The Enhancement of SMOKE to Process Multi-pollutant Inventories: Integration of Criteria and Toxic Pollutants

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Acknowledgements

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"Famous" Quotes from the Authors Regarding the Project

"This was more difficult than I thought…"

"This is very hard to explain"

EPA's Toxics and Criteria Modeling Systems Separate

- Photochemical vs Gaussian Grid
- SMOKE vs EMS-HAP
- NEI for Criteria vs NEI for HAPs

Issues:

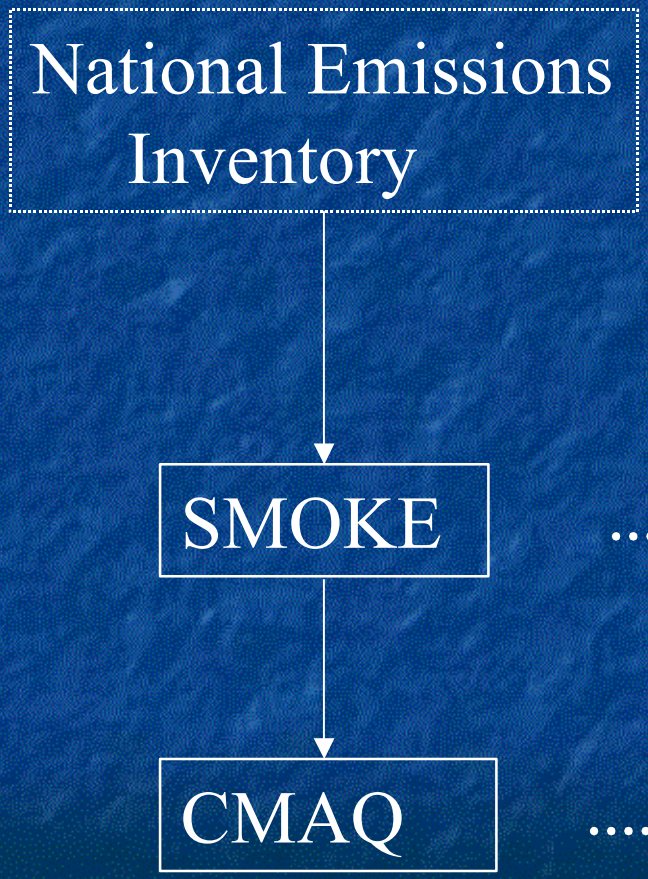
Sound Science

Consistency

Efficiency

EPA is moving towards one-atmosphere modeling to address these issues

One-Atmosphere Approach



COMMENTS:

Still two separate inventories for 1999: toxics (HAPs) & criteria

Modify to process multi-pollutant inventories

Add capabilities for toxics

SMOKE 1.5 Beta

- Released on March 14, 2003:

http://www.cmascenter.org/modelclear.html#smokewww.cmas.org/

- Includes MOBILE6
- Can process toxics and criteria inventories for onroad and nonroad mobile sources
  - Set up for CMAQ: CB4 and toxics CB4
  - Can utilize toxics VOC from toxics inventory without duplicating VOC mass

CMAQ's Toxics CB4

- Allows CMAQ to model 18 gaseous toxics from NATA – e.g., benzene, butadiene, formaldehyde, acetaldehyde, methylene chloride

Sample Model Species:

NAME	Comments
PAR	Same as in CB4
TOL	Same as in CB4
XYL	Same as in CB4
OLE	Same as in CB4

+

NAME	Chemistry Inside or Outside Mechanism	Comments
FORM	in	Contains only formaldehyde
FORMSUR		Non formaldehyde part of CB4 FORM
ALD2	in	Contains only acetaldehyde and those compounds that explicitly form acetaldehyde rapidly such as t-2-butene, c-2-butene,t-2-pentene.
ALD2SUR		Non-acetaldehyde part of CB4 ALD2. Includes higher-level aldehydes
BUTADIENE	in	1,3 butadiene
ACROLEIN	in	acrolein
BENZENE	out	benzene
MECL	out	Methylene chloride

