12
Test	subtests	Step 1 <sup>a</sup>	Step 2 <sup>b</sup>	Step 3 <sup>c</sup>	Step 4 <sup>d</sup>
NSPP-DT-1 <sup>e</sup>	5	√£	1	4	1
NSPP-DT-29	3	1	1	1	1
AMIT-DT-1 <sup>h</sup>	7	1	1	1	1
AMIT-DT-2 <sup>i</sup>	5	1	1	1	1
AMIT-PT-1-1	1	1	1	1	
AMIT-PT-1-2k	1	1	1	1	1
AMIT-5001 2	1	1	1	1	1
NSPP-DT-3 <sup>m</sup>	1				
AMIT-5002 <sup>n</sup>	1				

Table 6. Matrix showing data processing status

 ${}^{\mathcal{A}}\textsc{Dump}$  files from magnetic tapes by a utility program EZCOPY or UCHBUF.

<sup>b</sup>Convert raw data into engineering units.

<sup>C</sup>Tabulate data as a function of time and create a plot file for display. The monitored data vary from test to test, usually including vessel pressure, temperatures, heat fluxes, and sample volumes.

<sup>d</sup>Display key parameters as a function of time for single or multiple subtest.

<sup>e</sup>Heat and mass development tests.

<sup>7</sup>A check mark indicates that a processing step has been completed.

 $g_{\text{Same}}$  as NSPP-DT-1, but gas temperatures between torch delivery tube and vessel were measured.

<sup>h</sup>Same as NSPP-DT-2 in search of an optimal torch power while notice taining an adequate aerosol-generation rate.

<sup>2</sup>Aiming to minimize effects of radiation and background convection by modifying AMIT-DT-1 to include (1) a double-bended delivery tube, (2) an insulated vessel, and (3) a fast-scanning data logger.

 $^{j}\mathrm{A}$  preliminary heat test to study humidity response to torch power; test conducted with the AMIT vessel containing an initial relative humidity of ~50%.

<sup>k</sup>Same as AMIT-PT-1-1 but at a higher initial RH (~80%).

<sup>l</sup>Same as AMIT-PT-1-1 except with Fe<sub>2</sub>O<sub>3</sub> aerosol generation. Apart from routine heat monitoring, mass-related measurements were added: impactors, filters, and electrostatic precipitators.

<sup>m</sup>Same as AMIT-5001 but at NSPP operating conditions.

<sup>n</sup>Same as AMIT-5001 but at a higher initial RH of ~80%.

Capillary condensation is proposed to explain such observations. It would occur in a volume around the area of contact between two adjoining primary aerosol particles. Such a volume would possess a concave surface over which the vapor pressure of any condensed water would be significantly reduced below that for a plane surface. If condensation started in this contact region, further condensation could take place even if the environment were unsaturated.

Spheroidization of aerosol agglomerates is a complex process that may couple thermodynamics and dynamics. This progress report will focus on the thermodynamics of the capillary condensation occurring in the volume around the contact area of two identical adjoining particles. The complete discussion will include a derivation of the equation for capillary condensation, a numerical method to calculate equilibrium states and the time to reach significant growth, and a discussion of the application of this theory to spheroidization of aerosol agglomerates. However, only the derivation and input parameters will be reported here; the remaining portion of the work will be reported later.

#### 3.3.2 Thermodynamic formulation

This section will provide derivation of the growth equation and will list the conditions for condensation, equilibrium, and evaporation by capillary condensation.

3.3.2.1 Derivation of growth equation. The reference configuration of two identical aerosol primary particles embedded in an infinite water vapor environment is shown in Fig. 9. The volume formed around the area of contact can be fully characterized by the half-width  $a_1$ , a filling angle  $\phi$  of the condensed water ring, and a radius  $a_2$  of the concave intersurface between water and vapor.

In the formulation, the following assumptions were made:

1. particle surface is smooth,

m

- 2. wetting is perfect (i.e., the contact angle equals zero), and
- chemical/physical properties of the particle surface are not accounted for.

