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# VALIDATION OF CONTAIN CODE FOR SODIUM AEROSOL BEHAVIOR

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## ABSTRACT

Evaluation of the aerosol behavior is essential in the safety analyses of the LMFBRs. This is because, in the case of a sodium leak accident, radioactive materials could be released to the containment atmosphere, and they would behave together with the sodium aerosols during the accidents.

From 1988 to 1989, PNC participated in the Second International Sodium Aerosol Code Benchmark Study performed under the auspices of the Commission of EC in an attempt to validate the aerosol behavior module of the CONTAIN code. The other organizations participating in the study are CEA-France, KfK-W.Germany and UKAEA-U.K.

This paper describes an outline of the comparison between the test results and the calculational results made by PNC, whereas the international comparison is presented separately (Ref.1).

Results revealed that the suspended aerosol mass concentration and the aerodynamic mass median diameter obtained from both the pre- and post-test calculations agreed fairly well with the test results.

## INTRODUCTION

Postulated accidents in the LMFBRs would accompany the release of sodium oxide aerosols that contain the radioactive materials. Although most of these aerosols can be confined in the reactor containment system, leakage to the environment should be evaluated. From a viewpoint of reactor safety, therefore, the analysis of aerosol behavior within the containment is required for evaluating the radiological consequence following the LMFBRs accident.

A number of computer codes calculating the aerosol behavior have been developed and validated in each country. At PNC, the ABC-INTG code which was used for the safety analysis in the prototype fast breeder reactor Monju was developed (Ref.2), and the CONTAIN code which can analyze post-accident phenomena within the containment system has been developed under the collaboration with USNRC (Ref.3).

As a part of sodium aerosol study, PNC participated in the EC Benchmark Study to validate the aerosol behavior module of these codes. This study consisted of three stages: 1) pre-test blind calculation, 2) an aerosol release test, and 3) post-test calculation with the test information. The CONTAIN code was used for both the pre-test and post-test calculations since it can calculate the sodium fire and the aerosol behavior simultaneously. On the other hand, the ABC-INTG code was used only for the post-test calculation to perform a detailed parametric study.

## AEROSOL RELEASE TEST

For the benchmark study, an aerosol release test (sodium pool fire test) named TVMA (Ref.4) was conducted at CEA-Cadarache using a 400 $m^3$ concrete cell under air-filled atmospheric condition. A total weight of 111.2 kg sodium at 550 ℃ was burnt in a 1 $m^2$ pan for 90 minutes. After 90 minutes, a steel cover was placed over the pan and the aerosol release was cut off. During and after the sodium combustion, the concentration and particle size changes of the aerosol and the temperatures of various locations in the cell were measured for 10 hours.

The test conditions were provided as input data for the post-test calculation.

## PRE- AND POST-TEST CALCULATIONS BY THE CONTAIN CODE

### Pre-test Calculation

The CONTAIN code (Ref.3) is a integrated code which can analyze post-accident phenomena within the containment system, and can calculate the sodium fire and the aerosol behavior simultaneously. Its aerosol behavior model is based on the MAEROS code, and can calculate such aerosol processes as coagulation, deposition, leakage and additional sources in a spatially homogeneous confined atmosphere.

The pre-test calculation with the CONTAIN code was carried out as a simultaneous calculation of the aerosol behavior and the sodium fire. This means that an aerosol emission rate, a pool temperature, and a gas temperature and pressure were all calculated internally. This treatment differed from the other participants, whose codes were stand-alone aerosol codes and could not handle the simultaneous calculation.

The other input data for the pre-test calculation were derived from the special calculation for the test prerequisites and the information obtained in the previous sodium fire experiments. They are presented in Table I.

### Post-test Calculation

The post-test calculation, on the other hand, was carried out by taking account of the detailed test information, and some calculational conditions were revised by reflecting the test results:

(1) Initial conditions such as the pool temperature and gas conditions were adjusted to the actual test measurements.

(2) Measurements revealed that the gas and structure surface temperatures were higher than those of the pre-test analyses, suggesting that the generated heat is larger than the predictions. The larger heat generation could have been predicted assuming either the monoxide reaction or the sodium-water (vapor contents in the atmosphere) reaction at the pool surface. Based on our code experience, however, the peroxide reaction is the major sodium-oxygen reaction under the air-filled atmospheric condition. After some parametric calculations, it was decided to take the sodium-water reaction into consideration in the

post-test calculation (assuming the peroxide generation for the sodium-oxygen reaction as in the pre-test one).
In the calculation, it is assumed that the water vapor reaching the pool surface reacts with sodium, producing sodium-monoxide aerosols. However, those monoxides released from the pool are assumed to quickly react with the water vapor in the atmosphere producing hydroxides. Consequently, the apparent reaction becomes the hydroxide producing one.

