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Strategic Environmental Research and Development Program
Improving Mission Readiness Through Environmental Research

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Coagulation Simulation and Inference of Initial Particle Size Distributions

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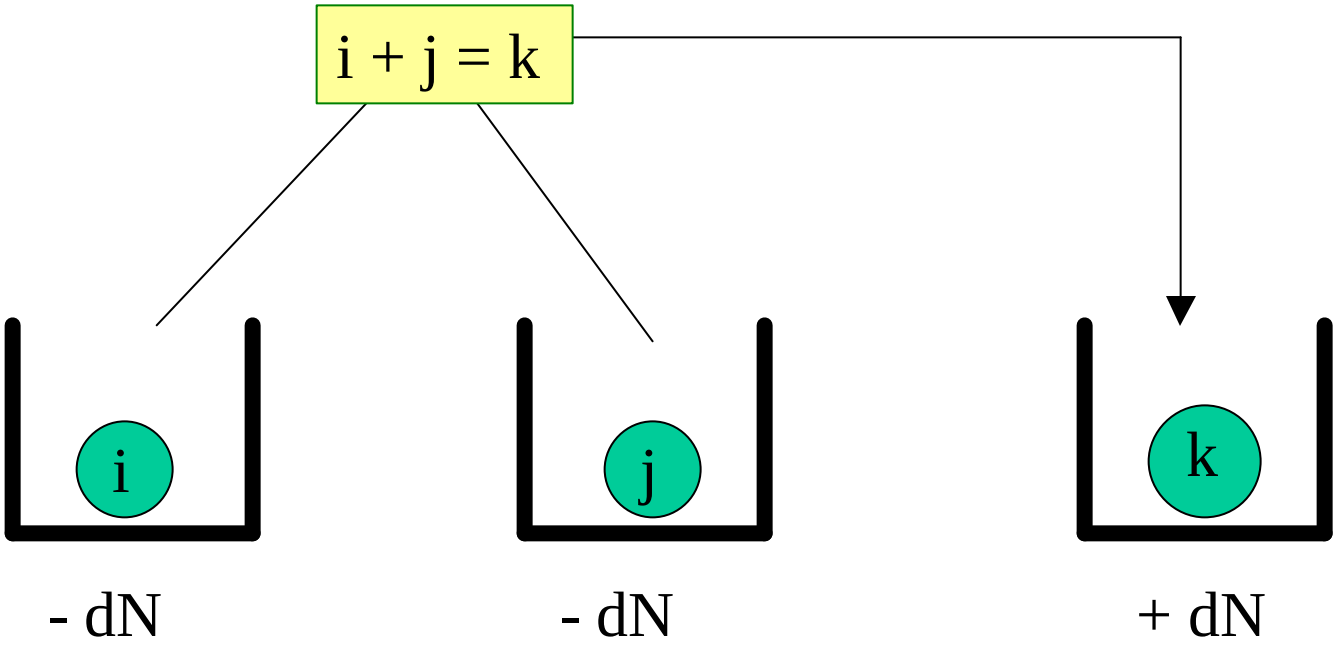
Background

- Particulate matter's adverse health effects
- Time delay for the measurement of particle size distribution
- Difficult to directly measure the particle size distribution at time zero
- How to know the particle size distribution at time zero

Objectives

- Develop a methodology to simulate the coagulation process
- Use the methodology developed to predict the particle size distribution at time zero

Coagulation Model



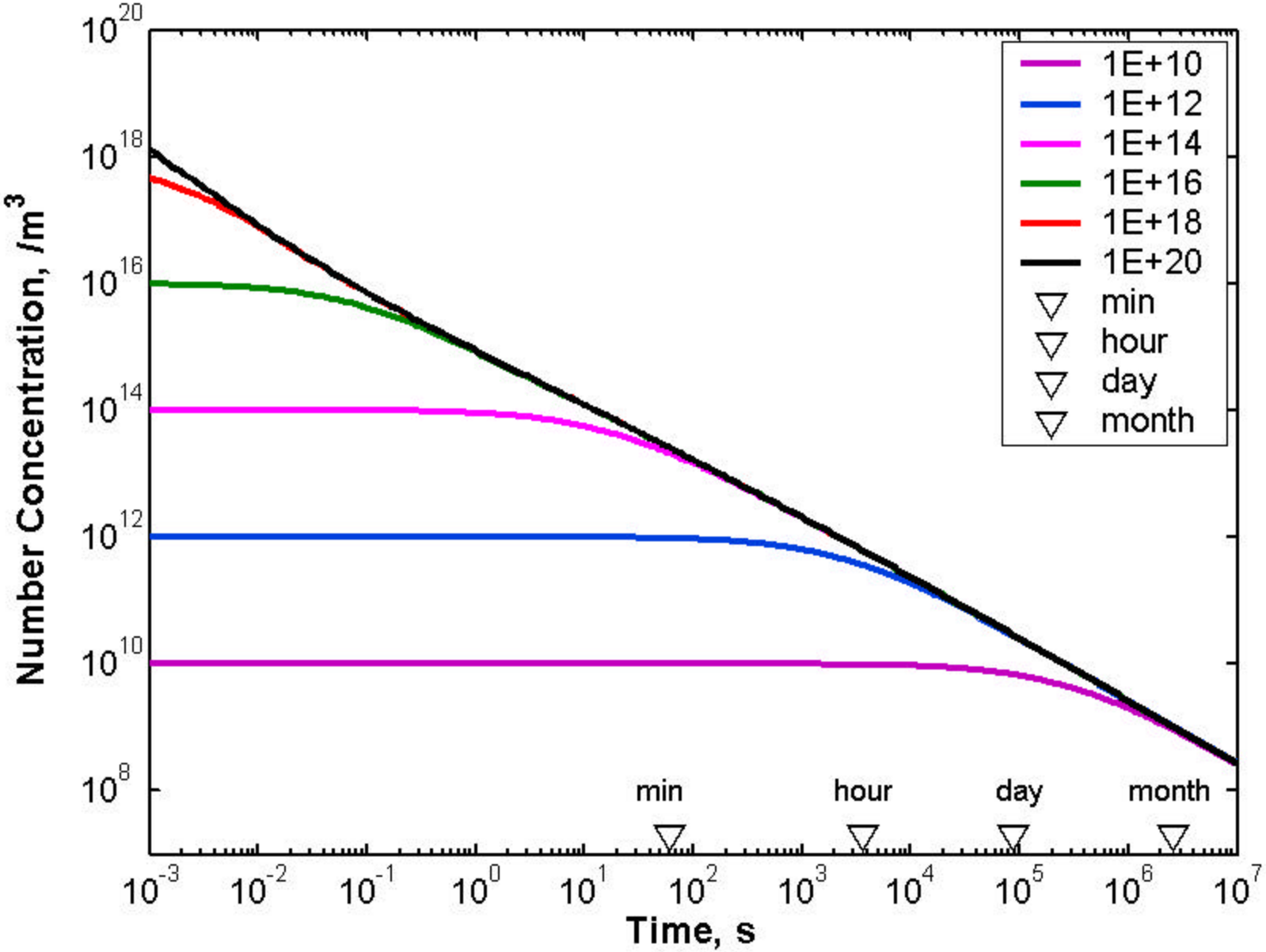
Particle of class i collides with particle of class j forming particle of class k, where the particle volume k equals volume i plus volume j.

