A general Overview of Aerosols in CMAQ

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Modal Approach

- CMAQ currently models the size distribution of aerosols using three lognormal sub-distributions called modes (Kenneth Whitby)

References:
1995 Binkowski - Shankar – RPM
1998 Ackermann et al. - MADE
2001 Schell et al. MADE-SORGAM
2003 Binkowski - Roselle – CMAQ
2005 Mathur et al. MAQSIP
2010 Kelly et al. Sea Salt

CMAQ Tri-Modal Representation of Mass

Mass Distribution vs Diameter [μm]

Aitken Mode ->

Accumulation Mode ->

Coarse Mode ->
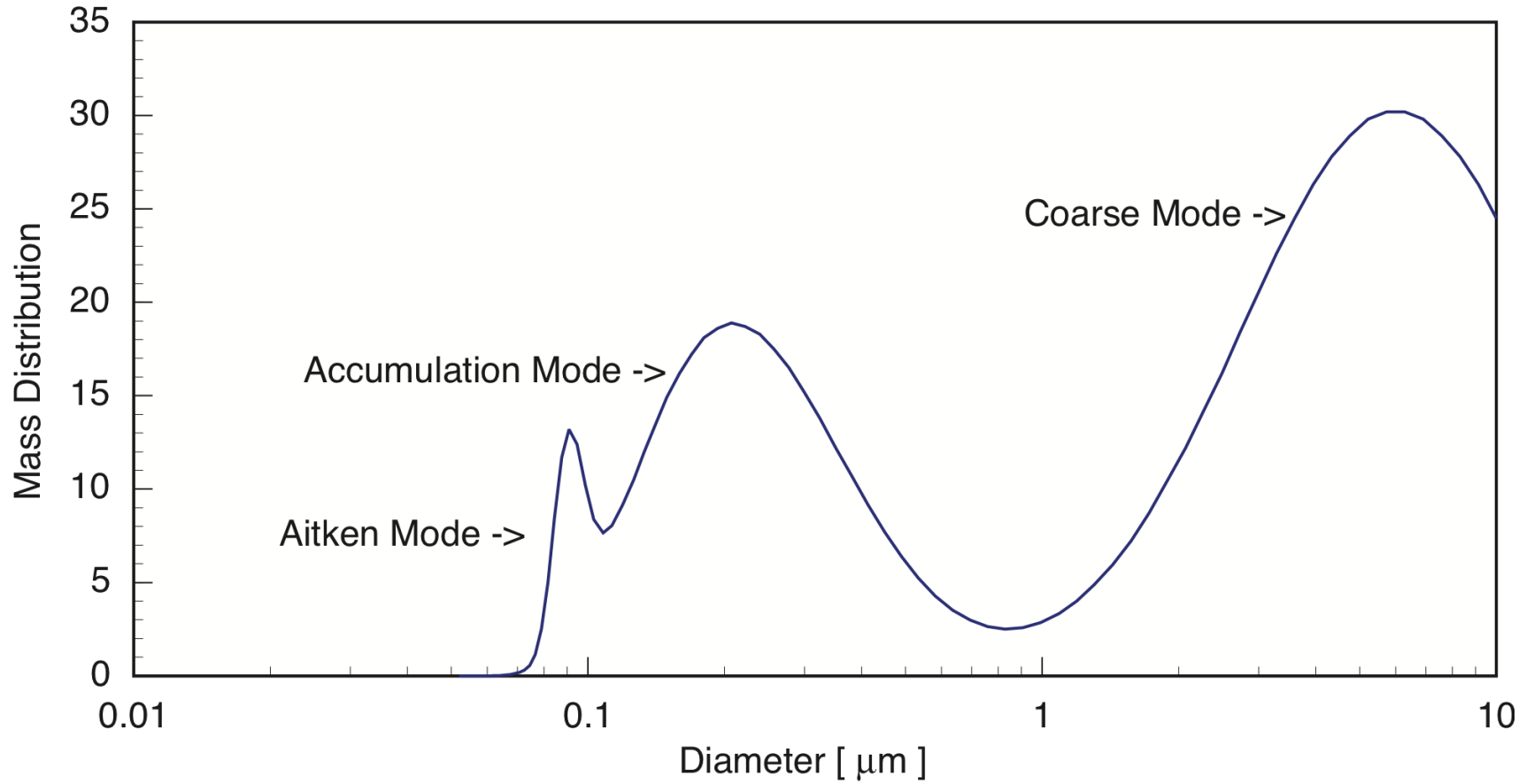
- Within each mode the History Variables are:

