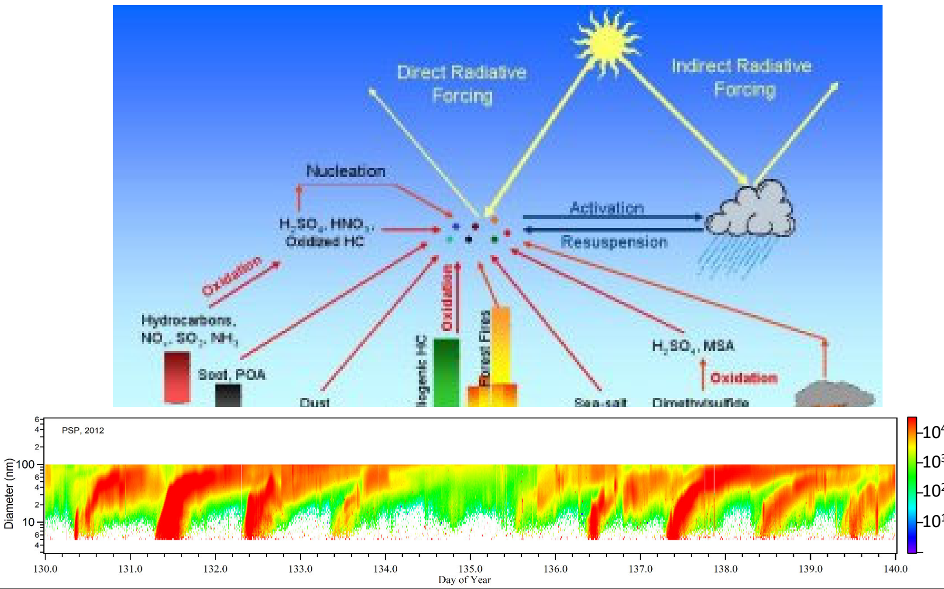
Lecture 11. New particle formation in the atmosphere



1

Nucleation Mechanisms

Unary Homogeneous Nucleation (UHN) — H_2O

Binary Homogeneous Nucleation (BHN) — $H_2O + H_2SO_4$

Ion-Mediated Nucleation (IMN) — $H_2O + H_2SO_4$ + Ions

Ternary Homogeneous Nucleation (THN) — $H_2O + H_2SO_4 + NH_3$

Ternary IMN (TIMN) — $H_2O + H_2SO_4 + NH_3$ + Ions

Ternary Nucleation with Amines — $H_2O + H_2SO_4$ + Amines

Organics-mediated Nucleation — $H_2O + H_2SO_4$ + Organics w/o ions

Pure Organics Nucleation — Organics w/o Ions

2

Key parameters controlling atmospheric new particle formation and implications

$J_{BHN} = J([H_2SO_4], RH, T)$

$J_{THN} = \ldots + [NH_3]$

$J_{ATHN} = \ldots + [Amines]$

$J_{IMN} = J([H_2SO_4], RH, T, Q, S_0)$

$J_{TIMN} = J([H_2SO_4], [NH_3], RH, T, Q, S_0)$

$J_{nucl\_org} = \ldots + [Organics] + ions$

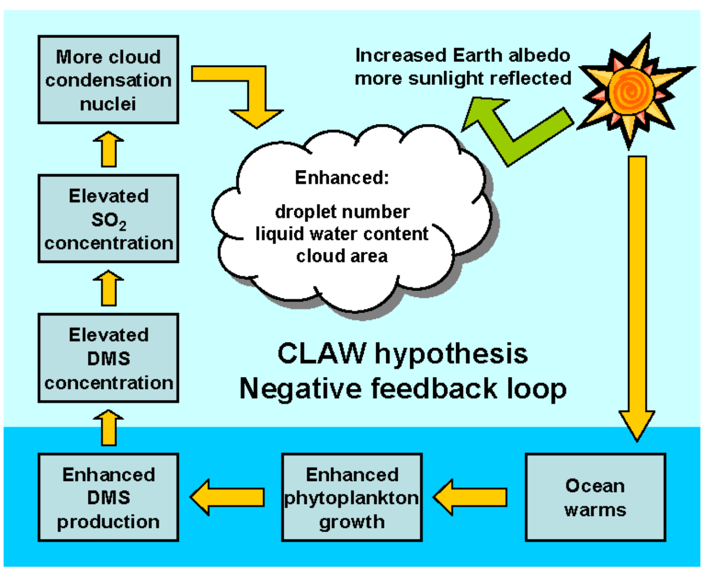
$J_{pure\_org} = [Organics] + ions$

…

3

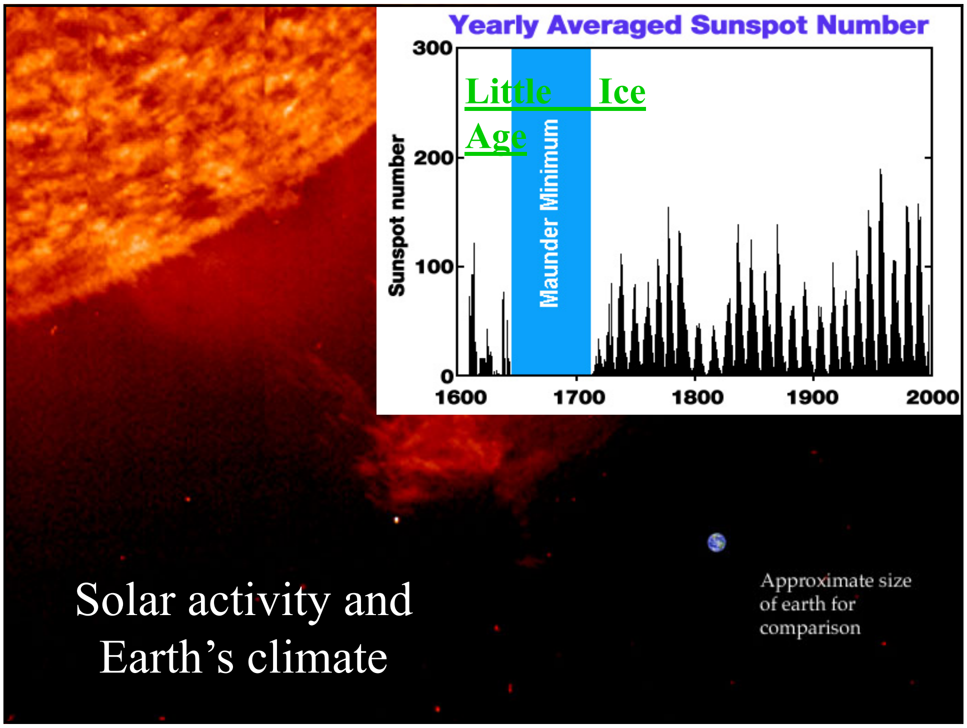
3

Negative climate feedback mechanism: CLAW hypothesis

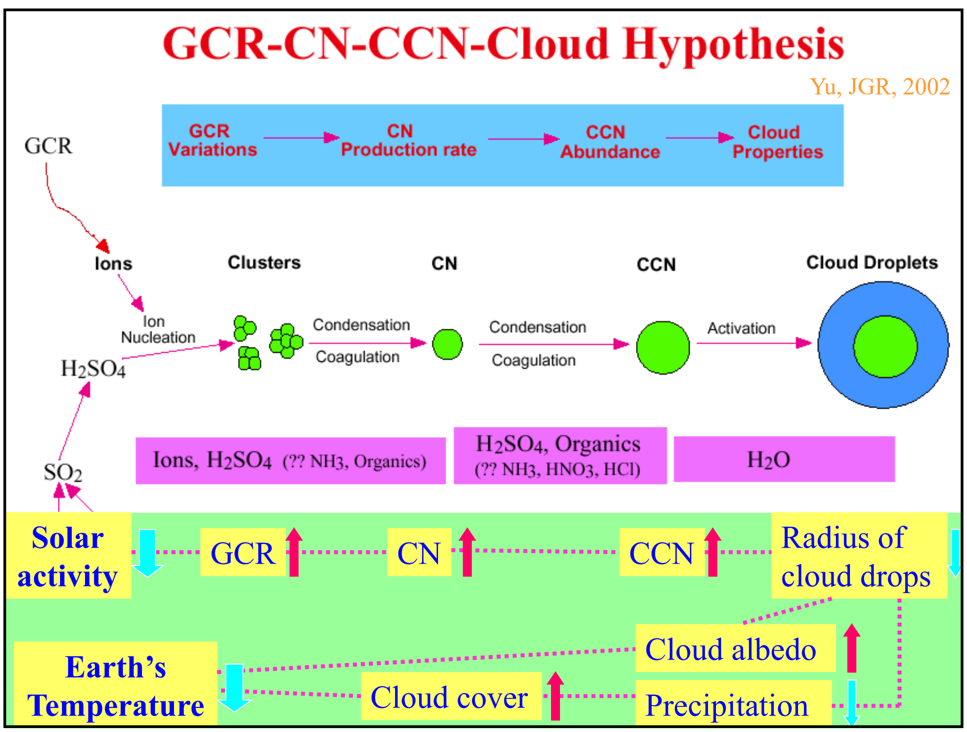


Charlson, R. J., J. E. Lovelock, M. O. Andreae, S. G. Warren, Oceanic phytoplankton, atmospheric sulphur, cloud albedo and climate, Nature, 326, 655-661, 1987.

