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Simulating nucleation characteristics

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Objectives

- New particle formation prediction capability
- Test new nucleation mechanisms
- Traces of nucleation mechanism in larger size particles
- Size of activated clusters

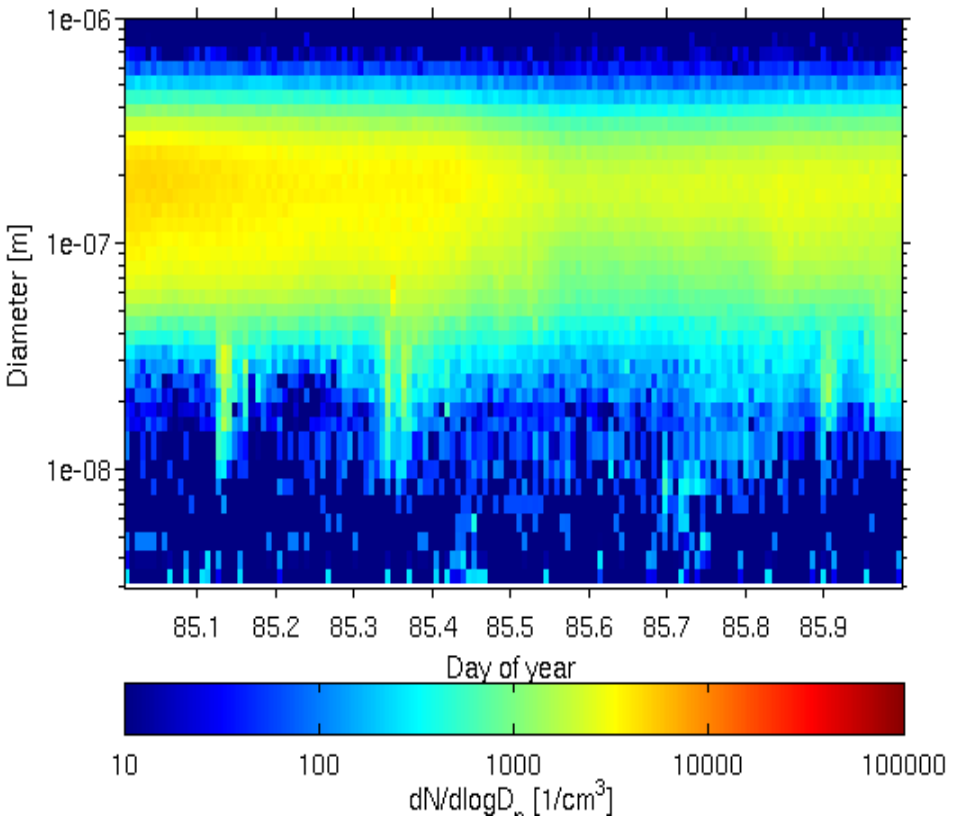
University of Helsinki Multicomponent Aerosol model (UHMA)

- sectional box model
- nucleation
- condensation (nano Köhler)
- coagulation
- dry deposition

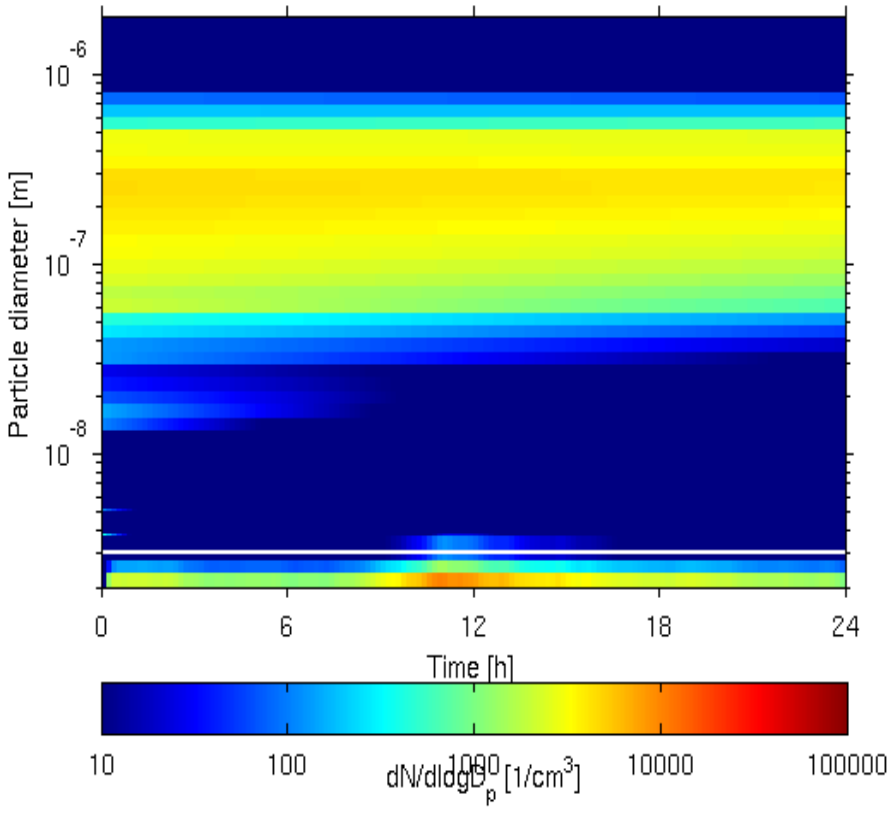
Korhonen et al., Atmos. Chem. Phys.,4 , 2004

