Correlation Confirmation on Removal Rate for Coagulating and Depositing Aerosols

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Contents

Introduction

Severe Accident Code Development

- **The severe accident analysis code, so called CINEMA, is being developed in the Korea**
- **Among various modules, SIRIUS tracks the fission product behabior in the plant. The key role of this code is to provide the quite accurate information about the radioactive materials such as the mass, size distribution, decay heat, activity and so on.**
- **The SIRIUS code has been developed to predict the behaviors of the radioactive materials in the reactor coolant system and in the containment under severe accident conditions.**

Aerosol Form of Radioactive Material Released from Core

- **In the situation of severe accidents, the radioactive materials retained in the pellet inside of the cladding can be released to the outside.**
- **The radioactive materials have tendency to transform its phase to aerosol from gaseous form. Hence the transport of these aerosol is very important to analysis of the safety of the nuclear power plant.**

Introduction

☐ Two Approaches for Aerosol Dynamcis

- **Sectional Method**
  - Approaches to the exact solution as the number of sections is increased
  - Generally considered to be more accurate than the log-normal codes(MAEROS, CONTAIN)
- **Lumped Model(or Log-Normal Method)**
  - Used in the early stage of the development of the aerosol dynamics
  - Initial Source and Size Distribution are approximated as log-normal distribution

☐ Dimensionless Numbers for Aerosol Dynamics

- **Capture both Advantages**
  - Computational Benefits and Sufficient Accuracy
- **Correlation Approximation**
  - The baseline idea is approximating correlation between integrodifferential equation of equation of aerosol coagulation and deposition such that the instantaneous rates of particle deposition are expressed in algebraic forms
- **Two Special Limiting Situations Considered**
  - One in which the aerosol cloud achieves a steady-state in the presence of a source and another in which the aerosol mass concentration continually decays by deposition in the absence of a source

Procedure for Calculating Dimensionless Mass and Removal Rate

☐ Two Major Dimensionless Numbers

$$\Lambda = \left(\frac{\gamma \varepsilon_0 \chi^2 \mu h^2}{\alpha K_0 g \rho} \right)^{1/2} \cdot \lambda \equiv \Lambda \left[\left(\frac{\gamma^9 g h^4 \varepsilon_0^5}{\alpha^3 K_0 \rho^3 \mu} \right)^{1/4} \cdot m \right]$$

$$\mathrm{M} = \left(\frac{\gamma^9 g h^4 \varepsilon_0^5}{\alpha^3 K_0 \rho^3 \mu} \right)^{1/4} \cdot m$$

☐ Actual Removal Rate in the Continuous and Discrete forms with the Effective Height

$$\lambda(t) = \frac{\int_0^\infty v n(v,t) u(v) dv}{h \int_0^\infty v n(v,t) dv}$$

$$u_{grav}(v(d_p)) = \frac{d_p^2 \rho_p g C_m}{18 \mu \chi}$$

$$\lambda(t) \approx \frac{\sum_{j=1}^{M} v_j u(v_j) n_j}{h \sum_{j=1}^{M} v_j n_j}$$

MELCOR 186 Reference Manual

$$u(v) = \frac{2}{9} \left(\frac{3}{4\pi} \right)^{2/3} \cdot \frac{\alpha^{1/3} g \rho v^{2/3}}{\chi \mu}$$

$$u(v) = B v^b$$

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Procedure for Calculating Dimensionless Mass and Removal Rate

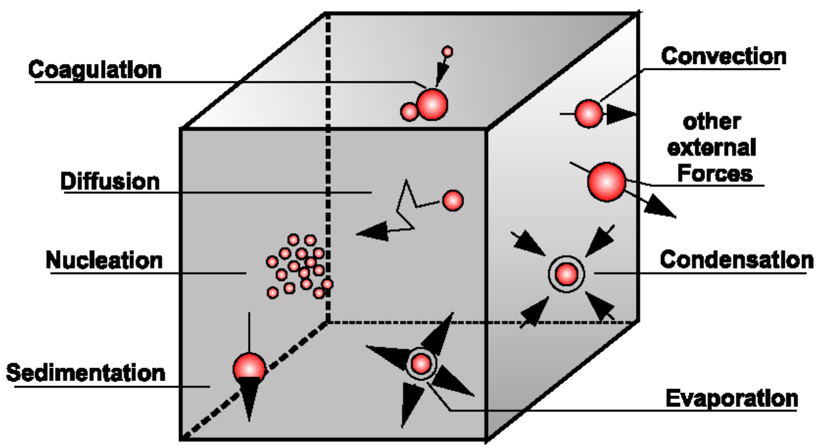
☐ Functional Relationship between dimensionless removal rate and mass