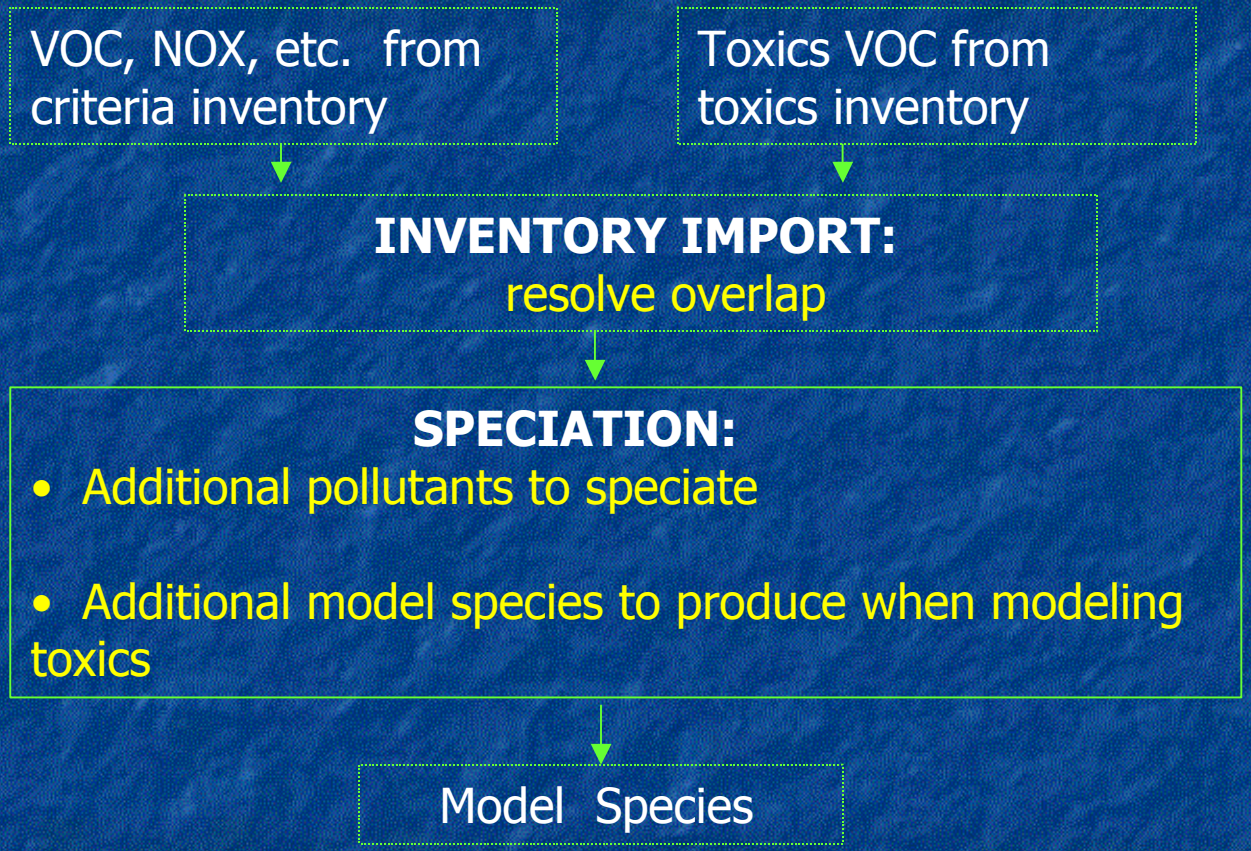
Aspects of the Design

- Importing the inventories
- Producing the necessary model species for CB4 and toxics CB4, using toxics inventory and without duplicating mass

Importing the Inventories

- Criteria and Toxics inventories imported as separate input files
  - Criteria uses same format
  - Toxics uses new “SMOKE-for-Toxics” format
- Onroad toxics and criteria emissions generated by using MOBILE6 in SMOKE, or fed in as “pre-computed” emissions
- User chooses which pollutants get carried forward and information on the toxics that overlap with VOC

