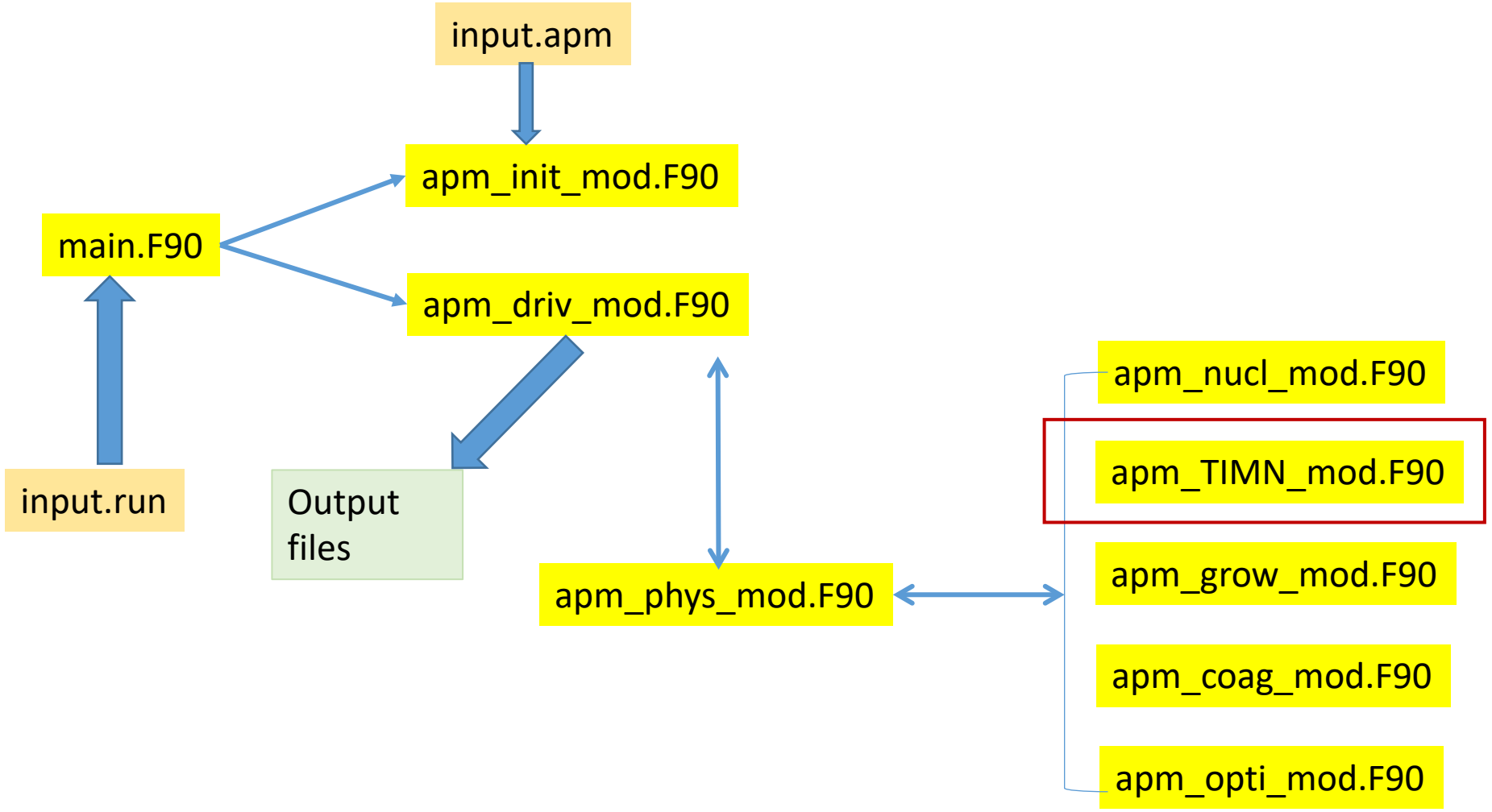
# Advanced Particle Microphysics (APM)

## Model: Nucleation

Hands-on computer lab


input.apm
apm_init_mod.F90
main.F90
apm_driv_mod.F90
input.run
Output files
apm_phys_mod.F90
apm_nucl_mod.F90
apm_TIMN_mod.F90
apm_grow_mod.F90
apm_coag_mod.F90
apm_opti_mod.F90

# Lookup tables of nucleation rates for BHN (*J*BHN), THN (*J*THN), BIMN (*J*BIMN), and TIMN (*J*TIMN)

six parameters controlling ***J*TIMN: sulfuric acid vapor concentration ([H2SO4]), ammonia gas concentration ([NH3]), temperature (*T*), relative humidity (RH), ionization rate (*Q*), and surface area of pre-existing particles (*S*)**. Compared to *J*TIMN, there is one fewer controlling parameter for both ***J*BIMN (no [NH3] dependence)** and ***J*THN (no *Q* dependence)**, while ***J*BHN only depends on four parameters ([H2SO4] *T*, RH, and *S*)**.

Geosci. Model Dev., 13, 2663–2670, 2020
https://doi.org/10.5194/gmd-13-2663-2020


Geoscientific Model Development
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**$H_2SO_4$–$H_2O$ 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[1], Alexey B. Nadykto[1,2,3], Gan Luo[1], and Jason Herb[1]

Yu et al., 2020. https://doi.org/10.5194/gmd-13-2663-2020

# Inputs and outputs

```
[jm332773@headnode7 APM-box-2025ATM515]$ vi input.apm
IFNUCL (see apm_phys_mod.F90 for options)
1
IFNH3
0
IFAG
1
IFCOAT, IFCOATBC (1=yes, 0=no)
1, 1
IFOPT (1=yes, 0=no;  Aerosol optical property calculation )
1
Z_R1,Z_SIGMA1,Z_R2,Z_SIGMA2 (BCOC size distribution parameters, Z_R in m)
4.0d-8,1.8,7.5d-8,1.8
DENBC (density of BC in kg/m3)
1800.0
~
```

Nucleation scheme

# Inputs and outputs

```
[jm332773@headnode7 APM-box-2025ATM515]$ vi input.run
TK (K),RH (%),XQ (ion pairs cm-3 s-1),CNH3(ppbv)
280., 80., 10., 3.0
MSO4,MBC,MOC,MDST,MSEA (ug/m3)
1.,0.2,2.,1.d-20,2.
PH2SO4max,PLVSOGmax  (# cm-3 s-1)
1.d5, 3.d5
dt(s), runhr (hr)
60., 120.
```

Parameters controlling nucleation

Time step and total runtime

# Outputs:

**output-CACID.txt [H2SO4] (#/cm3)**
**output-CLVSOG.txt [LVSOG] (#/cm3)**
**output-diameters.txt size bins of second particles**
**output-PACID.txt production rate of h2so4**
**output-PLVSOG1.txt production rate of lvsog**
**output-SP-PNSD.txt particle size distributions of second particles**
**output-TCS.txt total condensation sink**
**output-YJAVE.txt calculated nucleation rate**
**output-ZBEXT.txt total ext coef -- 550 nm**

```
cd APM_box_v5
cd APM-box-2025ATM515
vi input.apm
a.out
mv output*txt PLOT-NCL/
cd PLOT-NCL/
vi plot-APM-box-v5.ncl
ncl plot-APM-box-v5.ncl
```

e.g. Edit and save a file (input.apm):

vi input.apm

Press “i” to start edit mode

Press “Esc” to end edit mode

Shift+q or Shift + :

1) Save the edit and quit the file: type “wq!”

2) Directly quit the file : type “q!”

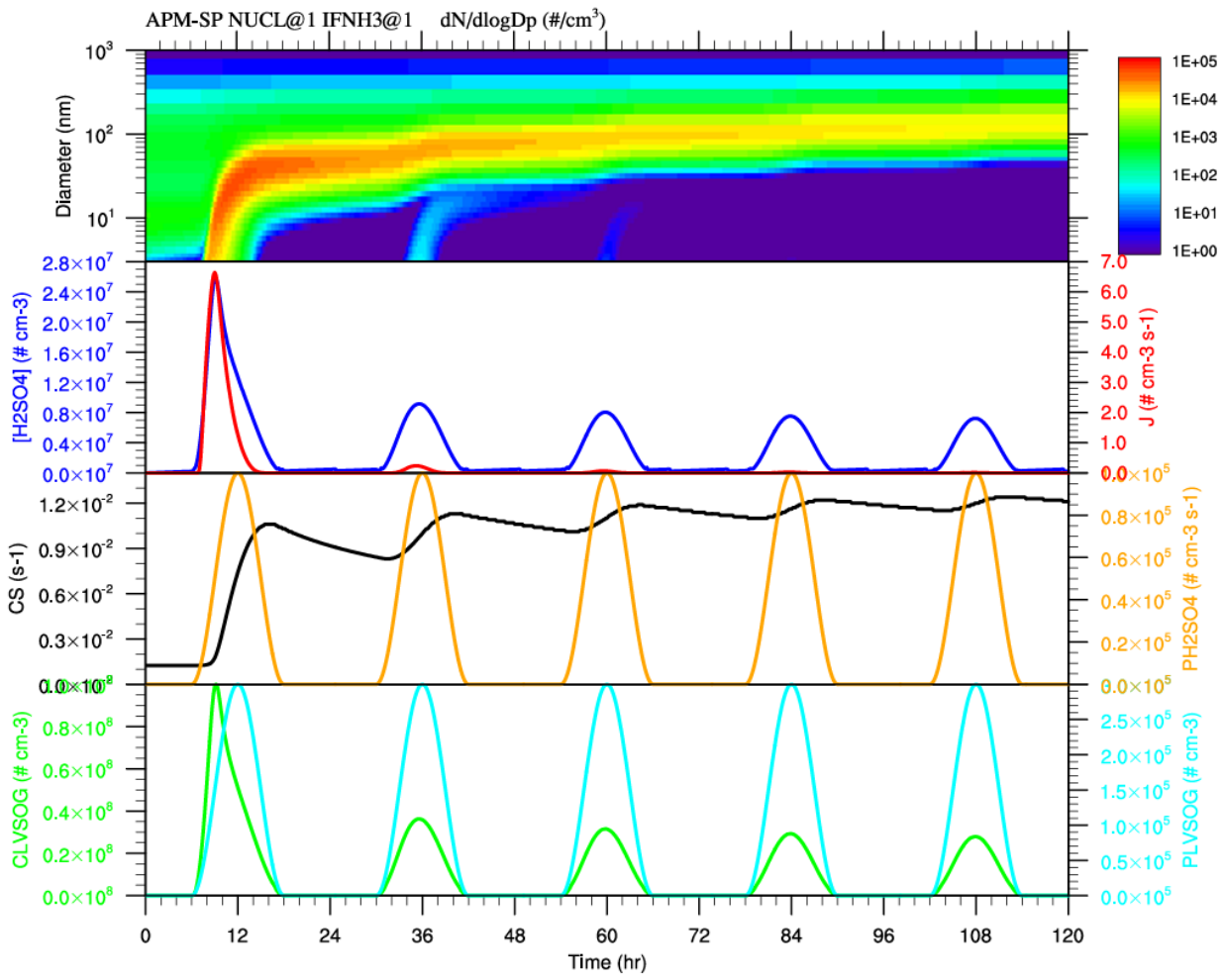
Model configuration

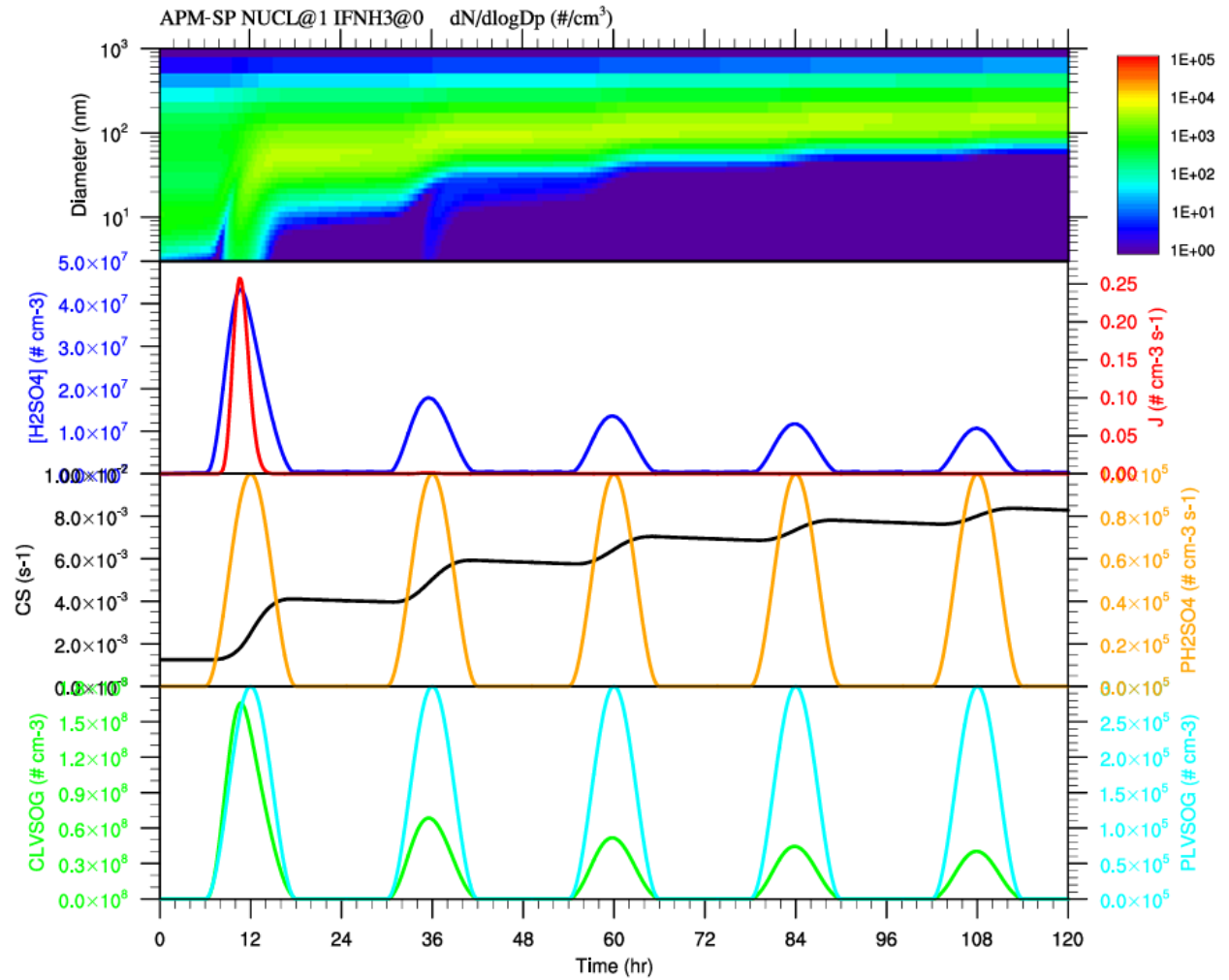
1) Nucleation schemes:

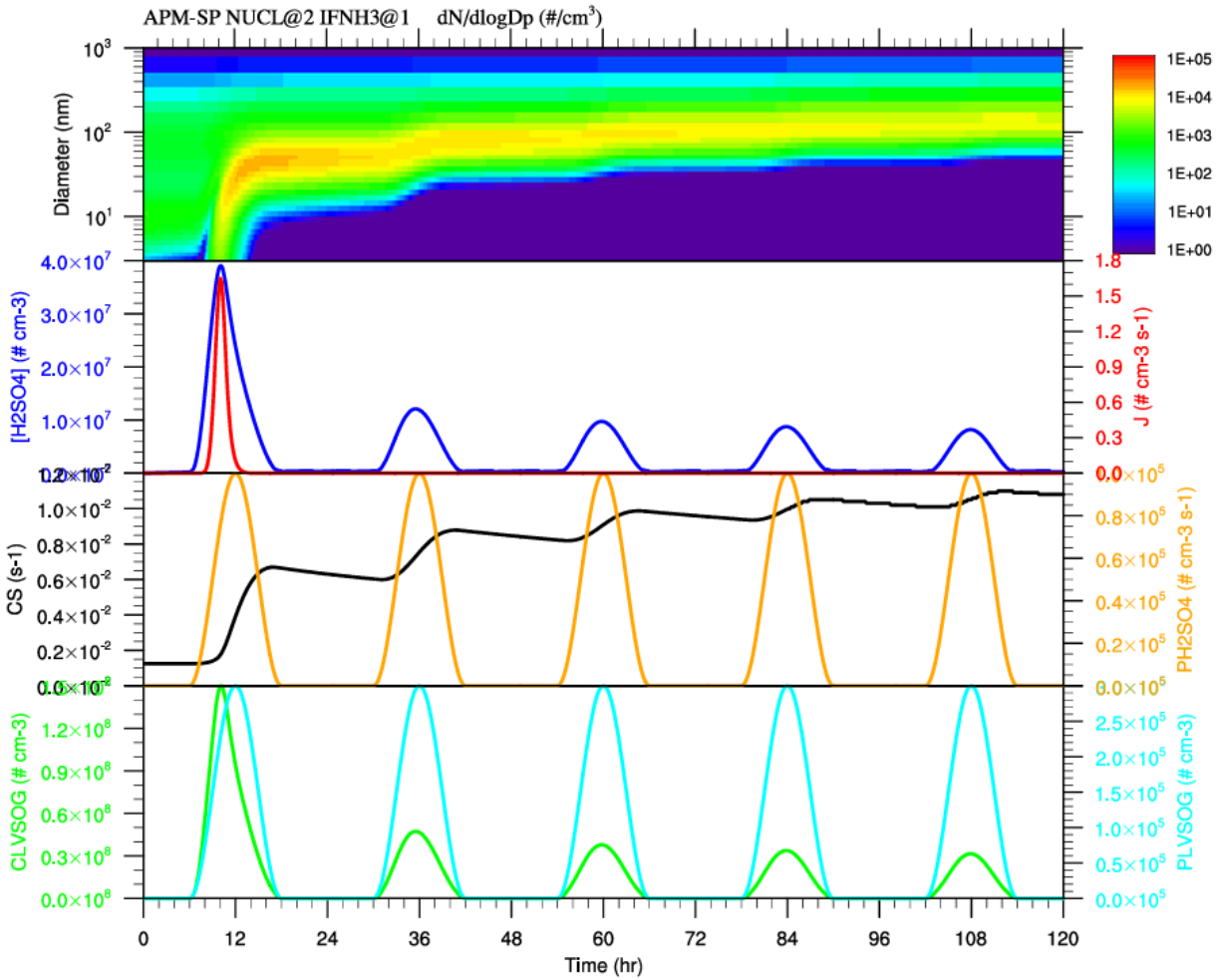
IFNUCL=1 (Ion-mediated nucleation)
IFNH3=0 BIMN
IFNH3=1 TIMN

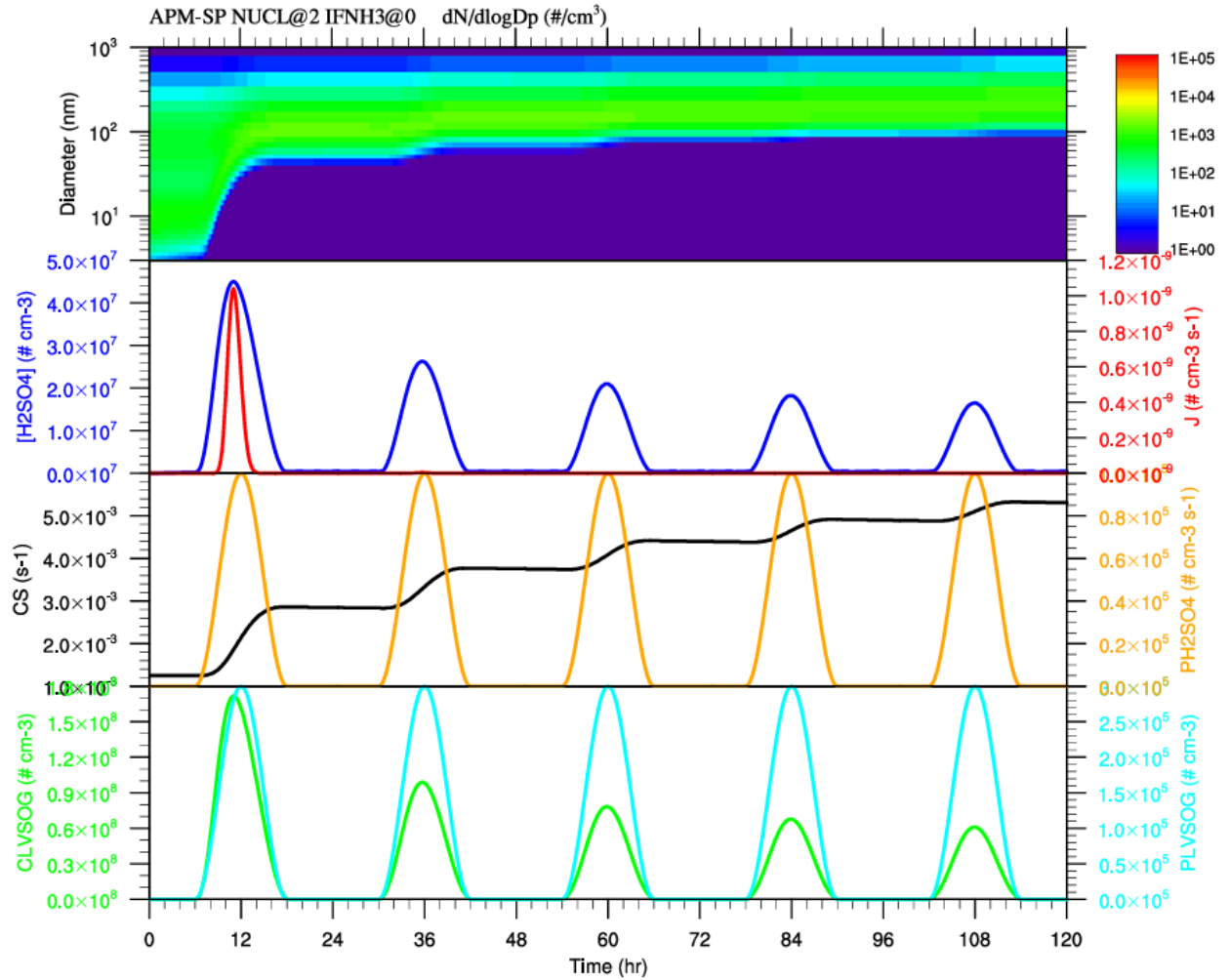
IFNUCL=2 (homogeneous nucleation)
IFNH3=0 BHN
IFNH3=1 THN

```
[jm332773@headnode7 APM-box-2025ATM515]$ vi input.apm
IFNUCL (see apm_phys_mod.F90 for options)
1
IFNH3
0
[jm332773@headnode7 APM-box-2025ATM515]$ vi input.run
TK (K),RH (%),XQ (ion pairs cm-3 s-1),CNH3(ppbv)
275., 70., 5., 3.0
[jm332773@headnode7 APM-box-2025ATM515]$ vi apm_phys_mod.F90
! Nucl
        IF(IFNUCL.EQ.1) THEN    ! IMN
          IF(IFNH3.EQ.0) THEN
           XNH3=1.d-20
           CALL YUJTIMN(CACID,RH,TK,XQ,XS,XNH3,YJ,YRSTAR)
          ELSEIF(IFNH3.EQ.1) THEN
           CALL YUJTIMN(CACID,RH,TK,XQ,XS,XNH3,YJ,YRSTAR)
          ELSE
           WRITE(6,*)"STOP at apm_phys_mod: Need to check IFNH3"
           STOP
          ENDIF
          IF((YJ*DT*10.).GT.(CACID/10.)) YJ= CACID/(DT*100.)
        ELSEIF(IFNUCL.EQ.2) THEN    ! KBHN (XQ=1.E-20)
          XQ=1.E-20
          IF(IFNH3.EQ.0) THEN
           XNH3=1.d-20
           CALL YUJTIMN(CACID,RH,TK,XQ,XS,XNH3,YJ,YRSTAR)
          ELSEIF(IFNH3.EQ.1) THEN
           CALL YUJTIMN(CACID,RH,TK,XQ,XS,XNH3,YJ,YRSTAR)
          ELSE
           WRITE(6,*)"STOP at apm_phys_mod: Need to check IFNH3"
           STOP
          ENDIF
```


APM-SP NUCL@1 IFNH3@1 dN/dlogDp (#/cm3)
Diameter (nm)
[H2SO4] (# cm-3)
J (# cm-3 s-1)
CS (s-1)
PH2SO4 (# cm-3 s-1)
CLVSOG (# cm-3)
PLVSOG (# cm-3)
Time (hr)


APM-SP NUCL@1 IFNH3@0 dN/dlogDp (#/cm3)
Diameter (nm)
[H2SO4] (# cm-3)
J (# cm-3 s-1)
CS (s-1)
PH2SO4 (# cm-3 s-1)
CLVSOG (# cm-3)
PLVSOG (# cm-3)
Time (hr)


APM-SP NUCL@2 IFNH3@1 dN/dlogDp (#/cm3)
Diameter (nm)
[H2SO4] (# cm-3)
J (# cm-3 s-1)
CS (s-1)
PH2SO4 (# cm-3 s-1)
CLVSOG (# cm-3)
PLVSOG (# cm-3)
Time (hr)


APM-SP NUCL@2 IFNH3@0 dN/dlogDp (#/cm3)
Diameter (nm)
[H2SO4] (# cm-3)
J (# cm-3 s-1)
CS (s-1)
PH2SO4 (# cm-3 s-1)
CLVSOG (# cm-3)
PLVSOG (# cm-3)
Time (hr)

# Hands-on computer lab

**BHN**

**1. stratosphere**

T=210 K, RH=0.6%,MSO4=0.06,MBC=1.d-3,MOC=8.d-3,MDST=1.d-20, MSEA=1.d-4, PH2SO4max=1.d3

**2. upper troposphere**

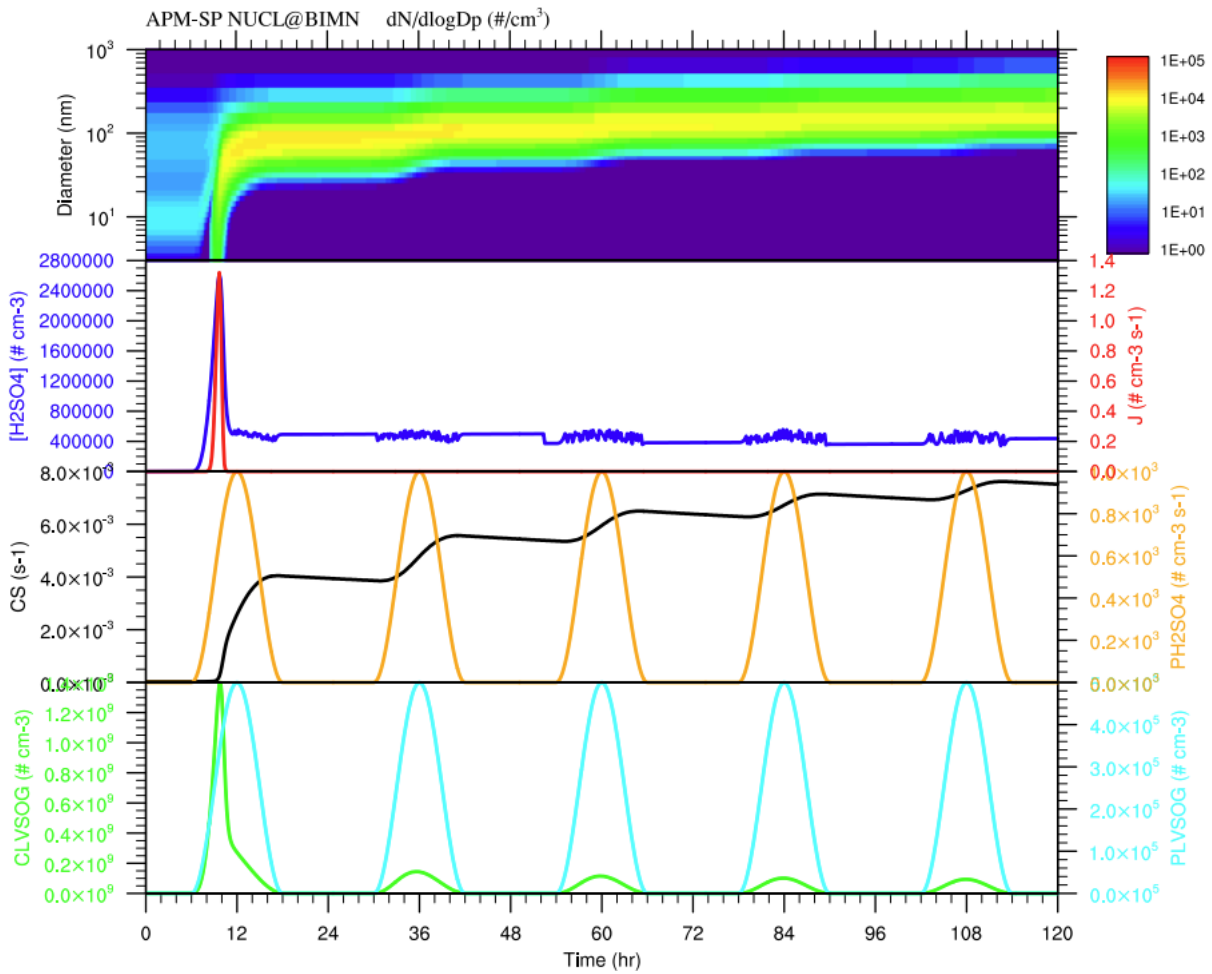
T=230 K, RH=50%,MSO4=0.4,MBC=0.01,MOC=0.04,MDST=1.d-20, MSEA=0.002,PH2SO4max=1.d4