- For Steady State with Source

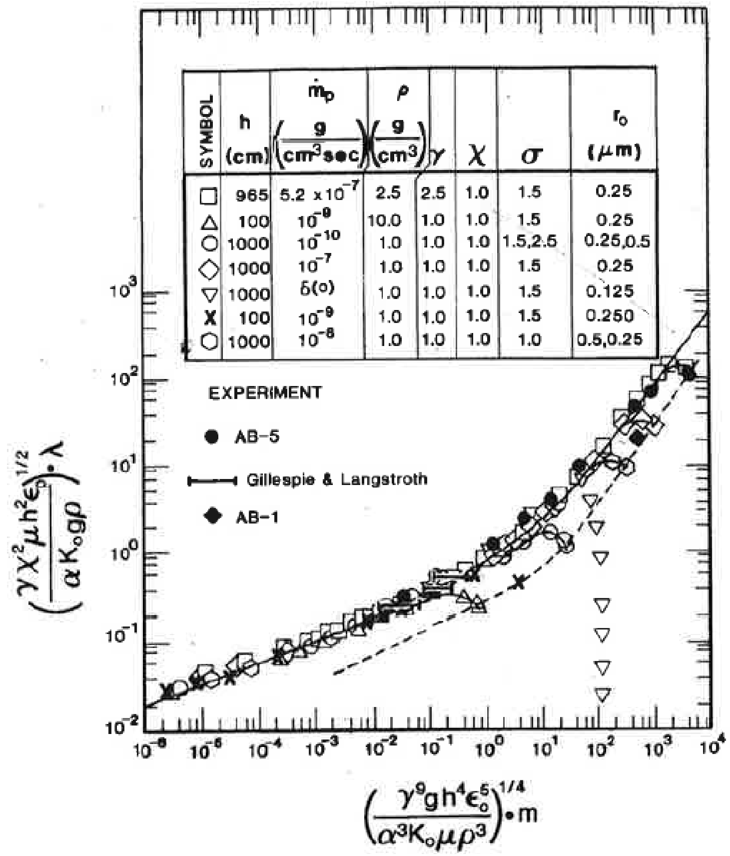
$$\Lambda_{SED}^{SS} = 0.266\mathrm{M}^{0.282}(1+0.189\mathrm{M}^{0.8})^{0.695}$$

- For decaying aerosol without Source

$$\Lambda_{SED}^{D} = 0.528\mathrm{M}^{0.235}(1+0.473\mathrm{M}^{0.754})^{0.786}$$



Modeling of Aerosol



Graph of Correlation by Epstein

Procedure for Calculating Dimensionless Mass and Removal Rate

☐ MAEROS Utilization

- **Based on the sectional method which is dividing the size spectrum into finite number of groups. The MAEROS code will provide us with the number density for each size group and system total mass for each case.**

$$\Lambda = \left(\frac{\gamma \varepsilon_0 \chi^2 \mu h^2}{\alpha K_0 g \rho} \right)^{1/2} \cdot \lambda$$

$$\mathrm{M} = \left(\frac{\gamma^9 g h^4 \varepsilon_0^5}{\alpha^3 K_0 \rho^3 \mu} \right)^{1/4} \cdot m$$