4

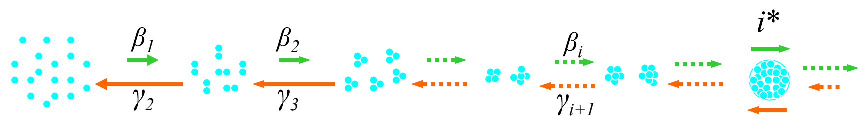

Yearly Averaged Sunspot Number
300
200
100
0
Sunspot number
Little Ice Age
Maunder Minimum
1600
1700
1800
1900
2000
Approximate size of earth for comparison
Solar activity and Earth's climate

5


GCR-CN-CCN-Cloud Hypothesis
Yu, JGR, 2002
GCR Variations
CN Production rate
CCN Abundance
Cloud Properties
GCR
Ions
Clusters
CN
CCN
Cloud Droplets
Ion Nucleation
Condensation
Coagulation
Condensation
Coagulation
Activation
H2SO4
SO2
Ions, H2SO4 (?? NH3, Organics)
H2SO4, Organics (?? NH3, HNO3, HCl)
H2O
Solar activity
GCR
CN
CCN
Radius of cloud drops
Cloud albedo
Earth's Temperature
Cloud cover
Precipitation

6

Water unary homogeneous nucleation



$$\frac{dn_{i+1}}{dt} = \delta_{i,1}\beta_i n_i - \gamma_{i+1}n_{i+1} - \beta_{i+1}n_{i+1} + \gamma_{i+2}n_{i+2}\,, \qquad i \geq 1$$

$\delta_{i,1} = 0.5$ if i=1
$\delta_{i,1} = 1$ if i≠1

Under quasi-steady state: $$J_{UHN} = \delta_{i,1}\beta_i n_i - \gamma_{i+1}n_{i+1}$$

Define a quantity f_i as, $$\delta_{i,1}\beta_i f_i = \gamma_{i+1}f_{i+1} \qquad \frac{J_{UHN}}{\delta_{i,1}\beta_i f_i} = \frac{n_i}{f_i} - \frac{n_{i+1}}{f_{i+1}}$$

$$J_{UHN}\sum_{i=1}^{i_L}\frac{1}{\delta_{i,1}\beta_i f_i} = \frac{n_1}{f_1} - \frac{n_{i_L+1}}{f_{i_L+1}}$$

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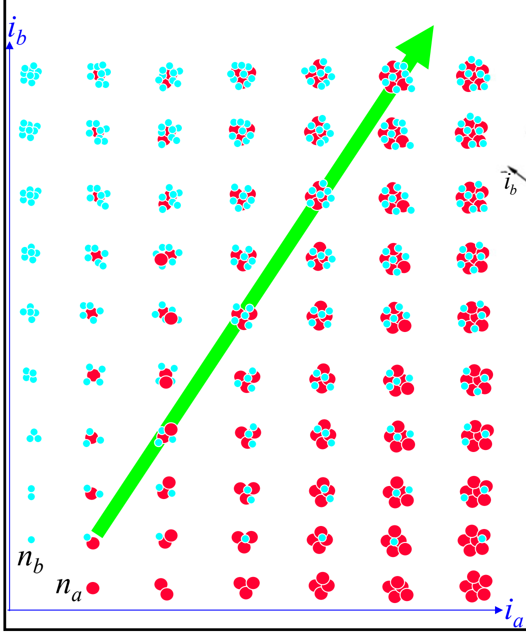
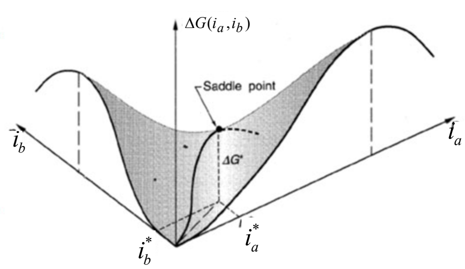
Binary homogeneous nucleation

Reiss, 1950; Doyle, 1961





$$J = C\exp\left(-\frac{\Delta G^*}{kT}\right) = K_{act}n^*$$

$$K_{act} = \frac{\beta_a\beta_b}{\beta_a\sin^2\theta + \beta_b\cos^2\theta}4\pi r^{*2} Z$$

$$n^* = (n_a + n_b)\exp(-\Delta G^*/kT)$$

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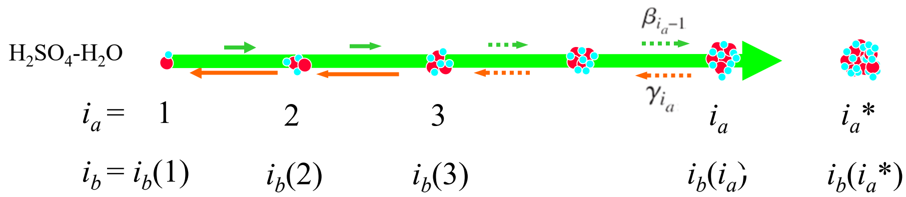
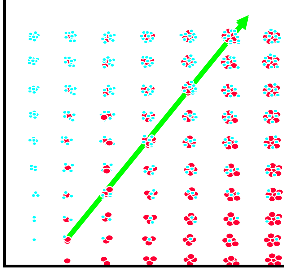
Kinetic Quasi-Unary Nucleation (KQUN)



(Yu, JCP, 2005a, 2007)

$$J_{KQUN} = n_1 \left(\sum_{i_a=1}^{i_L} \frac{f_1}{\delta_{i_a,1} \beta_{i_a} f_{i_a}} \right)^{-1} = 0.5 n_1 \left(\sum_{i_a=1}^{i_L} \frac{1}{\beta_{i_a} \prod_{j=1}^{i_a-1} \frac{\beta_j}{\gamma_{j+1}}} \right)^{-1}$$



$$\beta_{i_a} = \left(\frac{8\pi k_B T (m_1 + m_{i_a})}{m_1 m_{i_a}} \right)^{1/2} (r_1 + r_{i_a})^2 n_1 = k_{1,i_a} n_1$$

$$\gamma_{i_a} = \beta_{i_a-1} \exp\left(\frac{\Delta G_{i_a-1,i_a}}{RT} \right) = k_{1,i_a-1} n^s_{1,total} \exp\left(\frac{2\sigma v_a}{RT r_{i_a}} \right) = k_{1,i_a-1} F_{hy} n^s_{1,free} \exp\left(\frac{2\sigma v_a}{RT r_{i_a}} \right)$$

$$n_{i_a^*} = \frac{\beta_{i_a^*-1}}{\gamma_{i_a^*}} n_{i_a^*-1} = \frac{\beta_{i_a^*-1}}{\gamma_{i_a^*}} \frac{\beta_{i_a^*-2}}{\gamma_{i_a^*-1}} n_{i_a^*-2} = \ldots\ldots = \frac{\beta_{i_a^*-1}}{\gamma_{i_a^*}} \frac{\beta_{i_a^*-2}}{\gamma_{i_a^*-1}} \ldots\ldots \frac{\beta_2}{\gamma_3} \frac{\beta_1}{\gamma_2} n_1 = n_1^{i_a^*} \prod_{i_a=2}^{i_a^*} \frac{k_{1,i_a-1}}{\gamma_{i_a}}$$

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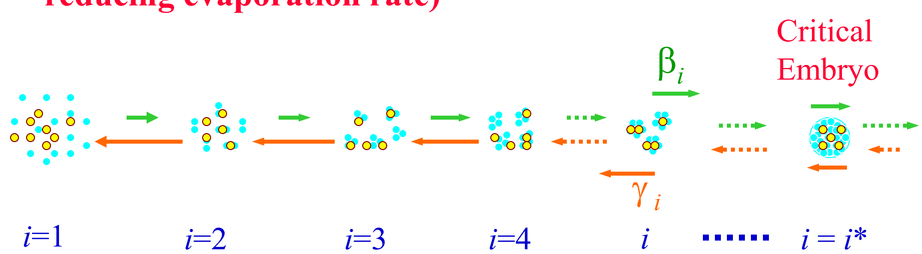
NH$_3$ may enhance nucleation by stabilizing clusters (i.e., reducing evaporation rate)



Classical Ternary H_2SO_4-H_2O-NH_3 nucleation

$$J = C \exp\left(-\frac{\Delta G^*}{kT} \right)$$

$$\Delta G = -n_1 kT \ln\left(\frac{P_1}{P_1^{sol}} \right) - n_2 kT \ln\left(\frac{P_2}{P_2^{sol}} \right) - n_3 kT \ln\left(\frac{P_3}{P_3^{sol}} \right) + 4\pi r^2 \sigma$$

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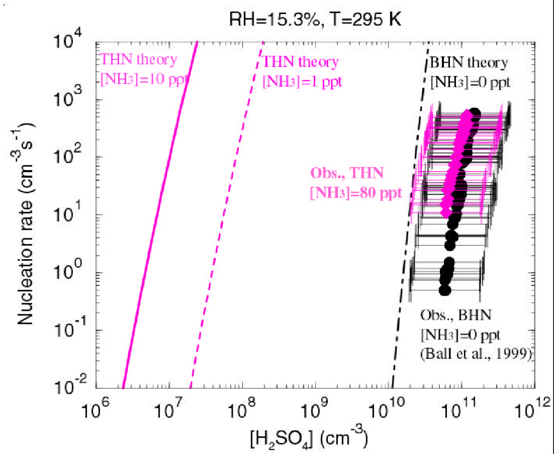
Effect of NH_3: Theory versus experiments

Enhancement of NH_3 on nucleation rate:

If the laboratory measurements are real, our study indicates that the effect of ammonia on H_2SO_4-H_2O homogeneous nucleation is very limited (Yu, JGR, 2006) .