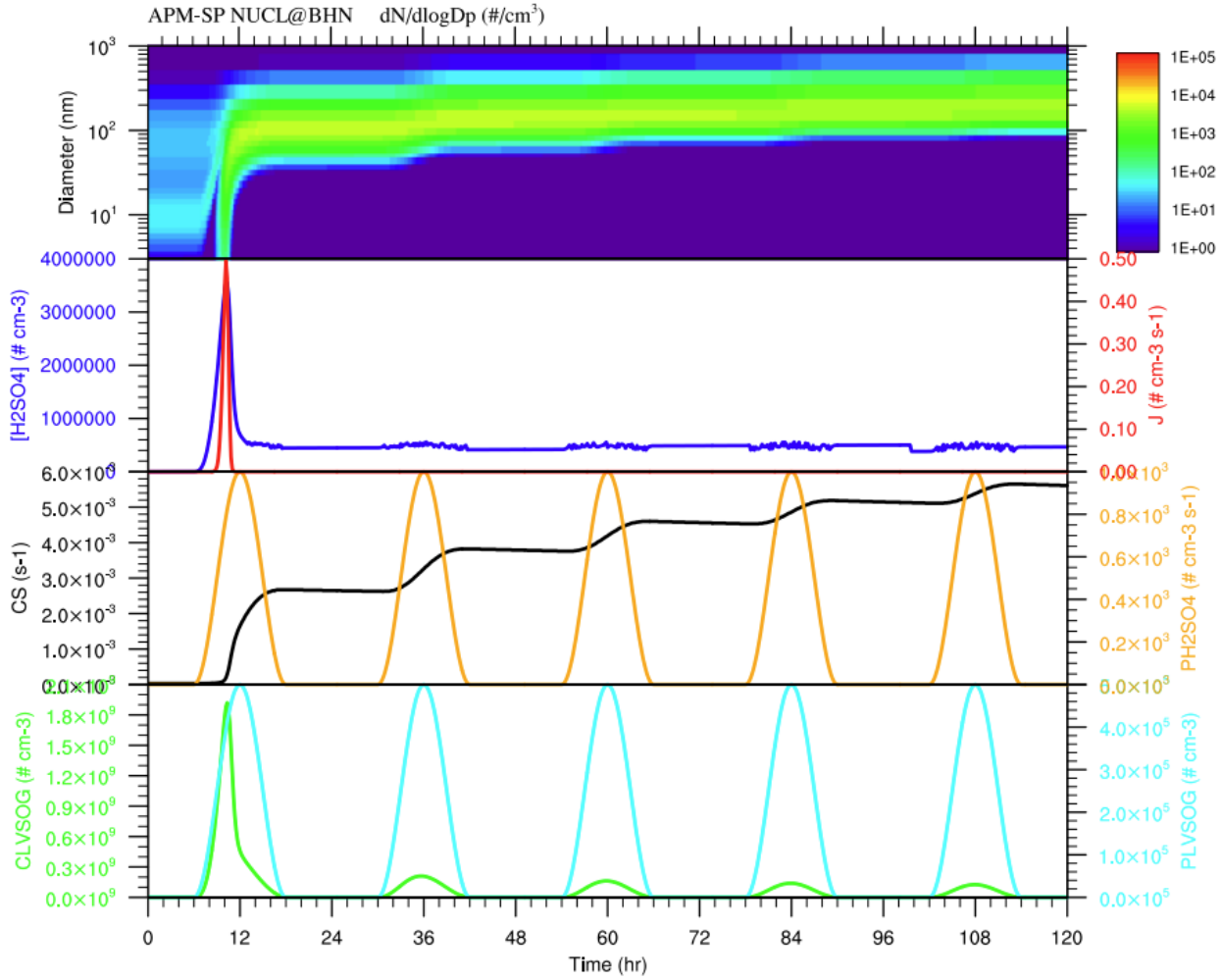
**3. near surface**

T=280 K, RH=80%, MSO4=1.,MBC=0.2,MOC=2,MDST=1.d-20, MSEA=2,PH2SO4max=1.d5

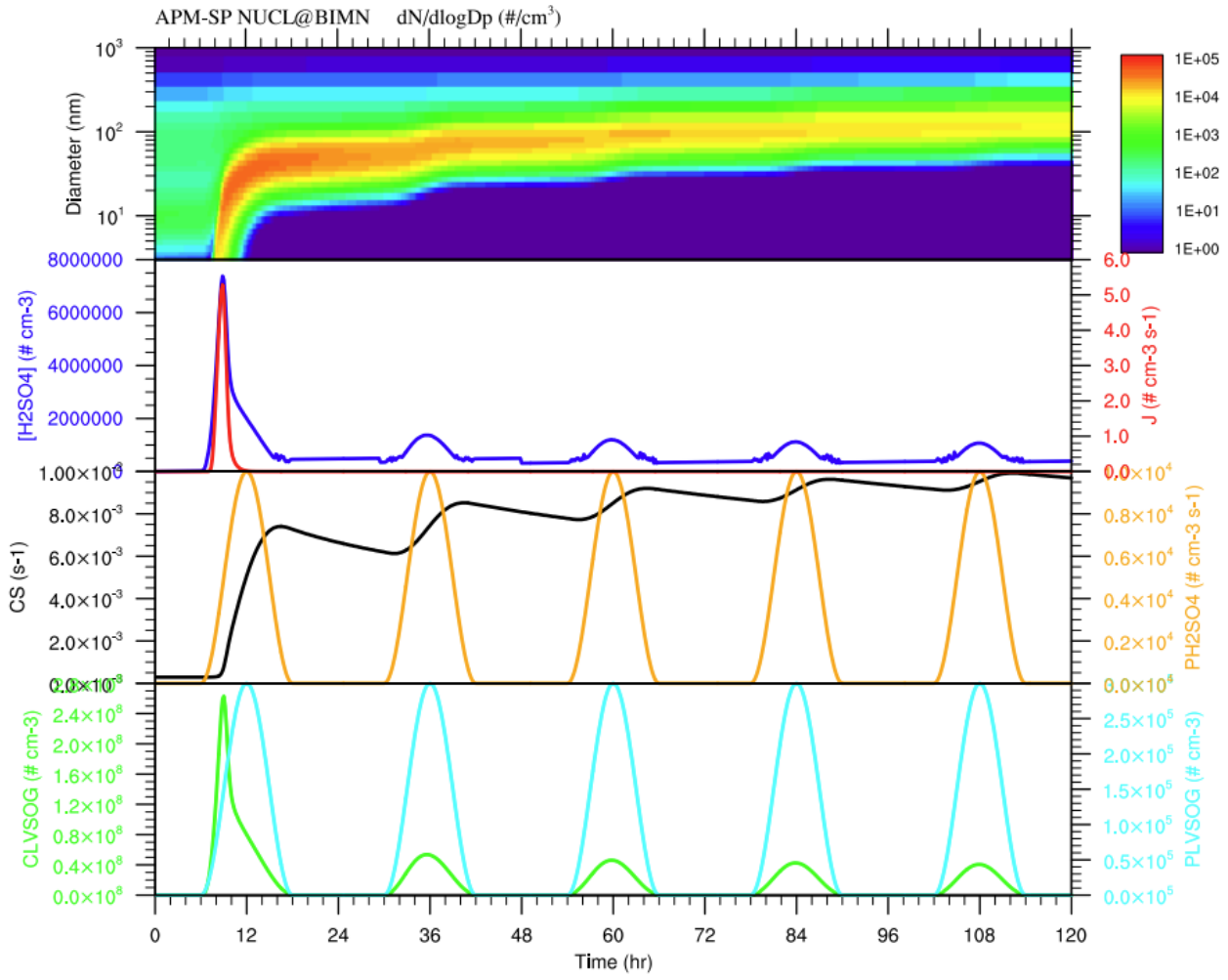
**BIMN:** assume ionization rate of 10 ion-pairs cm-3 s-1 .