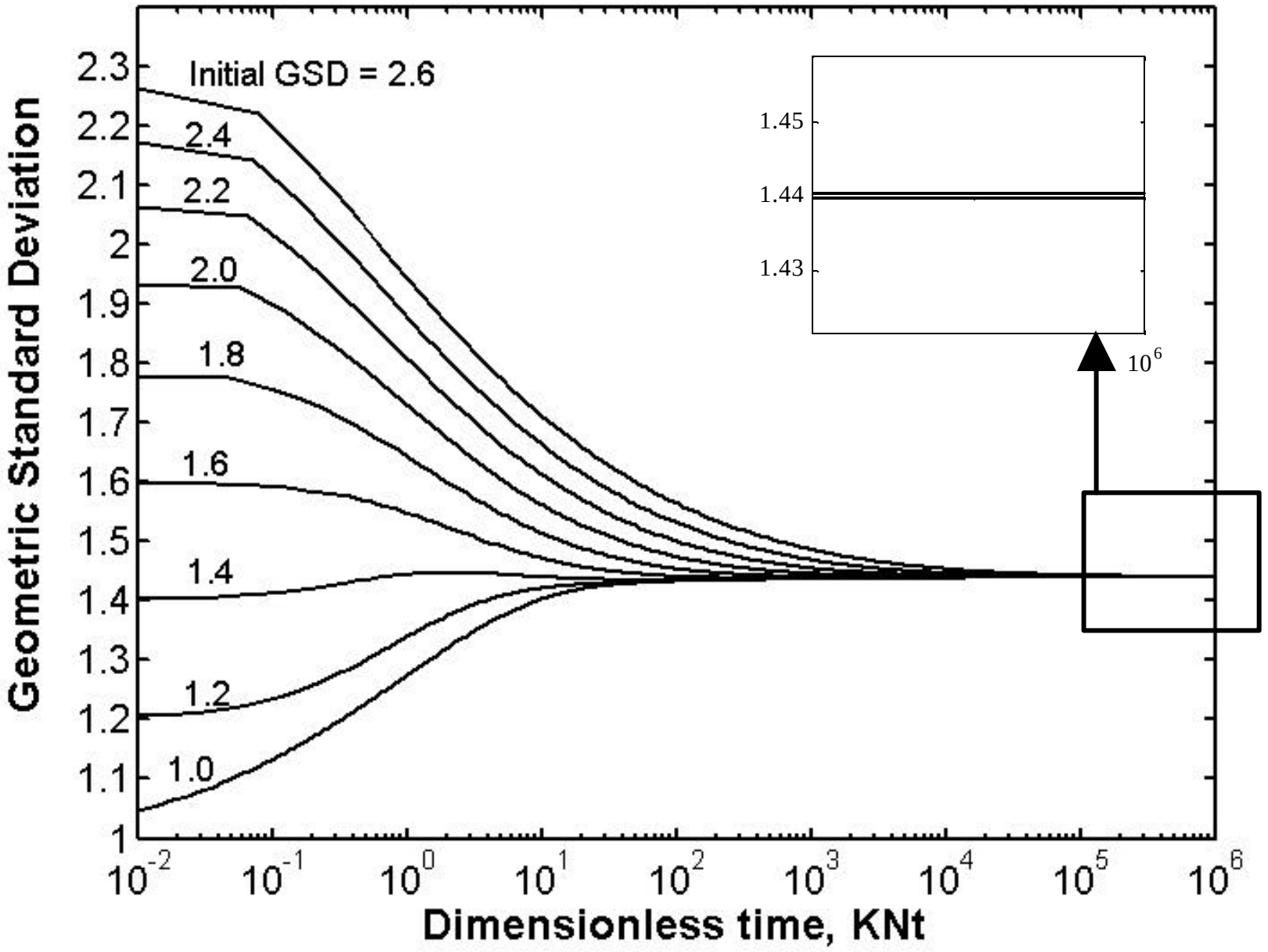
Coagulation Equations

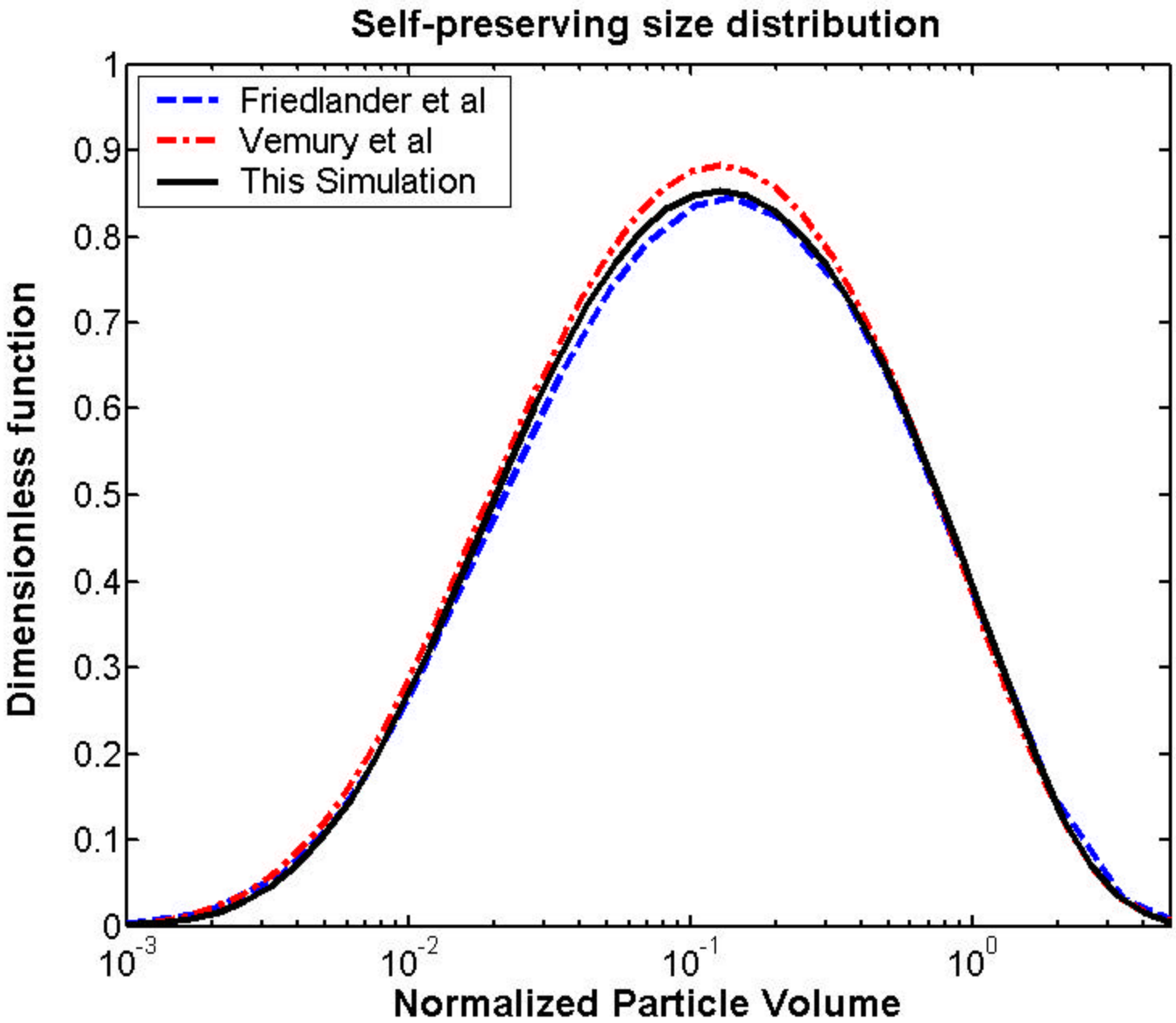
$$\left.\frac{dn(v_i,t)}{dt}\right|_{v_j} \; ? \; ? \; ? \; (v_i,v_j)n(v_i,t)n(v_j,t)$$

