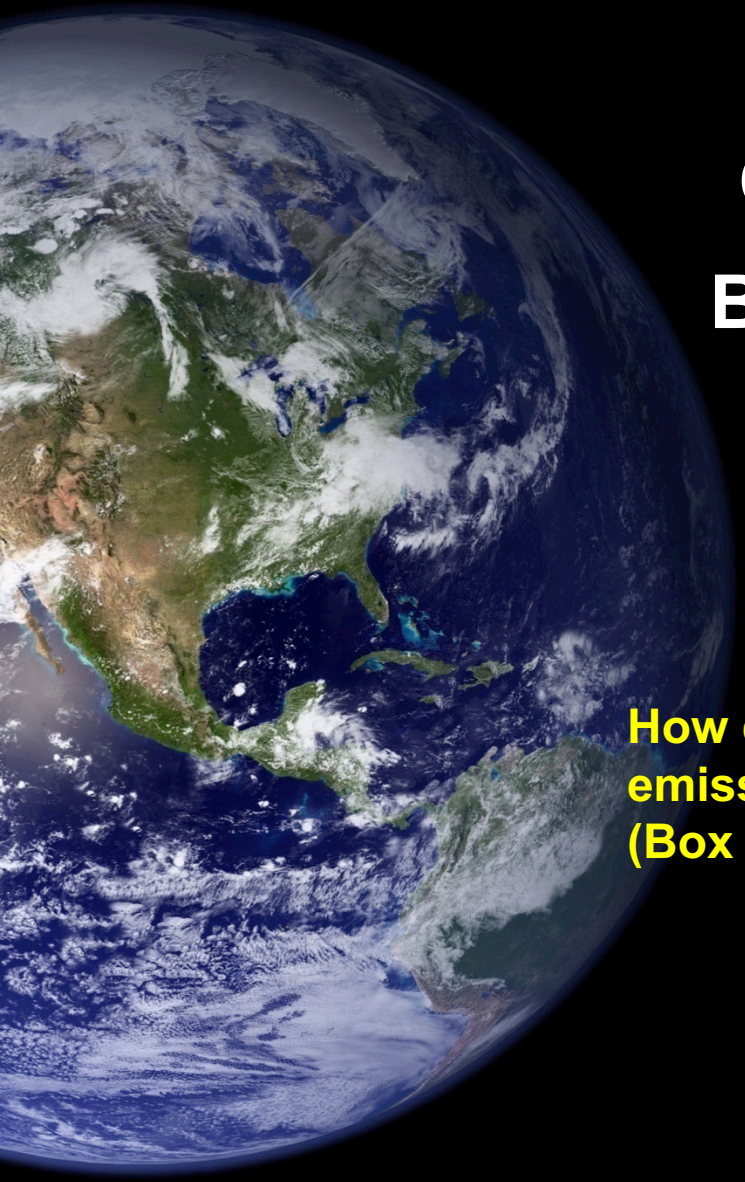
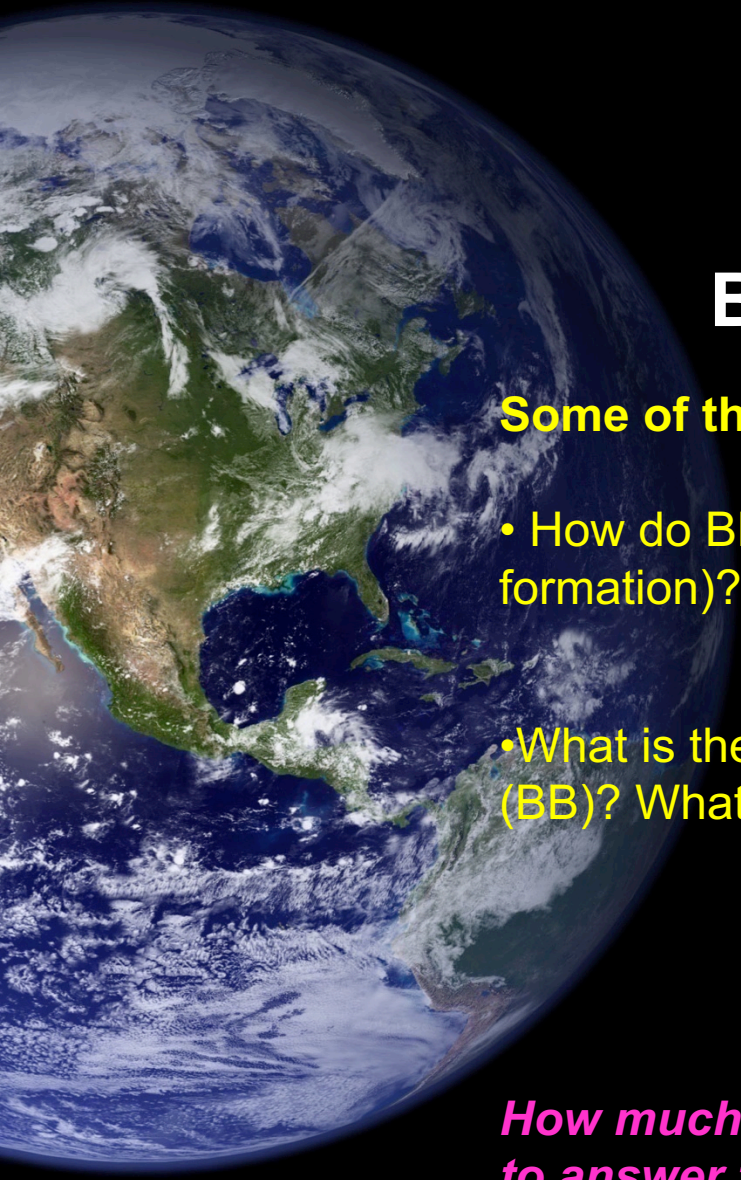


Chemical Mechanisms and Biomass Burning Emissions

John Orlando, NCAR ACOM
orlando@ucar.edu

How do we represent the chemistry of biomass burning emissions in models of varying degree of complexity (Box models, Lagrangian, Regional and Global,…) ??



Chemical Mechanisms and Biomass Burning Emissions

Some of the Science Questions: (plume evolution)

- How do BB plumes age photochemically (esp. wrt ozone formation)? NOx/VOC chemistry?

- What is the composition of SOA produced from biomass burning (BB)? What are their optical/hygroscopic properties?

How much chemical detail do we need in our mechanism(s) to answer these questions?