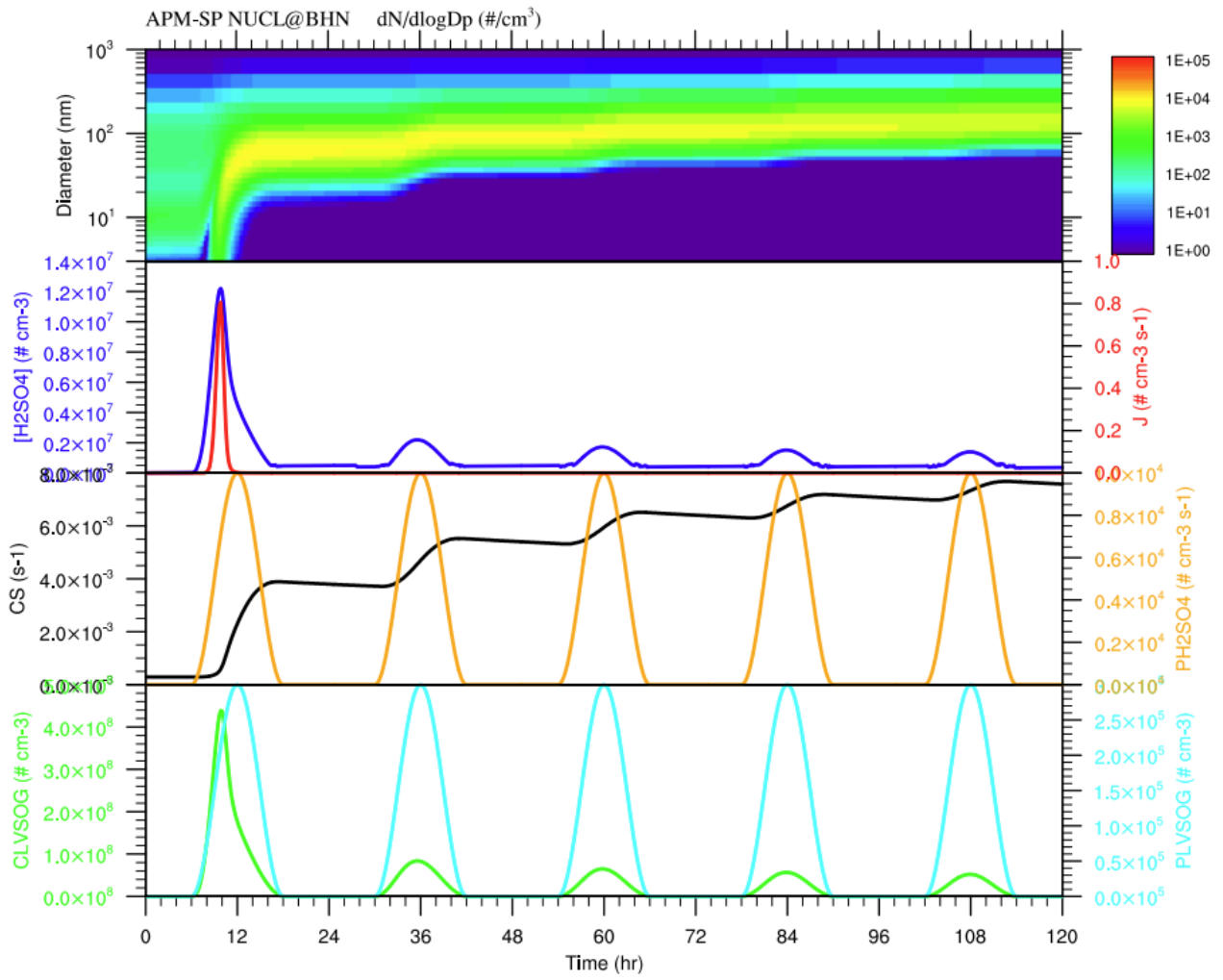
# 1.Stratosphere



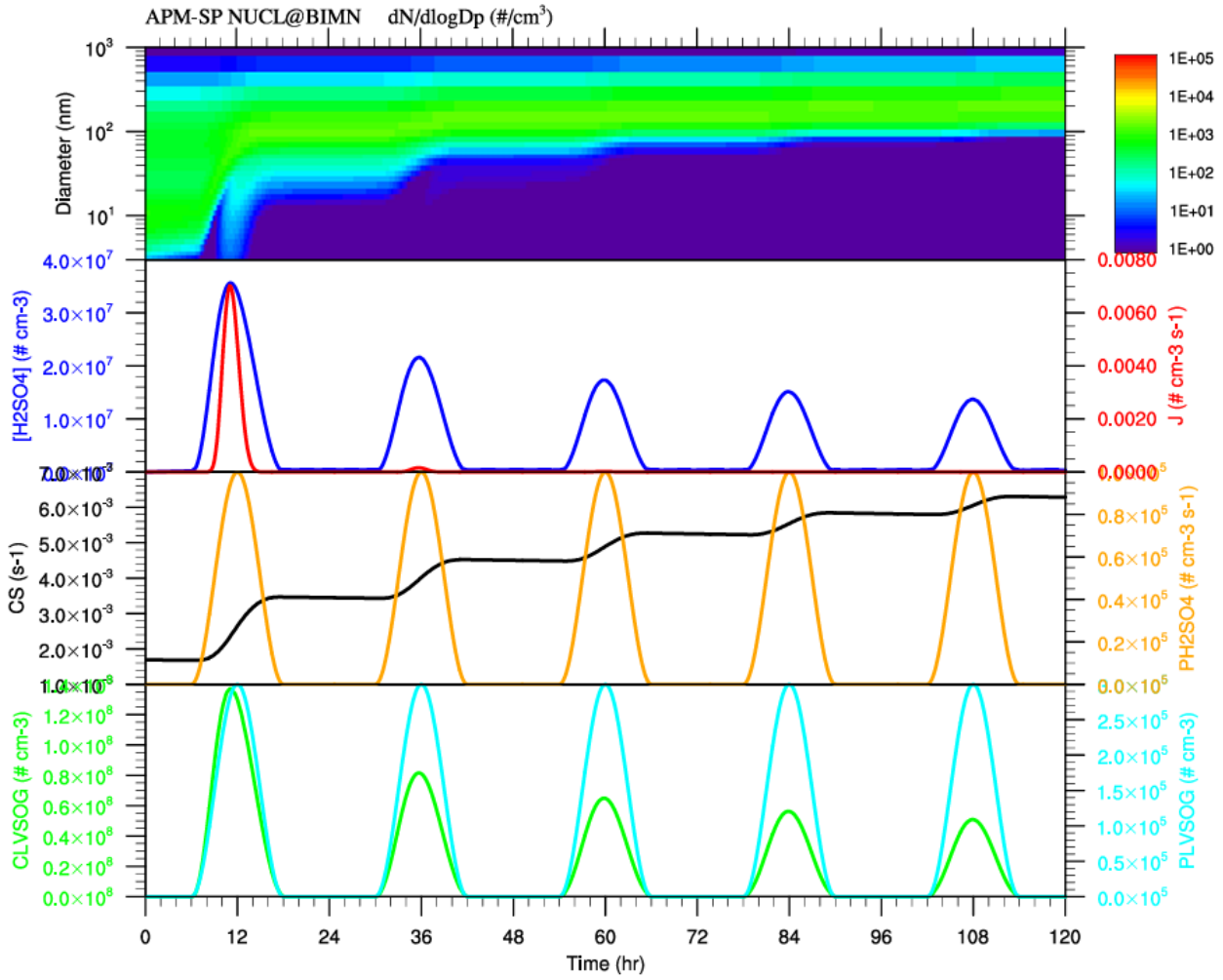



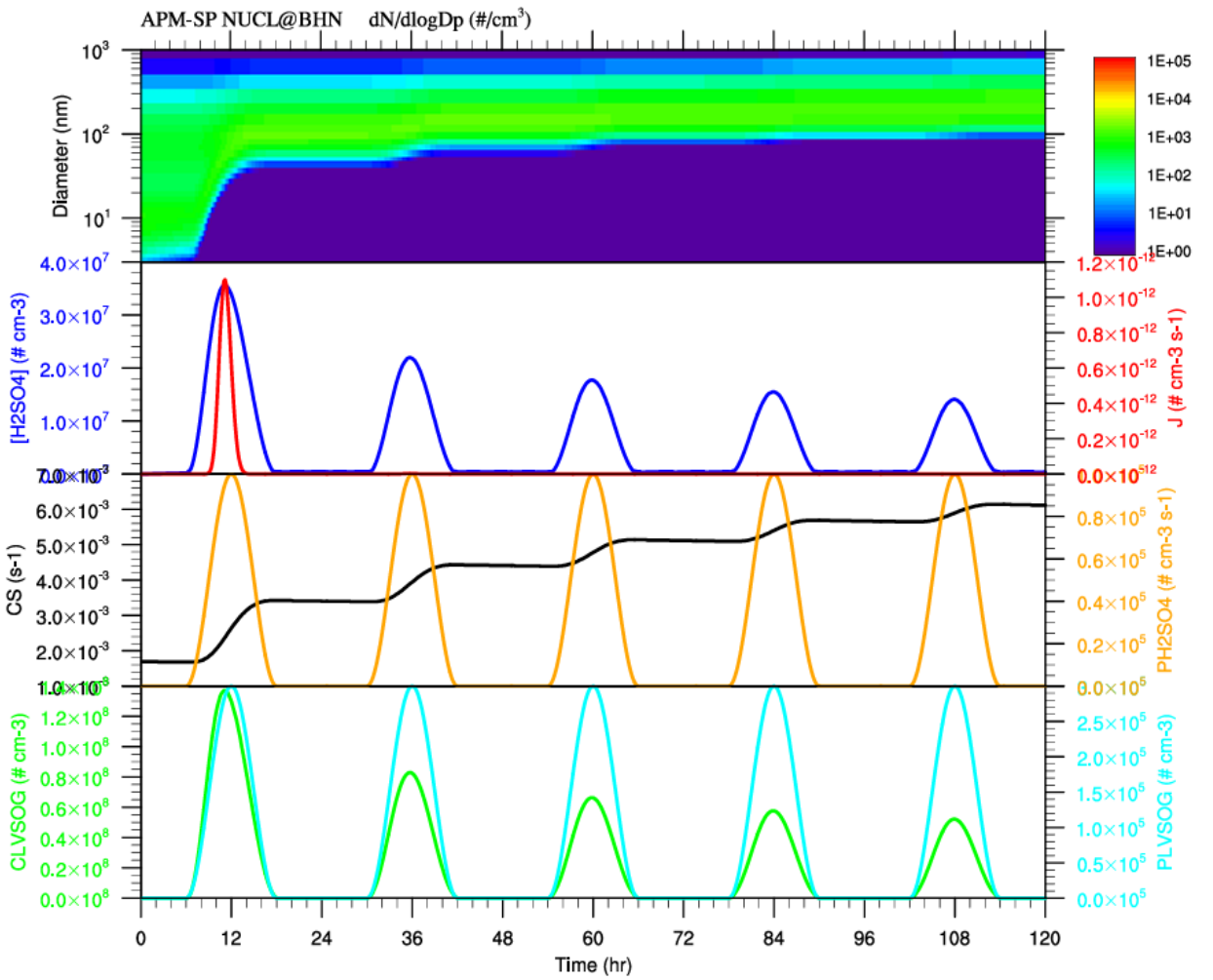
# 2.upper troposphere



# 3. near surface



# Advanced Particle Microphysics (APM)

## Model: Nucleation and growth

Hands-on computer lab

10/22/2025

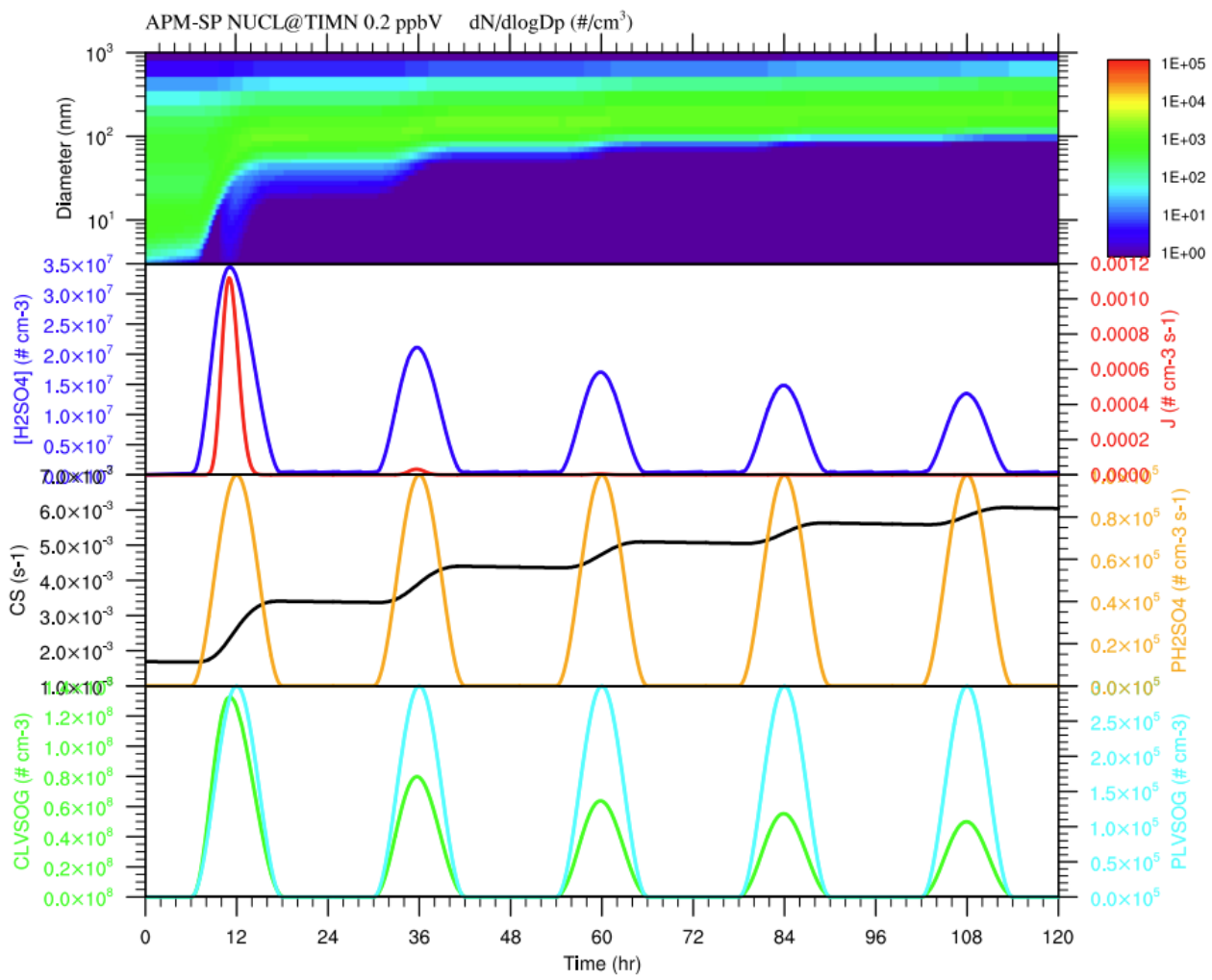
**THN**

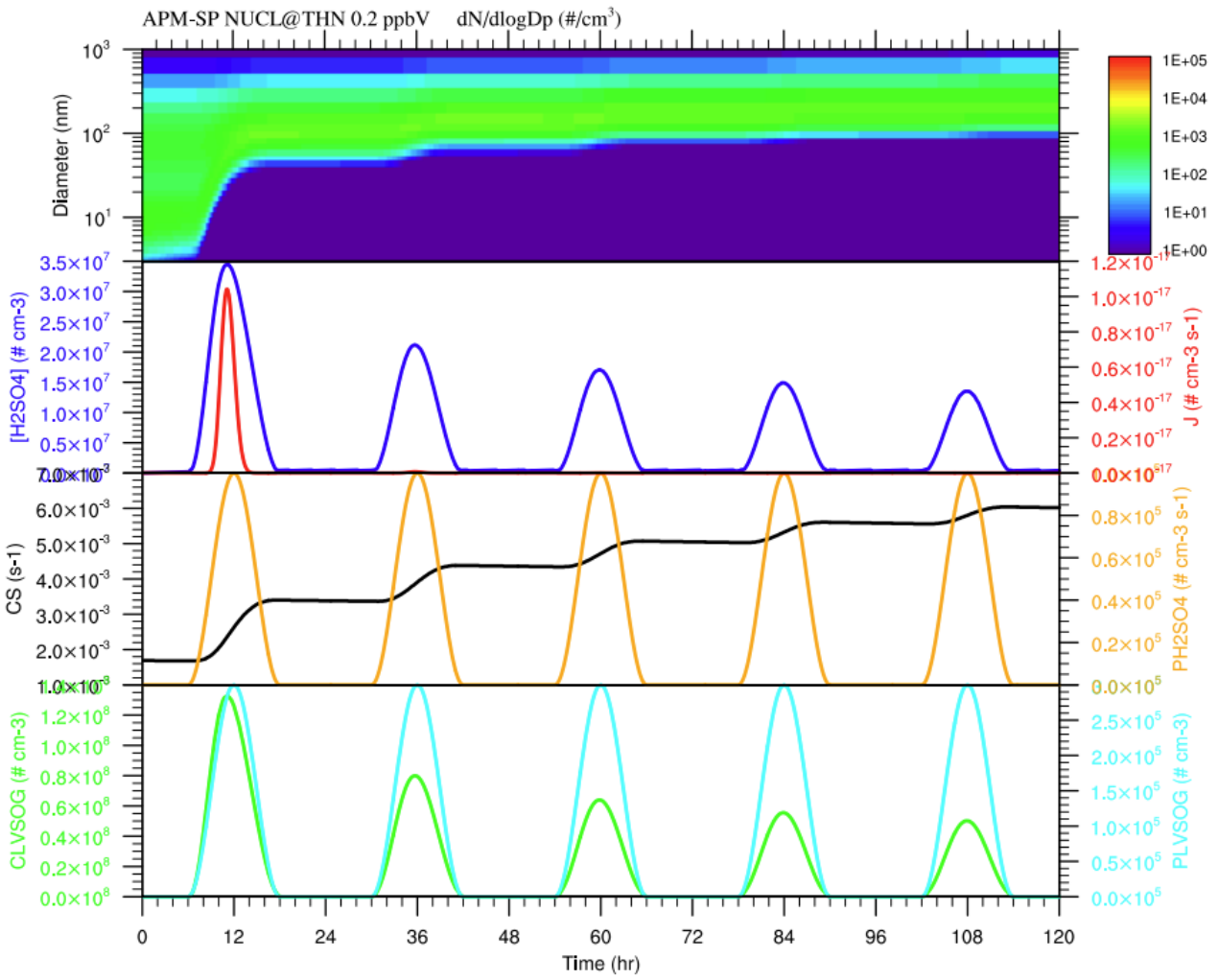
MSO4=1.,MBC=0.2,MOC=2,MDST=1.d-20,MSEA=2.

boundary atmosphere: (I) T=295 K, RH=80%;  (II) T=275 K, RH=80%
NH3=0.2, 5, and 40 ppbV

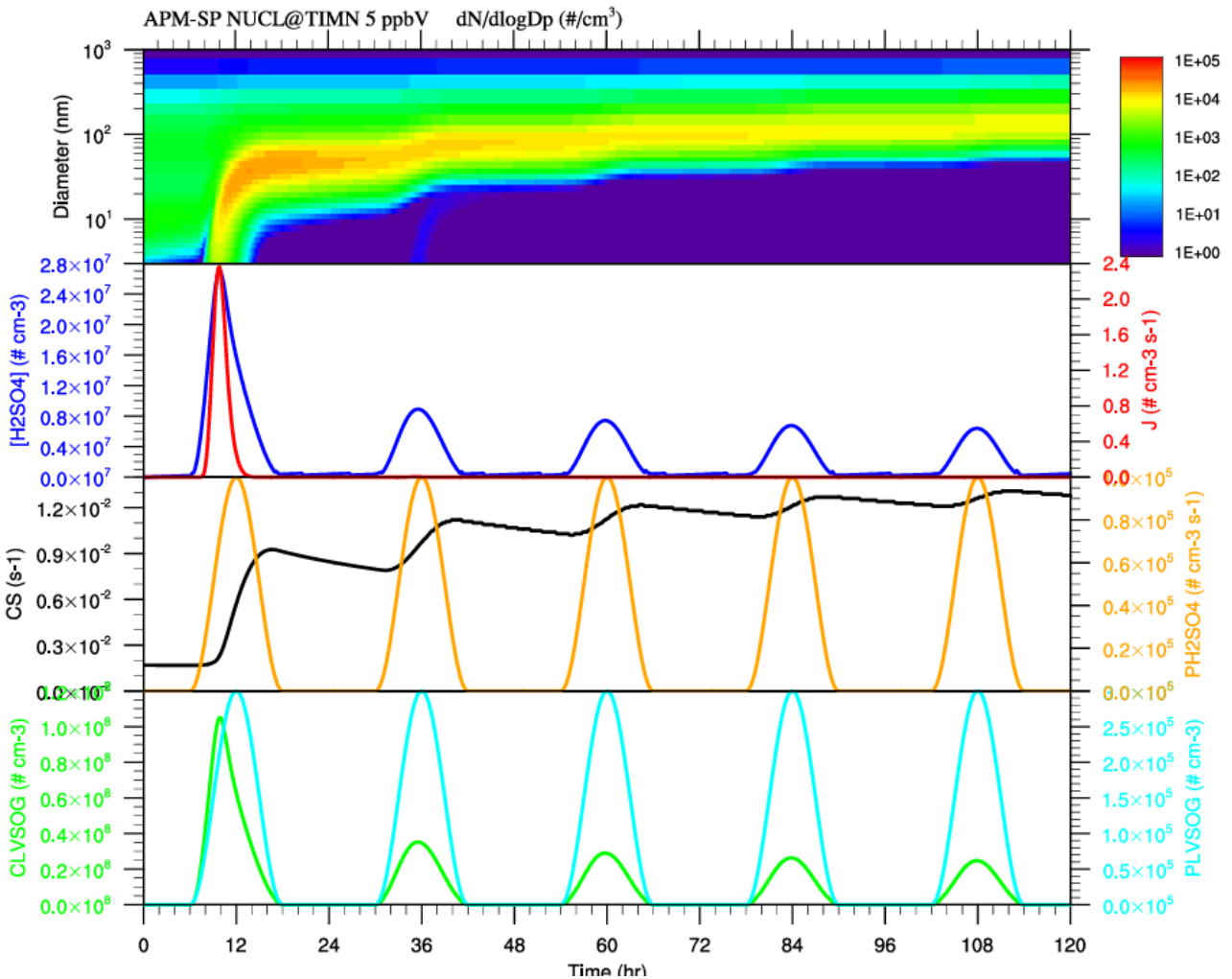
**TIMN:** assume ionization rate of 10 ion-pairs cm-3 s-1 .