New particle formation event prediction

DMPS



UHMA



Nucleation mechanisms

- Cluster activation concept *

$J = A \times [H_2SO_4]$

- "Kinetic" theory

$J = K \times [H_2SO_4]^2$

- Cluster activation by sulphuric acid **and** organics

$J = P \times [H_2SO_4] \times [org_P]$

- Cluster activation by sulphuric acid **or** organics

$J = Q \times ([H_2SO_4] + [org_Q])$

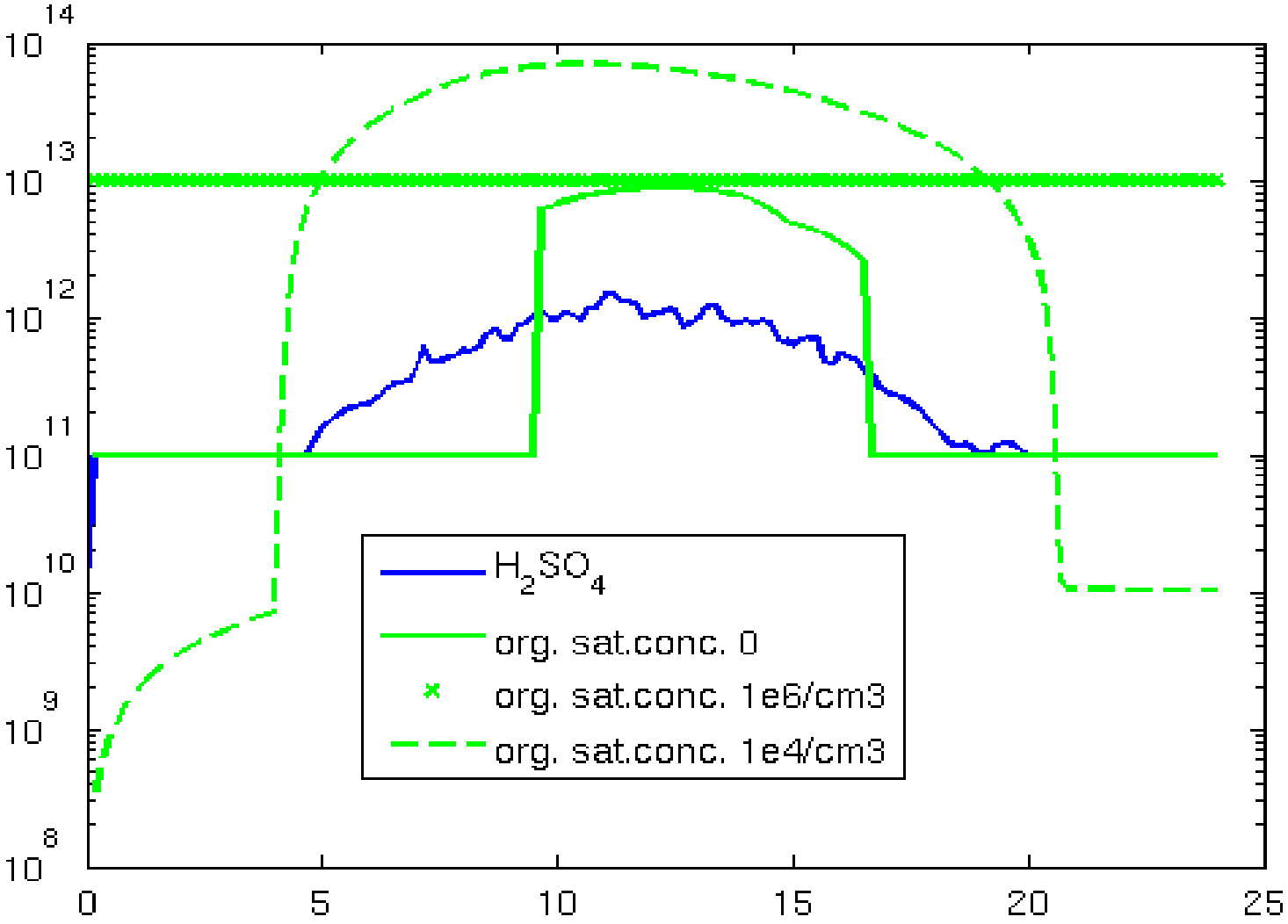
* Kulmala et al., Atmos. Chem. Phys., 6, 2006

Vapors

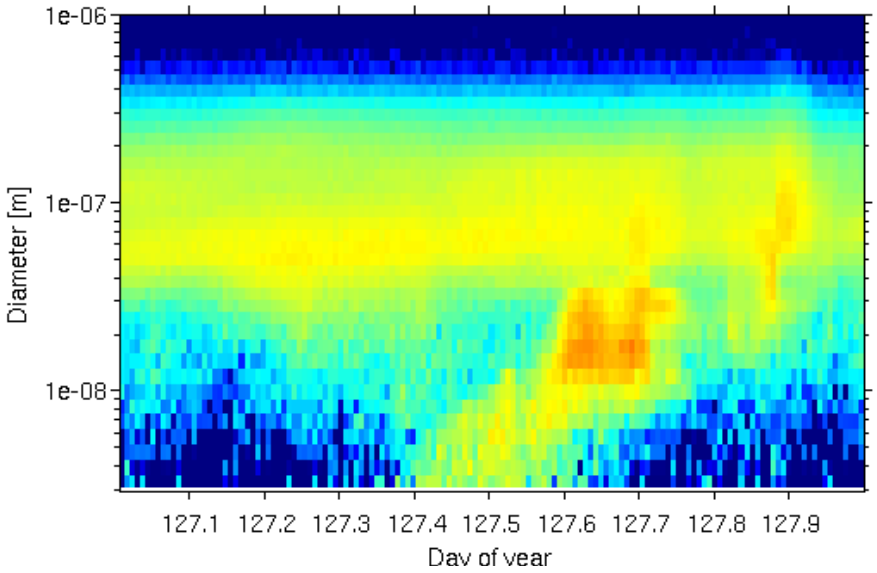
- Sulphuric acid read in from measurement data (CIMS*)
- A non-volatile organic vapor read in
  - growth rate of 2--4 nm particles not explained by H2SO4
  - profile from UVB
- Semi-volatile organics estimated from growth rate