With these simplifications. the capillary condensation may be regarded as a diffusion-controlled process with a driving force being the difference of vapor density between the environment and that over the concave water interface:

$$\frac{\mathrm{d}\mathbf{m}}{\mathrm{d}\mathbf{t}} = 4\pi \mathbf{r}_{\mathbf{k}} D \left[ \rho_{\mathbf{v}} - \rho_{\mathbf{v}}(\mathbf{r}) \right] , \qquad (1)$$

where D, m,  $r_k$ ,  $\rho_v$ , and  $\rho_v(r)$  represent, respectively, the water vapor diffusivity coefficient, condensed water mass, Kelvin radius, water vapor density of the ambient atmosphere, and that at the concave surface.

The mass, volume, and Kelvin radius of the water ring are related by

$$= \rho_{g} V$$
, (2)



Fig. 9. Reference configuration showing capillary condensation in the volume formed between two adjoining aerosol primary particles.

$$V = 2\pi r^3 f(\phi) , \qquad (3)$$

$$\frac{1}{r_{k}} = \frac{1}{2} \left( \frac{1}{a_{2}} - \frac{1}{a_{1}} \right) , \qquad (4)$$

where r and  $\rho_{\mbox{$\ell$}}$  are the particle radius and water density, respectively, and

$$f(\phi) = (\sec \phi - 1)^2 \left[ 1 - \left( \frac{\pi}{2} - \phi \right) \tan \phi \right] . \tag{5}$$

The volume expressed in Eq. (3) is that of the condensed water ring. The Kelvin radius defined in Eq. (4) is a harmonic mean of the half-width and radius of meniscus of the water ring and represents the characteristic length in the diffusion equation [Eq. (1)].

The equilibrium vapor pressure over the meniscus of the water ring is governed by the Kelvin equation. The equation states that vapor pressure  $P_v(r)$  over a concave surface is lower than that over a plane surface

and is represented by

$$\ln\left[\frac{P_{v}(r)}{P_{s}}\right] = -\frac{2\sigma M}{r_{k}\rho_{\ell}RT} , \qquad (6)$$

where, in addition, M,  $P_g$ , R, T, and  $\sigma$  denote water molecular weight, saturation vapor pressure over a plane surface, universal gas constant, gas temperature, and water surface tension, respectively.

By geometric relations, the half-width and radius of meniscus can be related to the filling angle as

$$a_1 = r \left( 1 + \tan \phi - \sec \phi \right), \tag{7}$$

$$a_2 = r (\sec \phi - 1) . \tag{8}$$

Combining Eqs. (1) through (8) yields the growth equation for capillary condensation

$$\frac{d\phi}{dt} = \frac{2r_k DMP_s}{r^3 \rho_{\ell} f'(\phi) RT} \left[ S - \exp\left(-\frac{2\sigma M}{r_k \rho_{\ell} RT}\right) \right], \qquad (9)$$

where  $f'(\phi)$  represents the first derivative of the function  $f(\phi)$  with respect to  $\phi$  and S signifies the saturation ratio (S =  $P_v/P_s$ ).

3.3.2.2 Existence of three distinct states. The growth equation reveals that three distinct states may exist, depending on the relative difference between water vapor pressures.

 Condensation (growth) would occur if the ambient vapor pressure is greater than the vapor pressure over the concave surface of the water ring;

$$\frac{d\phi}{dt} > 0$$
, if  $S > \exp\left(-\frac{2\sigma M}{r_k \rho_{\ell} RT}\right)$ . (10)

 An equilibrium state would be established if the vapor pressures were equal;

$$\frac{d\phi}{dt} = 0, \text{ if } S = \exp\left(-\frac{2\sigma M}{r_k \rho_{g} RT}\right). \tag{11}$$

3. Evaporation would occur when the condition in Eq. (10) is reversed.

#### 3.3.3 Solution method

The growth equation [Eq. (9)] is a nonlinear, first-order, ordinary differential equation and must be solved numerically. The solution method adopted is a standard IBM integrator called the Continuous System Modeling Program. Use of this well-established software can avoid unnecessary programming efforts in numerical integration, allowing concentration on physical formulation and result interpretation.