Chemical Mechanisms and Biomass Burning Emissions

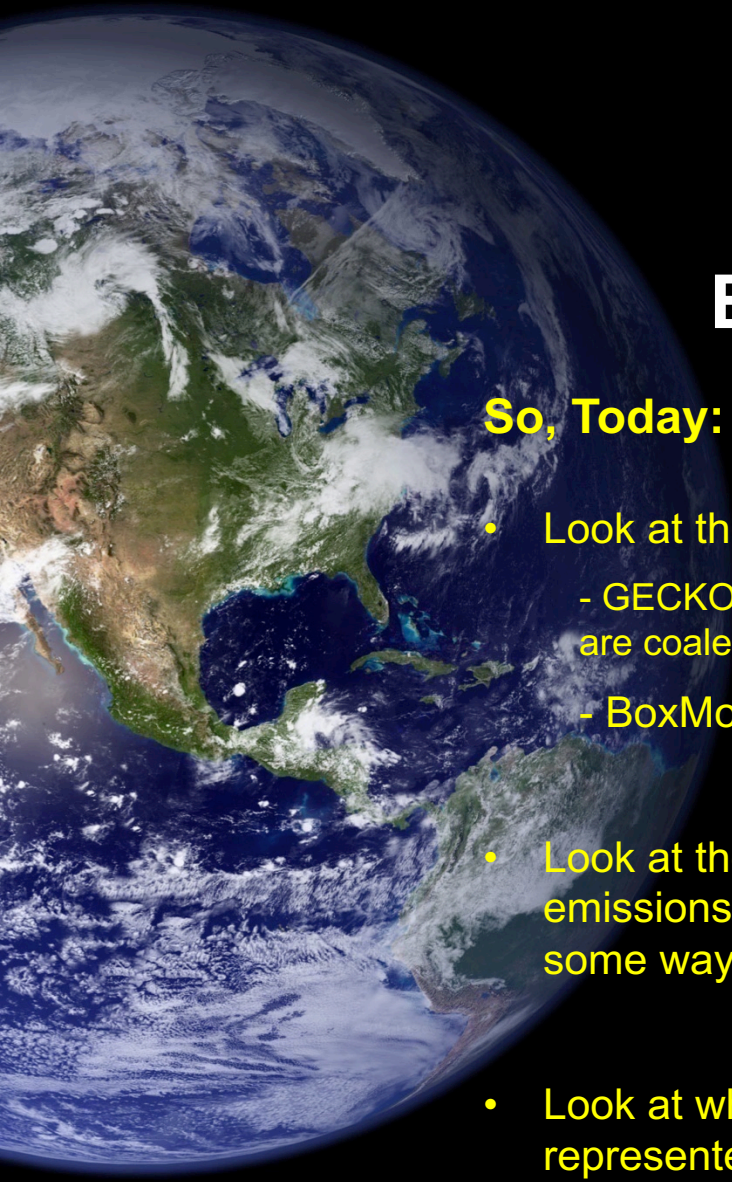
MECHANISTIC NEEDS MAY BE DIFFERENT FOR EACH QUESTION!!

Questions related to ozone, aged plumes may be simpler…

(OH reactivity, reactive N will be key factors)

than those related to SOA.

(need to track a larger, more complex and diverse set of OVOC in more detail)



Chemical Mechanisms and Biomass Burning Emissions

So, Today:

- Look at three mechanisms that vary in complexity.

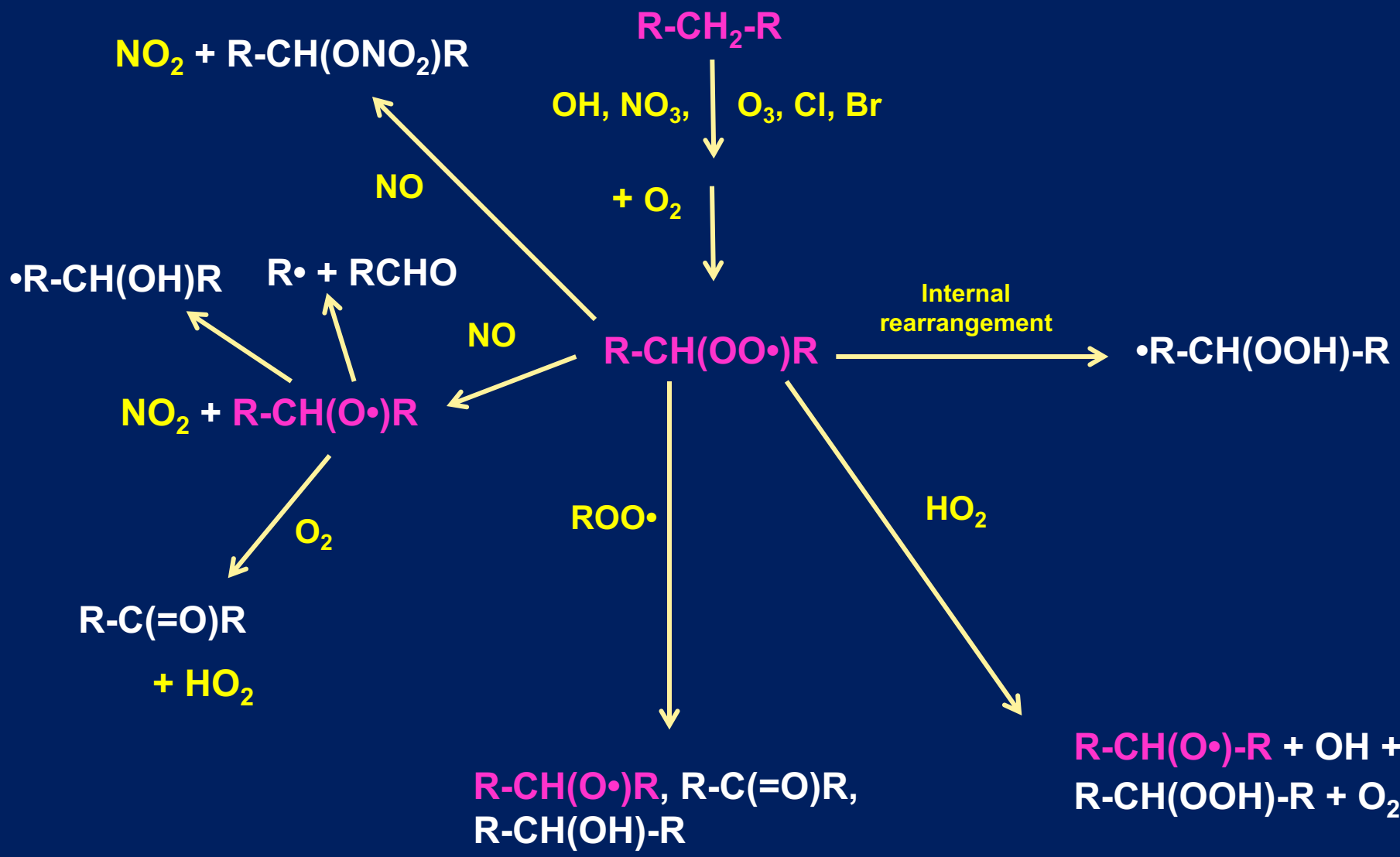
  - GECKO-A, 'hyper-explicit'; Leeds MCM, explicit; MOZART, lumped (These are coalescing…)

  - BoxMox

- Look at the top 25-50 OVOC emissions from BB (use black spruce emissions from Hatch et al., 2017 as a model). Categorize these in some way.

- Look at what we know about their chemistry, and how this is represented in current mechanisms.