$$\lambda(t) \approx \frac{\sum_{j=1}^{M} v_j u(v_j) n_j}{h \sum_{j=1}^{M} v_j n_j}$$

```
 TOTAL AEROSOLIZED MASS REMOVED SINCE LAST OUTPUT = 6.1815E-01 KG
 CUMULATIVE OVER ALL TIME =                         3.8691E+02 KG
          TOTAL SINCE LAST OUTPUT TIME
 CEILING (KG)    0.0000E+00
 WALLS (KG)      0.0000E+00
 FLOOR (KG)      6.1815E-01
 LEAKED (KG)     0.0000E+00
 TOTAL (KG)      6.1815E-01
 CUMULATIVE (KG) 3.8691E+02
1 COAGULATION ONLY, TWO COMPONENT EXAMPLE (3 MINUTES ON PC/AT)
 TIME = 6.4826E+03 SECONDS = 1.8007E+00 HOURS
 TEMPERATURE = 3.6075E+02 DEG K      PRESSURE = 1.4561E+05 N/M**2
 SECTION     DIAMETER RANGE (M)        KG/M**3     NUMBER/M**3       KG
   1     1.0000E-08 -- 1.4125E-08   0.0000E+00   0.0000E+00   0.0000E+00
   2     1.4125E-08 -- 1.9953E-08   0.0000E+00   0.0000E+00   0.0000E+00
   3     1.9953E-08 -- 2.8184E-08   0.0000E+00   0.0000E+00   0.0000E+00
   4     2.8184E-08 -- 3.9811E-08   0.0000E+00   0.0000E+00   0.0000E+00
   5     3.9811E-08 -- 5.6234E-08   1.1210E-44   8.4516E-26   9.5513E-42
   6     5.6234E-08 -- 7.9433E-08   1.1834E-34   3.1654E-16   1.0082E-31
   7     7.9433E-08 -- 1.1220E-07   7.0108E-23   6.6540E-05   5.9732E-20
   8     1.1220E-07 -- 1.5849E-07   5.4677E-16   1.8413E+02   4.6585E-13
   9     1.5849E-07 -- 2.2387E-07   7.9237E-12   9.4678E+05   6.7510E-09
  10     2.2387E-07 -- 3.1623E-07   2.9333E-09   1.2436E+08   2.4991E-06
  11     3.1623E-07 -- 4.4668E-07   1.2898E-07   1.9401E+09   1.0989E-04
  12     4.4668E-07 -- 6.3096E-07   1.6868E-06   9.0031E+09   1.4372E-03
  13     6.3096E-07 -- 8.9125E-07   1.0707E-05   2.0276E+10   9.1225E-03
  14     8.9125E-07 -- 1.2589E-06   3.9849E-05   2.6775E+10   3.3951E-02
  15     1.2589E-06 -- 1.7783E-06   8.9479E-05   2.1332E+10   7.6236E-02
  16     1.7783E-06 -- 2.5119E-06   1.2978E-04   1.0978E+10   1.1057E-01
  17     2.5119E-06 -- 3.5481E-06   1.4192E-04   4.2596E+09   1.2092E-01
  18     3.5481E-06 -- 5.0119E-06   1.3531E-04   1.4409E+09   1.1528E-01
  19     5.0119E-06 -- 7.0795E-06   1.3701E-04   5.1767E+08   1.1673E-01
  20     7.0795E-06 -- 1.0000E-05   2.1493E-04   2.8814E+08   1.8312E-01
                                    ----------   ----------   ----------
                  TOTAL             9.0080E-04   9.6937E+10   7.6748E-01

 TOTAL AEROSOLIZED MASS REMOVED SINCE LAST OUTPUT = 4.0525E-01 KG
 CUMULATIVE OVER ALL TIME =                         3.8732E+02 KG
          TOTAL SINCE LAST OUTPUT TIME
 CEILING (KG)    0.0000E+00
 WALLS (KG)      0.0000E+00
 FLOOR (KG)      4.0525E-01
 LEAKED (KG)     0.0000E+00
 TOTAL (KG)      4.0525E-01
 CUMULATIVE (KG) 3.8732E+02
```

Sample MAEROS Output

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Dissection of Removal Rate

☐ Decay Constant Definition

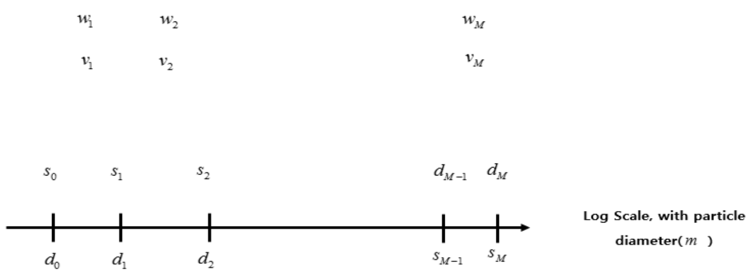
$$\lambda(t) = \frac{\int_0^\infty vn(v,t)u(v)dv}{h\int_0^\infty vn(v,t)dv}$$