Laboratory experiments

1-2 orders of magnitude (Ball et al., 1999: $[NH_3]$ = 80, 170 ppt)

< 1 order of magnitude (Kim et al., 1998: $[NH_3]$ = 0.71 -3.6 ppm; Christensen,1994; Diamond et al., 1985)

unobvious (Nolan, 1987)

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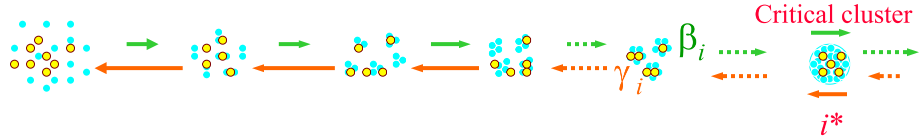
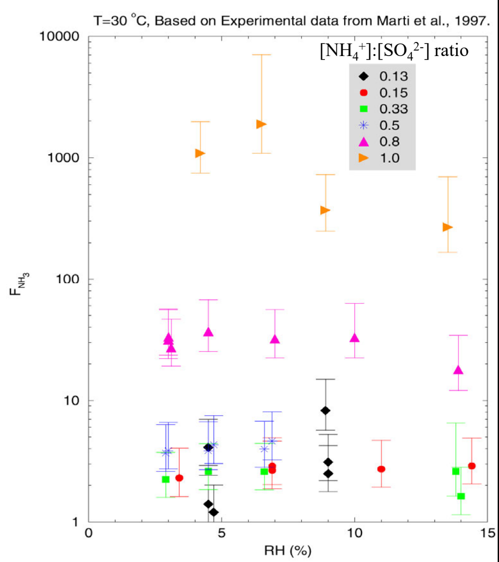


Kinetic THN (Yu, JGR, 2006)

$$\gamma_i^{\text{Ternary}} = \gamma_i^{\text{Binary}} / F_{\text{NH}_3}$$

F_{NH3} based on vapor pressure measurements: Depend strongly on the degree of neutralization.



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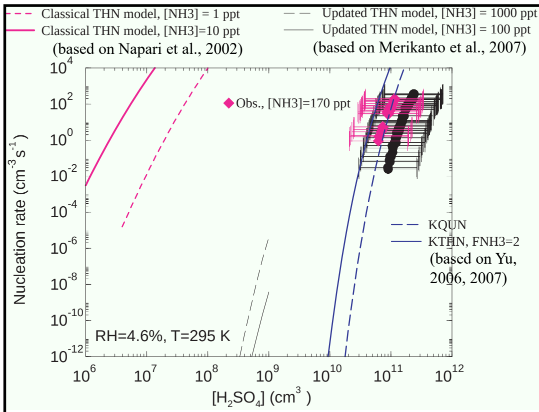
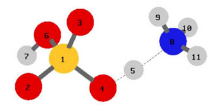


DFT PW91PW91/6-311++G(3df,3pd)
(Nadykto and Yu, 2006)



reaction	ΔH	ΔS	ΔG (kcal/mol)
$H_2SO_4+NH_3 \Leftrightarrow (H_2SO_4)(NH_3)$	-16.72	-30.01	-7.77 (~-8.5)[a]

([a] Hanson and Eisele, 2002)

Classical thermodynamics (based on liquid droplet model): most of the sulfuric acid in the atmosphere is bound to stable ammonium bisulphate clusters (Anttila et al., Boreal Env. Res., 2005, Merikanto et al., JGR, 2007).

Most of H_2SO_4 in the atmosphere is in the form of $(H_2SO_4)(H_2O)_n$, **not $(H_2SO_4)(NH_3)$.**

$(H_2SO_4)(NH_3)$ typically <0.1%

Nadykto et al., ACP, 2008.

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Understanding the role of ions in new particle formation in the atmosphere

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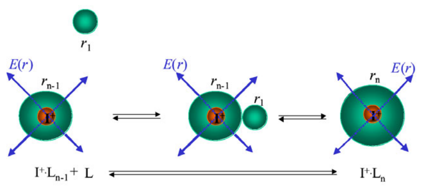
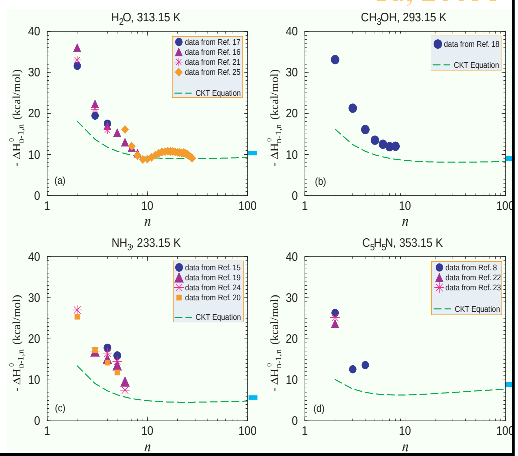
Classical ion induced nucleation theory

Classical Kelvin-Thomson (CKT) equation (Thomson, 1888):

$$\Delta G_{0,n}^{\text{charged}} = -nkT\ln\left(\frac{p}{p_{sat}}\right) + \sigma 4\pi r_n^2 - \frac{(qe)^2}{8\pi\varepsilon_0}\left(1-\frac{1}{\varepsilon_l}\right)\left(\frac{1}{r_0}-\frac{1}{r_n}\right)$$

Yu, 2005b





Fundamental inconsistency exists between the general form of the CKT expression and the properties of small cluster ions (Holland and Castleman, 1982).

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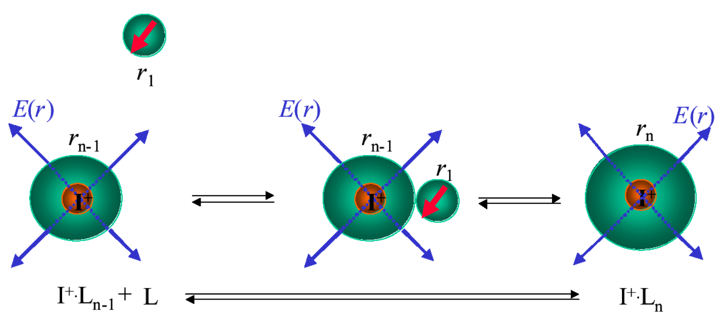
Dipole-charge interaction is important

Nadykto and Yu, 2004;
Yu, 2005b



Modified Kelvin-Thomson equation:

$$\Delta G_{0,n}^{\text{charged}} = -nkT\ln\left(\frac{p}{p_{sat}}\right) + \sigma 4\pi r_n^2 - \frac{(qe)^2}{8\pi\varepsilon_0}\left(1-\frac{1}{\varepsilon_l}\right)\left(\frac{1}{r_0}-\frac{1}{r_n}\right)$$
$$-\int_1^n \left\{\frac{1}{2}\alpha E_{n-1}^2 + kT\ln\left[\left(\exp\left(\frac{\mu_0 E_{n-1}}{kT}\right)-\exp\left(-\frac{\mu_0 E_{n-1}}{kT}\right)\right)/\left(2\frac{\mu_0 E_{n-1}}{kT}\right)\right]\right\}dn$$

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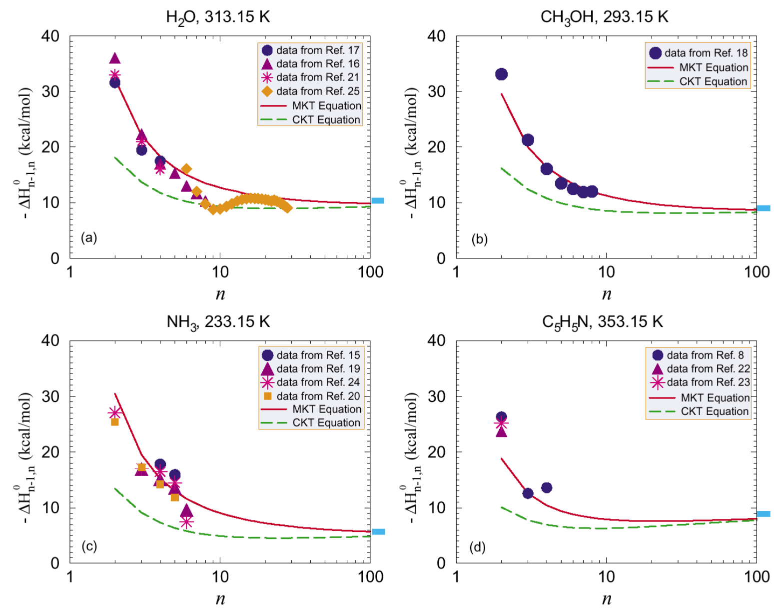
Clustering enthalpies for protonated clusters: $H^+X_{n-1} + X \rightarrow H^+X_n$