* Petäjä et al., ACPD, 2008

Vapors

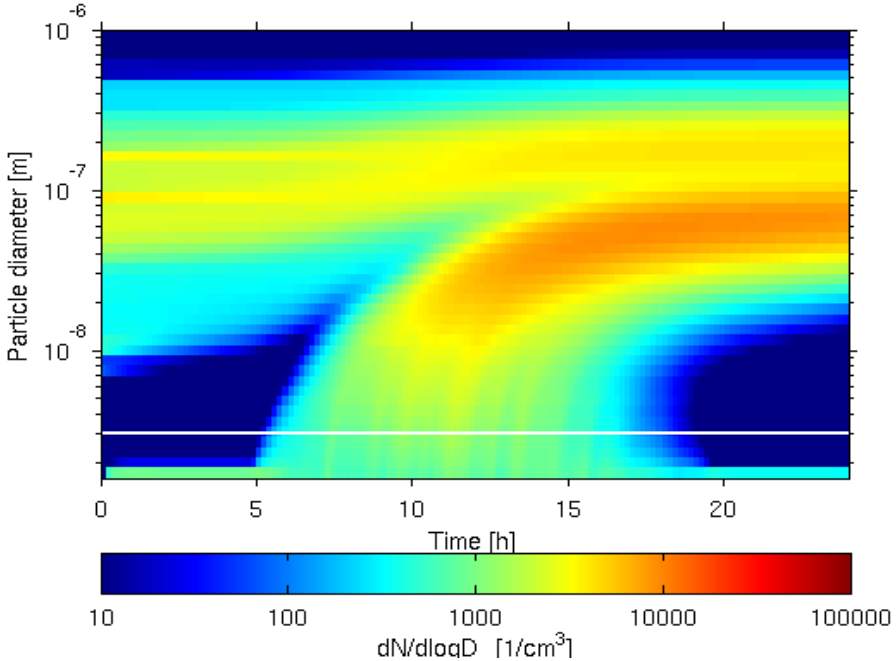

10^{14}
10^{13}
10^{12}
10^{11}
10^{10}
10^{9}
10^{8}
0
5
10
15
20
25
H_2SO_4
org. sat.conc. 0
org. sat.conc. 1e6/cm3
org. sat.conc. 1e4/cm3

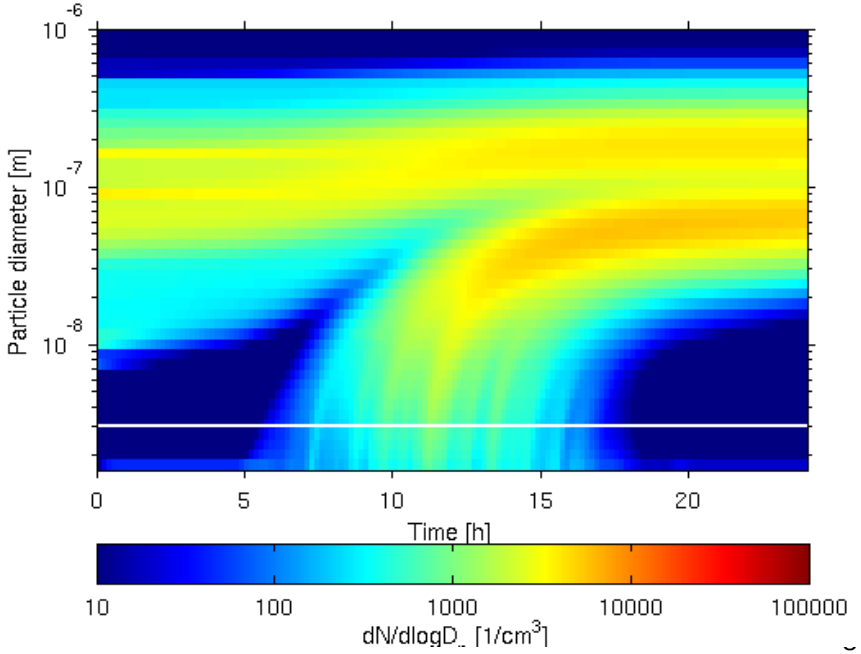
Nucleation mechanism (A & K)