(3) For the aerosol deposition, the thermophoretic deposition is calculated, while this deposition process was omitted in the pre-test calculation.

In the calculations with the CONTAIN code, since the sodium fire and the aerosol behavior were calculated simultaneously, the aerosol emission rate was calculated internally. The aerosol emission rate measured in the TVMA test, and those of the pre- and post-test calculations were 4.06, 3.80, and 3.97 (g/sec), respectively. The reason why the post-test calculational value became closer to the test data than pre-test one is that the calculation concerning the sodium pool combustion (including the temperature of sodium pool, gas, and wall) became closer to the test data by taking account of the sodium-water reaction. In either case, it can be said that these values are very close, and this simultaneous calculation is of advantage of the CONTAIN code.

The comparative results between the TVMA test and the pre- and post-test calculations are shown in Figures 1 through 4: (1) suspended aerosol mass concentration in the cell; (2) aerodynamic mass median diameter (AMMD); (3) settled aerosol mass on floor; (4) wall-deposited aerosol mass, respectively.

The test curves are obtained by linear interpolation between the experimental measurements averaging those of various locations and presented with dashed lines (Figures 1 and 2). Cumulative values at 10 hours in the test are plotted as a star mark in Figures 3 and 4. The pre- and post-test calculational results are presented with a dotted line and a solid line, respectively.

The comparison revealed that the suspended aerosol mass concentration, the aerodynamic mass median diameter, and the settled mass on the floor obtained from both calculations agreed fairly well with the test results (Figures 1, 2, and 3). However, disagreement was found in the pre-test calculational result of the wall-deposited aerosol mass. This was improved in the post-test calculation by taking account of the thermophoretic deposition. Nevertheless, the calculation still underestimates it by an order of magnitude (Figure 4). However, it should be noted that the suspended aerosol concentration is the major concern in respect of the safety analysis of the LMFBRs, and it is mostly governed by the floor settling process not by the wall deposition.

## RE-CALCULATION BY THE ABC-INTG CODE

After the post-test calculation, the calculational conditions were examined in detail to understand the reason of the smaller deposition mass. The aerosol behavior model of the CONTAIN code treats four deposition mechanisms onto the structure surfaces: (1) gravitational settling, (2) diffusiophoresis, (3) thermophoresis , and (4) particle diffusion. Among these mechanisms, diffusiophoresis and thermophoresis are the main mechanisms of the wall deposition. Therefore, the parameters regarding these two mechanisms were studied mainly.

The deposition rates due to diffusiophoresis (Rd) and thermophoresis (Rt) are expressed as follows:

$$Rd \propto \frac{D\,A}{V\,Dd} \qquad (1)$$

$$Rt \propto \frac{Bf\,A\,T}{V\,Dt} \qquad (2)$$

where, D=diffusion coefficient of aerosol particles, A=deposition area, V=vessel volume, Dd=diffusional boundary layer thickness, Bf=Brock's factor, T=temperature gradient between gas and wall, Dt=thermal boundary layer thickness.

The thermal boundary layer thickness (Dt) was evaluated by use of the following equation,

$$Dt=\frac{H}{Nu} \qquad (3)$$

where, H=height of the cell, and Nu=the Nusselt number.

From equation (3), Dt varies depending on the Nusselt number. Since the wall deposition by thermophoresis is in inverse proportion to Dt (eq.(2)), the disagreement might occur in estimating the Dt value.

Then to validate the ABC-INTG code (Ref.2), which is another aerosol behavior code and has the same model as CONTAIN, re-calculations were carried out for the following two cases:

(1)Case-A: The same calculational conditions as the post-test calculation with CONTAIN (Dt was internally calculated by use of the equation (3)). The aerosol emission rate, the pool and wall temperature, and the gas temperature and pressure were given as input data of the time table;

(2)Case-B: A fixed thermal boundary layer thickness (Dt=0.2cm) was used throughout the calculation. The other conditions were the same as Case-A.