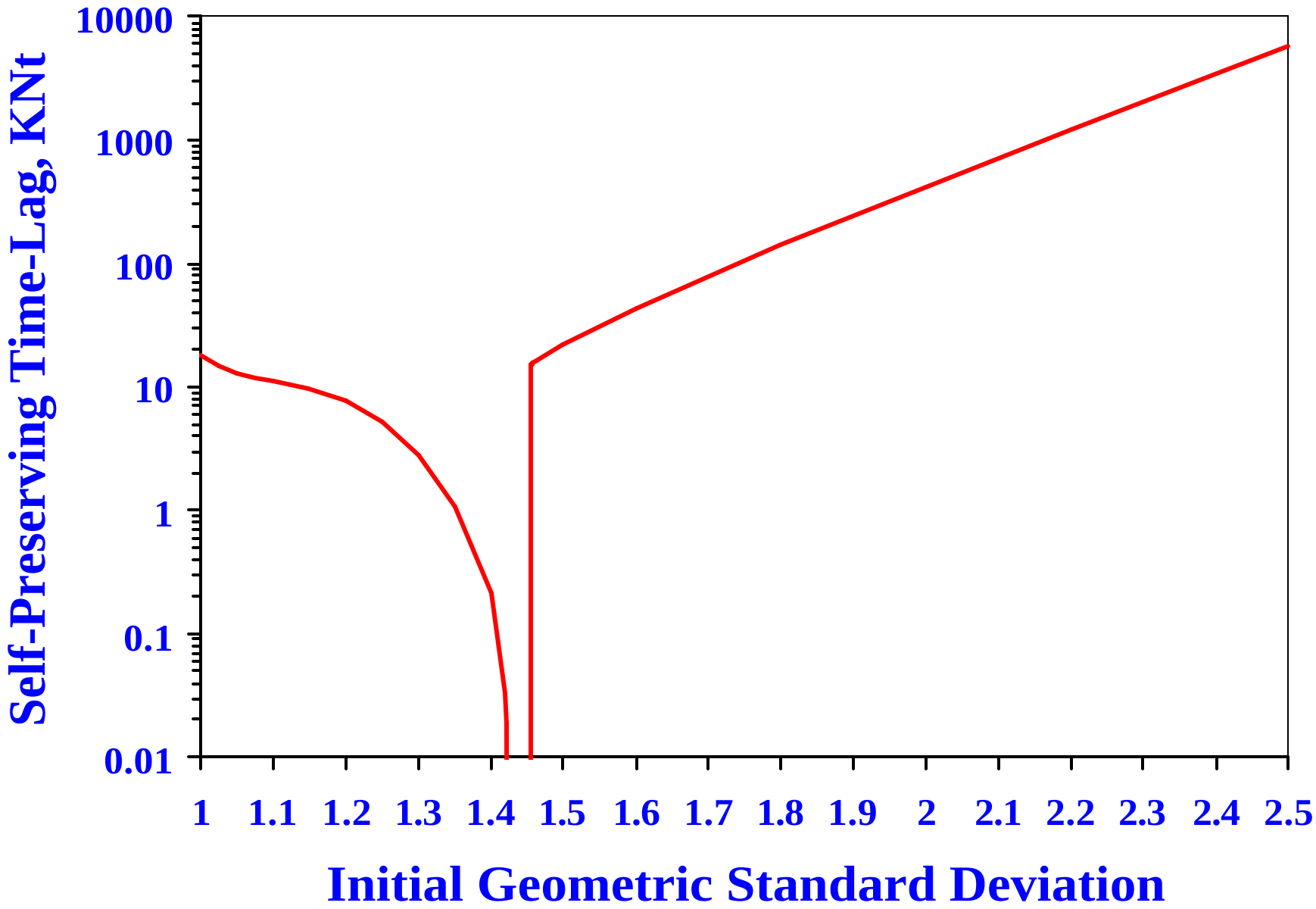
$$\left.\frac{dn(v_j,t)}{dt}\right|_{v_i} \; ? \; ? \; ? \; (v_i,v_j)n(v_i,t)n(v_j,t)$$

$$\left.\frac{dn(v_k,t)}{dt}\right|_{v_i,v_j} \; ? \; ? \; (v_i,v_j)n(v_i,t)n(v_j,t)$$