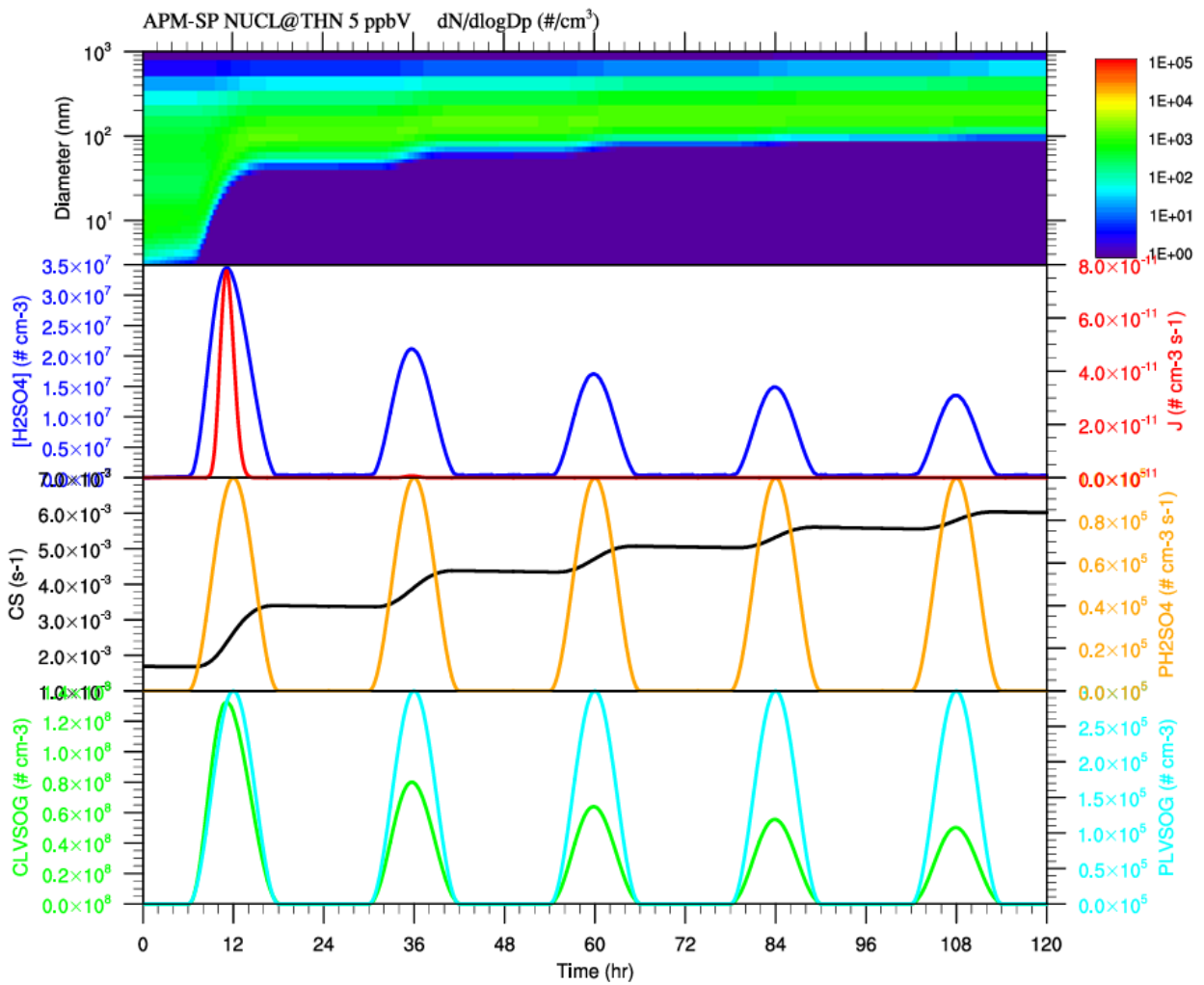
# (I) T=295 K, RH=80%， NH3=0.2ppbV



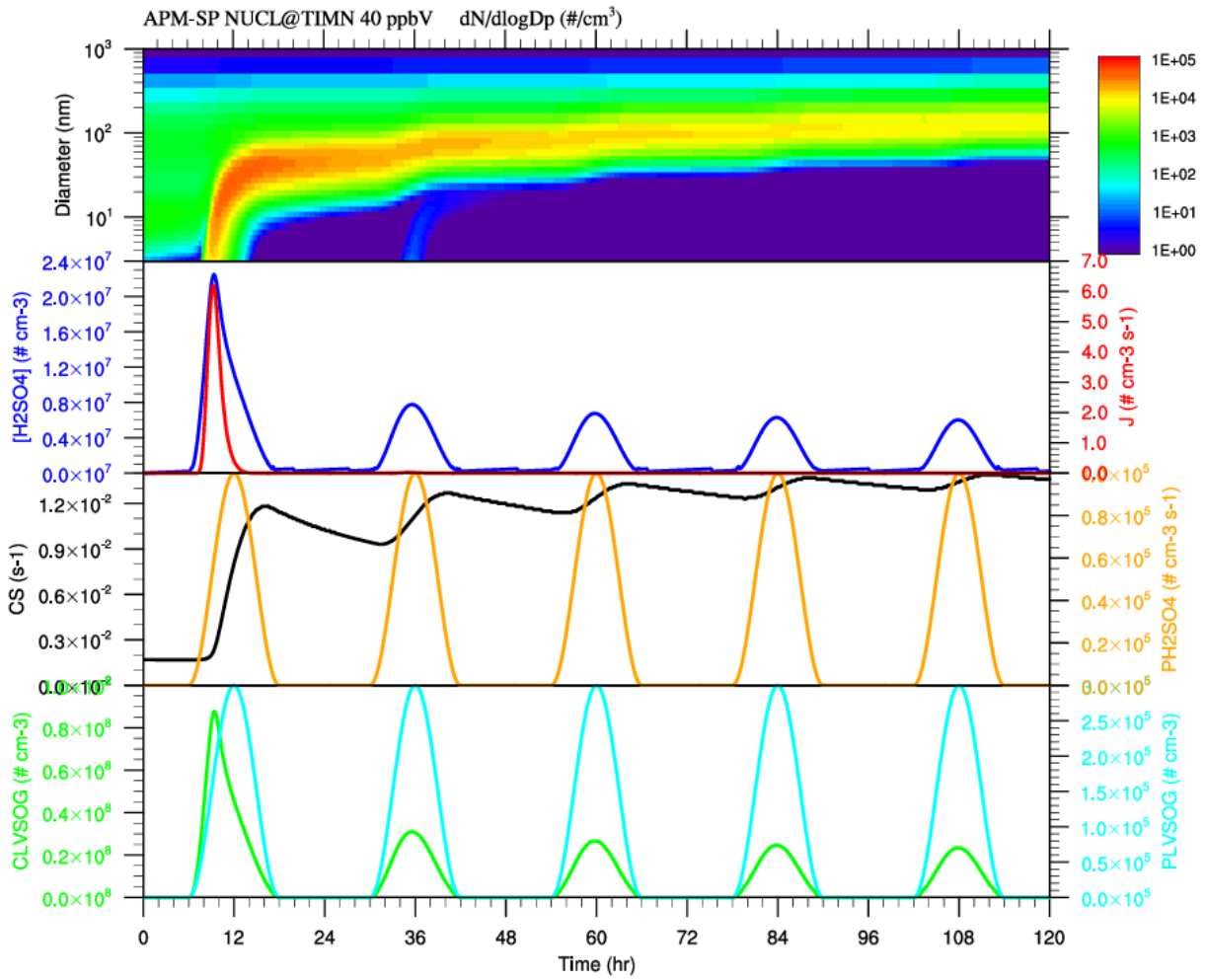



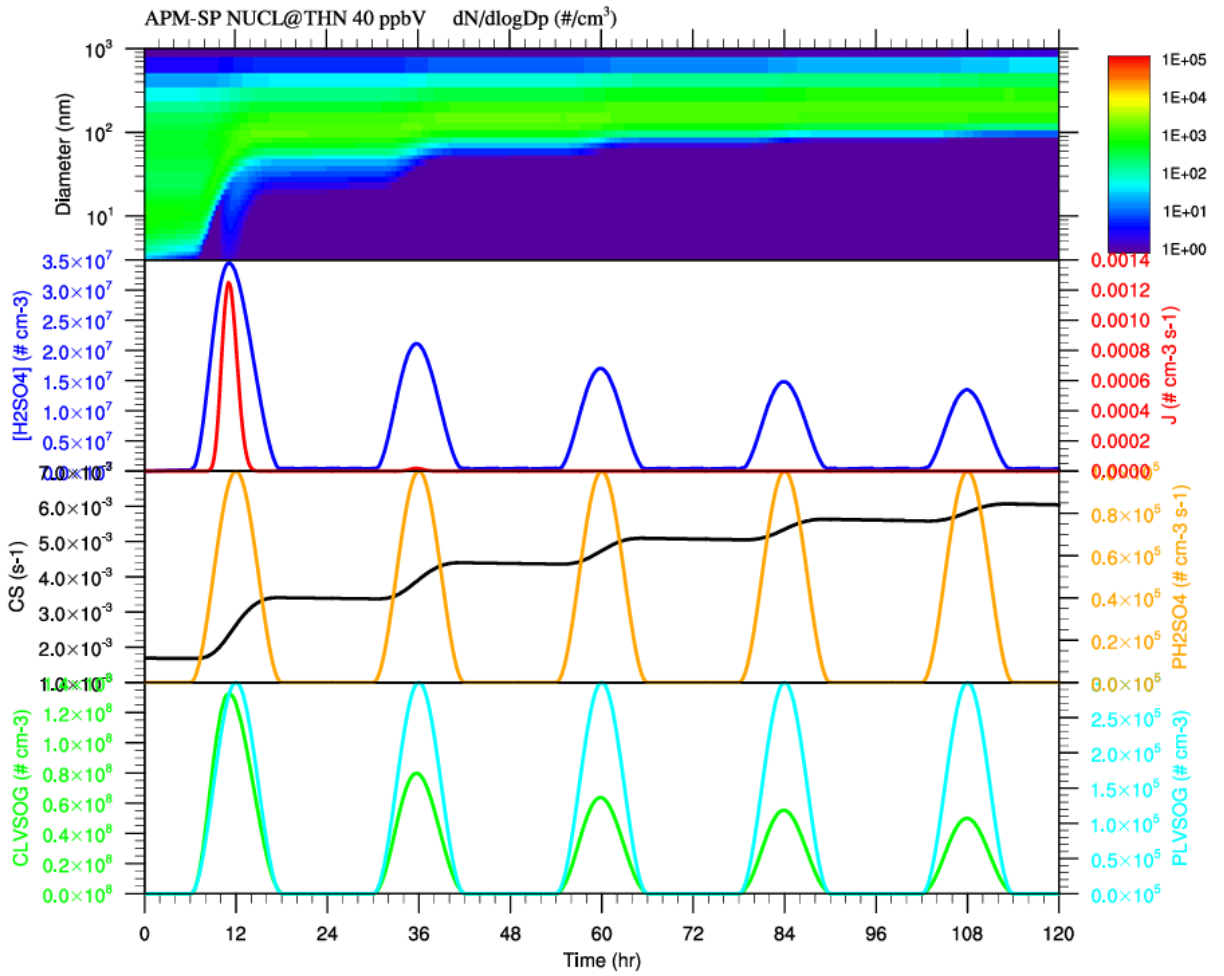
# (I) T=295 K, RH=80%， NH3=5ppbV



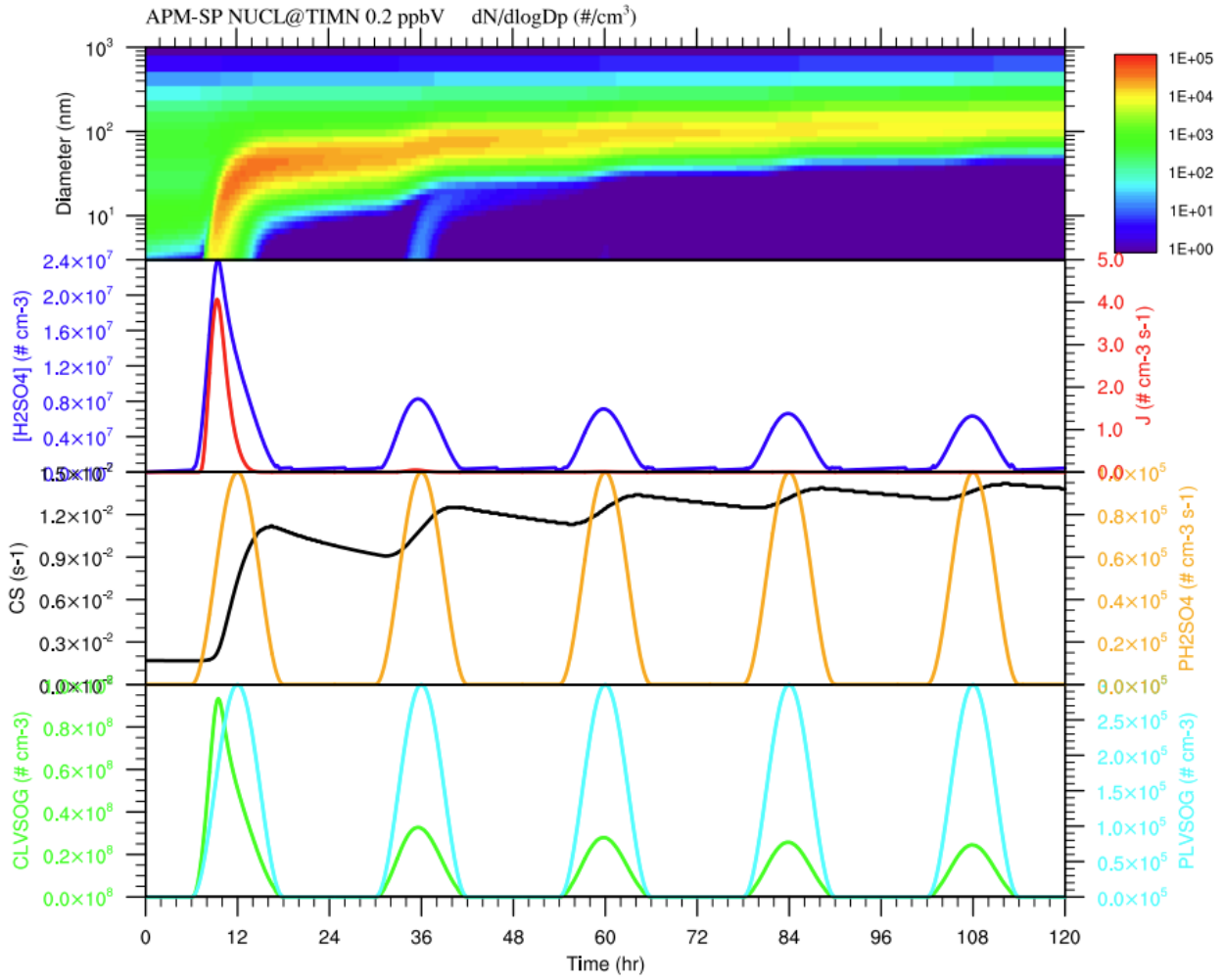



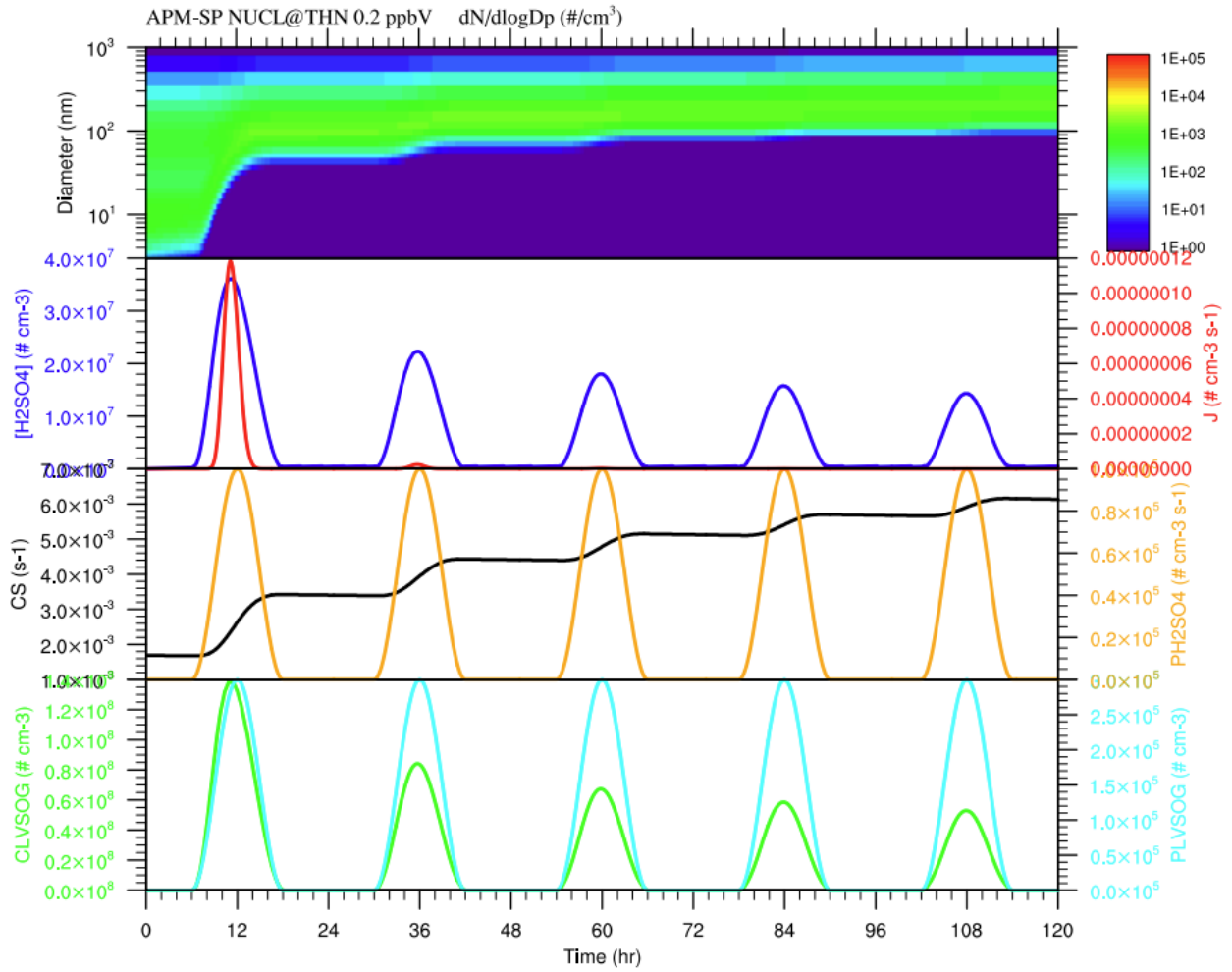
# (I) T=295 K, RH=80%， NH3=40 ppbV



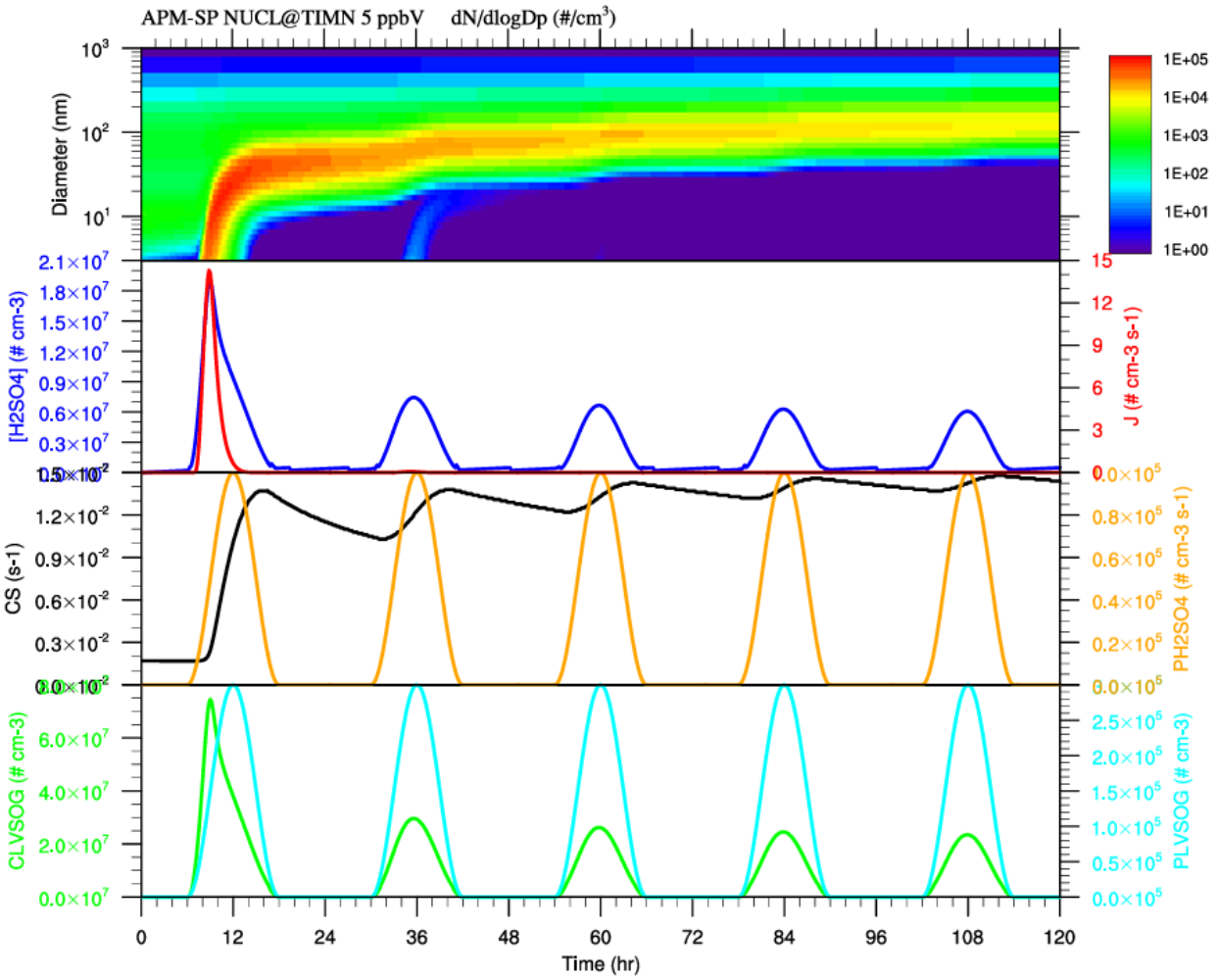