The results are shown in Figures 5 through 8 in the same way as the CONTAIN case. It was found that both results of the ABC-INTG calculations, except for the wall-deposited aerosol mass, were almost similar to the TVMA test data. The wall-deposited mass in Case-B became closer to the test data. Although in Case-A, Dt varied between 0.80 and 1.87 (cm) with the change of the Nusselt number, it was much larger than the value used in Case-B. Since the thermophoretic deposition mass rate is in inverse proportion to Dt, as mentioned previously, the wall deposition mass is smaller than the test data. Therefore, it can be suggested that Dt=0.2cm be most suitable for the TVMA test, at least.

## CONCLUSIONS

As a part of the EC benchmark study on sodium aerosol, PNC carried out the pre-test and post-test calculations by use of the CONTAIN and the ABC-INTG codes. The results are as follows:

(1) In the calculations with CONTAIN, the sodium fire and aerosol behavior were calculated simultaneously, and the aerosol emission rates of both pre- and post-test calculations were very close to the test data.
(2) Suspended aerosol mass concentration, aerodynamic mass median diameter, and settled aerosol mass obtained from both calculations agreed fairly well with the test data.
(3) Disagreement was found in the wall-deposited aerosol mass in the pre-test calculation. This was improved in the post-test calculation by taking account of the thermophoretic deposition mechanism.
(4) The best estimation of the wall deposition could be obtained using the fixed thermal boundary layer thickness parameter (Dt=0.2cm), instead of the Nusselt number correlation (which gives Dt=0.80 through 1.87 (cm) under the TVMA test condition).
(5) The calculational results by ABC-INTG agreed fairy well with the test data as those of CONTAIN did.
(6) The aerosol behavior modules of CONTAIN and ABC-INTG were validated in this study.

## ACKNOWLEDGMENTS

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# Table I
# Pre-test Calculation Input Data

## 1. Geometry

PLUTON containment (concrete vessel)

| | |
|---|---|
| •Basemat | 6 × 9 $m^2$ |
| •Height | 7.6 m |

## 2. Aerosol Source

| | |
|---|---|
| •Mass mean radius | 0.37 um |
| •Standard deviation ($\sigma$) | 1.5 |
| •Aerosol emission period | 90 min |
| •Density ($Na_2O_2$) | 2.8 $g/cm^3$ |

## 3. Aerosol Parameters

| | |
|---|---|
| •Collision efficiency | Pruppacher-Klett relation |
| •Dynamic shape factor | 1.0 |
| •Shape correction factor | 1.0 |
| •Density correction factor | 0.4 |
| •Thermal conductivity | 0.91 W/m•K |

## 4. Thermal Hydraulic Data

| | |
|---|---|
| •Thermal boundary layer thickness (=Dt) | 0.2 cm |
| •Diffusional boundary layer thickness (=Dd) | $10^{-3}$ cm |
| •Turbulent energy dissipation rate | $10^3$ $cm^2/s^3$ |