Producing the Model Species



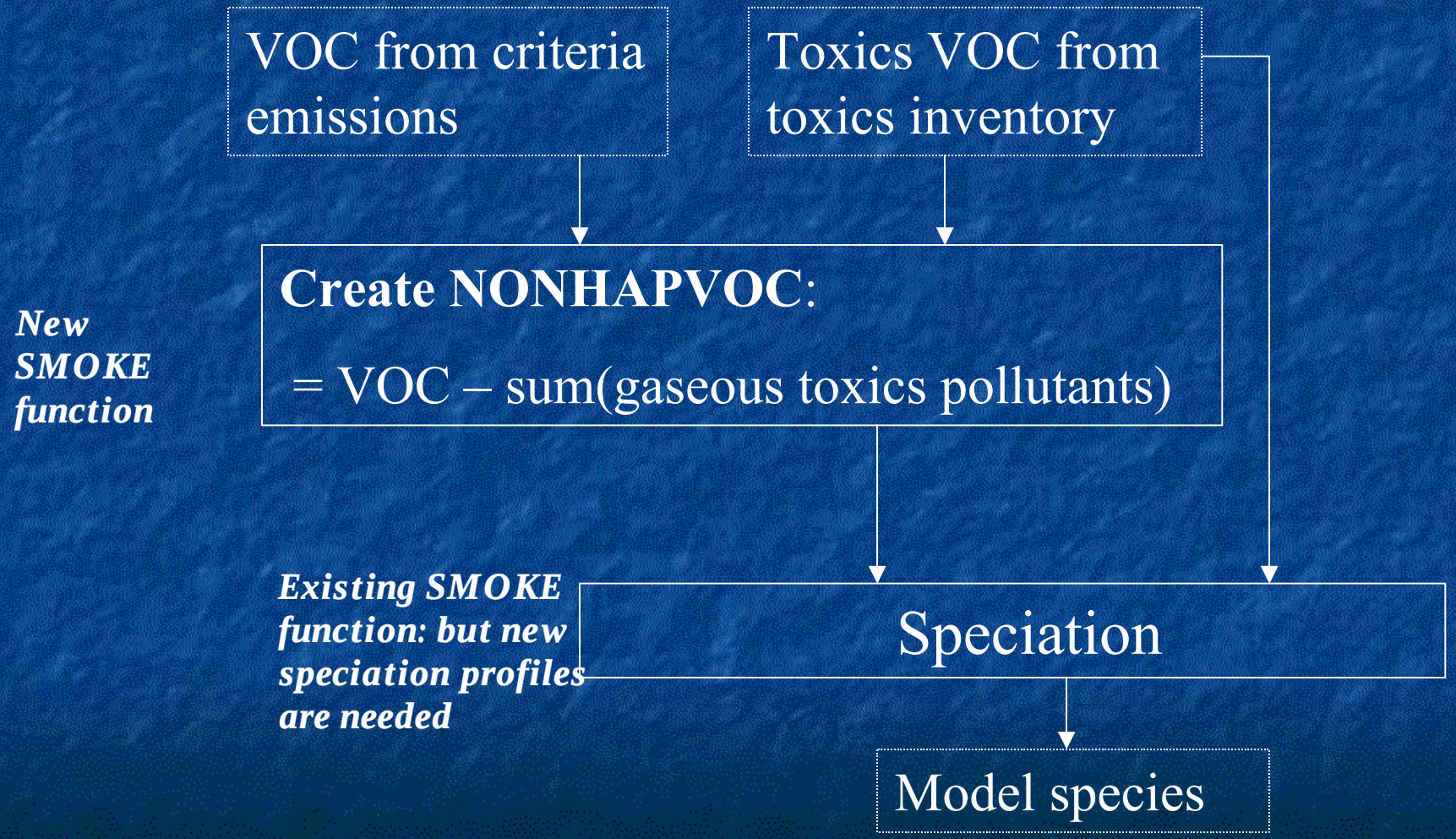
Note: even though we're not looking at particulates, addressing the VOC – HAP overlap will impact PM modeling

Two Ways to Address Overlap in Pollutants

- Integrate inventories, source by source
  - Use all toxics VOC from HAP inventory
  - Use only NONHAP from VOC inventory
  - Sum of toxics VOC + NONHAP = Total VOC from VOC inventory

- Don't Integrate inventories ("No-integrate")
  - Ignore toxics inventory when using CB4
  - Use toxics inventory for toxics model species only, when using toxics CB4. Remove toxics from VOC speciation profiles, in case of overlap.