($X = H_2O$, NH_3, CH_3OH, and C_5H_5N)

Yu, 2005b



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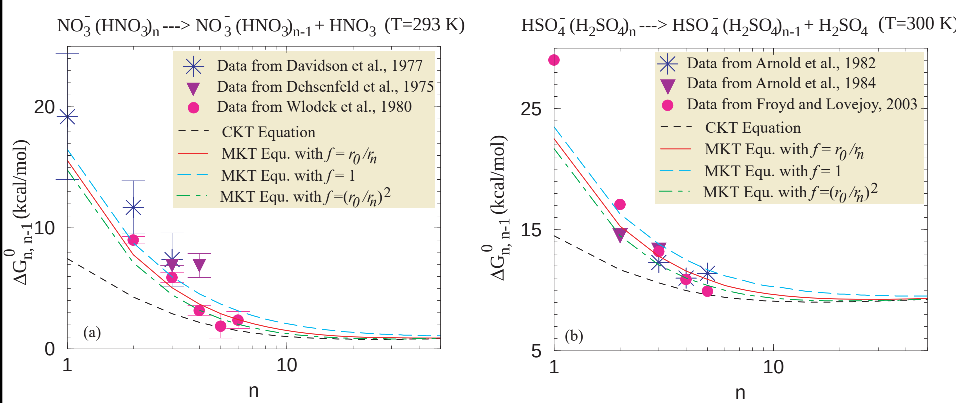

Yu, ACP, 2006

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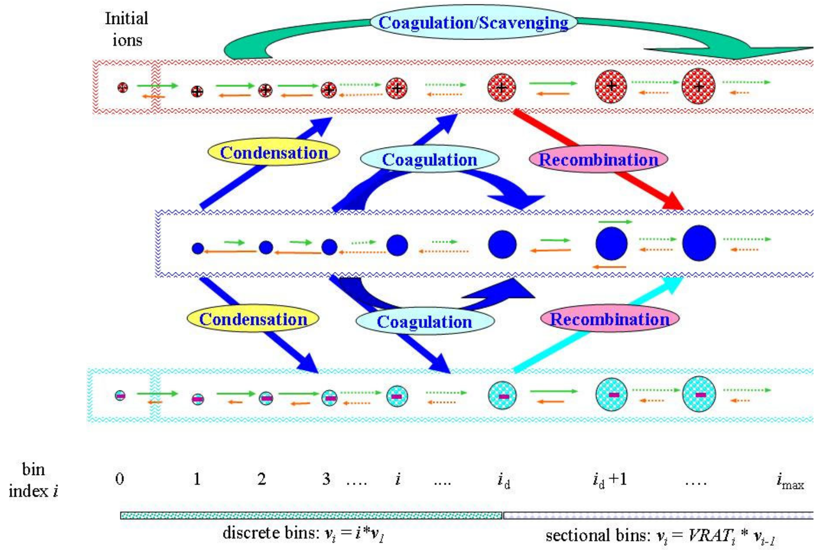
Ion-mediated nucleation (IMN) model



Yu, ACP, 2006

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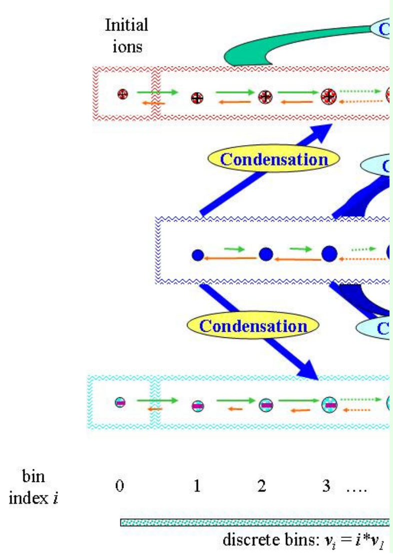
Ion-mediated nucleation (IMN) model



1. Compositions of small charged clusters were parameterized based on H_2O-ions clustering thermodynamic data from Froyd and Lovejoy (JPC, 2003).

2. Evaporation coefficients of H_2SO_4 molecules from charged clusters were calculated with Modified Kelvin-Thomson (MKT) equation which gives good agreement with ion-clustering thermodynamic data (Yu, JCP, 2005b; Yu, ACP, 2006).

3. Evaporation coefficients of H_2SO_4 molecules from neutral clusters were calculated with the most recent thermodynamic data for H_2SO_4-H_2O binary system and were constrained by multiple laboratory data sets (Yu, JCP, 2007).

Yu, ACP, 2006

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Ternary Ion-Mediated Nucleation (TIMN): Controlling Parameters

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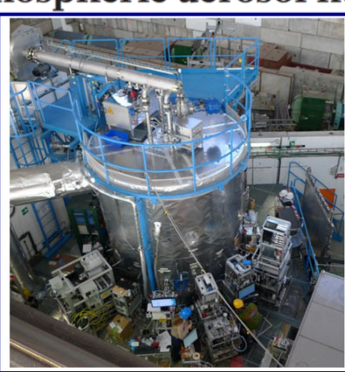
LETTER

Kirkby et al., Nature, 2011

doi:10.1038/nature10343

Role of sulphuric acid, ammonia and galactic cosmic rays in atmospheric aerosol nucleation

CERN CLOUD chamber



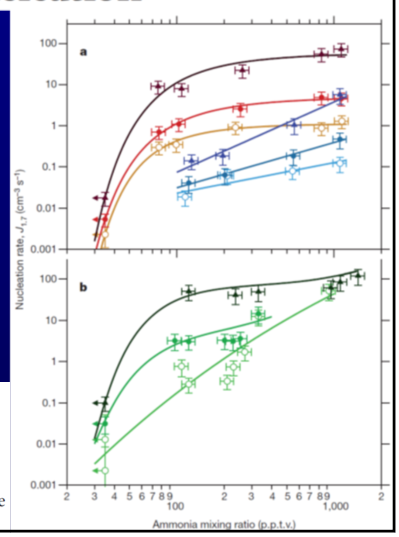


Figure 4 | Plots of nucleation rate against NH_3 concentration. Nucleation rates are shown as a function of ammonia mixing ratio. **a**, At 292 K and $[H_2SO_4] = 1.5 \times 10^8$ cm^{-3} (curves) and 4.3×10^7 cm^{-3} (straight lines); **b**, at 278 K and $[H_2SO_4] = 6.3 \times 10^7$ cm^{-3}. All measurements were made at 38% relative humidity. Triangles, J_{ch}; filled circles, J_{gcr}; open circles, J_n. The fitted lines are drawn to guide the eye. The bars indicate 1σ total errors, although the overall ammonia scale uncertainty of a factor 2 is not shown.

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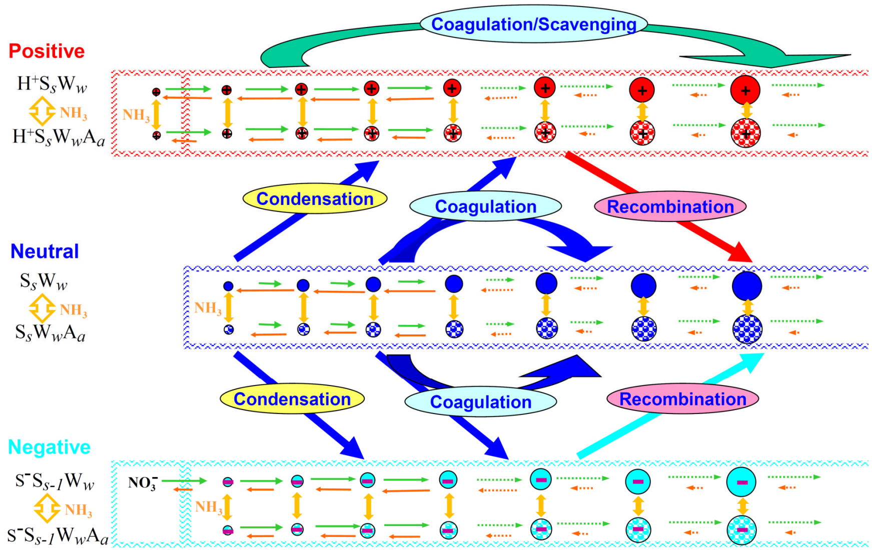
Kinetic-based H_2SO_4-H_2O-NH_3 ternary ion-mediated nucleation (TIMN) model