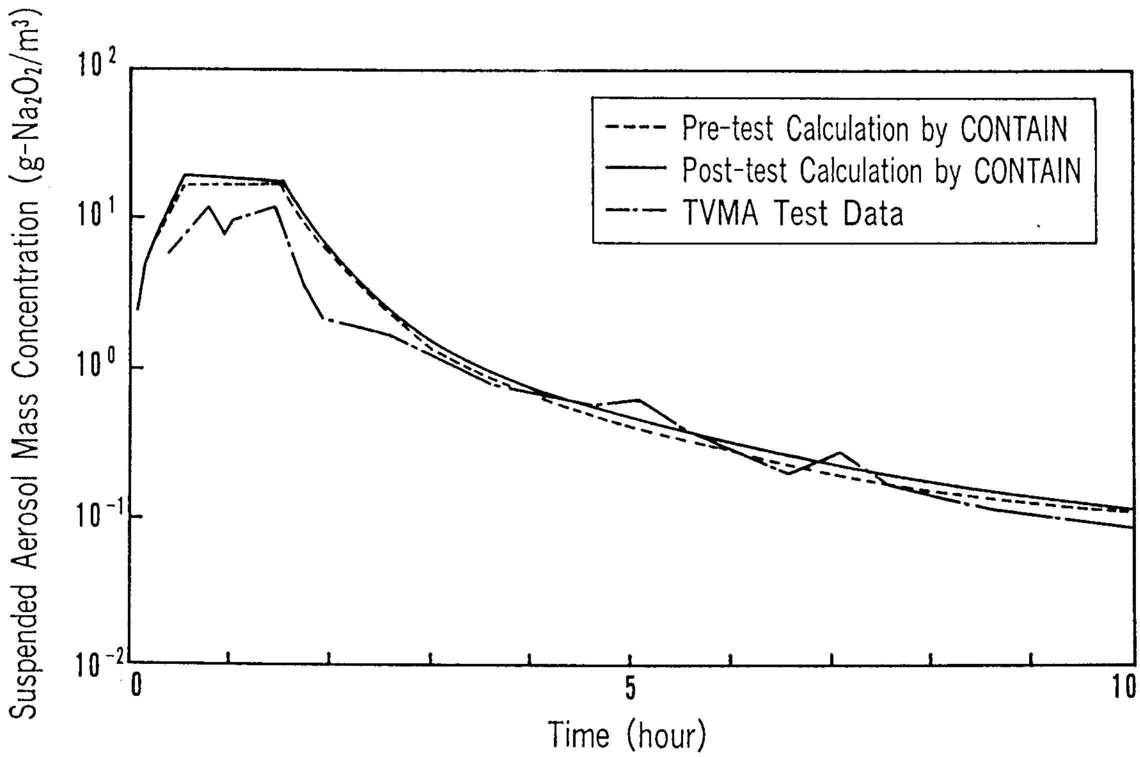


Figure 1 Comparison of Suspended Aerosol Mass Concentration between TVMA Test Data and Calculational Results by CONTAIN Code

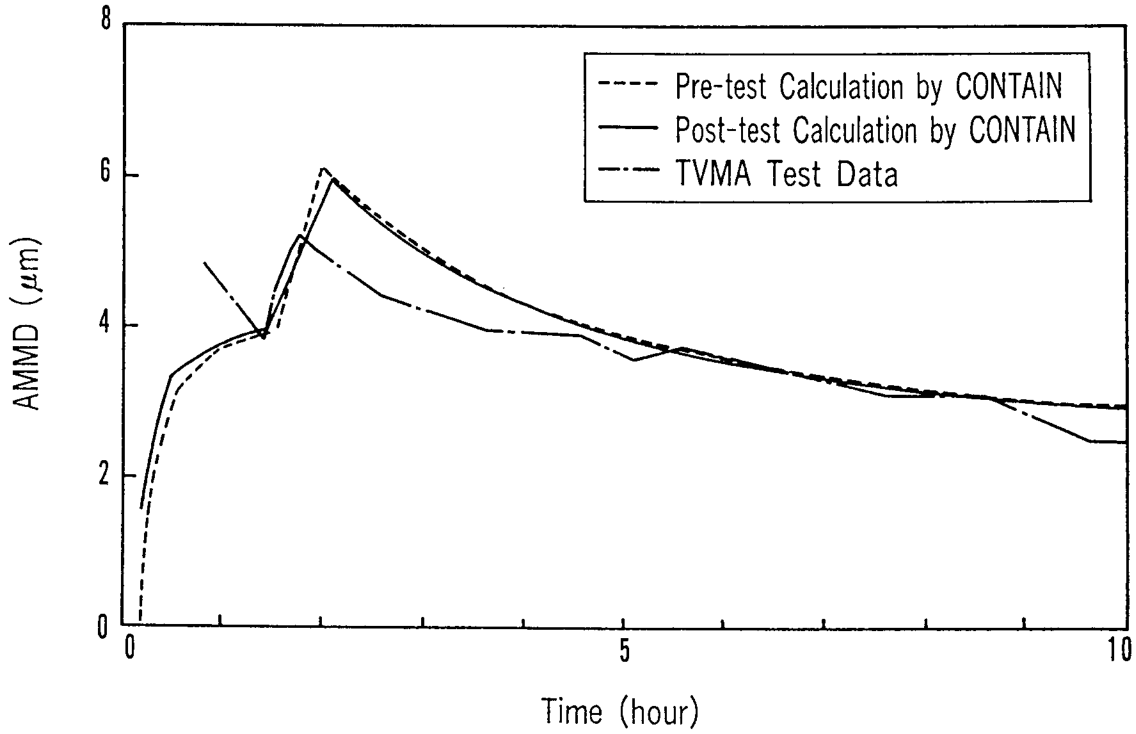


Figure 2 Comparison of Aerodynamic Mass Median Diameter (AMMD) between TVMA Test Data and Calculational Results by CONTAIN Code