☐ Discontinuous Form of Decay Constant

$$\lambda_{t_i} = \lambda(t_i) \qquad i = 0,1,\cdots,N$$

$$n_{t_i}(v) = n(v,t_i) \qquad i = 0,1,\cdots,N$$

$$n_{t_i}^{v_j} = n_{t_i}(v_j) \qquad i = 0,1,\cdots,N \qquad j = 1,2,\cdots,M$$



N:number of time interval

M:number of size interval

Number density with unit of #/m³ for j-th time step is used for

$$\lambda_{t_i} = \frac{\int_0^\infty vn_{t_i}(v)u(v)dv}{h\int_0^\infty vn_{t_i}(v)dv} \qquad \lambda_{t_i} \approx \frac{\sum_{j=1}^{M} v_j n_{t_i}^{v_j} u(v_j) w_j}{h\sum_{j=1}^{M} v_j n_{t_i}^{v_j} w_j}$$

$$v_j = \sqrt{s_{j-1}s_j} \qquad j = 1,2,\cdots,M$$

$$w_j = s_j - s_{j-1} \qquad j = 1,2,\cdots,M$$

$$s_j = \frac{1}{6}\pi d_j^3 \qquad j = 0,1,2,\cdots,M$$

MAEROS gives nw not n!

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Summary of Experiments for Numerical Simulation of the MAEROS Code

☐ MAEROS Input Preparation

Table I: Common Input Data for Sample Cases

	ABCOVE 5,6,7 and Additional Case (Case 1,2,3,4,5 and 6)
α	1.000E+00
μ (kg/(m*s))	1.565E-05
ε_o	1.000E+00
k(J/K)	1.380E-023
C_m	1.370E+00
g(m/s^2)	9.800E+00
B	2.222E-01
b	6.667E-01

Table II: Different Input Data for AB5,6 and 7

	γ	h (m)	χ	V (m^3)
AB5,6,7 (Case 1,2,3,4 and 5)	2.25	9.649	1.5	852
Zero Source (Case 6)	1.0	10.0	1.0	1000

Summary of Experiments for Numerical Simulation of the MAEROS Code

MAEROS Input Preparation

Table III: Initial Aerosol Data

	Initial GSD	Initial GMD (μm)	Initial Mass (kg/m^3)
AB5,6,7 (Case 1,2,3,4 and 5)	N/A	N/A	0.0
Zero Source (Case 6)	1.05	0.5	8.6487E-03

Case Identification

Table IV: Case Identification

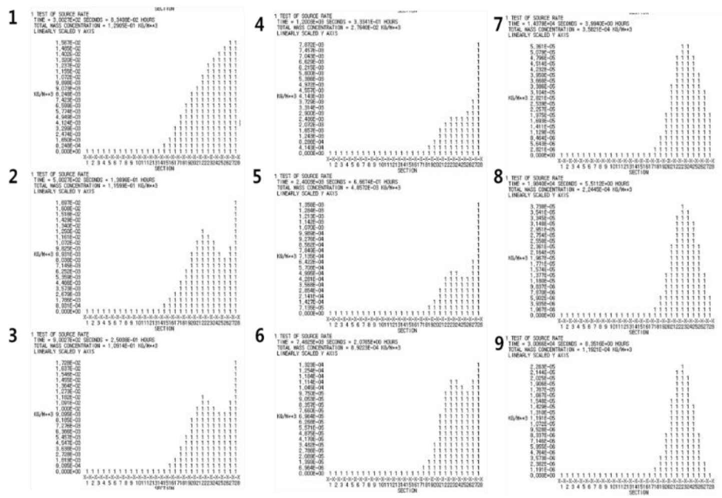
	Description
Case 1	ABCOVE5
Case 2	ABCOVE6 NaOH
Case 3	ABCOVE6 NaI
Case 4	ABCOVE7 NaOH
Case 5	ABCOVE7 NaI
Case 6	Values taken from the thesis of Epstein, 'Correlation of the Rate of Removal of Coagulating and Depositing Aerosols…'. For simulation of zero mass generation rate case