Integration Approach



The Creation of NONHAPVOC -example for hypothetical source

Criteria: VOC

FIPS	SCC code	tons
10001	2265002072	10.0

Toxics: Toxic VOC

FIPS	SCC code	HAP	tons
10001	2265002072	Benzene	1.0
10001	2265002072	Toluene	2.0
10001	2265002072	xylene	1.0
10001	2265002072	formaldehyde	2.0

SMOKE: Integrated Inventory

FIPS	SCC code	HAP	tons
10001	2265002072	NONHAPVOC	4.0
10001	2265002072	Benzene	1.0
10001	2265002072	Toluene	2.0
10001	2265002072	xylene	1.0
10001	2265002072	formaldehyde	2.0

To other processing steps

Speciation for the Integrated Approach

- SMOKE applies speciation profiles for NONHAPVOC and individual HAPs
- For a toxic modeled outside the mechanism (benzene), SMOKE maps the toxic to itself and its mechanism species

EXAMPLE PROFILES FOR TOXICS CB4

Number	Pollutant	Species	Split Factor	Divisor
1313A	NONHAPVOC	OLE	0.00127373705	1.0
1313A	NONHAPVOC	PAR	0.03439269933	1.0
1313A	NONHAPVOC	FORMSUR	0.00049291434	1.0
0000	BENZENE	BENZENE	1.00	78.11
0000	BENZENE	PAR	1.00	78.11
0000	BENZENE	NR	5.00	78.11
0000	FORM	FORM	1.00	30.03
0000	HEXANE	PAR	6.00	86.18

Practical Considerations for Integration

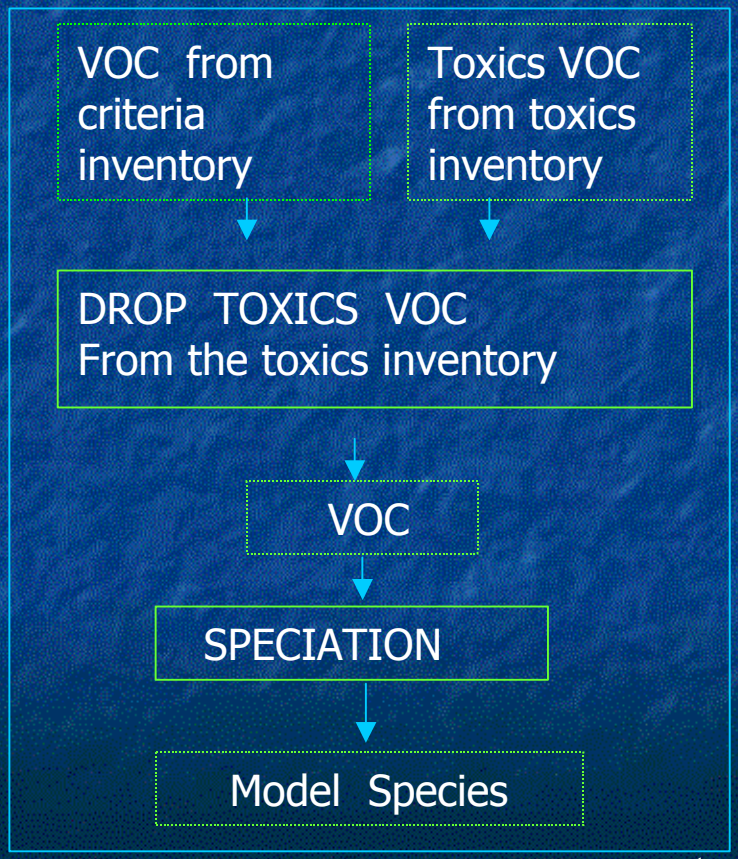
- **The emission sources must be exactly the same for the toxics and the VOC**
- **The methodology to estimate emissions should be consistent between the two inventories**

Both of these hold true for EPA-generated nonroad emissions and MOBILE6 generated emissions