Basic Hydrocarbon Oxidation Pathways

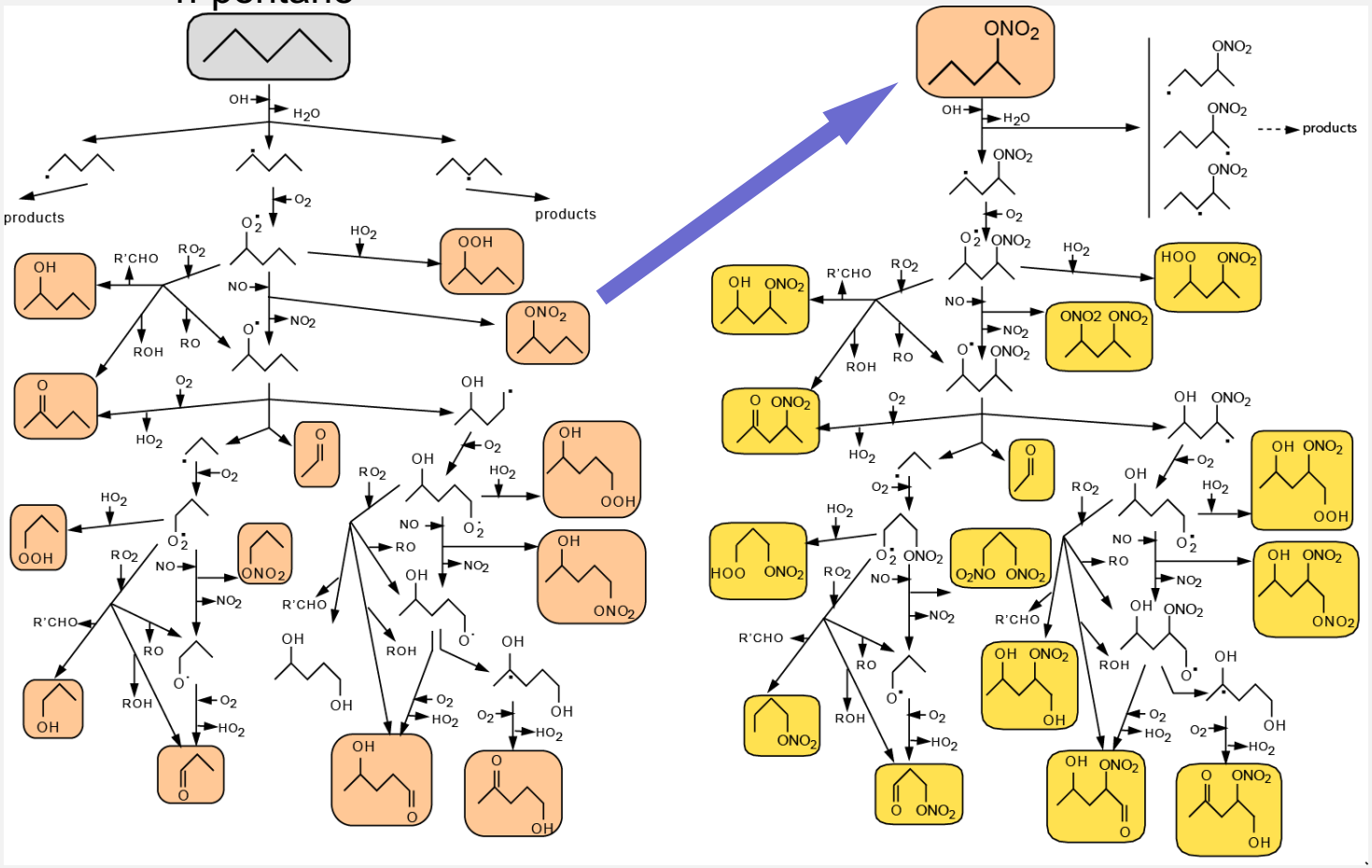


Chemical Mechanisms and Biomass Burning Emissions

GECKO-A

- A hyper-explicit, self-generating mechanism…
- Uses known chemistry, and augments unknowns with a set of ‘rules’ (Structure-Reactivity).
- Extremely detailed, excellent tool for box model studies, but not amenable for use in regional / global models.

rC Complexity: A small part of the mechanism for a small molecule

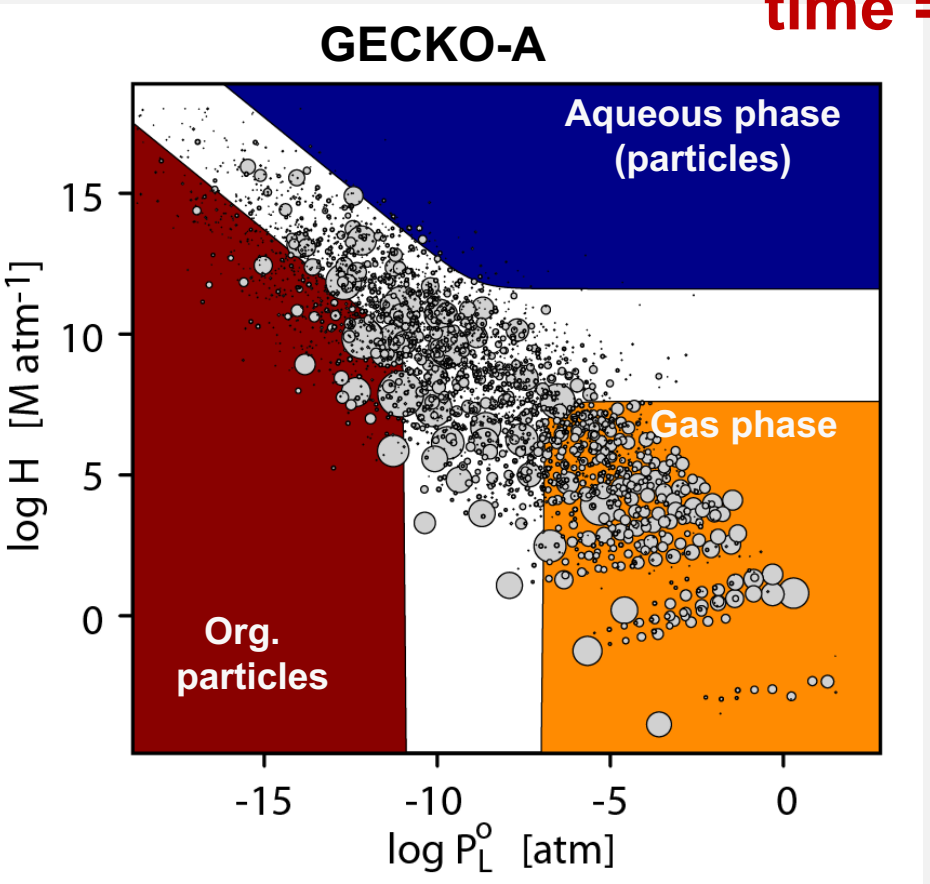


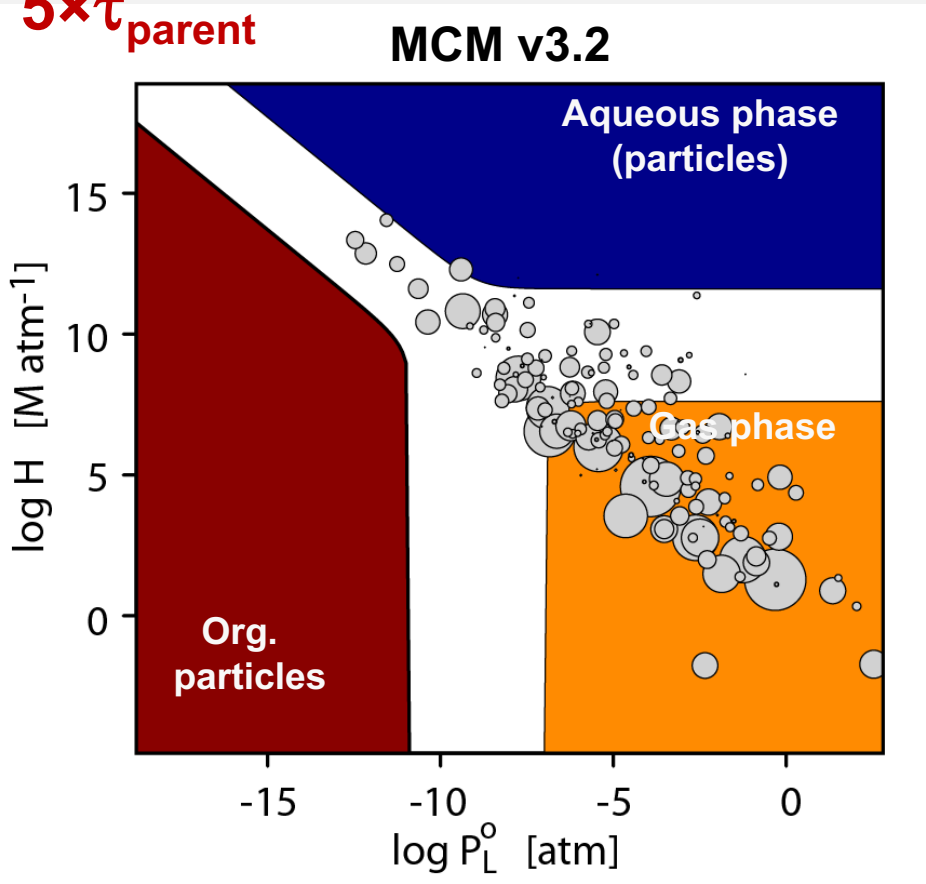
Parent hydrocarbon → 1st generation species → 2nd generation species → CO_2