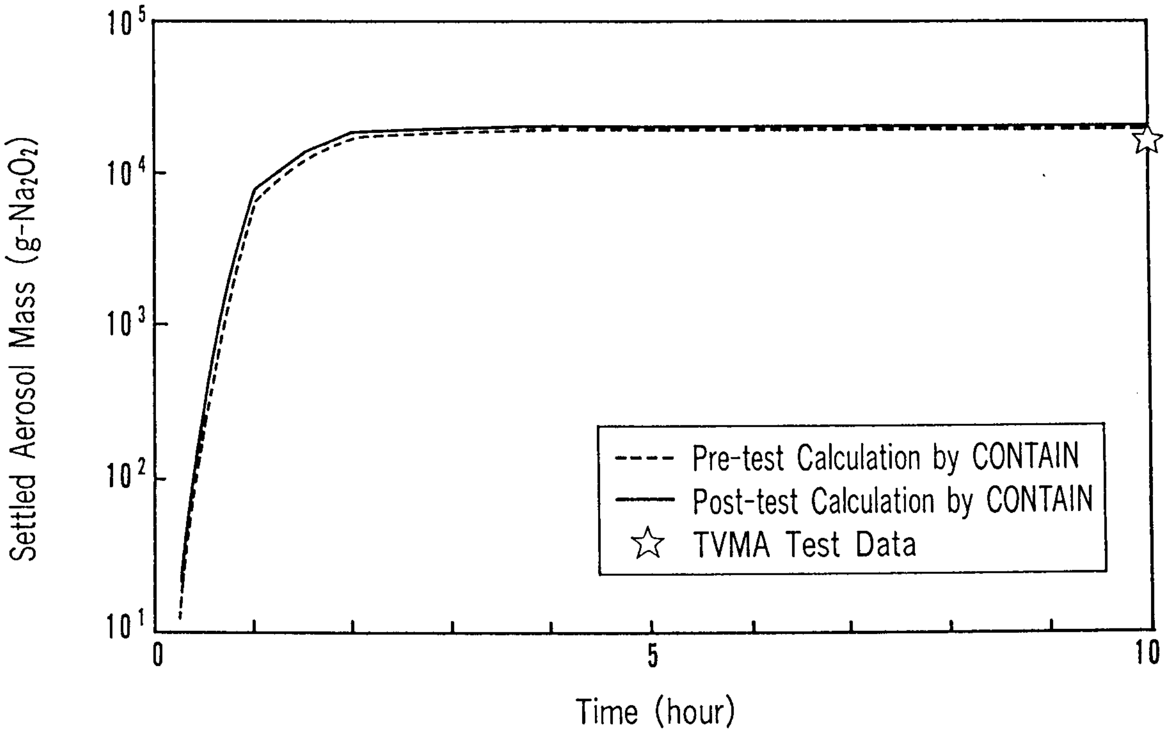


Figure 3 Comparison of Settled Aerosol Mass on Floor between TVMA Test Data and Calculational Results by CONTAIN Code