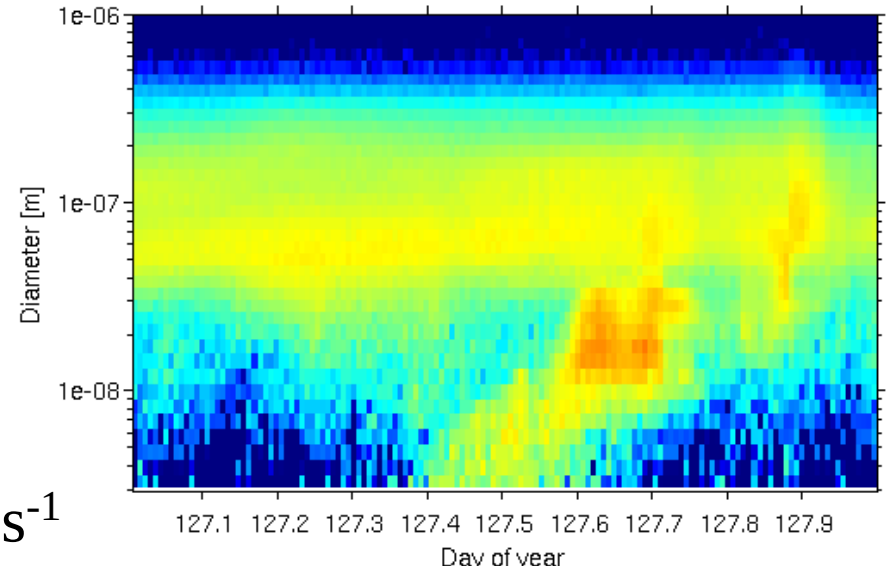
$A=10^{-6}\ s^{-1}$

$K=5x10^{-13}\ cm^{-3}s^{-}$



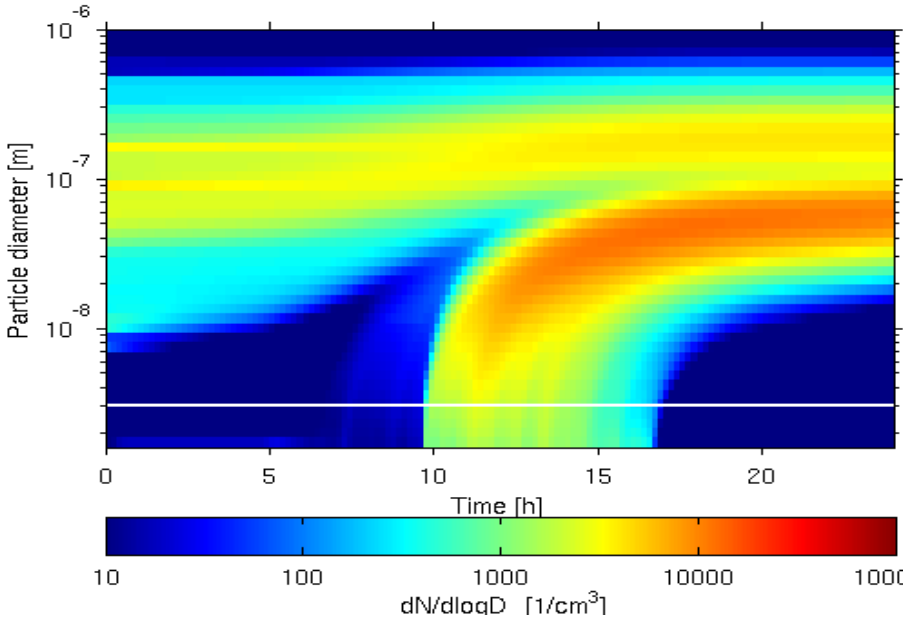


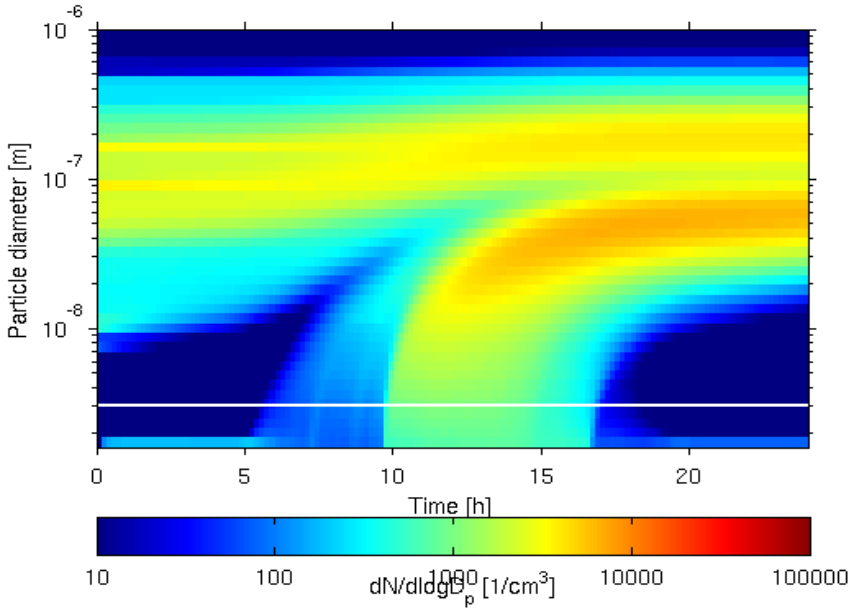
Nucleation mechanism (P & Q)