Yu et al., ACPD, 2018



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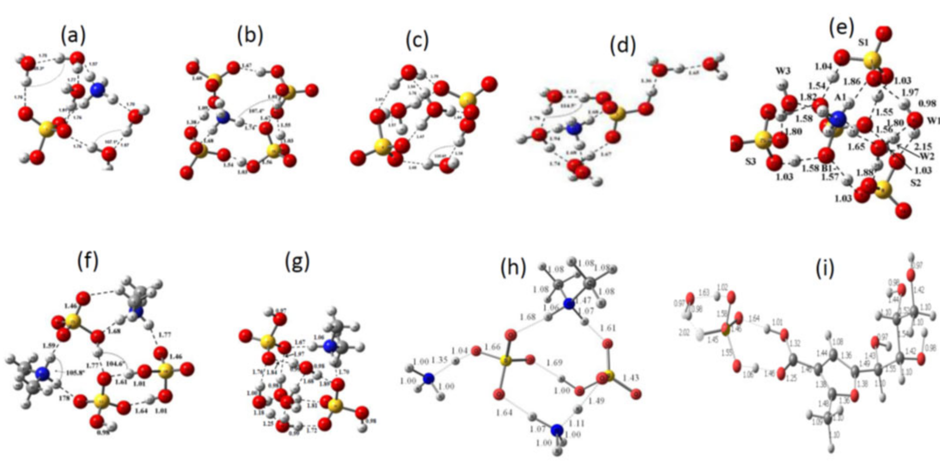
Quantum chemistry (QC) studies of neutral and charged clusters



Geometries of the most stable isomers of (a) $(NH_3)(H_2SO_4)(H_2O)_5$, (b) $(NH_3)_1(H_2SO_4)_4$, (c) $(H_3O^+)(H_2SO_4)_2(H_2O)_5$, (d) $(NH_4^+)(H_2SO_4)(H_2O)_6$, (e) $(HSO_4^-)(H_2SO_4)_3(NH_3)(H_2O)_3$, (f) $((CH_3)_2NH)_2(H_2SO_4)_3$, (g) $(H_2SO_4)_2[(CH_3)_2NH]_1(H_2O)_4$, (h) $(H_2SO_4)_2[(CH_3)_2NH]_2(NH_3)_2$, (i) $(C_{10}H_{14}O_7)$ (H_2SO_4) (H_2O), calculated at PW91PW91/6-311++G(3df,3pd) level of theory.

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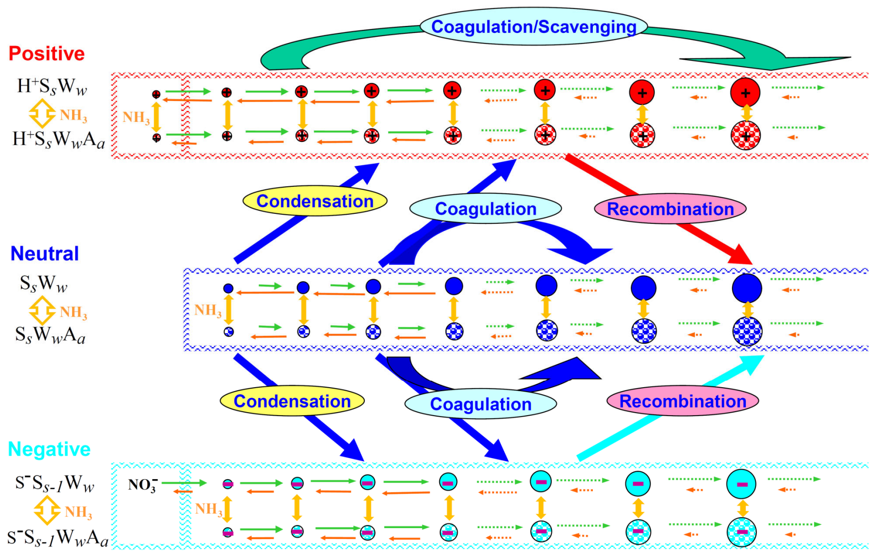
Kinetic-based H_2SO_4-H_2O-NH_3 ternary ion-mediated nucleation (TIMN) model

Yu et al., ACPD, 2018



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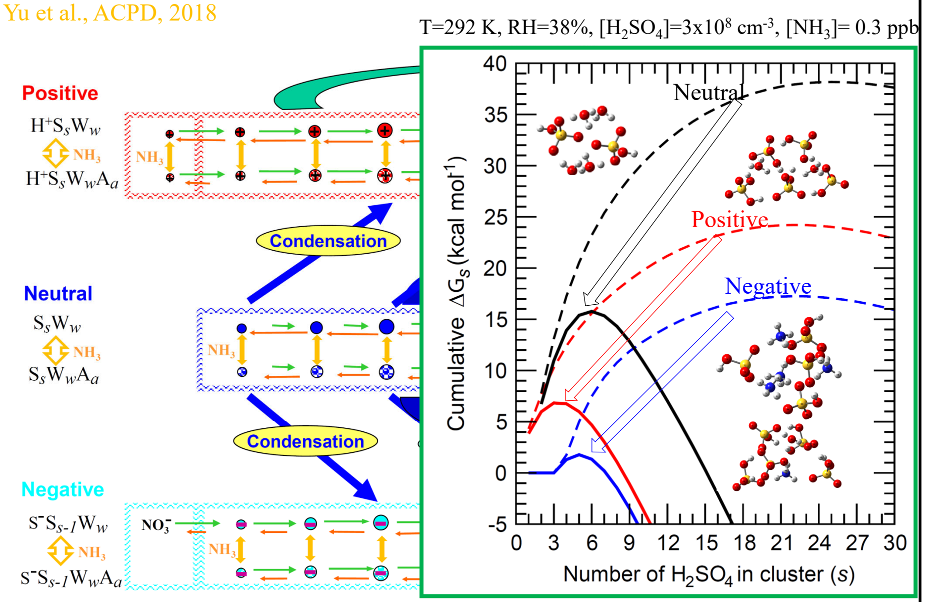
Kinetic-based H_2SO_4-H_2O-NH_3 ternary ion-mediated nucleation (TIMN) model

Yu et al., ACPD, 2018



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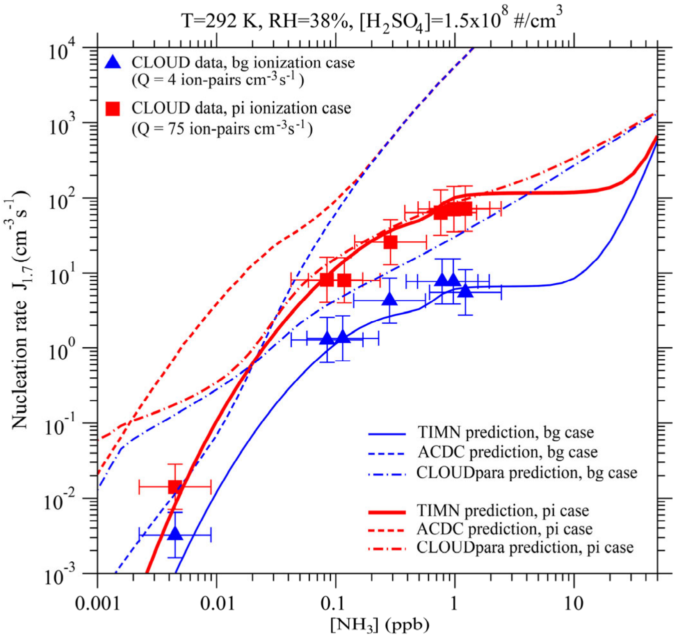

References: CLOUD data and CLOUDpara (Dunne et al., 2016)
ACDC (McGrath et al., 2012; Kürten et al., 2016)

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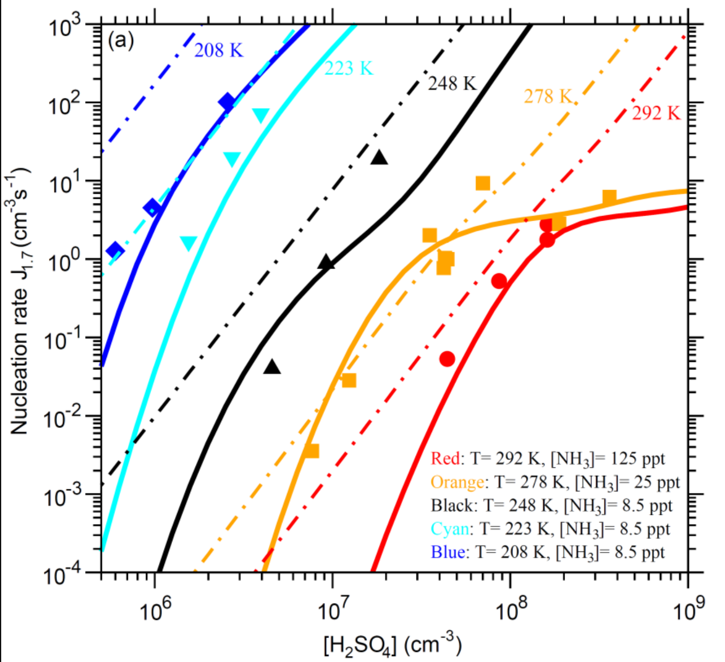
Symbols: CLOUD measurements, Solid lines: TIMN, Dot-dashed lines: CLOUDpara