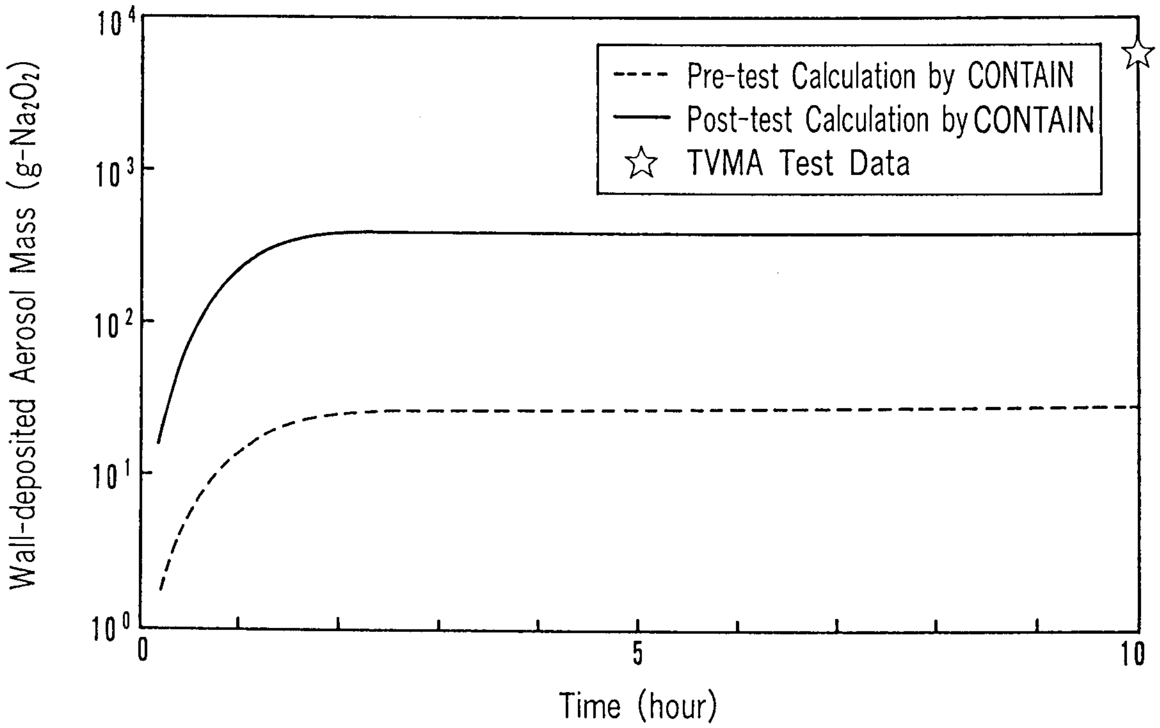


Figure 4 Comparison of Wall-deposited Aerosol Mass between TVMA Test Data and Calculational Results by CONTAIN Code

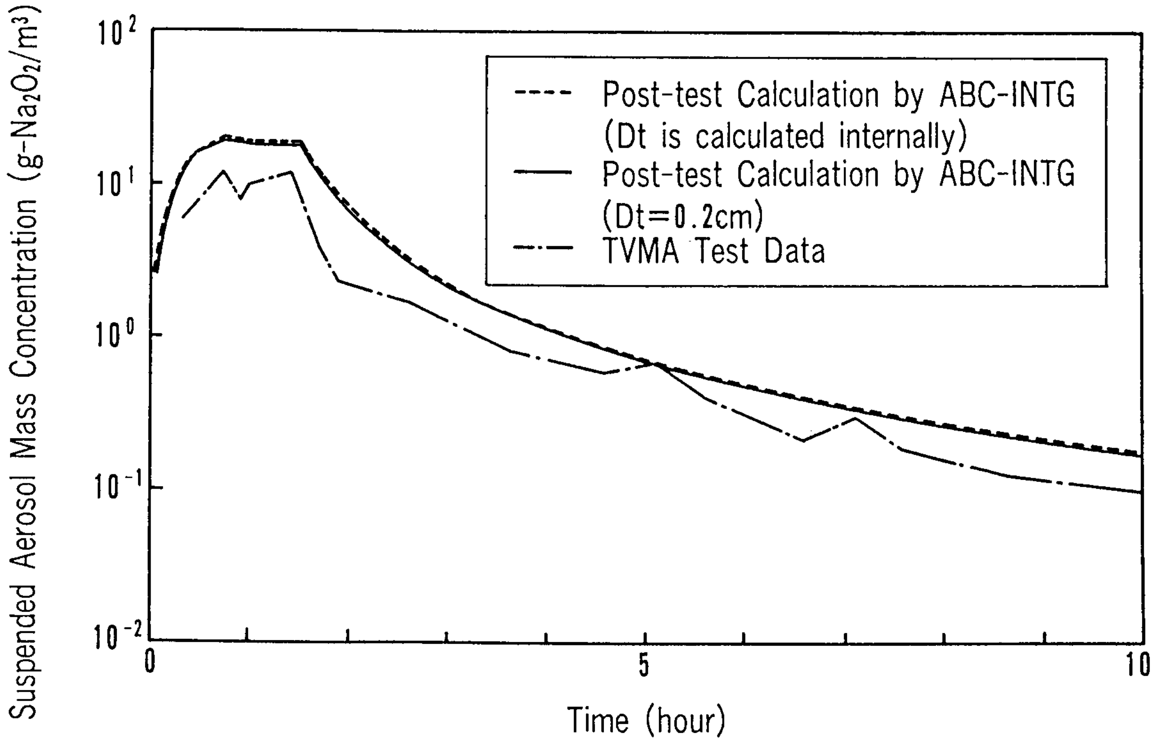


Figure 5 Comparison of Suspended Aerosol Mass Concentration between TVMA Test Data and Calculational Results by ABC-INTG Code