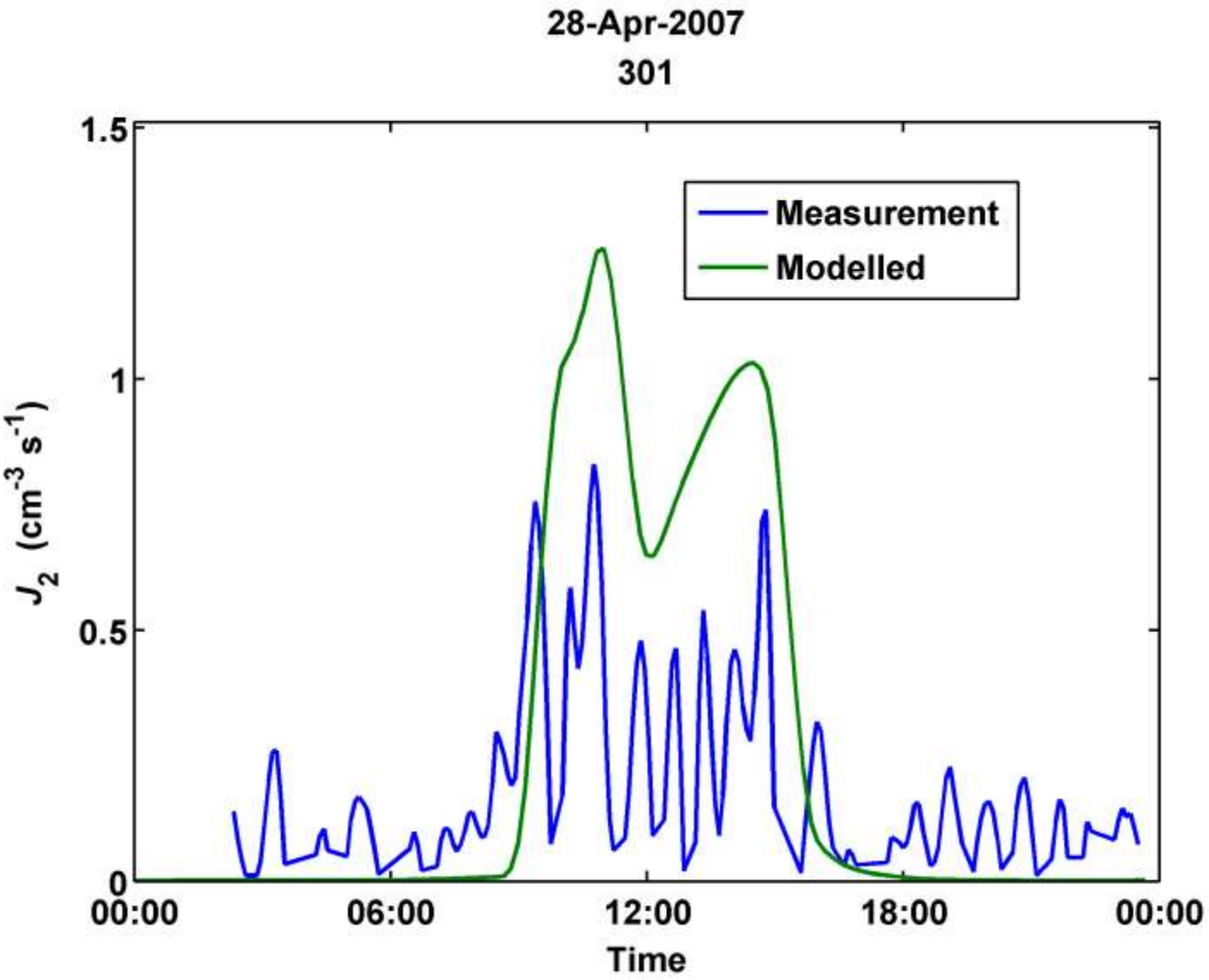
$P=2x10^{-13}\,cm^{-3}s^{-1}$

$Q=10^{-7}\,s^{-1}$





Formation rate comparison

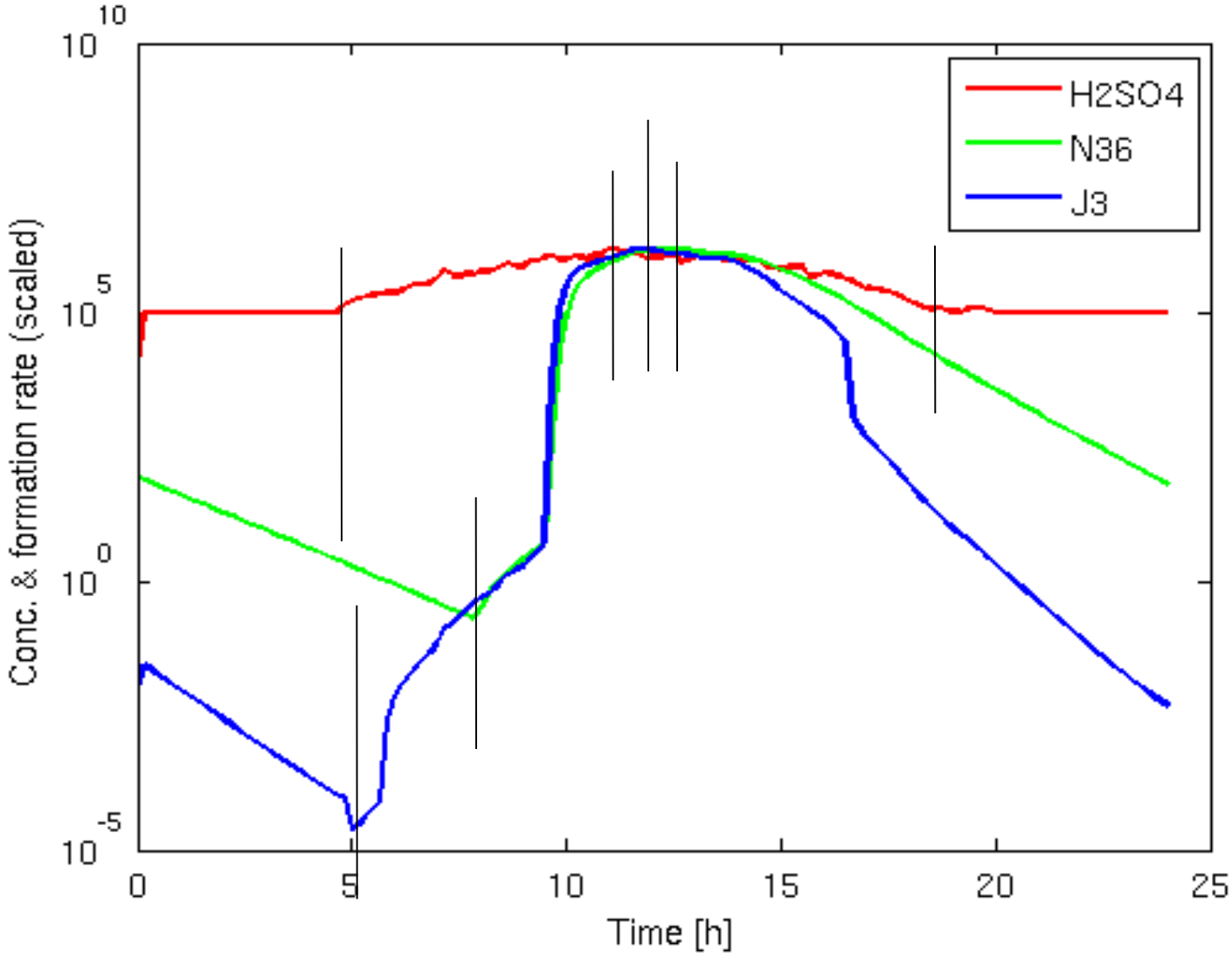


Tracing back the nucleation mechanism