TIMN (solid lines): Yu et al., ACP, 2018

CLOUDpara (dashed lines): Dunne et al., Science, 2016

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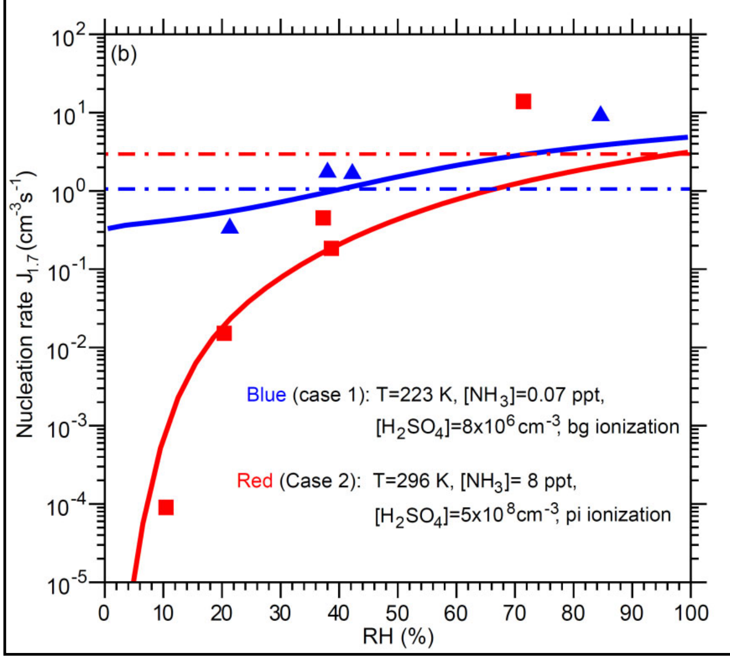

TIMN (solid lines): Yu et al., ACP, 2018

CLOUDpara (dashed lines): Dunne et al., Science, 2016

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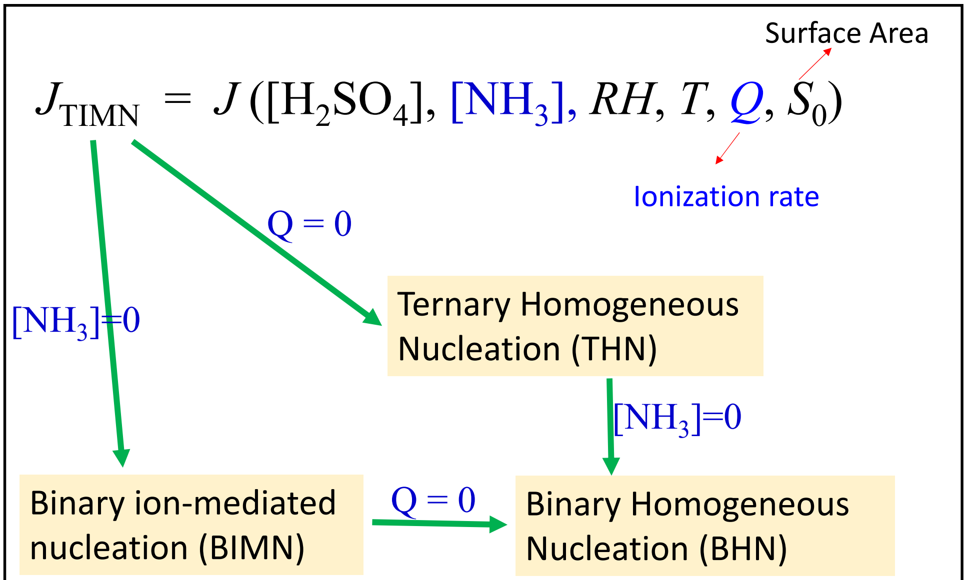
$$J_{\mathrm{TIMN}} = J([H_2SO_4], [NH_3], RH, T, Q, S_0)$$



6-dimensional TIMN lookup table

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Article

https://gmd.copernicus.org/articles/13/2663/2020/

Articles / Volume 13, issue 6 / GMD, 13, 2663–2670, 2020

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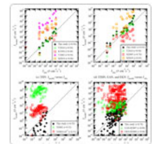
Development and technical paper | 17 Jun 2020

H_2SO_4–H_2O binary and H_2SO_4–H_2O–NH_3 ternary homogeneous and ion-mediated nucleation: lookup tables version 1.0 for 3-D modeling application



Fangqun Yu, Alexey B. Nadykto, Gan Luo, and Jason Herb

Abstract

Formation of new particles in the atmosphere has important implications for air quality and climate. Recently, we have developed a kinetically based H_2SO_4–H_2O–NH_3-ion nucleation model which well captures the absolute values of nucleation rates as well as dependencies of nucleation rates on NH_3 and H_2SO_4 concentrations, ionization rates, temperature, and relative humidity observed in the well-controlled Cosmics Leaving Outdoor Droplets (CLOUD) measurements. Here we employ the aforementioned recently developed kinetic nucleation model to generate nucleation rate lookup tables for H_2SO_4–H_2O binary homogenous nucleation (BHN), H_2SO_4–H_2O–NH_3 ternary homogeneous nucleation (THN), H_2SO_4–H_2O-ion binary ion-mediated nucleation (BIMN), and H_2SO_4–H_2O–NH_3-ion ternary ion-mediated nucleation (TIMN). A comparison of nucleation rates calculated using the lookup tables with CLOUD measurements of BHN, BIMN, THN, and TIMN is presented. The lookup tables cover a wide range of key parameters controlling binary, ternary, and ion-mediated nucleation in the Earth's atmosphere and are a cost-efficient solution for multidimensional modeling. The lookup tables and FORTRAN codes, made available through this work, can be readily used in 3-D modeling. The lookup tables can also be used by experimentalists involved in laboratory and field measurements for a quick assessment of nucleation involving H_2SO_4, H_2O, NH_3, and ions.

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https://zenodo.org/records/3483797

Lookup tables for H2SO4-H2O

zenodo.org/records/3483797

zenodo

Planned intervention: On Monday, October 6th, 06:30 UTC, Zenodo will be unavailable for 1-2 minutes to perform an upgrade to our compute cluster.

Published October 12, 2019 | Version 1.0.0 Dataset Open

Lookup tables for H2SO4-H2O binary and H2SO4-H2O-NH3 ternary homogeneous and ion-mediated nucleation

Fangqun Yu[1]

Show affiliations

2019/10/10

This directory contains fortran code and lookup tables for calculating
nucleation rate for the following four nucleation mechanims:
1. H2SO4-H2O binary homogenous nucleation (BHN),
2. H2SO4-H2O-NH3 ternary homogeneous nucleation (THN),
3. H2SO4-H2O-Ions binary ion-mediated nucleation (BIMN), and
4. H2SO4-H2O-NH3-Ions ternary ion-mediated nucleation (TIMN)

References:

1. Yu, F., Nadykto, A. B., Herb, J., Luo, G., Nazarenko, K. M., and Uvarova, L. A.: H2SO4-H2O-NH3 ternary ion-mediated nucleation (BHN): Kinetic-based model and comparison with CLOUD measurements, Atmos. Chem. Phys.,18, 17451-17474, https://doi.org/10.5194/acp-18-17451-2018, 2018.
2. Yu, F., Nadykto, A. B., Herb, and J., Luo, H2SO4-H2O binary and H2SO4-H2O-NH3 ternary homogeneous and ion-mediated nucleation: Lookup tables, in review, GMD, 2019.

Files included in the package:

YBHN/: BHN code and lookup table
YTHN/: THN code and lookup table
YBIMN/: BIMN code and lookup table
YTIMN/: TIMN code and lookup table

Lookup tables for H2SO4-H2O

zenodo.org/records/34

nucl_XXX_mod.f (XXX = BHN, THN, BIMN, TIMN): Stand alone module for XXX rate calculation.

mainXXX.f: Test program to demonstrate how the lookup table is used.

inputXXX.dat: Example input data for testing the code and lookup table.
outputXXX.dat: Example output after running the test code

Use "f95 *.f" to compile and get executable program a.out

To run the test program:

>a.out

For your reference, output of running the program on my workstation has been saved to outputXXX.dat.

I hope that the comments provided in the subroutines make the code self-explanatory. Contact me if you have questions.

Enjoy and have fun!