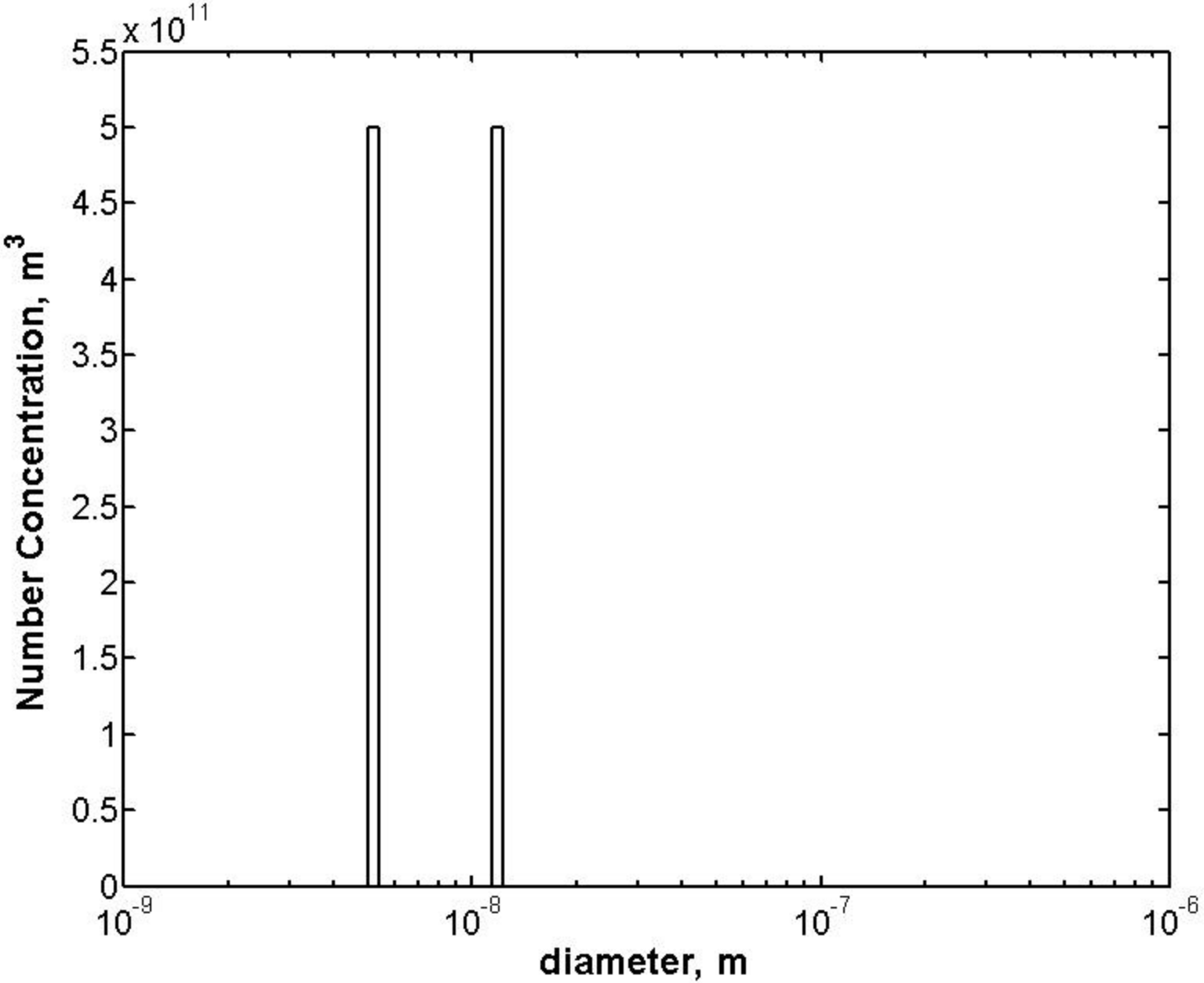

Number Concentration, /m3
Time, s
1E+10
1E+12
1E+14
1E+16
1E+18
1E+20
min
hour
day
month


Initial GSD = 2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
Geometric Standard Deviation
Dimensionless time, KNt
1.45
1.44