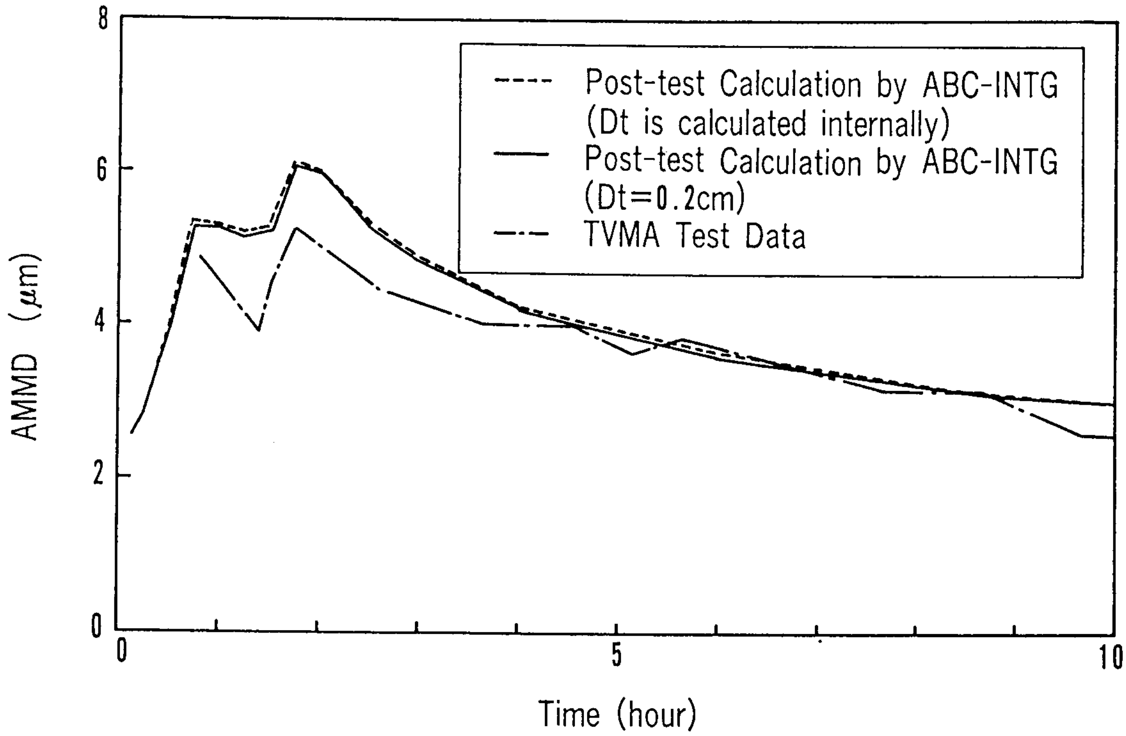


Figure 6 Comparison of Aerodynamic Mass Median Diameter (AMMD) between TVMA Test Data and Calculational Results by ABC-INTG Code