Fangqun Yu
SUNY-Albany
(fyu@albany.edu)

Files

Files (19.4 MB)

BHN-BIMN-THN-TIMN-LookupTables.tar.gz
md5:48fe9569eb9ba3375be13fba2e02db14

19.4 MB

Download

Additional details

Funding

U.S. National Science Foundation

Development, Validation, and Application of Multicomponent Atmospheric New Particle

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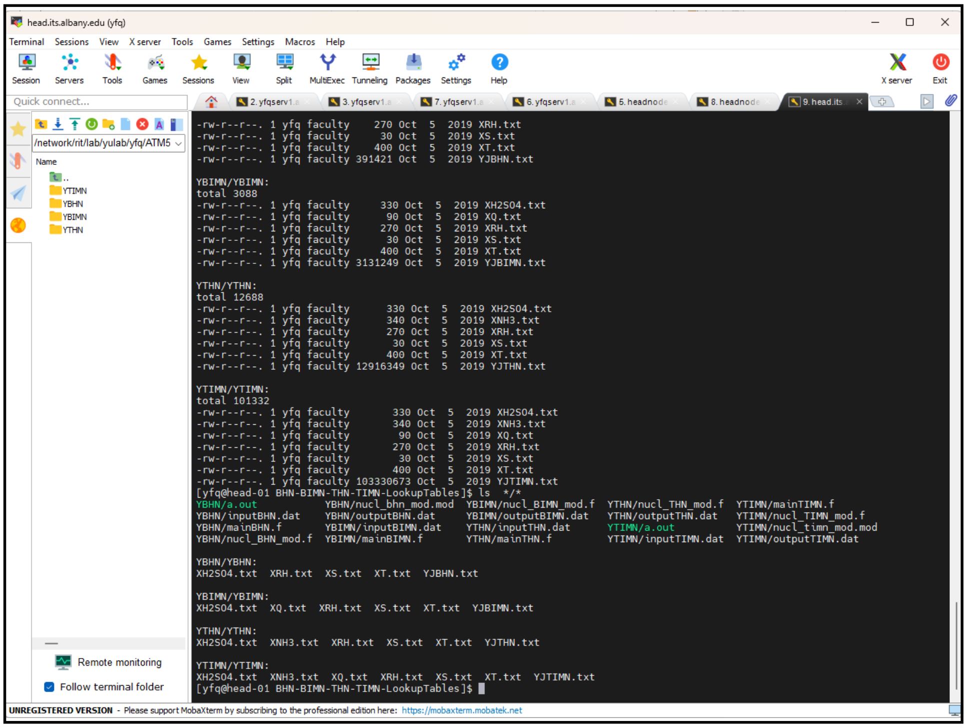
head.its.albany.edu (yfq)
/network/rit/lab/yulab/yfq/ATM5
YTIMN
YBHN
YBIMN
YTHN
-rw-r--r--. 1 yfq faculty   270 Oct 5 2019 XRH.txt
-rw-r--r--. 1 yfq faculty   30 Oct 5 2019 XS.txt
-rw-r--r--. 1 yfq faculty   400 Oct 5 2019 XT.txt
-rw-r--r--. 1 yfq faculty 391421 Oct 5 2019 YJBHN.txt
YBIMN/YBIMN:
total 3088
-rw-r--r--. 1 yfq faculty   330 Oct 5 2019 XH2SO4.txt
-rw-r--r--. 1 yfq faculty   90 Oct 5 2019 XQ.txt
-rw-r--r--. 1 yfq faculty   270 Oct 5 2019 XRH.txt
-rw-r--r--. 1 yfq faculty   30 Oct 5 2019 XS.txt
-rw-r--r--. 1 yfq faculty   400 Oct 5 2019 XT.txt
-rw-r--r--. 1 yfq faculty 3131249 Oct 5 2019 YJBIMN.txt
YTHN/YTHN:
total 12688
-rw-r--r--. 1 yfq faculty   330 Oct 5 2019 XH2SO4.txt
-rw-r--r--. 1 yfq faculty   340 Oct 5 2019 XNH3.txt
-rw-r--r--. 1 yfq faculty   270 Oct 5 2019 XRH.txt
-rw-r--r--. 1 yfq faculty   30 Oct 5 2019 XS.txt
-rw-r--r--. 1 yfq faculty   400 Oct 5 2019 XT.txt
-rw-r--r--. 1 yfq faculty 12916349 Oct 5 2019 YJTHN.txt
YTIMN/YTIMN:
total 101332
-rw-r--r--. 1 yfq faculty   330 Oct 5 2019 XH2SO4.txt
-rw-r--r--. 1 yfq faculty   340 Oct 5 2019 XNH3.txt
-rw-r--r--. 1 yfq faculty   90 Oct 5 2019 XQ.txt
-rw-r--r--. 1 yfq faculty   270 Oct 5 2019 XRH.txt
-rw-r--r--. 1 yfq faculty   30 Oct 5 2019 XS.txt
-rw-r--r--. 1 yfq faculty   400 Oct 5 2019 XT.txt
-rw-r--r--. 1 yfq faculty 103330673 Oct 5 2019 YJTIMN.txt
[yfq@head-01 BHN-BIMN-THN-TIMN-LookupTables]$ ls */*
YBHN/a.out YBHN/nucl_bhn_mod.mod YBIMN/nucl_BIMN_mod.f YTHN/nucl_THN_mod.f YTIMN/mainTIMN.f
YBHN/inputBHN.dat YBHN/outputBHN.dat YBIMN/outputBIMN.dat YTHN/outputTHN.dat YTIMN/nucl_TIMN_mod.f
YBHN/mainBHN.f YBIMN/inputBIMN.dat YTHN/inputTHN.dat YTIMN/a.out YTIMN/nucl_timn_mod.mod
YBHN/nucl_BHN_mod.f YBIMN/mainBIMN.f YTHN/mainTHN.f YTIMN/inputTIMN.dat YTIMN/outputTIMN.dat
YBHN/YBHN:
XH2SO4.txt XRH.txt XS.txt XT.txt YJBHN.txt
YBIMN/YBIMN:
XH2SO4.txt XQ.txt XRH.txt XS.txt XT.txt YJBIMN.txt
YTHN/YTHN:
XH2SO4.txt XNH3.txt XRH.txt XS.txt XT.txt YJTHN.txt
YTIMN/YTIMN:
XH2SO4.txt XNH3.txt XQ.txt XRH.txt XS.txt XT.txt YJTIMN.txt
[yfq@head-01 BHN-BIMN-THN-TIMN-LookupTables]$
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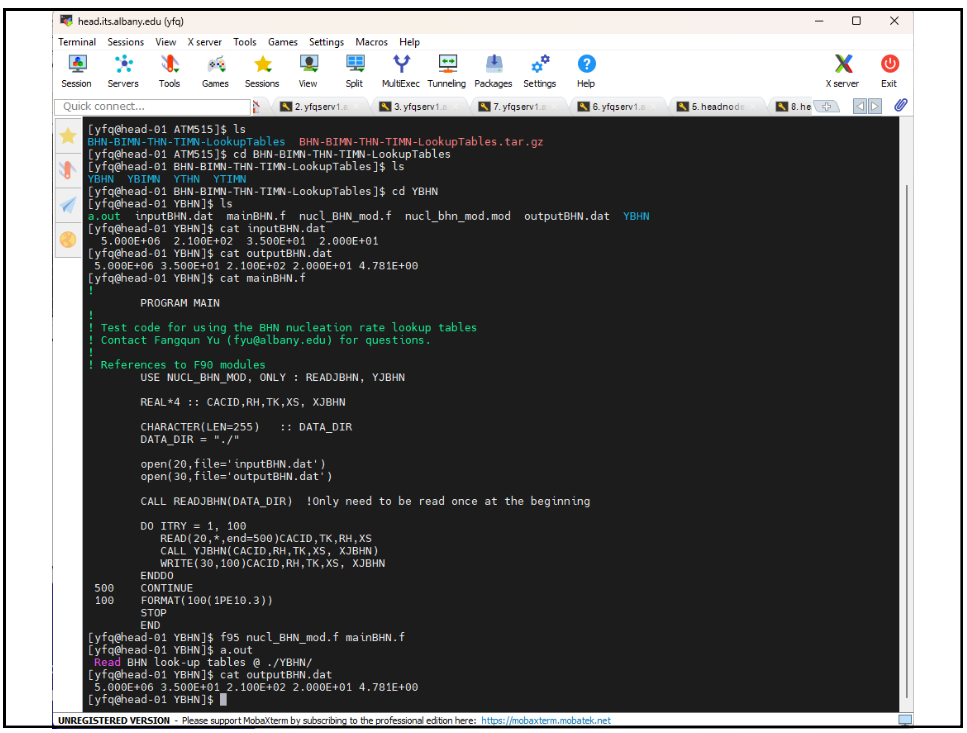
head.its.albany.edu (yfq)
[yfq@head-01 ATM515]$ ls
BHN-BIMN-THN-TIMN-LookupTables BHN-BIMN-THN-TIMN-LookupTables.tar.gz
[yfq@head-01 ATM515]$ cd BHN-BIMN-THN-TIMN-LookupTables
[yfq@head-01 BHN-BIMN-THN-TIMN-LookupTables]$ ls
YBHN YBIMN YTHN YTIMN
[yfq@head-01 BHN-BIMN-THN-TIMN-LookupTables]$ cd YBHN
[yfq@head-01 YBHN]$ ls
a.out inputBHN.dat mainBHN.f nucl_BHN_mod.f nucl_bhn_mod.mod outputBHN.dat YBHN
[yfq@head-01 YBHN]$ cat inputBHN.dat
5.000E+06 2.100E+02 3.500E+01 2.000E+01
[yfq@head-01 YBHN]$ cat outputBHN.dat
5.000E+06 3.500E+01 2.100E+02 2.000E+01 4.781E+00
[yfq@head-01 YBHN]$ cat mainBHN.f
!
PROGRAM MAIN
!
! Test code for using the BHN nucleation rate lookup tables
! Contact Fangqun Yu (fyu@albany.edu) for questions.
!
! References to F90 modules
USE NUCL_BHN_MOD, ONLY : READJBHN, YJBHN
REAL*4 :: CACID,RH,TK,XS, XJBHN
CHARACTER(LEN=255)   :: DATA_DIR
DATA_DIR = "./"
open(20,file='inputBHN.dat')
open(30,file='outputBHN.dat')
CALL READJBHN(DATA_DIR) !Only need to be read once at the beginning
DO ITRY = 1, 100
READ(20,*,end=500)CACID,TK,RH,XS
CALL YJBHN(CACID,RH,TK,XS, XJBHN)
WRITE(30,100)CACID,RH,TK,XS, XJBHN
ENDDO
500   CONTINUE
100   FORMAT(100(1PE10.3))
STOP
END
[yfq@head-01 YBHN]$ f95 nucl_BHN_mod.f mainBHN.f
[yfq@head-01 YBHN]$ a.out
Read BHN look-up tables @ ./YBHN/
[yfq@head-01 YBHN]$ cat outputBHN.dat
5.000E+06 3.500E+01 2.100E+02 2.000E+01 4.781E+00
[yfq@head-01 YBHN]$
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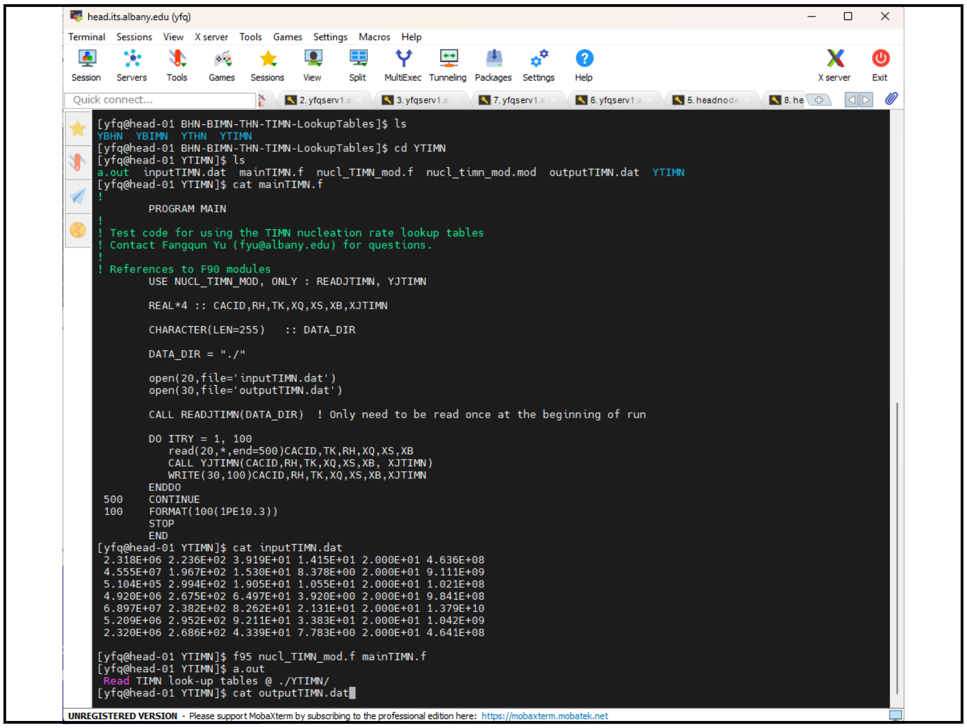