Tabl~ 7 lists water surface tension and saturation vapor pressure as functions o. temperature. The range of the temperatures represents the prevailing gas temperatures within the AMIT (~ $30^{\circ}$ C) and NSPP (~ $100^{\circ}$ C) vessels in which aerosol-moisture interactions occur.

Table 7. Surface tension and saturation vapor pressure

		fo	r wate	r
T		σ		Ps
(K)	( N/	/m)	)	(kPa)
373	5.89	×	10-2	101.29
353	6.26	×	10-2	47.33
333	6.62	×	10-2	19.91
313	6.46	×	10-2	7.38
303	7.12	×	10-2	4.24
293	7.28	×	10-2	2.34
283	7.42	×	10-2	1.23

3.4 Computer Code Activities

M. L. Tobias

#### 3.4.1 Experimental data processing

Because of changes in data acquisition equipment used in connection with the AMIT program and LACE experiment port work, a number of *ad hoc* changes have been necessary in the data is essing codes. An example of this occurred in one of the experimental runs where the data for a sweep of the sensor channels was recorded in two incomplete segments. A special code had to be constructed to splice the segments together, taking into account the fact that not all of the data records were broken and that one of the numbers in a sweep had been split in two.

#### 3.4.2 Correction of aerosol sample volumes

The task of correcting the sample volume values for the 400-, 500-, and 600-series of aerosol-in-steam experiments in the NSPP has been completed. As has been reported earlier,<sup>2</sup> the absolute values of aerosol mass concentrations reported were not correct. It was expected that the normalized mass concentration values, done on the basis of  $C/C_{max}$ , would be much less affected, however; this appears to be the case for the 400-series results. Work continues on applying the new sample volume values to the 500- and 600-series.

The new sample volume calculation procedure includes a printout of the clock times for the start and stop of the sampling process. This information is useful in ruling out spurious sampling indications because it enables comparison with the raw data records, which clearly show when sampling was actually being done. The calculations themselves have been improved to use the average of vessel conditions at the beginning and end of sampling instead of at the beginning alone. Furthermore, those vessel pressure gage readings that are below atmospheric pressure have been included. It was formerly believed that these readings were inaccurate, but comparisons with a new transducer placed on the vessel have shown that they can be used with confidence in analyzing past experimental results.

#### 3.4.3 Code development and implementation

The CONTAIN code has been successfully used for pretest predictions of the forthcoming LA-1 LACE test. This has necessitated changing the code from single- to double-precision operation on the IBM machines. While the single-precision version of the program was adequate for the test calculations supplied with the code, it failed to function for certain combinations of aerosol parameters. The change to double-precision eliminated this difficulty. Additionally, it was necessary to enlarge one of the machine space parameters to enable operation with more than 20 size bins.

During the course of this work, some questions have arisen concerning the code treatment of water condensation on aerosols. These questions have been brought to the attention of the code originators who are currently studying them.

Some CONTAIN calculations of the condensation of steam on a stagnant aerosol have been carried out in collaboration with Prof. S. K. Loyalka of the University of Missouri. The purpose of these calculations is to compare code results with analytical solutions to the problem. The model used in the code was an aerosol of unit density with a very high value of  $\chi$  and a very low value of  $\gamma$  to prevent settling and coagulation. This aerosol was placed in a supersaturated steam atmosphere. So far, deposition rates of the water on the aerosol have been calculated to be extremely high. Of particular interest will be comparisons of the change in aerosol size distribution.

## 3.4.4 LACE experiment LA-1 predictions using CONTAIN

Pretest predictions have been made for various assumptions of aerosol parameters to determine their effect on the final result. These parameters are listed in Table 8.

Comparisons of single- and double-precision results for cases 2 and 3 show no significant differences;  $\chi$  and  $\gamma$  changes are much more important. Details will be reported in a later document.

Case	x	Y	Number of size bins	Precision
1	1.0	1.0	20	Double
2	1.5	7.0	20	Single
3	1.5	7.0	20	Double
4	1.5	7.0	30	Double
5	1.1	3.0	20	Single
6 <sup>a</sup>	1.0	3.0	20	Double

# Table 8. Values of parameters used in CONTAIN pretest predictions for LACE experiment LA-1

<sup>a</sup>Standard calculation.

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