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





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?





MECHANISTIC NEEDS MAY BE DIFFERENT FOR EACH

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)





#### 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**







### **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





### Dodecane oxidation – oxidation trajectories



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



### SOA Lifecycle Studies with GECKO-A







### 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.





### **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<sup>+</sup> 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<sup>+</sup> (O)VOCs now identified from BB studies (e.g., Hatch et al. 2017)

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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)

 $C_3H_6$ **BIGALK BIGENE** 

 $C_3H_8$ **XYLOL TERPROD1** 







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?





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alpha-Pinana	2-methyl phenol	Cyclohexene, 4-methyl-	Tetradecane	CBH14 isomer
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Propylene	1-Pentone	n-Gutane	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-	Virylcyclopentane	2,3-Pentanedione	C10H12 laomer
Acetaldehyde	Methyl benzofuran isomer	2-Heptene, (E)-	2-Heptanone	C7H12 isomer
Actalein	Hydroxyacetone	Danzene, 1-ethyl-2-methyl-	2-Butanone, 3-methyl-	C7H12 isomer
Terpinolene	Cadinadiene isomer	Benzene, 1,2,3,5-tetramethyl-	Acetophenone	C7H12 isomer
Ketana Fragmenta	1H-Pyrole, 2-methyl-	2-Cyclopentene-1,4-clone	Pyridine	C10H18 lapmer
2-Hydraxy-3-Methyl-2-Cyclopenterione	Futan, 2-ethyl-5-methyl-	1-Euten-3-yne, 2-methyl-	1.4-Pentadien-3-one	C11H12 isomer
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Alpha terpinene	Beta-Phellandrene	Pentane	Carbon suboxide	C10H12 laomer
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Deta-Pinene	1H-Pyrole, 3-metryl-	1-Haxen-3-yne	3-Methylpytidazine	C7H12 isomer
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Deta-pyronene	Furan, 2-ethyl-	1-Butene, 2-ethyl-3-methyl-	Butanenitrie, 2-methyl-	C7H10 isomer
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Hutene	2-Hexane, (E)-	4-Methylaniscle	Formaldehyde	C10H14 isomer - non-aromatic
Pyrtole	Germacrene D	Fenchyl acetate	Methanol	C10H14 isomer - non-aromatic
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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 (a-Pinene)
Formaldehyde	Ethylene	1,3-Cyclopentadiene
Acetaldehyde	1,3-Butadiene	Limonene
Methanol	1,3-Cyclopentadiene	1,3-Butadiene
Terpenes (a-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-Cvclopentadiene	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		
I UTITIC ACIU	1,3-Cyclopentadiene, 1-methyl-	Terpinolene
Hydroxyacetone	Propyne	Ketene Fragments
		2-Hydroxy-3-Methyl-2-
1,3-Cyclopentadiene	alpha-Pinene	Cyclopentenone
		Catechol (Benzenediols);
Toluene	Furan, 2-methyl-	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
Ontenting (Demonstration) Mathematica	4.0 Curlebrandland	4 Duture
Catechol (Benzenediols); Methylfurfural	1,3-Cyclonexadiene	1-Butene
Acetonitirile	2-Euran methanol	Xylenol (2.5-Dimethyl phenol)
1.3-Cyclonentadiene	Terninolene	1 3-butadiene
alnha-Pinene	Methyl vinyl ketone	Indene
Unknown	Furan 2 5-dimethyl-	Furan 2 5-dimethyl-
Phenol	Styrene	Butenvne
Nanhthalene	1 3 Pentadiana (7).	Europ
Inknown	2-Dentene (E)	2-Euran methanol
Euran 2-methyl-	Dhenol	Propupe
2 3-Butanedione	Methylalyoval	Phonol
imonana	1-Hevene	Cadinadiana isomer
Linonene	I-LIAYONG	Caunaciene Isomer
Butene	Alpha terpinene	1.4-Cyclobexadiene 1-methyl-
		r, - cyclonoxidaene, - metry-
1,3-butadiene	Xylenol (2,5-Dimethyl phenol)	Methyl-Naphthalenes
n-Butane	2-Butenal	i-Butene
Tricyclene	trans-2-Butene	Pyrrole
Under notes	4.4. Overlah averdiana 4. avertheid	

### ACOM / ACCORD BIOMASS BURNING WORKSHOP – July, 2017

Black Spruce emissions, Hatch et al., 2017





		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











#### 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)





#### **TERPENES**

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





#### 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?).











#### **CYCLOPENTADIENES**



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





A few concluding thoughts:

Hatch et al, 2017: Names numerous furan derivatives (furfural, 2-Me-furan, 2-furan methanol) and 1,3cyclopentadiene 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???