NCAR

Dodecane oxidation – oxidation trajectories

time = $5 \times \tau_{parent}$





Phase partitioning (> 99 %) assuming:
- C_{OA} = 10 µg m^{-3}, $MW_{aerosol}$ = 200 g mol^{-1}
- LWC = 10 µg m^{-3} (deliquescent particle)

NCAR

SOA Lifecycle Studies with GECKO-A

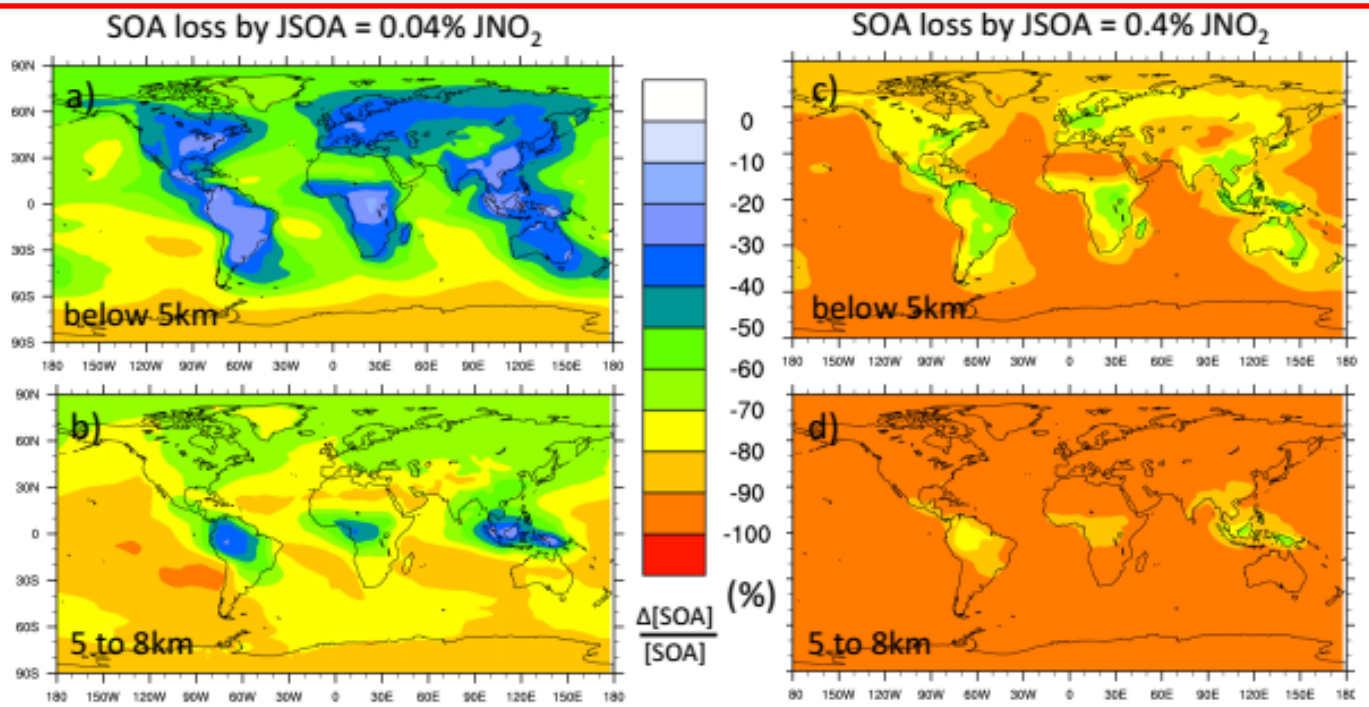


Figure 8. Relative reductions (%) in SOA concentrations due to particle-phase photolysis in the lower **(a, c)** and upper **(b, d)** troposphere. Two in-particle photolysis rates are considered, i.e., J_{SOA} of 0.04 % J_{NO_2} (left side) and J_{SOA} of 0.4 % J_{NO_2} (right side).

Hodzic et al., 2015

www.atmos-chem-phys.net/15/9253/2015/ Atmos. Chem. Phys., 15, 9253–9269, 2015

Chemical Mechanisms and Biomass Burning Emissions

Leeds MCM

- A very detailed, extremely useful, publicly available and often-used mechanism
- Explicit – each molecule is a ‘real’ species, no lumping
- Hand-written, so necessarily ‘cuts off’ the chemistry at some point… not every last pathway included.
- Not easily extendable (by users) to new compounds / pathways.

Chemical Mechanisms and Biomass Burning Emissions

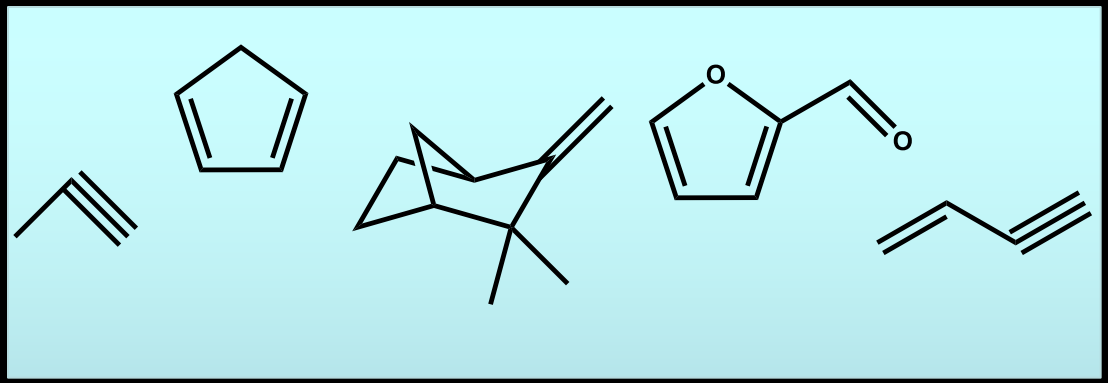
MOZART T-1

- The NCAR/ACOM mechanism used in CESM, WACCM, CAM-Chem, and (optionally) WRF-Chem.
- Heavily 'lumped' and simplified.
- (e.g., explicit chemistry for C1-C3 species; larger alkanes, alkenes lumped into one species).
- Similar in size, complexity and style to GEOS-Chem, RACM, SAPRC (100^{+} species, 200 rxns.)
- SOA production is done in parallel to the gas-phase chemistry (VBS).

- ***This is where the sausage gets made:*** 800 cpds., 60 species to use as surrogates.