1.43
10^6

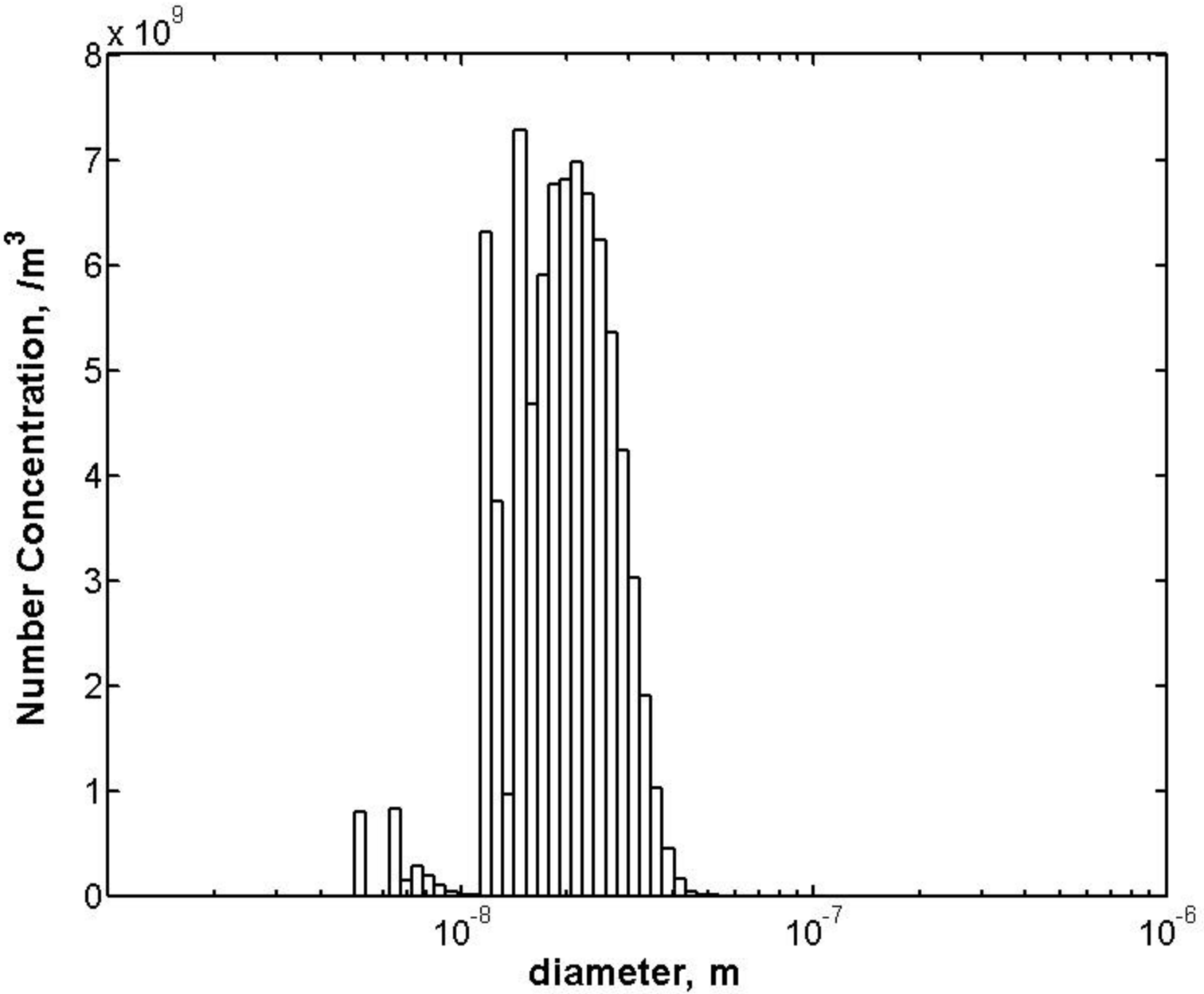

Self-preserving size distribution
Friedlander et al
Vemury et al
This Simulation
Dimensionless function
Normalized Particle Volume
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
10^-3
10^-2
10^-1
10^0