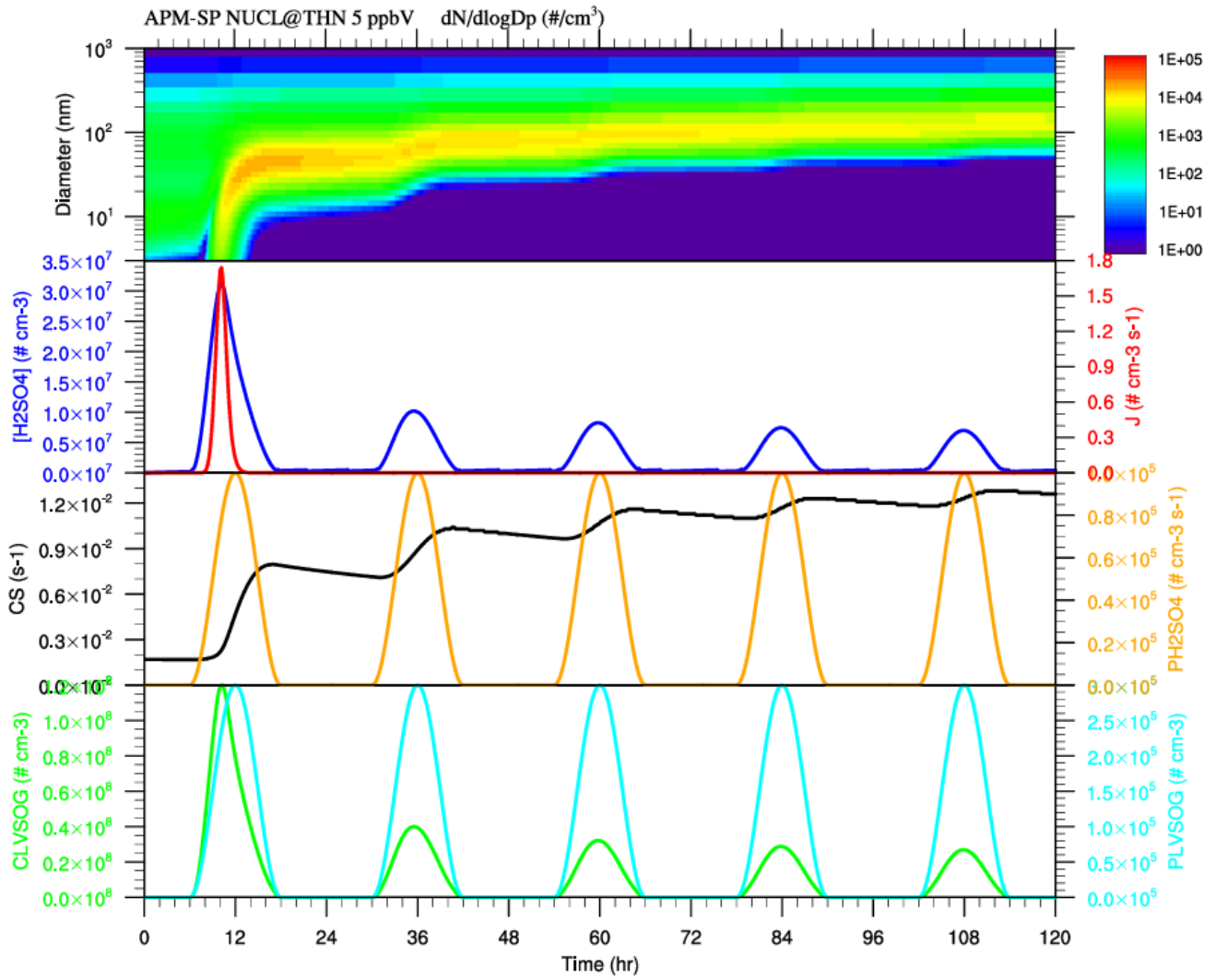
# (II) T=275 K, RH=80%, NH3=0.2ppbV



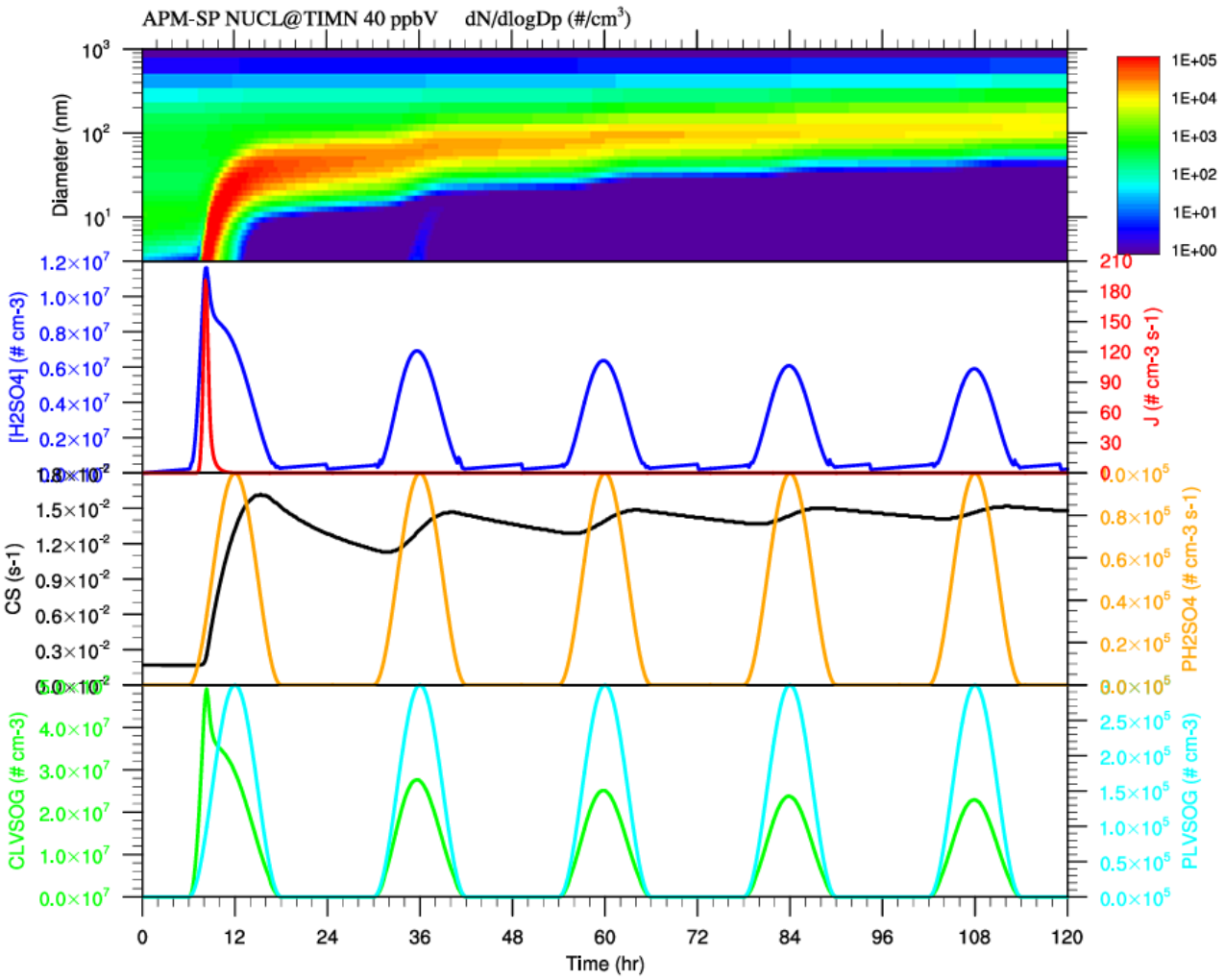



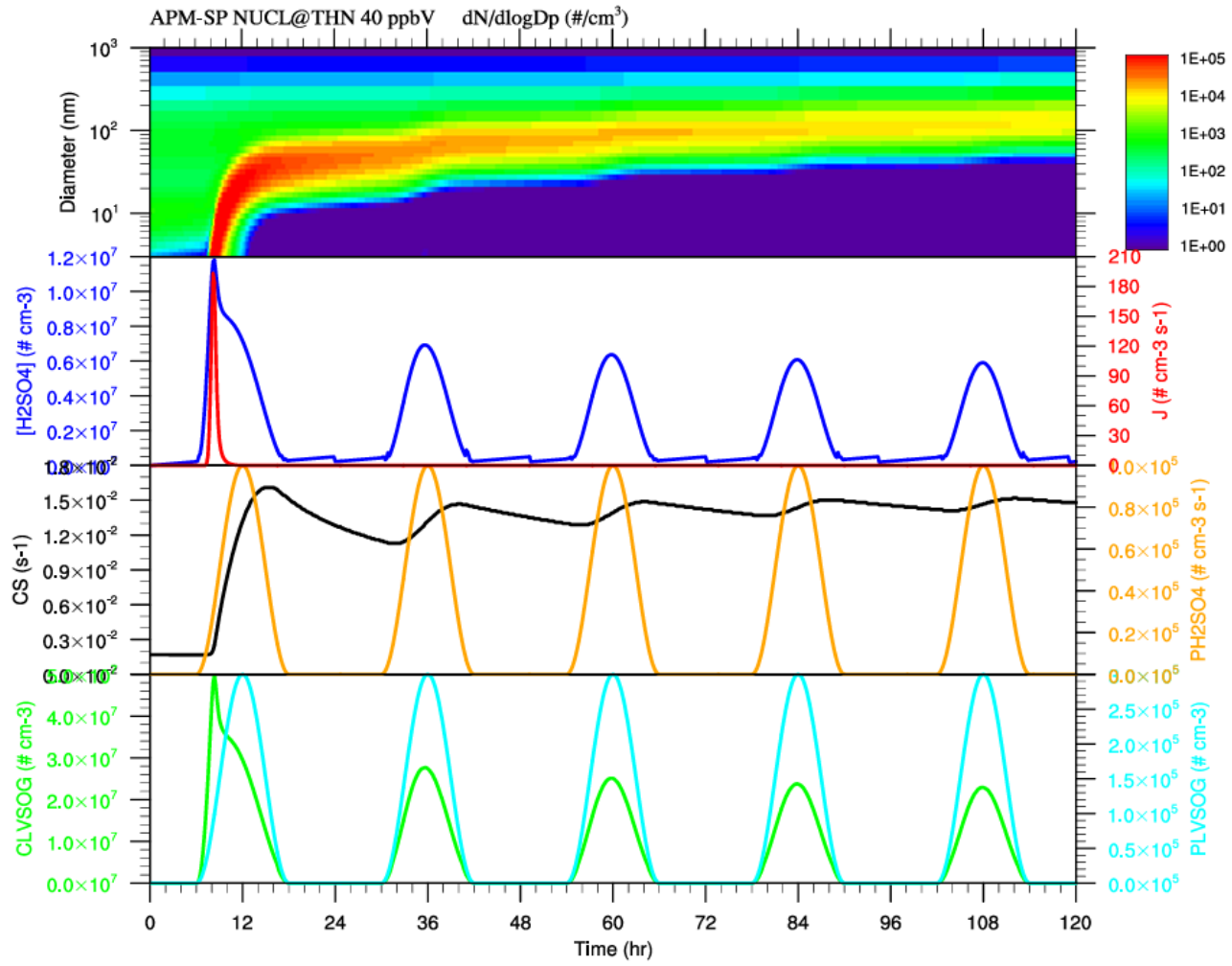
# (II) T=275 K, RH=80%, NH3=5ppbV



# (II) T=275 K, RH=80%, NH3=40ppbV



# NUCLEATION SCHEME: TIMN ($H_2O$ + $H_2SO_4$ + $NH_3$ + Ions)

input.run :
T=275 K, RH=80%, $NH_3$=5ppbV

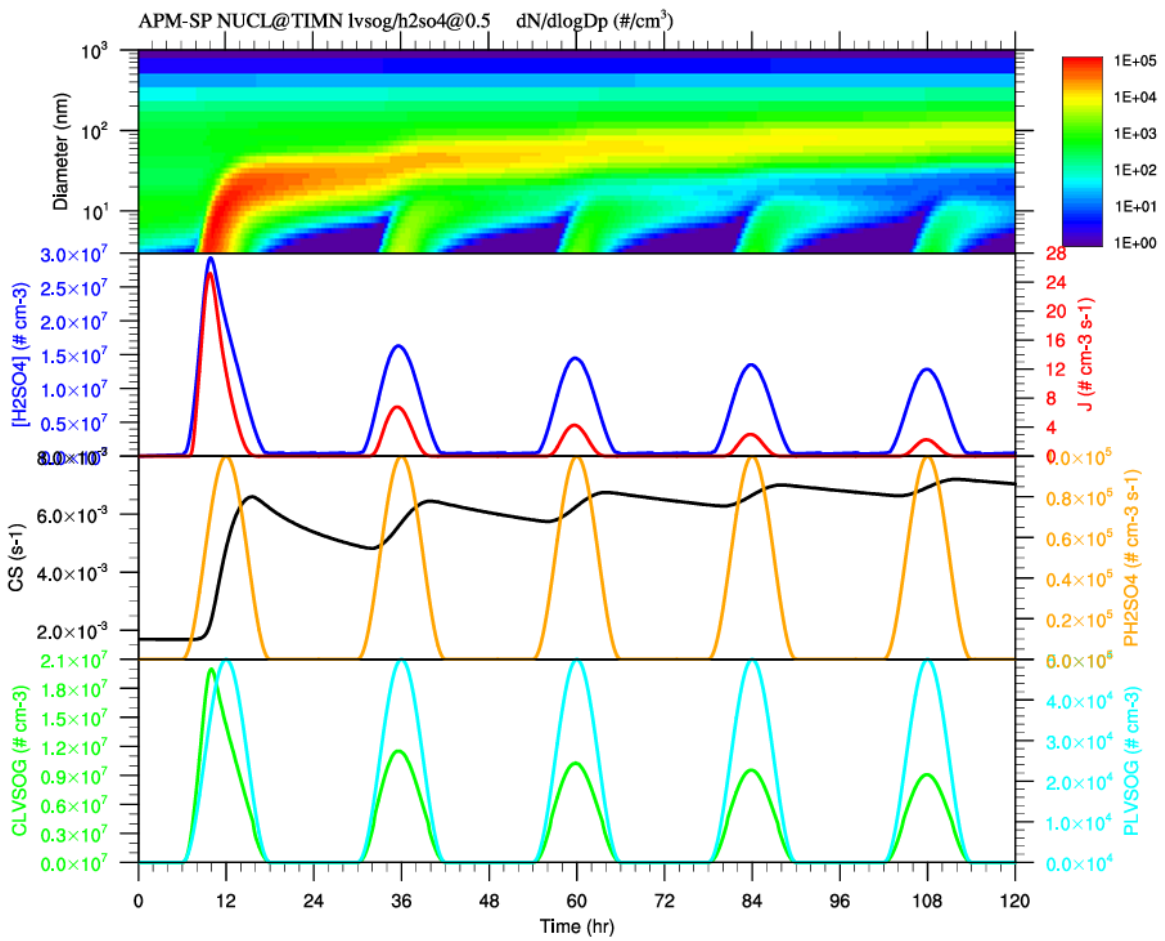