The essence of the problem:

There are about 800^{+} (O)VOCs now identified from BB studies (e.g., Hatch et al. 2017)



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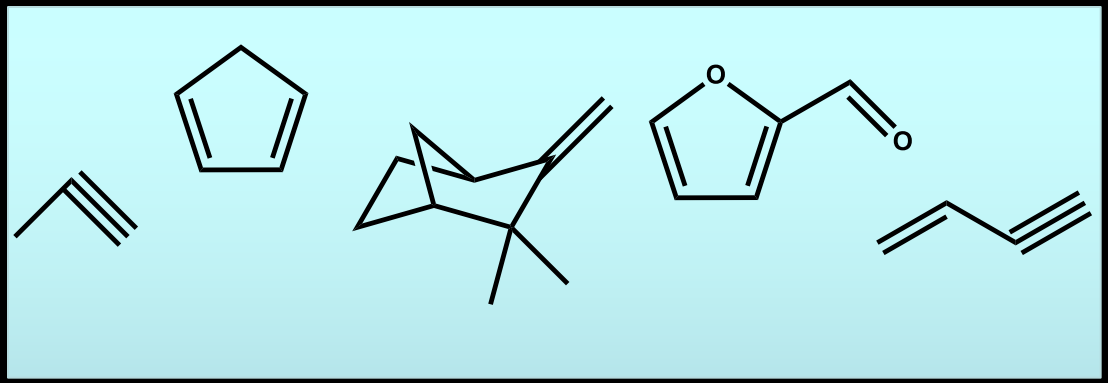
There are about 800^{+} (O)VOCs now identified from BB studies (e.g., Hatch et al. 2017)



There are only 60 or so in typical mechanisms used in regional / global models. (Emmons et al., in prep; Emmons et al., 2010; Lamarque et al., 2012)

C_3H_6	C_3H_8
BIGALK	XYLOL
BIGENE	TERPROD1

Chemical Mechanisms and Biomass Burning Emissions

For complex species that do not exist in simple mechanisms, must ‘lump’.

What criteria do we use for this lumping?

- OH reactivity?
- Type of products that get formed, and their reactivity?
- SOA formation potential?
- Nitrate yield?
- *Toxicity?*