Summary of Experiments for Numerical Simulation of the MAEROS Code

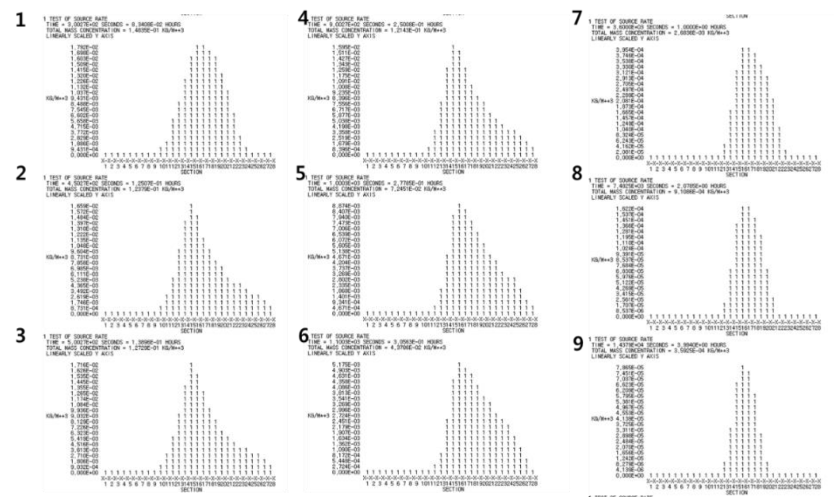
☐ Range of Size to Simulate

- Before Modification : From 0.01E-06 to 10.0E-06m
- After Modification : From 0.01E-06 to 250.0E-06m

☐ Effect of Changing Aerosol Size Range



Before Modification



After Modification

- If the upper limit of the size range is below from certain value, the missing particles occurs although actually the particles which have bigger size than value of upper size limit exist.

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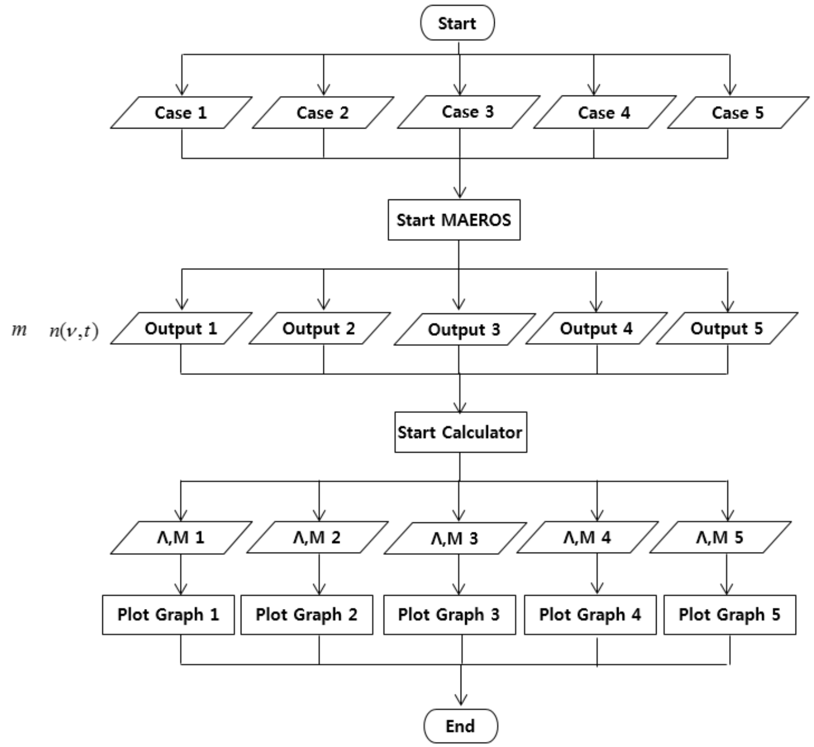
Summary of Experiments for Numerical Simulation of the MAEROS Code

Material Densities for Cases

- The material densities, ρ(kg/m^3), for cases are 2500, 2450, 3670, 2130, 3670, 1000, respectively. In Table III, it can be found that there are no aerosols for ABCOVE experiments at the beginning.