Self-Preserving Time-Lag, KNt
10000
1000
100
10
1
0.1
0.01
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2
2.1
2.2
2.3
2.4
2.5
Initial Geometric Standard Deviation

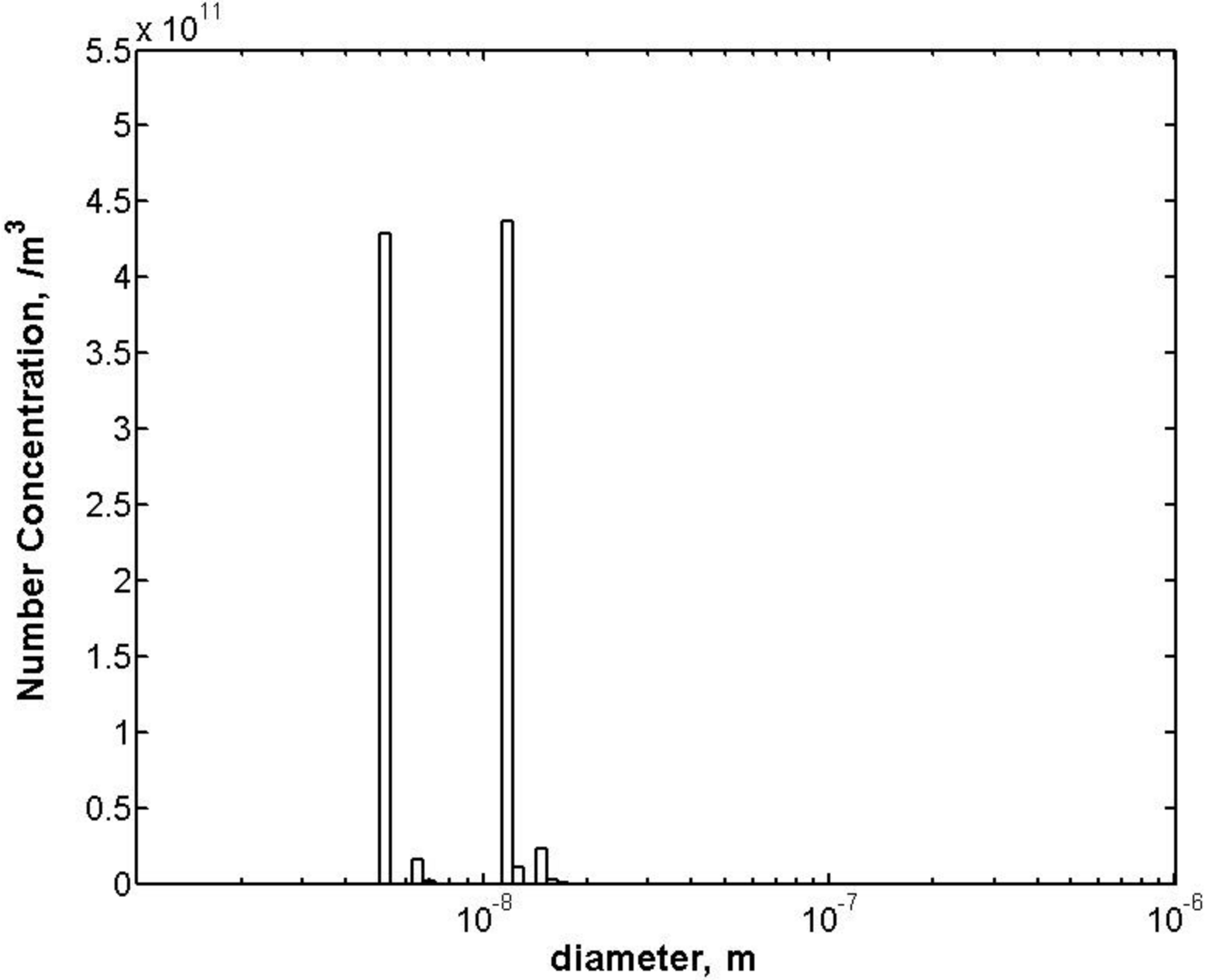
Initial Particle Size Distribution



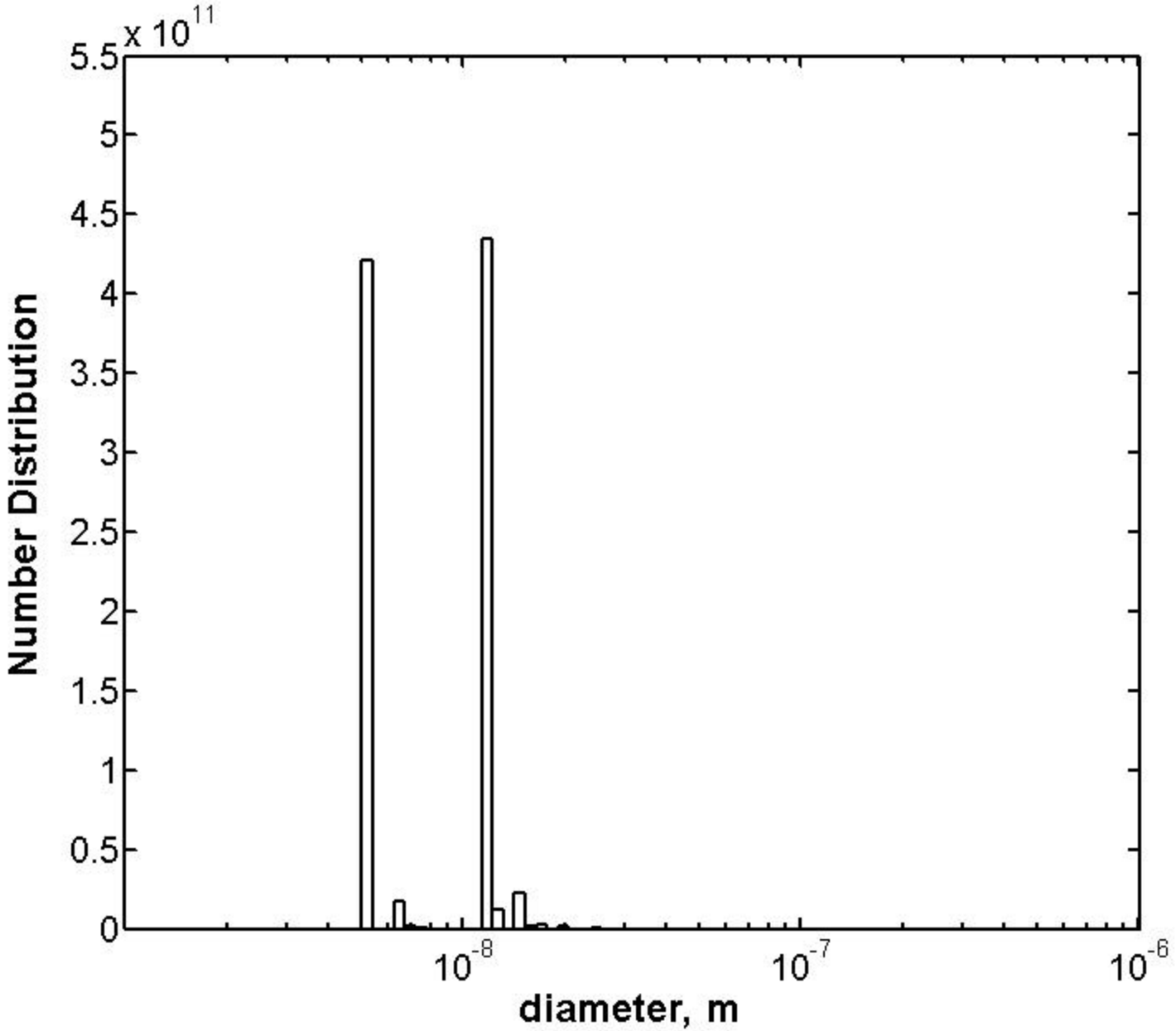