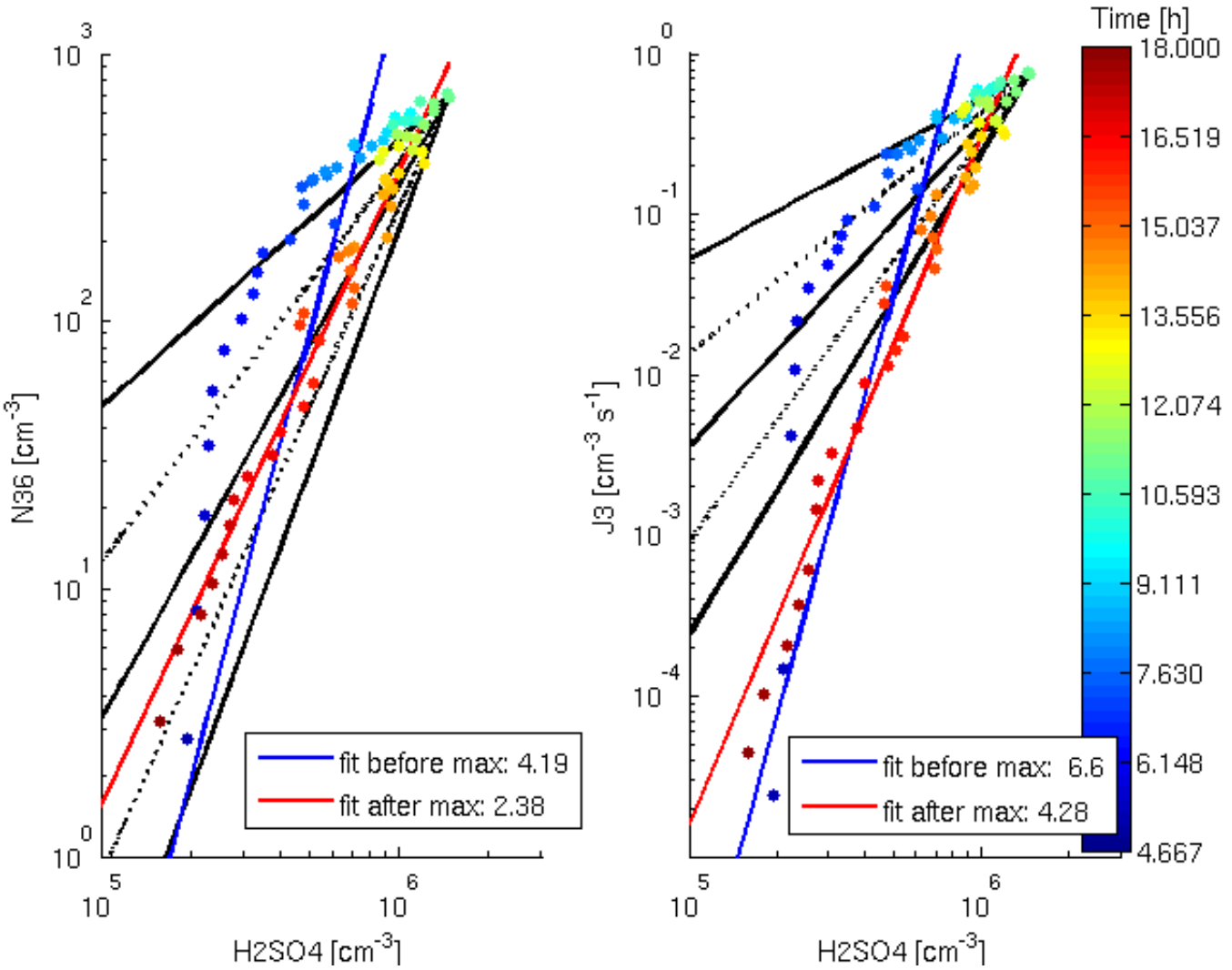
- Data analysis has suggested
  - $N_{3\text{-}6}\ (t) \sim ([H2SO4](t\text{-}dt_1))^{n1}$
  - $J_3\ (t) \sim ([H2SO4](t\text{-}dt_2))^{n2}$