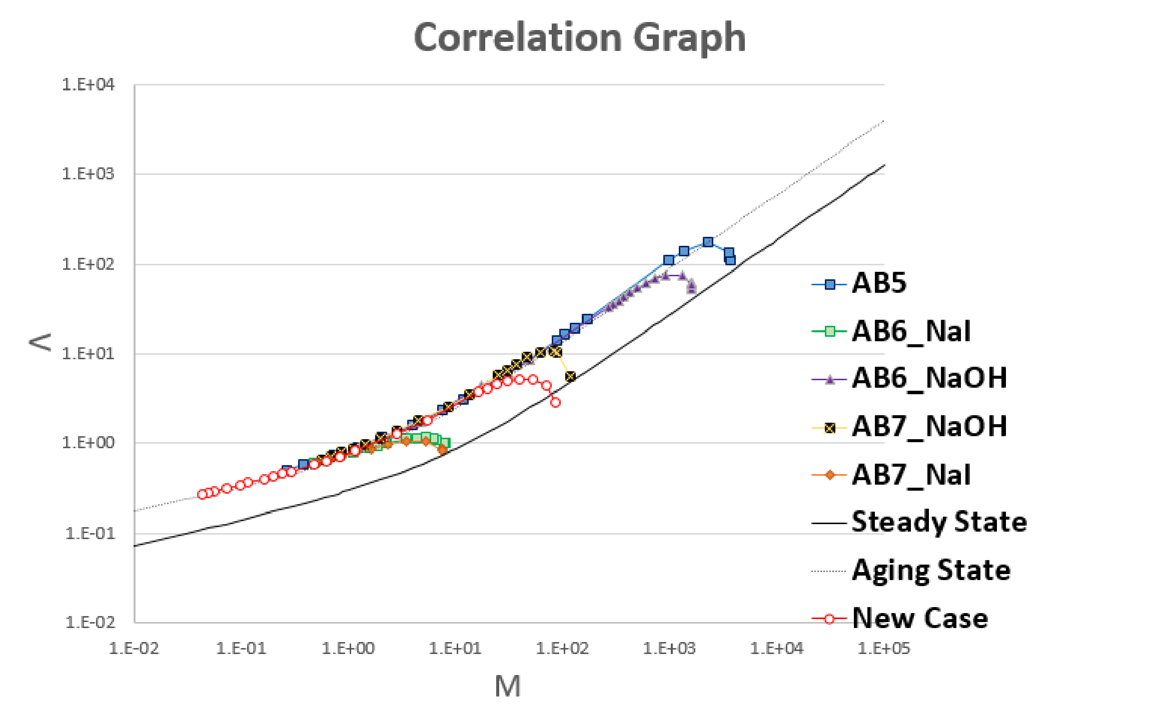
Calculation Flow Chart



Summary of Experiments for Numerical Simulation of the MAEROS Code

❑ Numerical Result

- By using the MAEROS outputs and definition of dimensionless number of Epstein, the pairs of dimensionless mass and removal rate could be calculated. Also, the MAEROS outputs are compared with the MELCOR simulation. As a result the consistency was found for both result.



Summary of Experiments for Numerical Simulation of the MAEROS Code

□ Explanation

- **All ABCOVE experiments have no initial aerosol and it is supplied by some mass source continuously for certain duration of time. Then after some time elapsed, each experiment reach the steady-state which have fixed size distribution shape and no change in system total mass. So every case approaches to the steady-state owing to the mass supply. Suddenly the source turned off. Then the particles which have large size disappear very fast. Then the removal rate decreases with the decreasing system total mass. This start with the aging aerosol line in the figure in the previous page. So the line of aging aerosol means that the line itself is turning point that the removal rate is decreasing, conversely.**
- **It was found that all of the experiment is following the previous explanation. Also, by just changing a few variables such as collison shape factor, effective height, particle settling shape factor and material density.**

Summary

☐ Conclusion

- The Epstein's correlation was confirmed from the sample runs.
- The most important factor to identify a case from the other cases is mass supplying rate(or source strength). Although the ABCOVE experiments have almost same condition except for the material density, initial source distribution, source strength, the results are much from each other. With this fact, it can be concluded that the most effective factors are distinct from each other.
- The dimensionless removal rate and system total mass have correlation.