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Understanding the role of organics in new particle formation in the atmosphere

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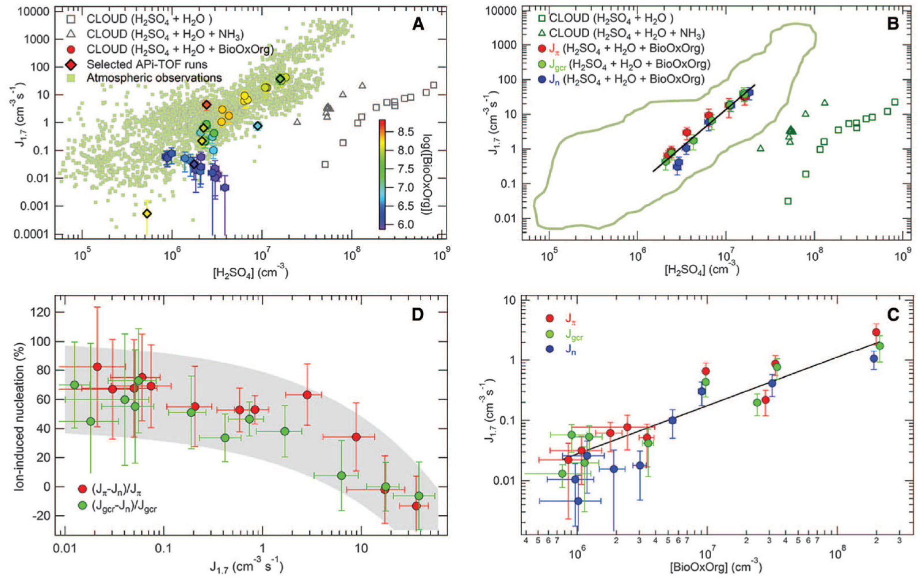

Oxidation Products of Biogenic Emissions Contribute to Nucleation of Atmospheric Particles
Francesco Riccobono *et al.*
Science **344**, 717 (2014);
DOI: 10.1126/science.1243527

$$J = k_m[H_2SO_4]^2[BioOxOrg]$$

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Impact of temperature dependence on the possible contribution of organics to new particle formation in the atmosphere

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[2]Department of Applied Mathematics, Moscow State University of Technology "Stankin", Vadkovsky 1, Moscow 127055, Russia

Correspondence to: Fangqun Yu (fyu@albany.edu)

Received: 12 September 2016 – Discussion started: 19 October 2016
Revised: 1 March 2017 – Accepted: 2 March 2017 – Published: 18 April 2017

Table 1. The changes in enthalpy (ΔH), entropy (ΔS), and Gibbs free energy (ΔG) for the formation of a $(C_{10}H_{14}O_7)(H_2SO_4)_2$ cluster under the standard condition ($P = 1$ atm, $T = 298$ K).

	ΔH (kcal mol^{-1})	ΔS (cal mol^{-1} K^{-1})	ΔG (kcal mol^{-1})
$C_{10}H_{14}O_7 + H_2SO_4 + H_2SO_4 \rightleftharpoons (C_{10}H_{14}O_7)(H_2SO_4)_2$	−38.30	−75.45	−15.81

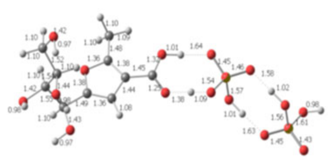
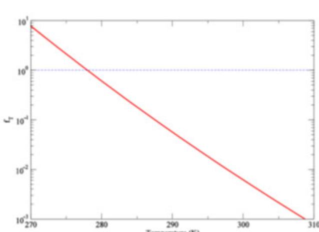


Figure 1. The equilibrium geometry of the most stable isomers of the heteromolecular trimer composed of $(C_{10}H_{14}O_7)(H_2SO_4)_2$ obtained at the PW91PW91/6-311++G(3df,3pd) level of theory. The bonding lengths are in Ångstroms.



$$J_{\text{Nucl-OrgT}} = J_{\text{Nucl-Org}} f_T$$

$$f_T = \exp\left[\frac{\Delta H}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right],$$

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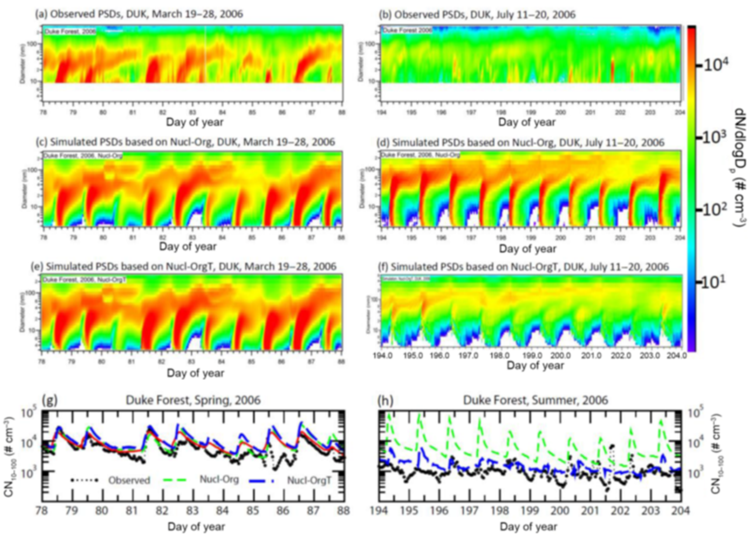

Figure 7. The particle size distributions (PSDs) observed **(a, b)** and simulated based on the Nucl-Org **(c, d)** and Nucl-OrgT **(e, f)** schemes during two 10-day periods in March **(a, c, e)** and July **(b, d, f)** 2006 in Duke Forest (DUK), along with a time series of the concentration of condensation nuclei between 10 and 100 nm (CN_{10-100}) **(g, h)**.

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