Chemical Mechanisms and Biomass Burning Emissions

Black Spruce emissions, Hatch et al., 2017

Compound Name				
Terpenes (α-Pinene)	1-Nonene	a-Myrcene	Benzene,1-ethynyl-2-methyl-	C8H12 isomer
1,3-Cyclopentadiene	1,2-Butadiene, 2,3-dimethyl-	Benzene, 1-propenyl-	Benzene, 1-methyl-4-propyl-	C10H18 isomer
Limonene	2,4-Cyclopentadiene-1-one	C10H16 isomer	C10H22 isomer	C10H12 isomer
1,3-Butadiene	Caryophyllene	Butenal, 2-methyl-	p-Cymene	C10H14 isomer - non-aromatic
Camphene	Naphthalene, 1-methyl-	Benzene, 5-ethyl-1,3-dimethyl-	2,3-Butanedione	C10H10 isomer
Beta-Myrcene	1,3-Pentadiene, 2-methyl-, (E)-	Propane	2-Pentanone	C7H12 isomer
Isoprene	1-Butene, 3-methyl-	C10H16 isomer	Cyclohexanone	C7H12 isomer
Santene	4-Methylstyrene	2-Butenal, 2-methyl-	Cyclohexene, propyl-	C8H14 isomer
Hydroxymethylfurfural	2,4-Hexadiene, (E,E)-	1,3-Butadiyne	Benzene, 1-propynyl-	C7H10 isomer
1,3-Cyclopentadiene	Benzaldehyde	Heptenal	Cyclohexene, 1,4-dimethyl-	C7H10 isomer
alpha-Pinene	2-methyl phenol	Cyclohexene, 4-methyl-	Tetradecane	C8H14 isomer
2-Furan Methanol	o-Xylene	Furan, 2,3-dihydro-5-methyl-	Cyclopentane, ethyl-	C8H10 isomer (non-aromatic)
Ethylene	2-Cyclopenten-1-one, 2-methyl-	Furan, 4-methyl-2-propyl- (or C8H12O isomer)	Benzene, 1,4-diethyl-	C8H12 isomer - non-aromatic
Propylene	1-Pentene	n-Butene	Cyclopentane, methyl-	C7H12 isomer
3-Carene	1-Decene	Benzene, 2-propenyl-	Furan, tetrahydro-	C10H14 isomer - non-aromatic
1,3-Cyclopentadiene, 1-methyl-	Furan, 2,3-dimethyl-	Vinylcyclopentene	2,3-Pentanedione	C10H12 isomer
Acetaldehyde	Methyl benzofuran isomer	2-Heptene, (E)-	2-Heptanone	C7H12 isomer
Acrolein	Hydroxyacetone	Benzene, 1-ethyl-2-methyl-	2-Butanone, 3-methyl-	C7H12 isomer
Terpinolene	Cadinadiene isomer	Benzene, 1,2,3,5-tetramethyl-	Acetophenone	C7H12 isomer
Ketene Fragments	1H-Pyrrole, 2-methyl-	2-Cyclopentene-1,4-dione	Pyridine	C10H18 isomer
2-Hydroxy-3-Methyl-2-Cyclopentenone	Furan, 2-ethyl-5-methyl-	1-Buten-3-yne,2-methyl-	1,4-Pentadien-3-one	C11H12 isomer
Catechol (Benzenediolic): Methylfurfural	1-Butene, 2,3-dimethyl-	C10H16 isomer	Isobutyronitrile	C7H10 isomer
2-Furanone	1H-Indene, 1-methyl-	2-Hexene, 3-methyl-, (Z)-	1-Butyne, 3-methyl-	C10H18 isomer
Furan, 2-methyl-	o-Guaiacol	Cyclopentene, 3-ethyl-	C_5 Diketone isomer	C10H18 isomer
1,3-Cyclopentadiene, 5-methyl-	octane	Propanal	Cyclopentane	C11H18 isomer
Styrene	1,5-Hexadien-3-yne	Decane	Butanenitrile, 3-methyl-	C10H12 isomer
Alpha terpinene	Beta-Phellandrene	Pentane	Carbon suboxide	C10H12 isomer
1,3-Pentadiene, (E)-	Biomylene	2-Propenoic acid, methyl ester	3-Butyn-2-one	C10H14 isomer - non-aromatic
Furfural	p-Cymene	1,3,5-Cycloheptatriene	Benzonitrile	C12H22 isomer
Beta-Pinene	1H-Pyrrole, 3-methyl-	1-Hexen-3-yne	3-Methylpyridazine	C7H12 isomer
Naphthalene	Allo-ocimene or a-pyronene	C10H16 isomer	Acetic acid, methyl ester	C7H12 isomer
Beta-pyronene	Furan, 2-ethyl-	1-Butene, 2-ethyl-3-methyl-	Butanenitrile, 2-methyl-	C7H10 isomer
1,3-Cyclohexadiene	Benzene, 1,2,3-trimethyl-	2-Octene, (Z)-	Pentane, 2,3,3-trimethyl	C10H10 isomer
gamma pyronene	Tricyclene	3-Penten-2-one, (E)-	Dimethyl Sulfide	C10H14 isomer - non-aromatic
1-Butene	Methyl benzofuran isomer	1-Pentene, 4-methyl-	Ethyl Acetate	C8H12 isomer - non-aromatic
Xylenol (2,5-Dimethyl phenol)	1,12-Tridecadiene	3-Penten-1-yne, (E)-	Propanenitrile	C10H12 isomer
1,3-butadiene	3-Penten-1-yne, (Z)-	Indane	Methyl propionate	Unknown
Indene	1,5-Hexadiene	m-Cymene	Butanenitrile	C7H10 isomer
Furan, 2,5-dimethyl-	Naphthalene, 2-ethenyl-	1,3-Dimethyl-4-ethylbenzene	Formic acid, ethyl ester	C11H16 isomer
Butenyne	1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-[E,E]]-	2-Cyclohexen-1-one	Acetonitrile	C7H12 isomer
Furan	2-Pentene, 3-methyl-, (Z)-	1-Penten-3-yne, (E)-	3-methyl-2-butyl nitrate	C8H12 isomer
2-Furan methanol	Benzaldehyde, 3-methyl-	Benzene, 1-butynyl-	2-Butyl nitrate	C7H12 isomer
Propyne	1,6-Heptadiene	2-Methyl-2-heptene	2-pentyl nitrate	C10H18 isomer
Phenol	Vinylfuran	2H-Pyran, 3,4-dihydro-	3-pentyl nitrate	Pentanenitrile, 4-methyl-
Cadinadiene isomer	a-Cubebene	Furan, 2-(2-propenyl)-	n-propyl nitrate	C10H12 isomer
1,4-Cyclohexadiene, 1-methyl-	1,2-propadiene	2-Nonene, (E)-	Ethyl chloride	C10H10 isomer
Methyl-Naphthalenes	Cyclohexene, 1-methyl-	Benzene, pentyl-	Ethyl nitrate	C11H12 isomer
i-Butene	2-Hexene, (E)-	4-Methylanisole	Formaldehyde	C10H14 isomer - non-aromatic
Pyrrole	Germacrene D	Fenchyl acetate	Methanol	C10H14 isomer - non-aromatic
1,3-Pentadiene, (Z)-	Benzene, 1-propenyl-	1,4-Pentadiene, 3-methyl-	Methanethiol	C10H12 isomer
1-Hexene	Furan, 2,3,5-trimethyl-	nonane	Formic Acid	C7H8 isomer
Guaiacol (2-Methoxyphenol)	2-Propynal	Benzene, 4-ethyl-1,2-dimethyl-	Hydrogen Cyanide	C11H14 isomer
2-Pentene, (E)-	3-Cyclopenten-1-one	Octanal	Carbon Disulfide	C11H16 isomer
Sabinene	Furan, 2,4-dimethyl-	Furan, 2,5-dihydro-	Methyl chloride	C7H10 isomer
Alpha-Phellandrene	Cyclohexene, 3-methyl-	Heptane	Carbonyl sulfide	C8H12 isomer
1,3-Pentadiene, 2-methyl-, (Z)-	2,3-Dihydrofuran	Furan, 2-propyl-	Methyl nitrate	C7H8 isomer
Methyl vinyl ketone	1,10-Undecadiene	4-Nonene, (Z)-	Tribromomethane	C10H14 isomer - non-aromatic
m&p-Xylene	2,5-Dimethyl phenol	Furan, 3-ethyl-	methyl iodide	C8H14 isomer
1,3-Cyclopentadiene, 5,5-dimethyl-2-propyl-	Ethylbenzene	Benzene, 1-ethyl-4-methyl-	Unknown	C8H12 isomer
Toluene	trans-1,4-Hexadiene	Benzeneacetaldehyde	C8H12 isomer	C7H10 isomer
2-Methyl-1-butene	Benzene, 1,2,4-trimethyl-	i-Butene	C7H10 isomer	C10H12 isomer
Cyclohexene	Copaene	2-Butenal, 3-methyl-	C7H10 isomer	C7H10 isomer
2-Butenal	Acetylene	3-Octene, (E)-	C9H16 isomer	Unknown
trans-2-Butene	Butenal, 3-methyl-	Benzene, 2-ethyl-1,4-dimethyl-	C9H16 isomer	C10H18 isomer
Naphthalene	a-Methylstyrene	Acetic acid ethenyl ester	C9H16 isomer	C10H12 isomer
1-Heptene	1,4-Pentadiene, 2-methyl-	Hexane	C10H18 isomer	Assorted HCs inc. Dihydronaphthalene
4-Methyl-1,3-pentadiene	Cyclopentene, 3-methyl-	1,2-Dimethyl-3-ethylbenzene	C9H16 isomer	Phenylethyne
Cyclohexene, 4-ethenyl-1,4-dimethyl-	Glycolaldehyde	5-Hexen-2-one	C9H14 isomer	C8H10 isomer
Cyclopentene, 1-methyl-	a-Cadalene	Benzene, propyl-	C9H16 isomer	C9H14 isomer
1-Undecene	1,7-Octadiene	2-Ethylacrolein	C7H10 isomer	C7H10 isomer
Cyclopentene	Benzofuran, -dimethyl- (isomer)	Tridecane	C9H18 isomer	C9H14 isomer
2-Cyclopenten-1-one	Butenal	Benzene, butyl-	C9H16 isomer	C8H8 isomer
(E)-Ocimene	Cyclopentene, 4,4-dimethyl-	Acetic acid, 2-propenyl ester	C10H18 isomer	C7H12 isomer
Methacrolein	Propanal, 2-methyl-	1-Butene, 2-ethyl-3-methyl-	C8H10 isomer (non-aromatic)	C10H20 isomer
1,11-Dodecadiene	1H-Pyrrole, 2,5-dimethyl-	Ethene	C8H14 isomer	C7H10 isomer
Methylglyoxal	3-Hexene, (E)-	1-Heptene, 2-methyl-	C9H16 isomer	C8H12 isomer
2-Pentene, 2-methyl-	2-Hexene, 3-methyl-, (Z)-	2-Pentenal, (E)-	C10H18 isomer	C10H12 isomer
2-Pentene, (E)-	Salicylaldehyde	Methacrylonitrile	C10H14 isomer - non-aromatic	4-Penten-1-yne
1-Dodecene	Fenchene	2-Pentyne	C9H18 isomer	Cyclopentanone
Benzene, 1-ethenyl-3-methyl-	Acetic Acid	3-Butenenitrile	C11H22 isomer	1-Hexene, 5-methyl-
Allo-ocimene or a-pyronene	Methyl benzofuran isomer	2-Pentene, 4-methyl-	C8H12 isomer - non-aromatic	Benzene, 1-methyl-2-propyl-
3-Buten-2-one, 3-methyl-	4-Phenylbut-3-ene-1-yne	1-Hexene, 4-methyl-	C8H14 isomer	2-Hexanone
3+4-methyl phenol	1,9-Decadiene	Biphenyl	C8H14 isomer	C_6 Diketone isomer
1,3-Hexadiene,c&t	Naphthalene, 1,3-dimethyl-	1-Penten-3-one	C8H14 isomer	Thiophene
Bornyl acetate	3-Furaldehyde	3-Heptene, (E)-	C8H10 isomer (non-aromatic)	Benzene, 1,3,5-trimethyl-
Cadinadiene isomer	Benzene, 1-ethyl-3-methyl-	4-Penten-2-one	C11H20 isomer	C10H16 isomer
Cadinadiene isomer	C10H16 isomer	Benzene, 1-methyl-3-propyl-	C10H14 isomer	2-Heptene, (Z)-
Benzofuran	C10H16 isomer	Benzene, (1-methylbutyl)-	C8H14 isomer	5-Methylenecyclooctene-1,3-diene
Gamma terpinene	2-Propen-1-ol	Anisole	C8H14 isomer	2-Octene, (E)-
Acenaphthylene	1H-Pyrrole, 1-ethyl-	Dimethyl Sulfide	C8H12 isomer	Furan, 2-acetyl-
cis-2-Butene	Hexanal	Ethyl acetate	C7H12 isomer	1,13-Tetradecadiene
1,3-Pentadiene, 3-methyl-, (Z)-	1,4-Hexadiene, (Z)-	Undecane	C11H20 isomer	Furan, 3-methyl-
2,4-Hexadiene, (E,Z)-	C10H16 isomer	Dodecane	C11H12 isomer	1-Tetradecene
1H-Pyrrole, 1-methyl-	Pentanal	Benzene, hexyl-	C8H12 isomer	Benzene
Cyclohexene, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	Naphthalene, 1-ethyl-	Acrylonitrile	C11H12 isomer	Calamenene
1-Octene	1,3-Dimethyl-1,4-cyclohexadiene	Acetone	C8H12 isomer	1-Tridecene
1,4-Pentadiene	3-Penten-2-one, (E)-	Benzene, isopropyl-	C8H14 isomer	1,8-Nonadiene
5-Methyl furfural	3,5-Dimethylcyclopentene	2-Butanone	Unknown	Naphthalene, 2-methyl-