☐ Future Works

- Take dimensionless time into account.
- Utilize this result to predict size distribution as well.
- Literary reviews

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Appendix A. Sample MAEROS Input for ABCOVE 5

MAEROS input

```
1 = NUMBER OF CASES
TEST OF SOURCE RATE
SECTIONS   COMPONENTS  NUMBER-OUTPUTS  NUMBER-SOURCES  STATUS
   28          1            20              6             0
CONDENSE  TP-TABLE  NEWCOEF  STORE  AUTO-BOUNDARIES  INITIAL  SOURCES
   0          20       1        0          1             1        1
PLOTS  PLOT-COMPONENTS  ROWS  COLUMNS  MIN-CONC.  MAX-CONC.
  1          0           20     50        0.        1.
CEILING/V  FLOOR/V  WALL/V  CHI  DIFFUSION-THICK  Particle-material-density
   0.      .103638     0.   1.5       1.E-5           2.5E3
LEAK-RATE  GAMMA  STICK  TGRAD-C  TGRAD-F  TGRAD-W   THERMAL COND. G/P
   0.       2.25    1.      0.       0.       0.              .05
RHO-C RHO-F  RHO-W  VFRAC-C  VFRAC-F  VFRAC-W  VGRAD-C  VGRAD-F  VGRAD-W
1.E3  1.E3   1.E3    0.        0.        0.        0.        0.       0.
TURBDS  VOLUME  MOLECULAR-WT  ROUND-OFF  REL-ERROR  INITIAL STEAM CONC.
.001      852.       28.8         1.E-6       0.003         0.0
TGAS1   TGAS2    PGAS1    PGAS2
290.15  700.15   1.E5     3.E5
SMALLEST-DIAMETER  LARGEST-DIAMETER
   .01E-6              25.E-5
INITIAL-MASS-CONC.(KG/M**3)   MEAN-DIAMETER   GEO-STAND.-DEV.
         0.0                   4.0E-7            1.1
TIME  VAPOR-SOURCE-RATE (KG/S)/ AEROSOL SOURCE RATE (LOG-NORMAL)(KG/S)
0.       0.
0.  0.5E-6  1.5
TIME  VAPOR-SOURCE-RATE (KG/S)/ AEROSOL SOURCE RATE (LOG-NORMAL)(KG/S)
12.9     0.
0.  0.5E-6  1.5
TIME  VAPOR-SOURCE-RATE (KG/S)/ AEROSOL SOURCE RATE (LOG-NORMAL)(KG/S)
13.      0.
0.445  0.5E-6  1.5
TIME  VAPOR-SOURCE-RATE (KG/S)/ AEROSOL SOURCE RATE (LOG-NORMAL)(KG/S)
885.0    0.
0.445  0.5E-6  1.5
TIME  VAPOR-SOURCE-RATE (KG/S)/ AEROSOL SOURCE RATE (LOG-NORMAL)(KG/S)
885.1    0.
0.  0.5E-6  1.5
TIME  VAPOR-SOURCE-RATE (KG/S)/ AEROSOL SOURCE RATE (LOG-NORMAL)(KG/S)
200000.0  0.
0.  0.5E-6  1.5
OUTPUT TIMES (SECONDS)
300.27  450.27 500.27  900.27 1000.27 1100.27 1200.27  2400.27 2800. 3200. 3600.  7482.45
 14378.53 19840.41 30065.85 43664.33 61325.25 81202.66 111191.46 132225.02
TIME  TEMPERATURE (K)  PRESSURE (PA)
   300.27    587.8707          0.2372901E6
   450.27    605.44            0.2443819E6
   500.27    610.8609          0.24657E6
   900.27    599.4837          0.2419776E6
  1000.27    486.0336          0.1961841E6
  1100.27    461.6464          0.1863403E6
  1200.27    451.606           0.1822875E6
  2400.27    401.9348          0.1622379E6
  2800.      393.4694          0.1588208e6
  3200.      386.9271          0.15618e6
  3600.      381.7545          0.1540921e6
  7482.45    357.4802          0.1442938E6
 14378.53    347.2311          0.1401568E6
 19840.41    339.423           0.137005E6
 30065.85    339.423           0.1369115E6
 43664.33    326.2268          0.1316784E6
 61325.25    315.6111          0.1273933E6
 81202.66    310.5922          0.1253674E6
111191.46    305.0869          0.1231451E6
132225.02    302.9817          0.1222953E6
```