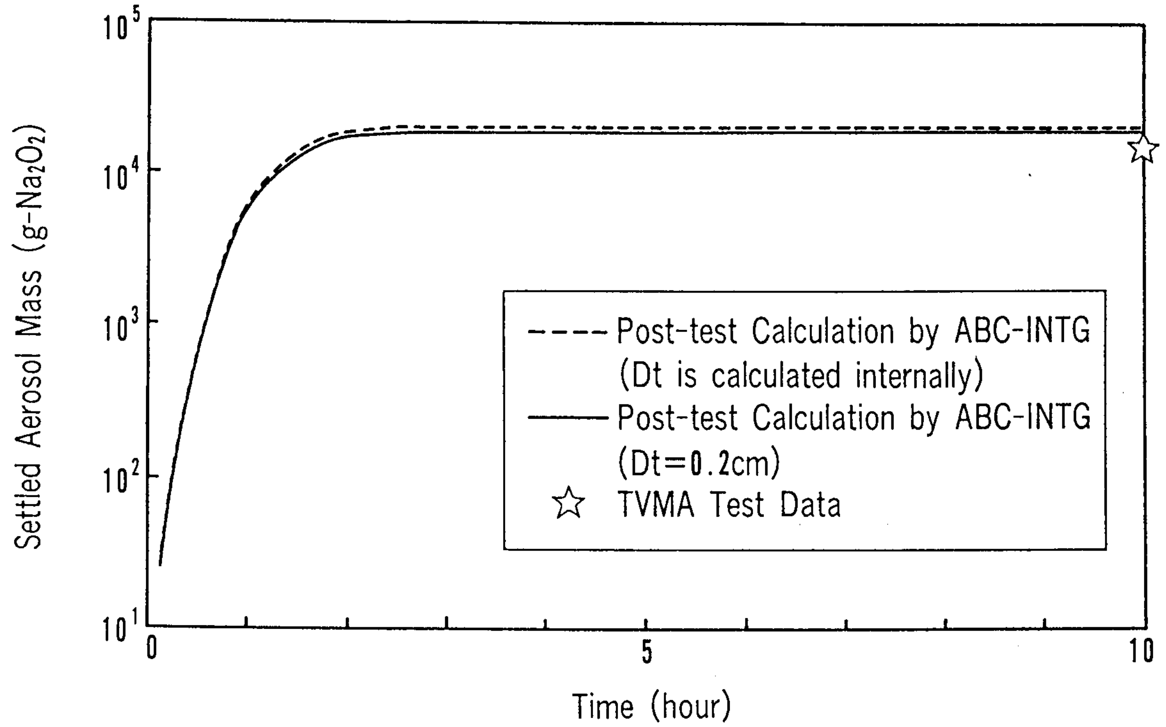


Figure 7 Comparison of Settled Aerosol Mass on Floor
between TVMA Test Data and Calculational Results by ABC-INTG Code

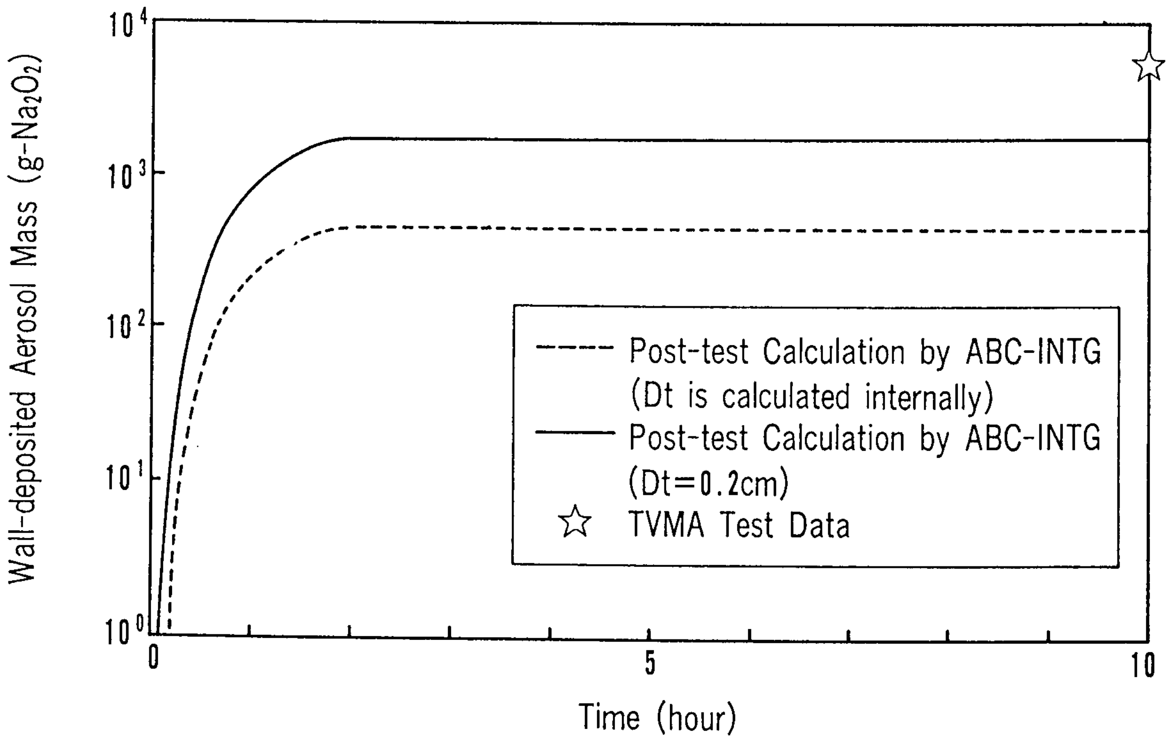


Figure 8 Comparison of Wall-deposited Aerosol Mass
between TVMA Test Data and Calculational Results by ABC-INTG Code