$PH_2SO_4$max,PLVSOGmax (# $cm^{-3}$ $s^{-1}$)

1) 1.d5, 5.d4
2) 1.d5, 1.d5
3) 1.d5, 1.d6

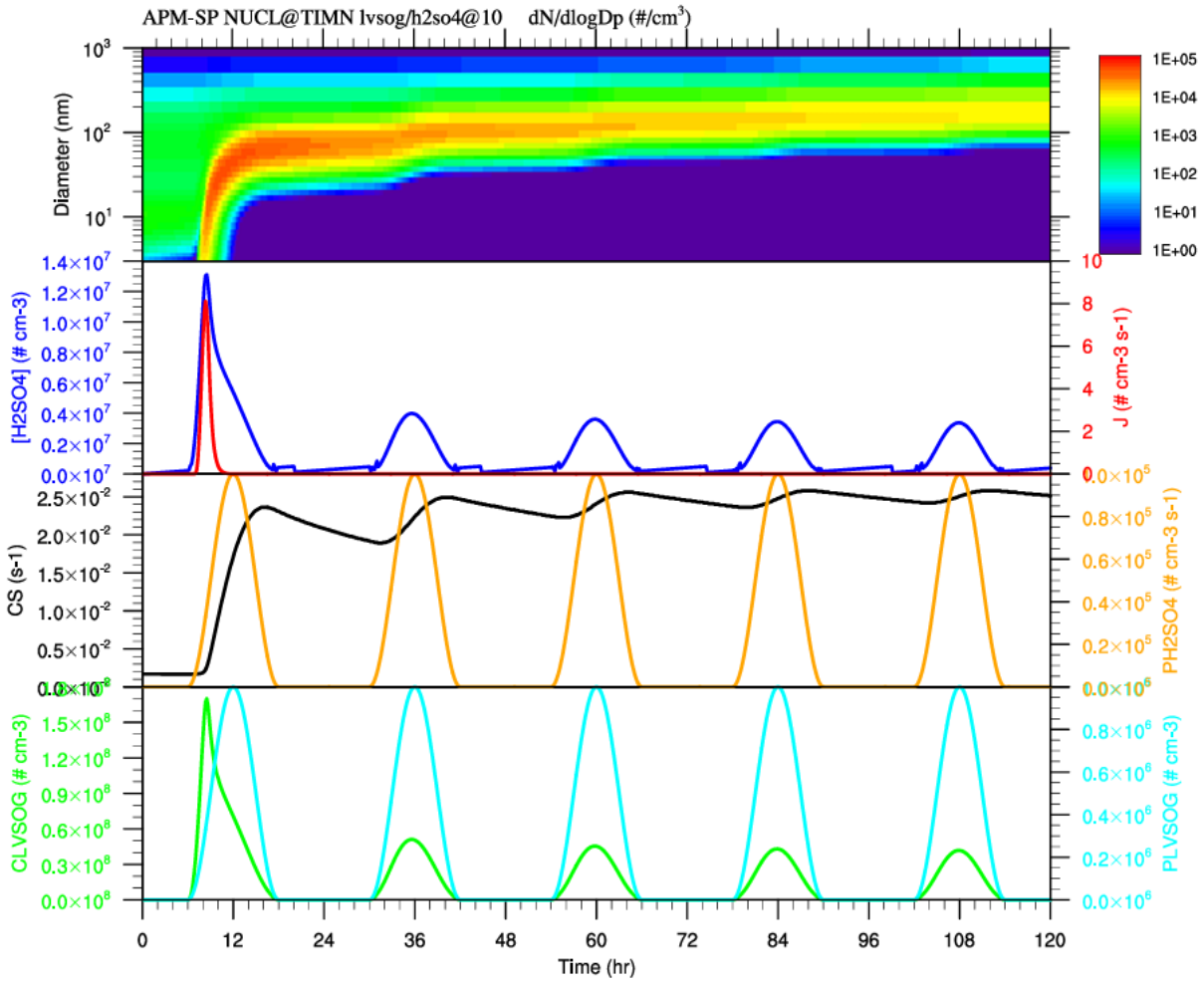
4) 1.d4, 5.d4
5) 1.d4, 5.d3

# PH2SO4max,PLVSOGmax (# cm-3 s-1)

## 1.d5, 5.d4

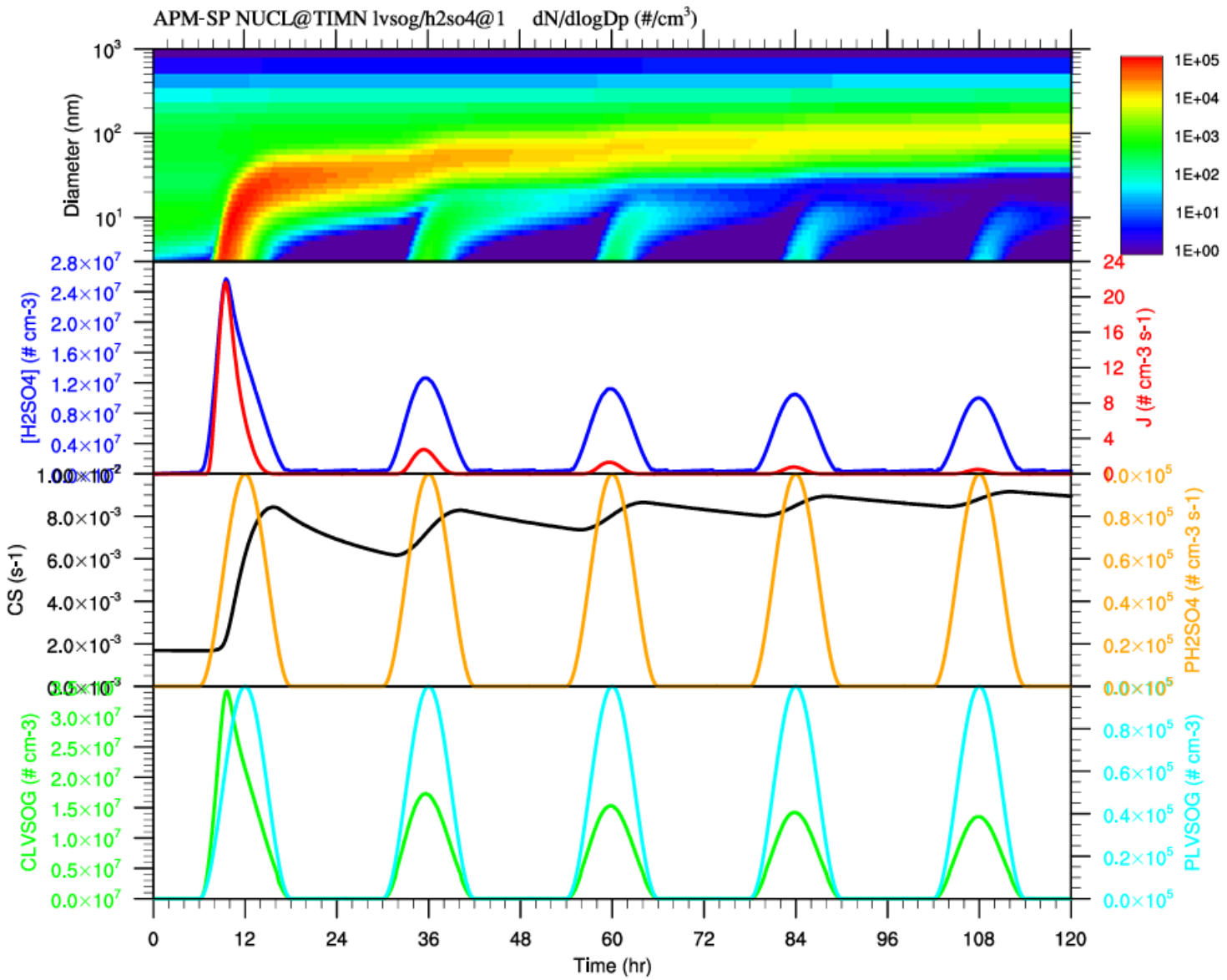



## 1.d5, 1.d5



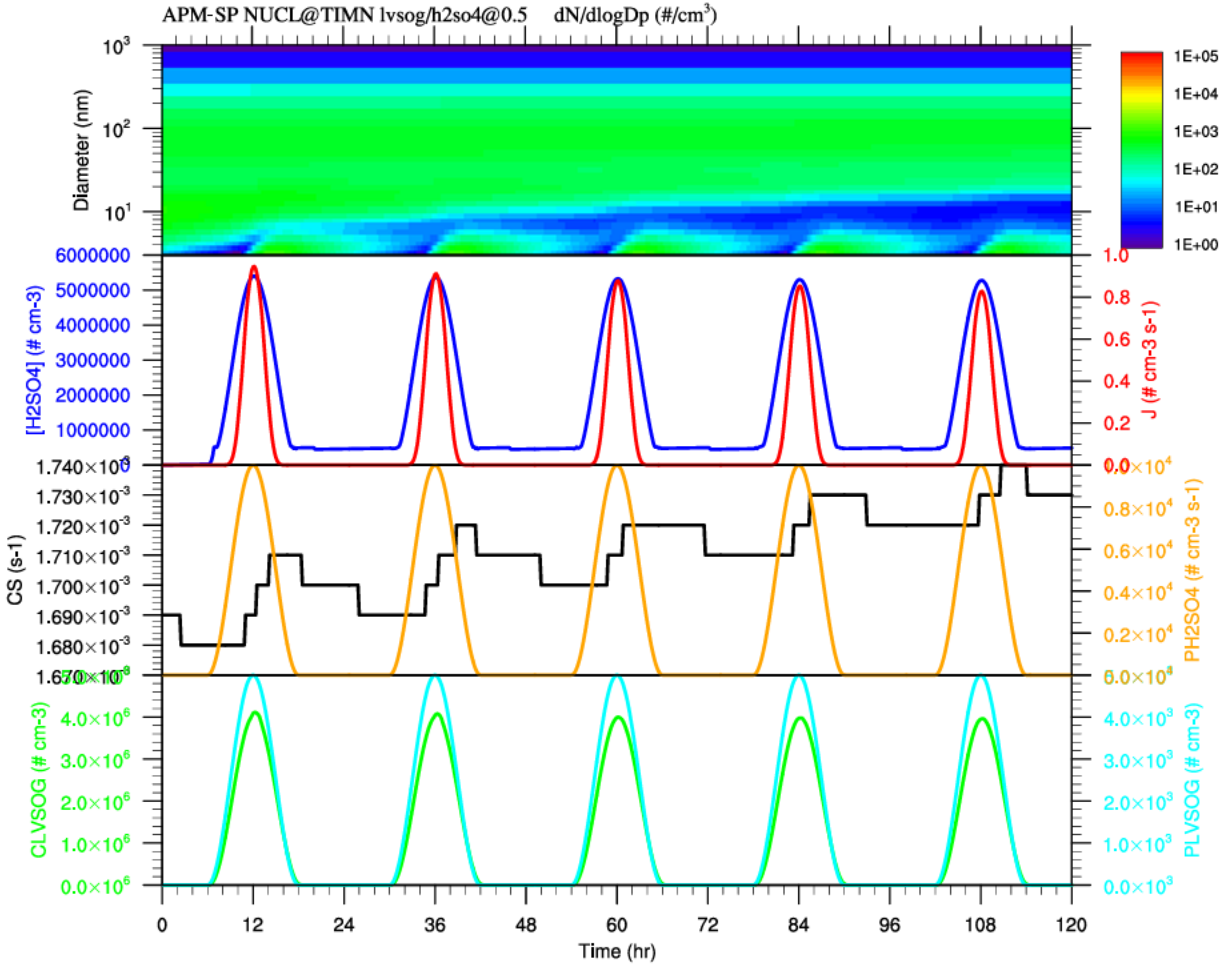
# PH2SO4max,PLVSOGmax (# cm-3 s-1)