Black Spruce emissions, Hatch et al., 2017

Chemical Mechanisms and Biomass Burning Emissions

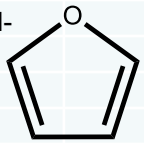
BY EMISSIONS	BY OH REACTIVITY	BY SOA POTENTIAL
Ethylene	Terpenes (α-Pinene)	Terpenes (α-Pinene)
Formaldehyde	Ethylene	1,3-Cyclopentadiene
Acetaldehyde	1,3-Butadiene	Limonene
Methanol	1,3-Cyclopentadiene	1,3-Butadiene
Terpenes (α-Pinene)	Acetaldehyde	Camphene
Ketene Fragments	Ketene Fragments	Beta-Myrcene
Acetylene	Propylene	Isoprene
Acetic Acid	Formaldehyde	Santene
Propyne	Isoprene	Hydroxymethylfurfural
Propylene	Acrolein	1,3-Cyclopentadiene
Unknown	1,3-Cyclopentadiene	alpha-Pinene
Acrolein	Limonene	2-Furan Methanol
Ethane	2-Furan Methanol	Ethylene
1,3-Butadiene	Camphene	Propylene
Hydrogen Cyanide	Hydroxymethylfurfural	3-Carene
Benzene	Beta-Myrcene	1,3-Cyclopentadiene, 1-methyl-
Acetone	2-Furanone	Acetaldehyde
Propane	Santene	Acrolein
Formic Acid	1,3-Cyclopentadiene, 1-methyl-	Terpinolene
Hydroxyacetone	Propyne	Ketene Fragments
1,3-Cyclopentadiene	alpha-Pinene	2-Hydroxy-3-Methyl-2-Cyclopentenone
Toluene	Furan, 2-methyl-	Catechol (Benzenediols); Methylfurfural
Camphene	1-Butene	2-Furanone
Isoprene	1,3-butadiene	Furan, 2-methyl-
Unknown	2-Hydroxy-3-Methyl-2-Cyclopentenone	1,3-Cyclopentadiene, 5-methyl-
Methylglyoxal	Catechol (Benzenediols); Methylfurfural	Styrene
2-Furanone	1,3-Pentadiene, (E)-	Alpha terpinene
1-Butene	Furfural	1,3-Pentadiene, (E)-
Glycolaldehyde	Butenyne	Furfural
Methyl vinyl ketone	Furan	Beta-Pinene
Furfural	1,3-Cyclopentadiene, 5-methyl-	Naphthalene
2-Furan Methanol	3-Carene	Beta-pyronene
Butenyne	i-Butene	1,3-Cyclohexadiene
Furan	Pyrrole	gamma pyronene
Catechol (Benzenediols); Methylfurfural	1,3-Cyclohexadiene	1-Butene
Acetonitirile	2-Furan methanol	Xylenol (2,5-Dimethyl phenol)
1,3-Cyclopentadiene	Terpinolene	1,3-butadiene
alpha-Pinene	Methyl vinyl ketone	Indene
Unknown	Furan, 2,5-dimethyl-	Furan, 2,5-dimethyl-
Phenol	Styrene	Butenyne
Naphthalene	1,3-Pentadiene, (Z)-	Furan
Unknown	2-Pentene, (E)-	2-Furan methanol
Furan, 2-methyl-	Phenol	Propyne
2,3-Butanedione	Methylglyoxal	Phenol
Limonene	1-Hexene	Cadinadiene isomer
i-Butene	Alpha terpinene	1,4-Cyclohexadiene, 1-methyl-
1,3-butadiene	Xylenol (2,5-Dimethyl phenol)	Methyl-Naphthalenes
n-Butane	2-Butenal	i-Butene
Tricyclene	trans-2-Butene	Pyrrole
Unknown	1,4-Cyclohexadiene, 1-methyl-	1,3-Pentadiene, (Z)-

Chemical Mechanisms and Biomass Burning Emissions

Categories			
Simple Species	**Biogenic**	**Furan derivatives**	**Cyclopentadienes**
Ethylene	Isoprene	Hydroxymethylfurfural	1,3-Cyclopentadiene
Propylene	1,3-Butadiene	2-Furan Methanol	1,3-Cyclopentadiene, 1-methyl-
Acetaldehyde	Limonene	2-Furanone	
Acrolein	Camphene	Furan, 2-methyl-	
	Beta-Myrcene		
	alpha-Pinene		
	Santene		

Black Spruce emissions, Hatch et al., 2017

Chemical Mechanisms and Biomass Burning Emissions

Categories			
Sim[illegible]pecies	Biogenic	Furan derivatives	Cyclopentadienes
Ethylene	Isoprene	Hydroxymethylfurfural	1,3-Cyclopentadiene
Propylene	(1,3-Butadiene)	2-Furan Methanol	1,3-Cyclopentadiene, 1-methyl-
Acetaldehyde	Limonene	2-Furanone	
Acrolein	Camphene	Furan, 2-methyl- 	
	Beta-Myrcene		
	alpha-Pinene		
	Santene		

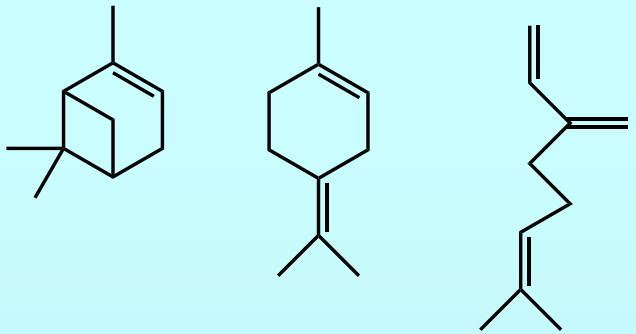
Chemical Mechanisms and Biomass Burning Emissions

ISOPRENE; (1,3-Butadiene)

- **Lab Chemistry:** characterized in gory detail.
- **GECKO-A:** Needs initial steps hard-wired, but runs hyper-explicit chemistry from there.
- **Leeds MCM:** Very much up-to-date…
- **MOZART:** Evolving, but reasonably up-to-date (though simplified)
  - NB: Can connect gas-phase products (IEPOX) to aq. SOA formation (E. Marais, GEOS-Chem, 2016)

Chemical Mechanisms and Biomass Burning Emissions

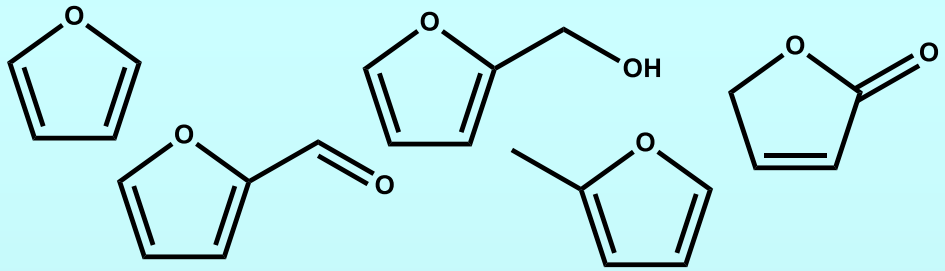
TERPENES



- **Lab Chemistry:** initial steps ok, details not known. SOA yields measured (empirical?).
- **GECKO-A:** Initial steps driven by MCM, then hyper-explicit from there.
- **Leeds MCM:** Fairly detailed representation for some, nothing for others.
- **MOZART:** Initial steps included, products 'lumped'.