PSD after 10,000 s of coagulation



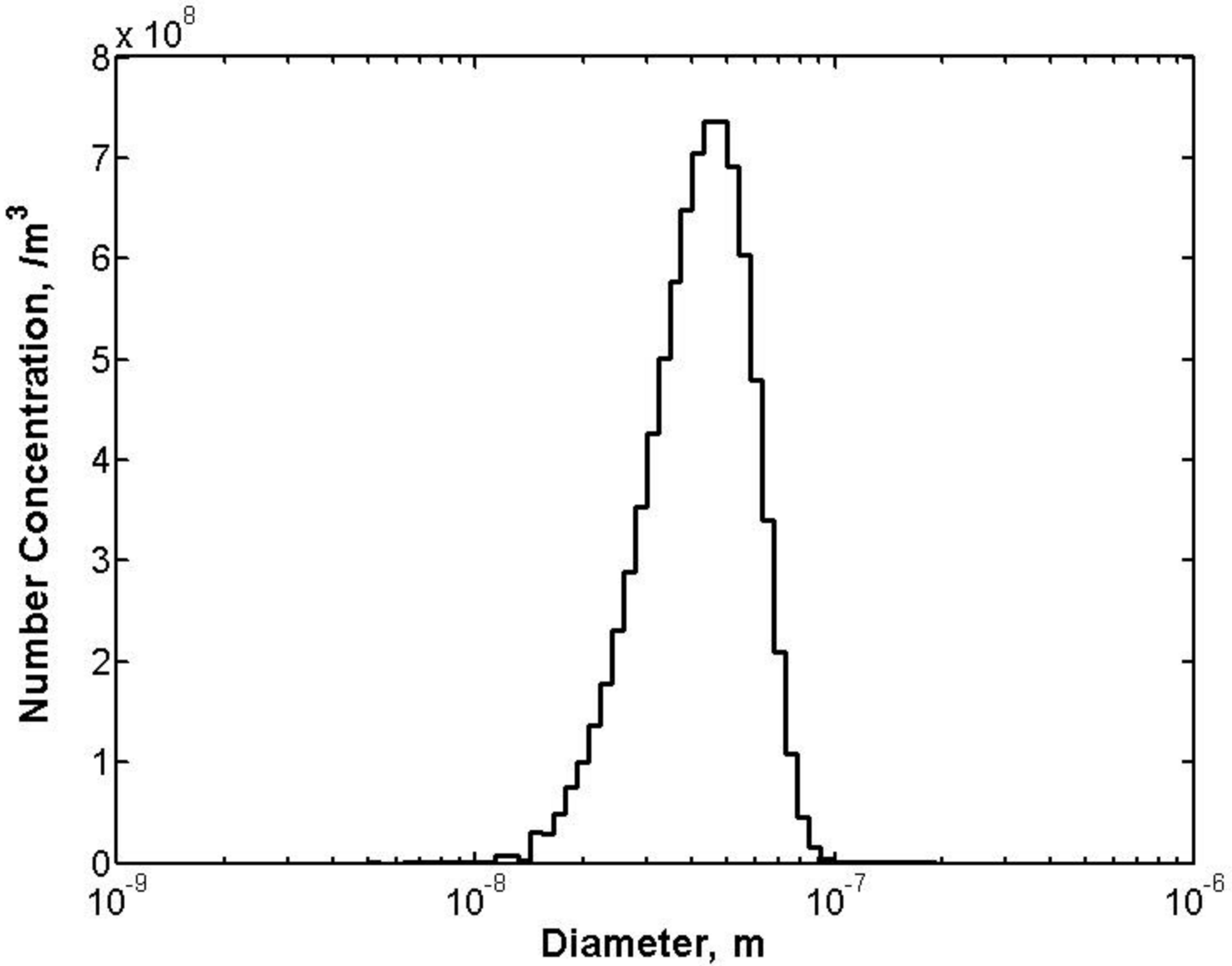
Initial PSD predicted by marching back



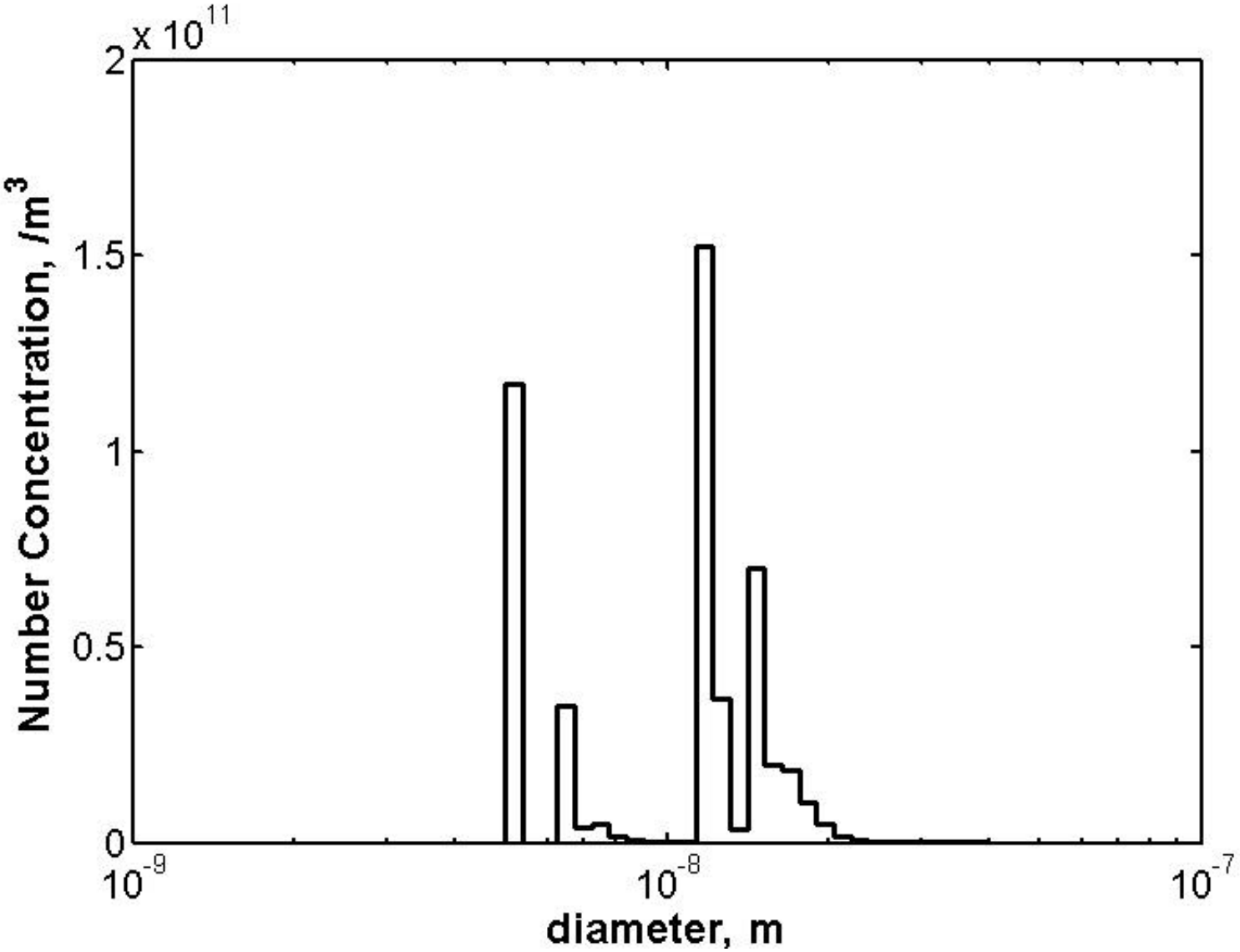
Predicted Initial PSD, with ?1% error Added



PSD After 1E5 Seconds of Coagulation



Initial PSD Predicted: Marching Back 1E5 s



Conclusions

- **The method proposed here makes the coagulation simulation very simple**
- **Back calculation could obtain initial particle size distribution**
- **The methodology has been used for soot oxidation simulation**

Acknowledgements

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