1.d5, 1.d6

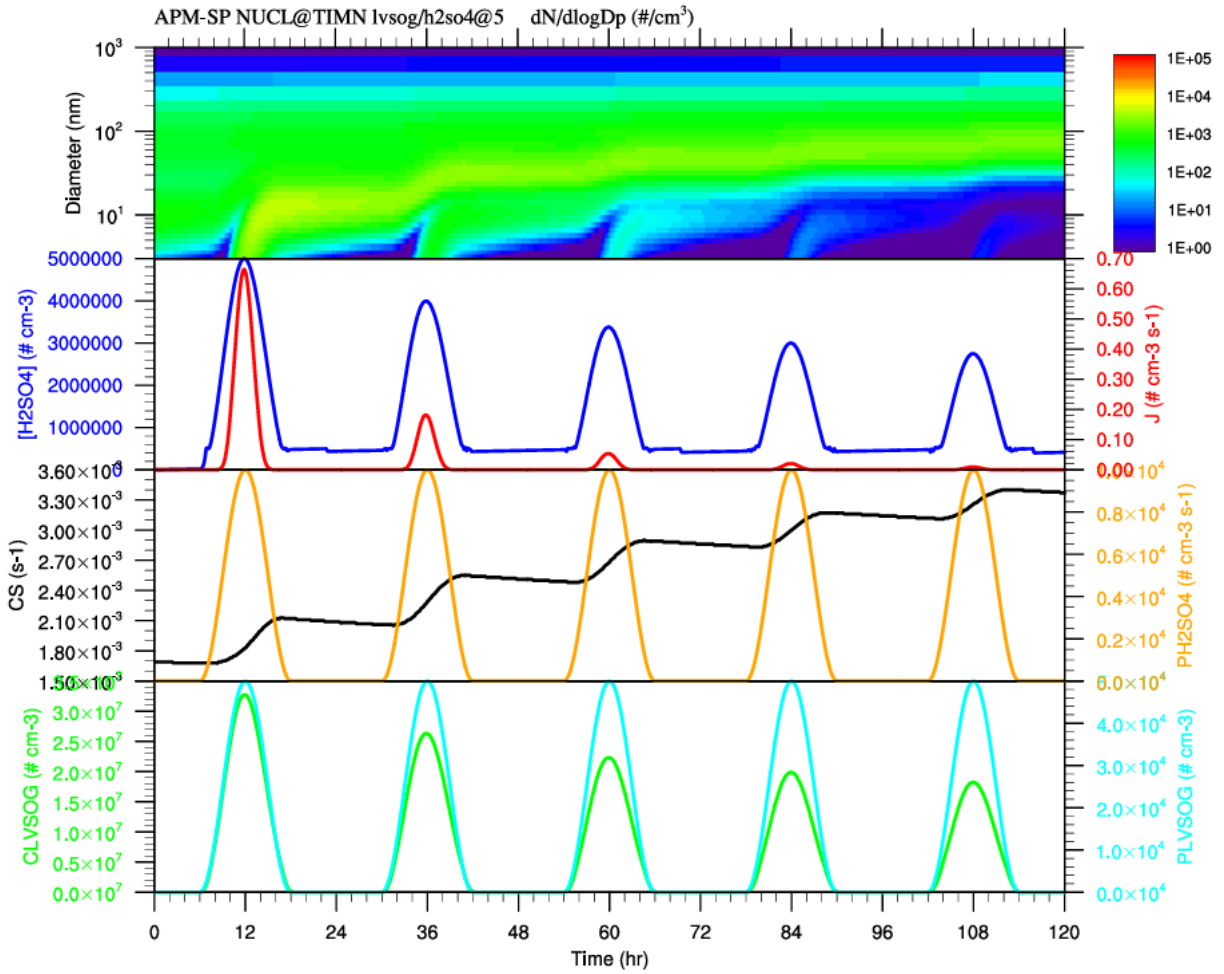


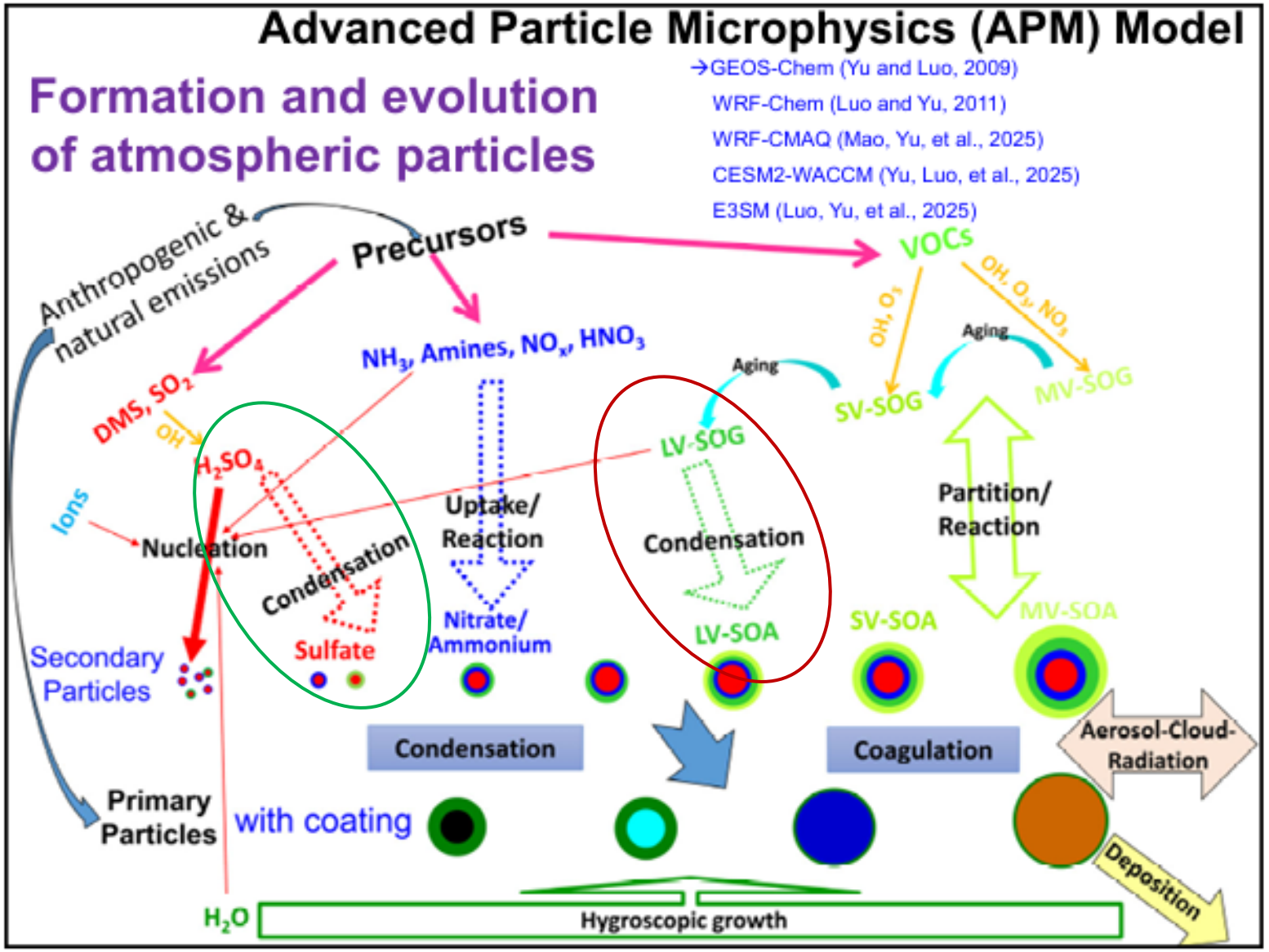
# PH2SO4max,PLVSOGmax (# cm-3 s-1)

## 1.d4, 5.d4




## 1.d4, 5.d3




Advanced Particle Microphysics (APM) Model
Formation and evolution of atmospheric particles
→GEOS-Chem (Yu and Luo, 2009)
WRF-Chem (Luo and Yu, 2011)
WRF-CMAQ (Mao, Yu, et al., 2025)
CESM2-WACCM (Yu, Luo, et al., 2025)
E3SM (Luo, Yu, et al., 2025)
Anthropogenic & natural emissions
Precursors
VOCs
OH, O3
OH, O3, NO3
Aging
Aging
NH3, Amines, NOx, HNO3
DMS, SO2
OH
H2SO4
SV-SOG
MV-SOG
LV-SOG
Ions
Nucleation
Condensation
Uptake/ Reaction
Condensation
Partition/ Reaction
Nitrate/ Ammonium
Sulfate
LV-SOA
SV-SOA
MV-SOA
Secondary Particles
Condensation
Coagulation
Aerosol-Cloud-Radiation
Primary Particles
with coating
Deposition
H2O
Hygroscopic growth

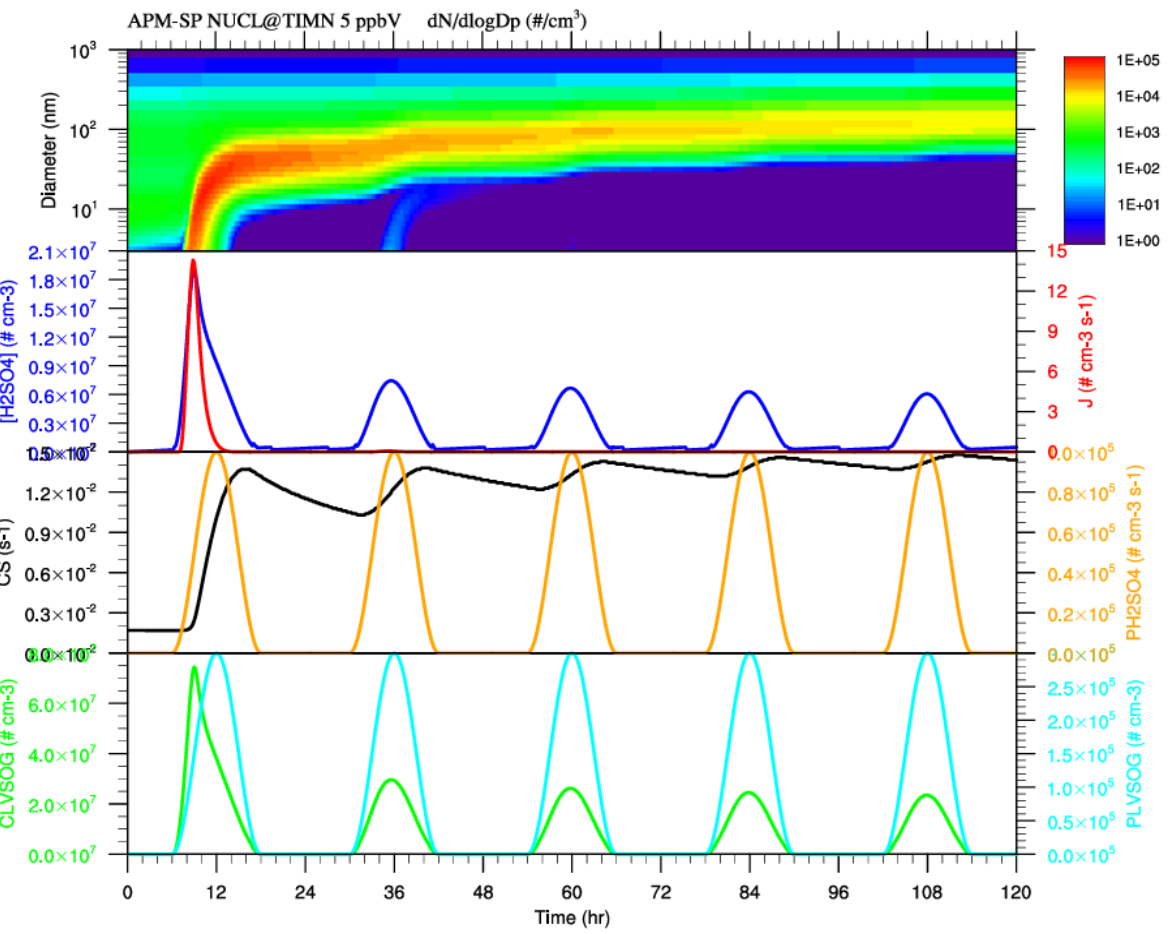


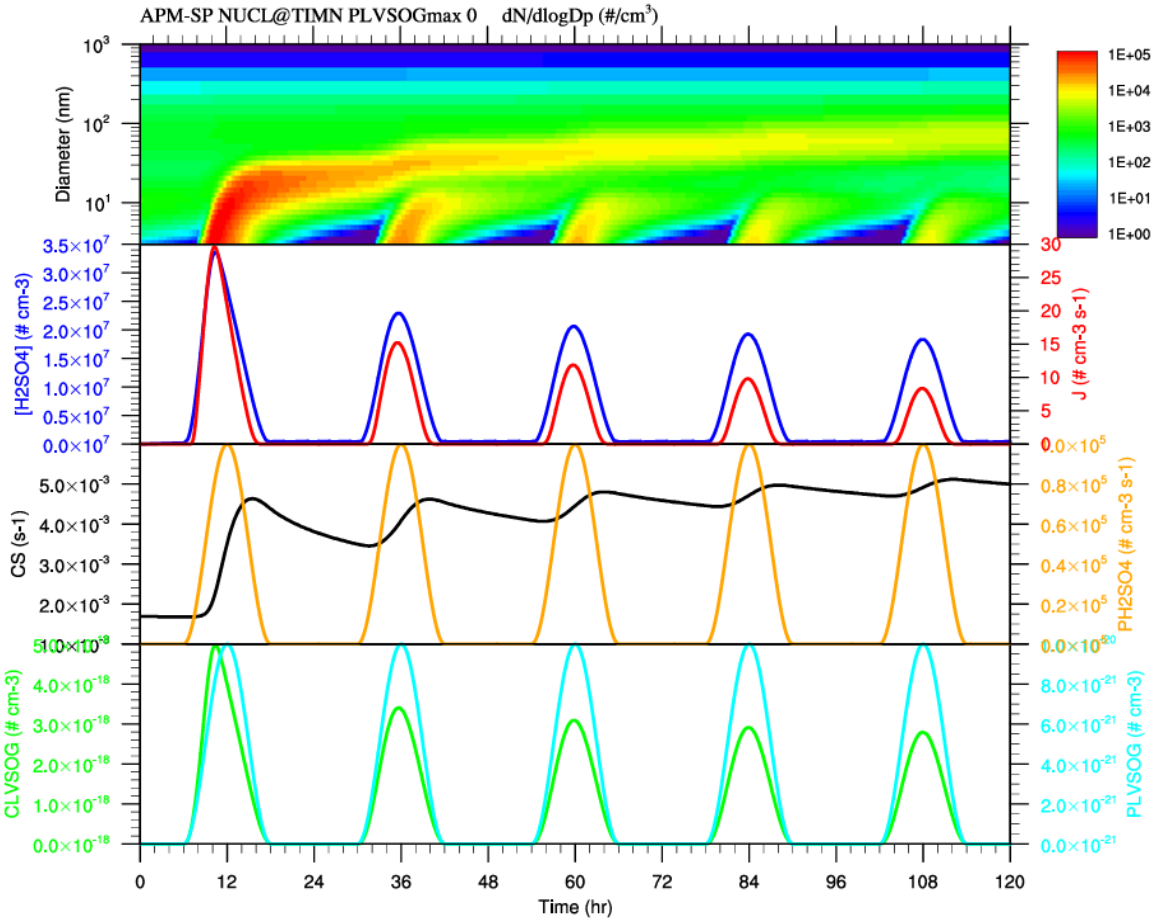
Yu, 2011

H2SO4 is the only condensing gas

T=275 K, RH=80%, NH3=5ppbV

when LV-SOG condensation is considered, nucleation events are shorter and generate fewer new particles.




This is a result of increased particle surface area and reduced [H2SO4] associated with enhanced growth rates.