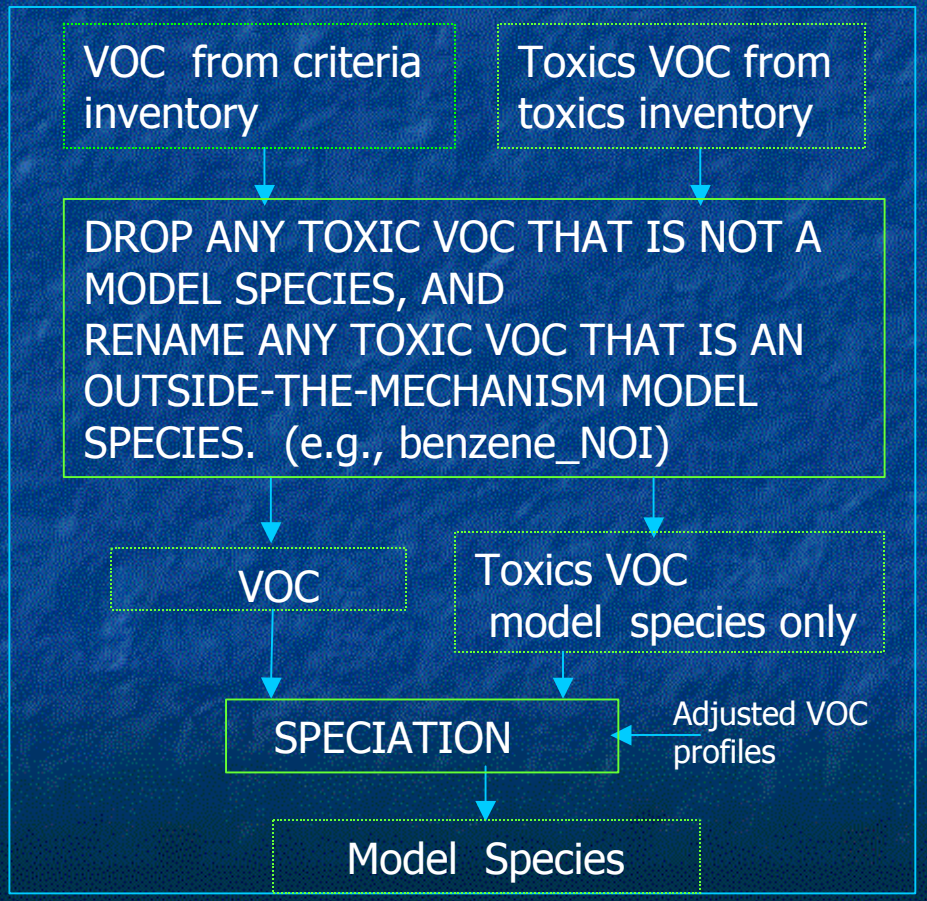
Generally, these don't hold true for stationary sources, and may not hold true for State-generated Mobile estimates

No-integrate Case

- CB4: Ignore toxics



- Toxics CB4: Use toxics only for toxics model species



Pollutants resulting from the No-integrate Case -example for hypothetical source

Criteria: VOC

FIPS	SCC code	tons
10001	2265002072	10.0

Toxics: Toxic VOC

FIPS	SCC code	HAP	tons
10001	2265002072	Benzene	1.0
10001	2265002072	Toluene	2.0
10001	2265002072	xylene	1.0
10001	2265002072	formaldehyde	2.0

SMOKE: Inventory, No-integrate

FIPS	SCC code	Pollutant	tons
10001	2265002072	VOC	10.0
10001	2265002072	Benzene	1.0
10001	2265002072	formaldehyde	2.0

To other processing steps

Speciation For The No-integrate Case

- SMOKE speciates VOC; profiles designed to remove the inside-the-mechanism toxics model species (e.g., formaldehyde)
- SMOKE maps the toxics inventory pollutants to the toxics CB4 explicit toxics model species
- For a toxic modeled outside the mechanism, SMOKE maps the toxic to itself, but not its mechanism species

EXAMPLE SPECIATION PROFILES FOR THE NO-INTEGRATE CASE

0307	TOG	ALD2SUR	0.00010234648	1
0307	TOG	ETH	0.00681283422	1
0307	TOG	NR	0.01503804958	1
0307	TOG	OLE	0.00126649899	1
0307	TOG	PAR	0.03791738749	1
0000	FORM	FORM	1.00	30.03
0000	BENZENE_NOI	BENZENE	1.00	78.11

Preliminary Testing

SMOKE Run Times for Toxics CB4 (1.4 GHz PC processor using Linux)

- Annual/national run for nonroad sources: ~3 days (single processsor, Linux).
- Annual/national run using MOBILE6.2 in SMOKE: ~18 days (weekly temperature averaging and spatial averaging)

Impact on Model Species

- For onroad mobile sources, use of toxics results in less non-reactive and generally a larger increase in FORM than other model species

Summary

- EPA is advancing towards one-atmosphere modeling using toxics and criteria inventories
- EPA's mobile source methods used for 1999 NEI allow opportunity for integration
- SMOKE 1.5 Beta allows for integration of mobile source toxics and criteria inventories for CMAQ/CB4 and CMAQ/toxics CB4
- Tests show less non reactive species produced when integrating toxics & criteria for onroad mobile sources

Future

- SMOKE 2.0 will add stationary source capability
- Wider integration will be possible when inventories become more consistent