- 1. Modal mass by species
- 2. Modal number
- 3. Modal surface area

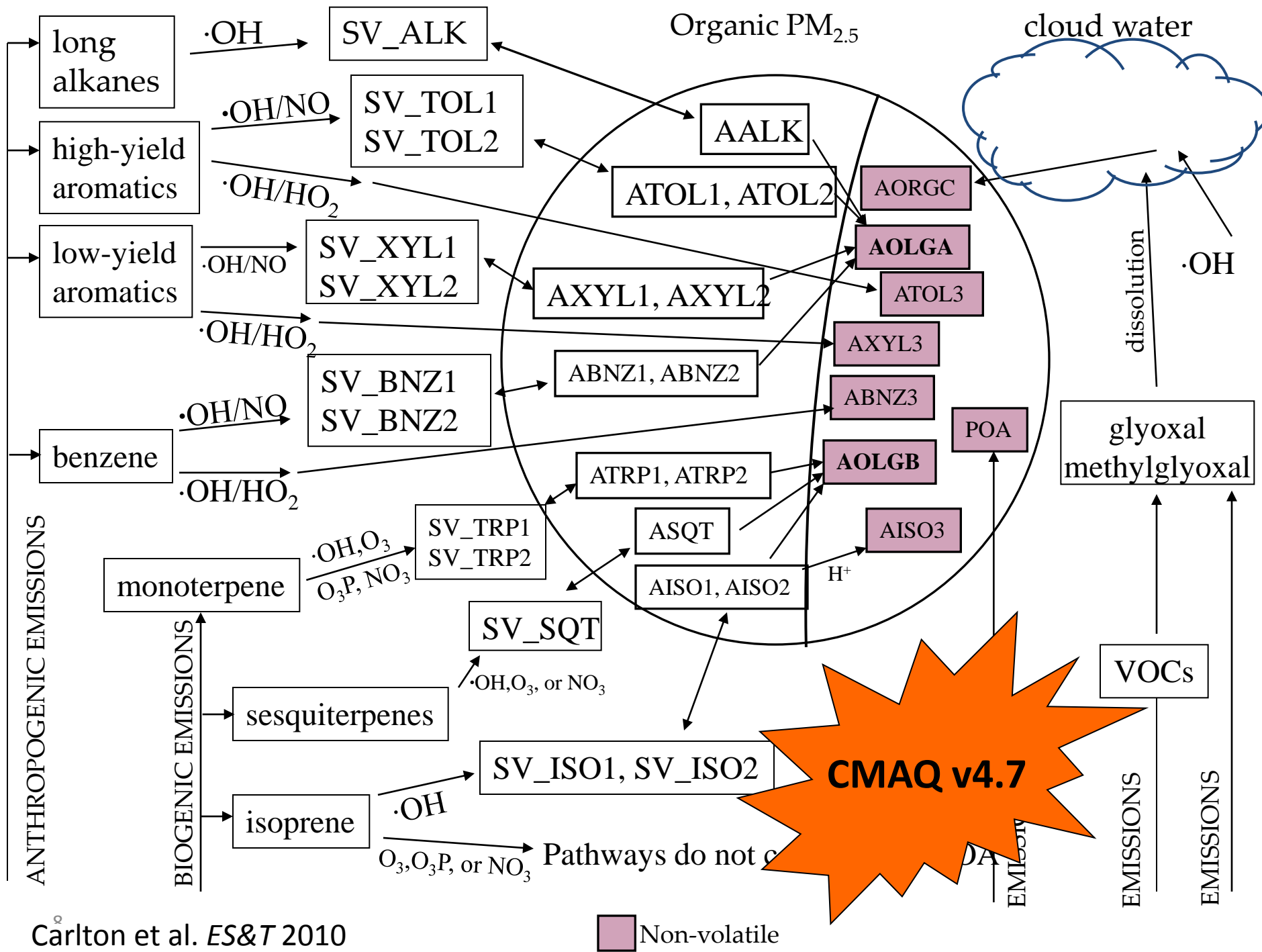These three History Variable are sufficient to diagnose the:

Modal Geometric Mean Diameter for the Number distribution

Modal Geometric Standard Deviation

- A system of three analytical differential equations (number, surface area, mass) calculates Intra-modal and Inter-modal Coagulation for Condensational Growth for each Mode.

Modal Species

- Aitken Mode: sulfate, nitrate, ammonium, elemental carbon, water,

- organics (Primary only)

- Accumulation Mode: sulfate, nitrate, ammonium, elemental carbon, water, organics (Primary and Secondary), sodium, chloride.

- Coarse Mode: sulfate, nitrate, ammonium, sodium, chloride, water

Organic PM$_{2.5}$

cloud water

long alkanes → ·OH → SV_ALK

high-yield aromatics → ·OH/NO → SV_TOL1 SV_TOL2

high-yield aromatics → ·OH/HO$_2$ →

low-yield aromatics → ·OH/NO → SV_XYL1 SV_XYL2

low-yield aromatics → ·OH/HO$_2$ →

benzene → ·OH/NO → SV_BNZ1 SV_BNZ2

benzene → ·OH/HO$_2$ →

monoterpene → ·OH,O$_3$ / O$_3$P, NO$_3$ → SV_TRP1 SV_TRP2

sesquiterpenes → ·OH,O$_3$, or NO$_3$ → SV_SQT

isoprene → ·OH → SV_ISO1, SV_ISO2

isoprene → O$_3$,O$_3$P, or NO$_3$ → Pathways do not c...

AALK

ATOL1, ATOL2

AXYL1, AXYL2

ABNZ1, ABNZ2

ATRP1, ATRP2

ASQT

AISO1, AISO2

AORGC

AOLGA

ATOL3

AXYL3

ABNZ3

AOLGB

AISO3

POA

H$^+$

dissolution

·OH

glyoxal methylglyoxal

VOCs

ANTHROPOGENIC EMISSIONS

BIOGENIC EMISSIONS

EMISSIONS

EMISSIONS

EMISSIONS

CMAQ v4.7

Carlton et al. *ES&T* 2010

Non-volatile

- Thank You.

- Any questions.