e.g. Sihto et al., Atmos. Chem. Phys., 2006

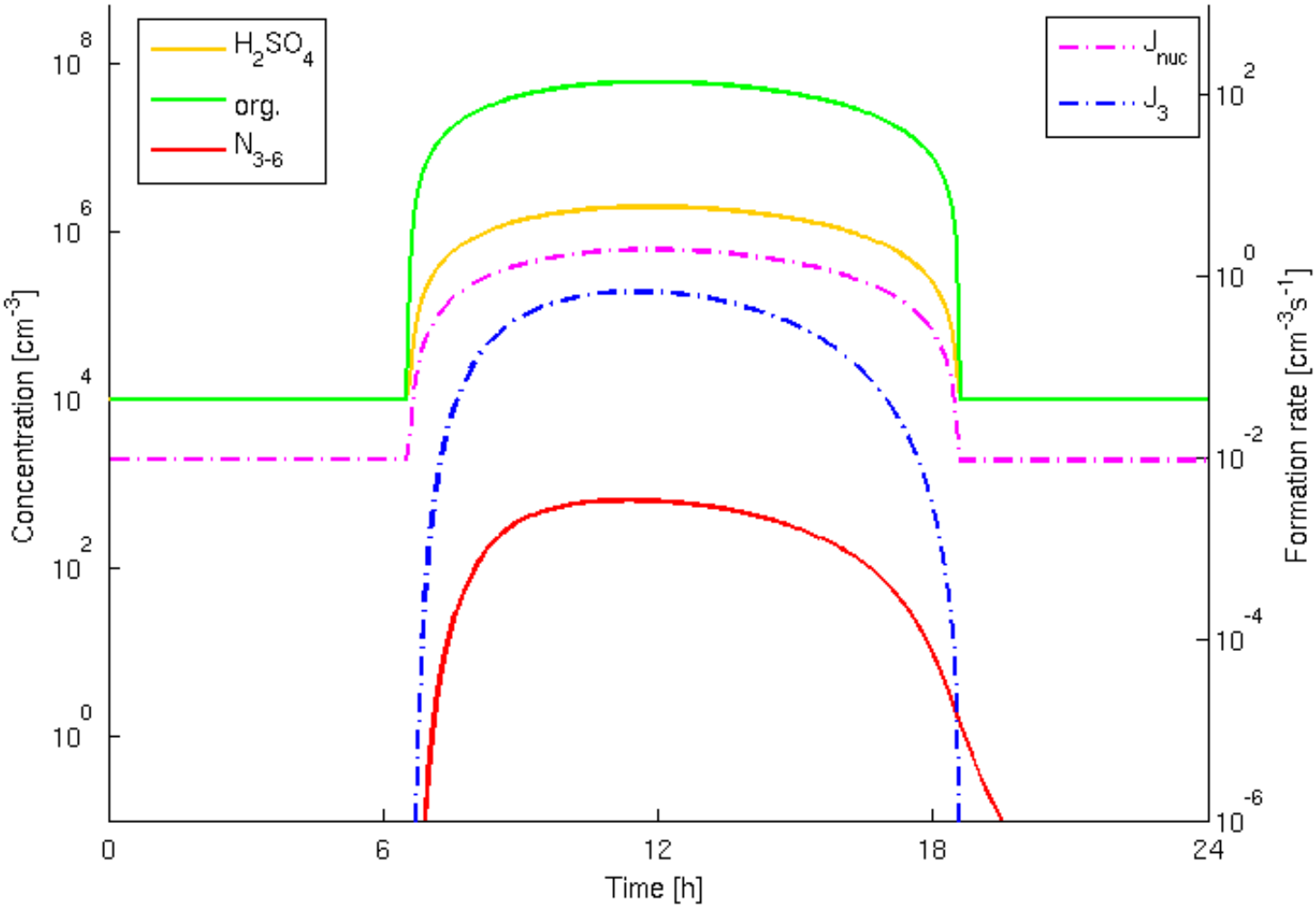
The method for determining time delay



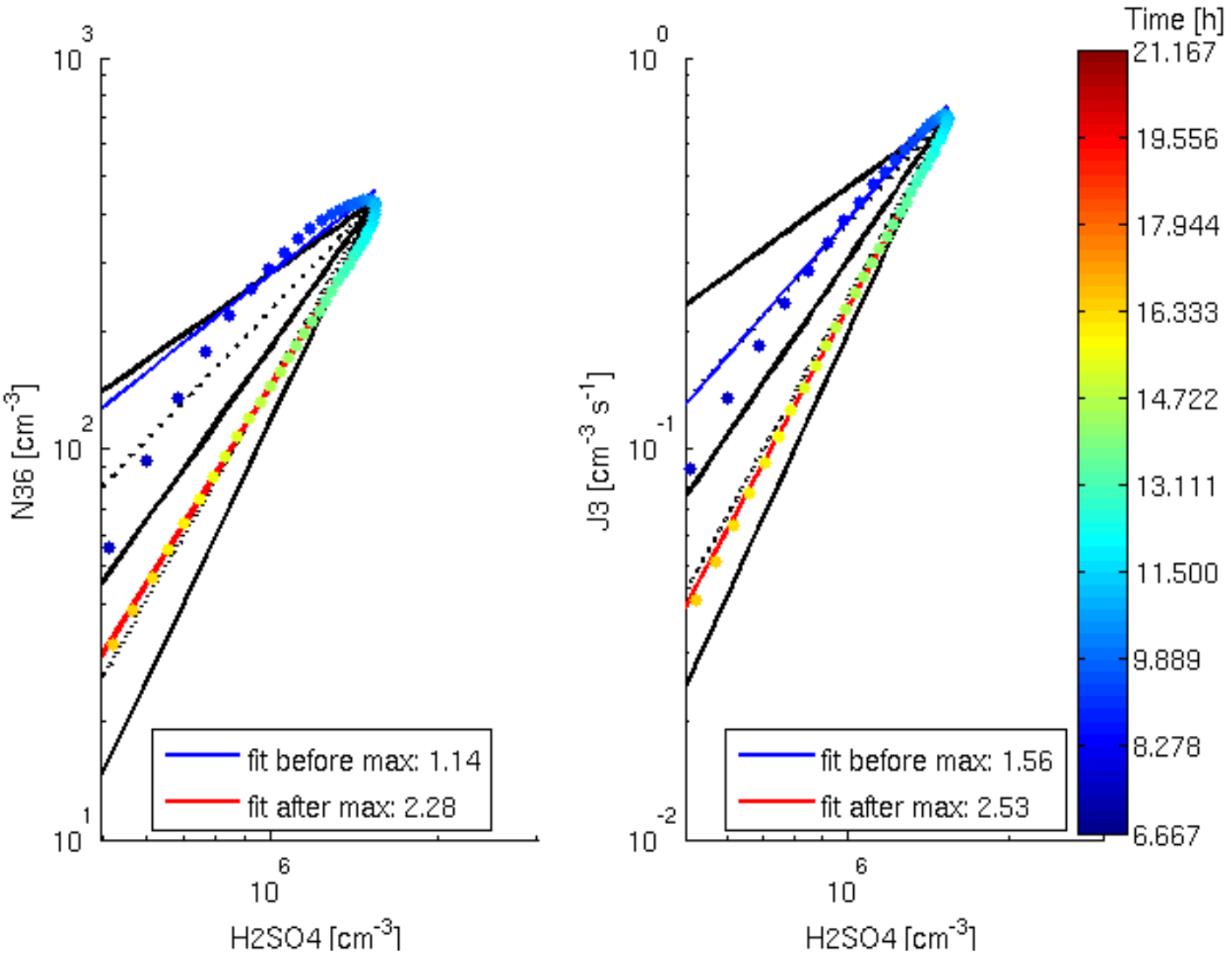
The method for determining exponents



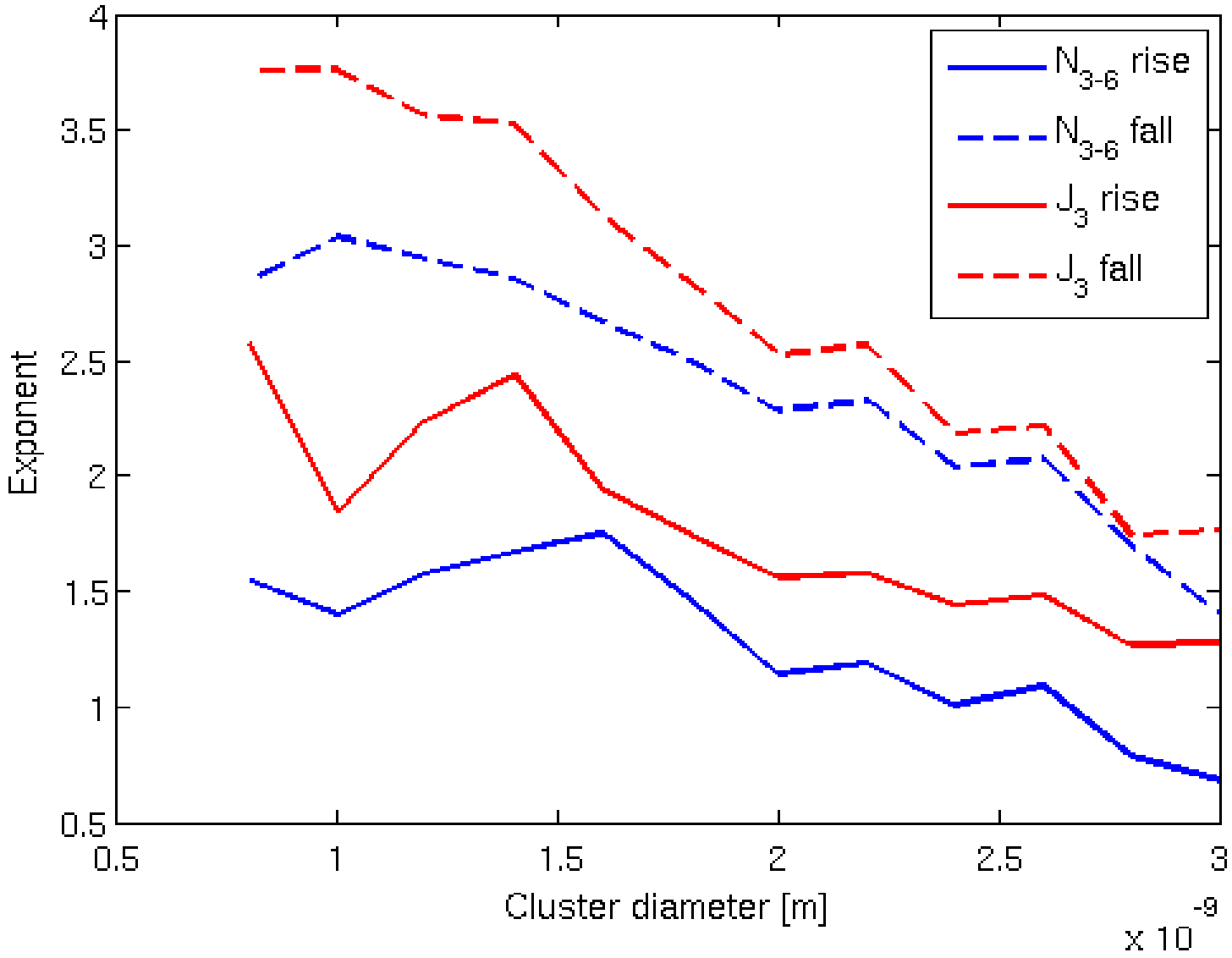
Simulated input



Exponents for simulated input case (A)



Cluster diameter effect (A)



Conclusions

- Event / non-event prediction successful
- All tested nucleation mechanisms provide reasonable results with some differences
- growth still difficult to model correctly
- Exponents smaller before event maximum
- The greater the initial cluster diameter, the smaller the exponents n_{J3} and $n_{N3\text{-}6}$