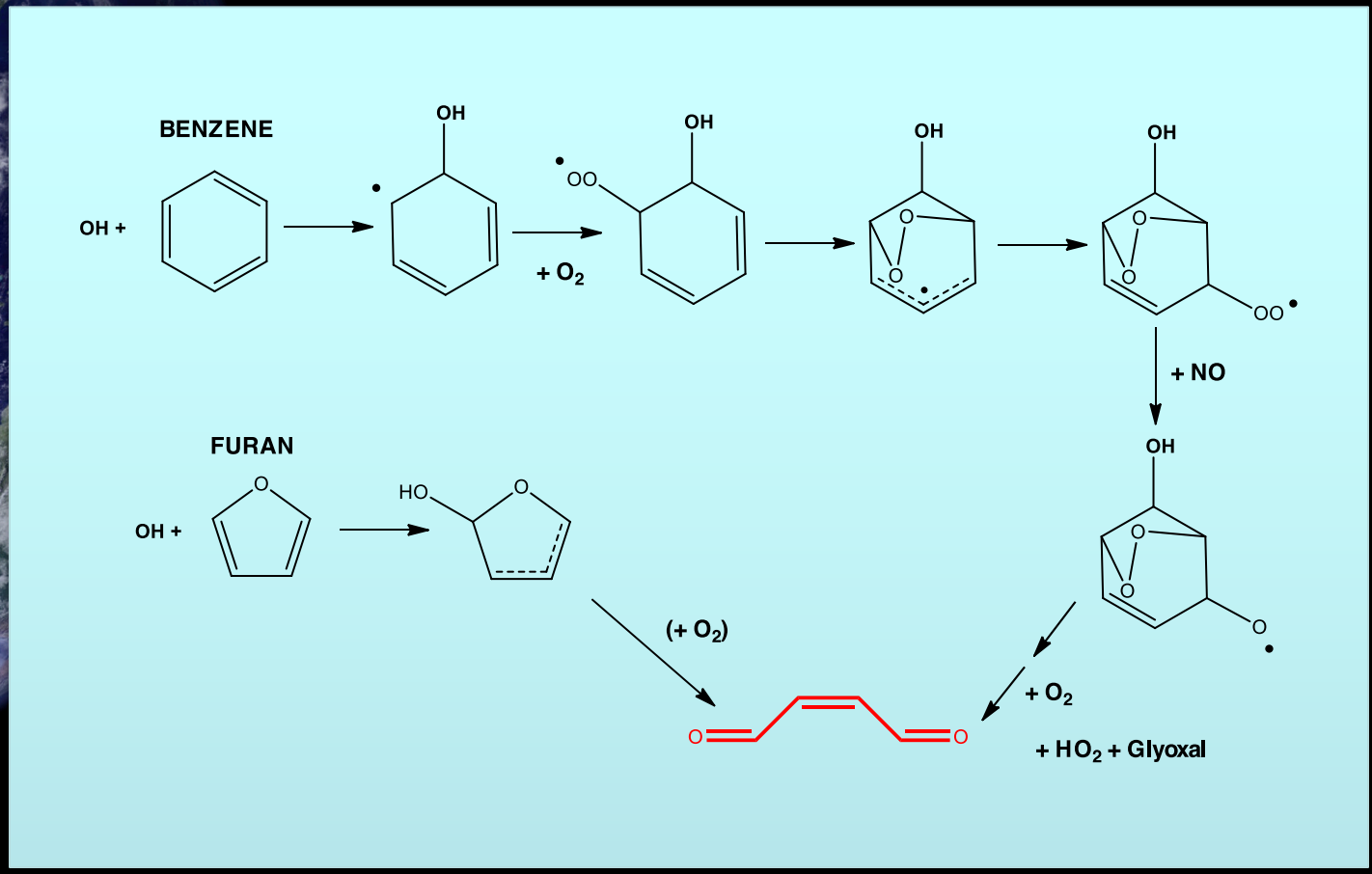
Chemical Mechanisms and Biomass Burning Emissions

FURAN AND DERIVATIVES



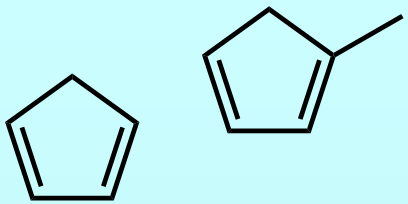
- **Lab Chemistry:** some initial steps known, details very uncertain. *(Parallels to aromatics, though!)*
- SOA yields not well studied at all.
- **GECKO-A:** Not currently dealt with
- **Leeds MCM:** Not dealt with.
- **MOZART:** Not dealt with (yet?).

Chemical Mechanisms and Biomass Burning Emissions

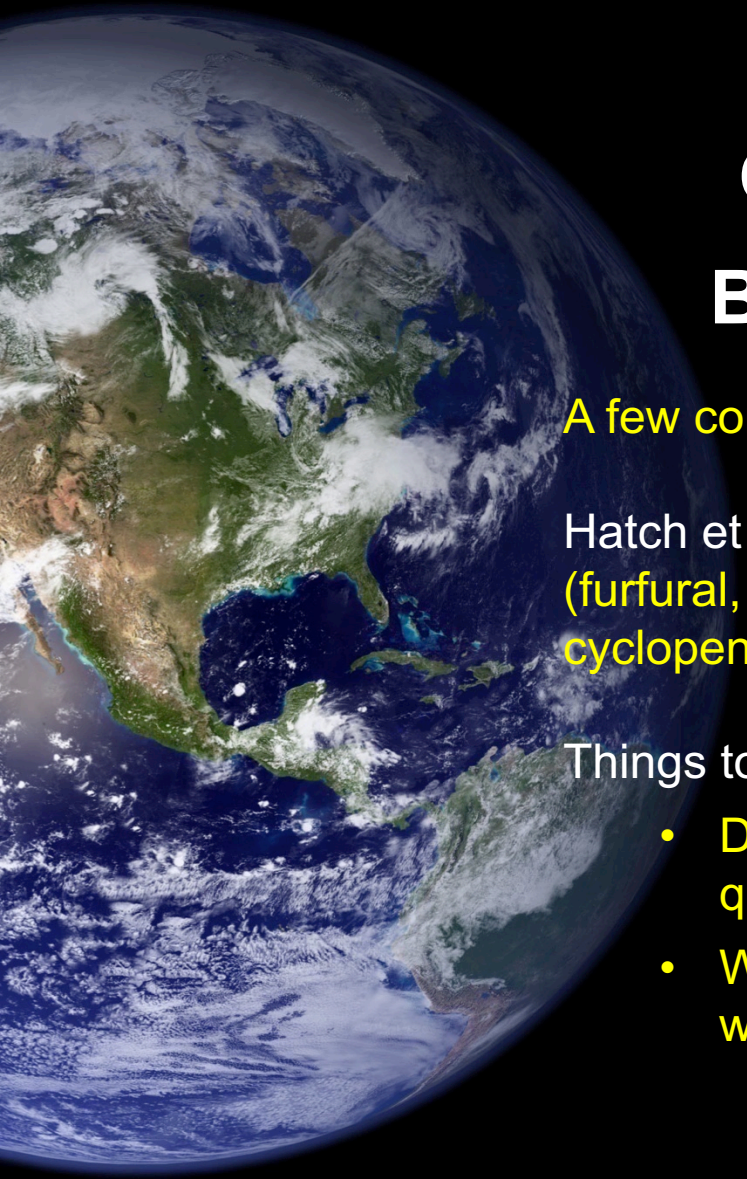


Chemical Mechanisms and Biomass Burning Emissions

CYCLOPENTADIENES



- Not studied in lab…SOA yields unknown.
- Not so easy, probably can make some reasonable guesses, but… *caveat emptor.*



Chemical Mechanisms and Biomass Burning Emissions

A few concluding thoughts:

Hatch et al, 2017: Names numerous furan derivatives (furfural, 2-Me-furan, 2-furan methanol) and 1,3-cyclopentadiene as key candidates for further study.

Things to think about these next couple of days:

- Do we have the mechanisms we need to answer the questions we have? If not, what is needed?
- Would a BB extension to MOZART be useful? What would it include?

Questions???