ELECTRIC POWER RESEARCH INSTITUTE

SCICHEM Development Update

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Some Introductory Notes

- A new SCICHEM version is forthcoming in a few months
- A prior version SCICHEM has been described in previous presentations at this conference; this version has some of but not all the enhancement of the future version
- As such, it has seen limited distribution as a "pre-release" version

- This presentation will provide an update on the status of SCICHEM development

SCICHEM: Origin

- An overview of the SCICHEM system has been provided earlier in this conference
- Detailed presentations on SCICHEM have been given at past EPA Modeling Conferences and past CMAS Modeling Conferences, as well as other venues

- SCICHEM development started in the late 1990s
- All existing versions of SCICHEM are based on a 1998 version of the SCIPUFF model

SCICHEM: Early Testing and Availability

- Testing and evaluation of past SCICHEM versions has been documented in EPRI reports
  - These EPRI reports are publicly and freely available at EPRI.com
  - Contact the EPRI Customer Assistance Center for information on how to download these reports (as well as many other EPRI reports) and a "legacy" version of SCICHEM

SCICHEM: The APT Branch

- In the 2000s, EPRI embedded the SCICHEM model into the EPA CMAQ model as a plume-in-grid module for sub-grid treatment of industrial plumes
- This PiG version of SCICHEM is known by the name "Advanced Plume Treatment" or APT, i.e. CMAQ-APT
- A version of CMAQ-APT was publicly released via the CMAS Center based on CMAQ4.6
- This version was based on the sectional MADRID aerosol treatment

SCICHEM: The APT Branch (Continued)

- Further development of APT continued using CMAQ 4.7.x as the host model
  - Added the option of modal aerosol treatment consistent with EPA's CMAQ AERO modules
  - Added the ability to run in parallel processors
  - UNC tested this version and provided useful feedback to model development
  - CMAQ-APT based on CMAQ4.7.1 was not released publicly as development efforts focused on releasing APT with CMAQ5.0 as the host model
  - This will be released soon in a interim release of CMAQ5.x in upcoming months

SCICHEM: SCIPUFF and APT in the 2000s

- The chemistry elements of SCICHEM underwent refinement through continued development of APT in the 2000s
- Similarly, the transport and dispersion elements of SCICHEM underwent refinement though continued development of SCIPUFF in the 2000s

- Evaluation of APT and SCIPUFF during this period has been documented in the peer-reviewed scientific literature

- However, this branching of the code has led to an effort to reconcile the two codes into one uniform code for the standalone dispersion model

Reconciliation of SCIPUFF and SCICHEM

- At the end of this reconciliation, there will be only one standalone model
- However, the two names will remain in order to emphasize whether chemistry is “on” or “off”
- The SCIPUFF/SCICHEM equivalency may be thought of as:
  - SCIPUFF is SCICHEM with chemistry off
  - SCICHEM is SCIPUFF with chemistry on

User Considerations of SCICHEM

- The pre-release version of SCICHEM does not have a graphics user interface (GUI)
  - The release version will include a basic GUI
- The release version will be available in Windows and Unix/Linux versions (which can also be run from a command line interface)

- The release version will be able to take advantage of multiple cores on a single machine
- It will include user manuals and documentation on evaluation and testing, as well as a test case

Availability of SCICHEM

- The new release of SCICHEM will become available to the community in upcoming months
- The model will be free, open-source and public-domain
- As derivative products of SCICHEM may be developed, EPRI will remain the "custodian" of the "core" SCICHEM model
  - Sage Management and ENVIRON are acknowledged as the current model developers

Distribution of SCICHEM and Comments

- Distribution of the "core" SCICHEM model will be through EPRI.com and through other linked portals
  - Potential portals include the websites of the model developers, CMAS Center and EPA Model Clearinghouse
- We encourage the community to test, evaluate and apply the model as appropriate and to provide feedback that will allow for future refinements

Selected SCICHEM Enhancements

Selected SCICHEM Enhancements

1. ***Allocatable Arrays***
   - Size limits are set in ini files
   - Code does not have to be recompiled
2. ***Nested meteorology grid***
   - High resolution terrain and meteorology can be used in nested grid
3. ***Improve convective boundary layer diffusion***
   - represent non-Gaussian vertical diffusion
   - "two-stream" model for skewness of vertical velocity pdf

Selected Enhancements (continued)

4. ***Dense gas effects***
   - Takes account of dense gas and ground interaction
5. ***Simple flashing liquid model***
   - Instantaneous release of cryogenic liquids due rupture of pressurized tank treated as two-phase mixture
6. ***Simple liquid pool model***
   - Evaporation based on mass transfer theory with consideration for different modes of heat transfer

Selected Enhancements (continued)

4. ***New sampler file format capabilities***
   - Moving samplers
   - Line of sight sampler
   - Integrated concentration
   - Time averaged concentration
   - Meteorological samplers for outputting meteorological data

Skew Turbulence in the Convective Boundary Layer

Convective Layer Diffusion

- Vertical diffusion in convectively-driven turbulence is non-Gaussian
- PDF of vertical velocity fluctuations is skewed
  - $$S = \left\langle w^3 \right\rangle \Big/ \left\langle w^2 \right\rangle^{3/2}$$
- Can be represented by two "streams"
  - narrow, high velocity updrafts
  - wide, low velocity downdrafts

Two-stream Model

- Represent skew-*w* PDF with 2 Gaussians
- From Luhar et al. (*Atmos. Env.*,**30**,1996)

$$\bar{w}_d = -m\sigma_d, \qquad \bar{w}_u = m\sigma_u$$

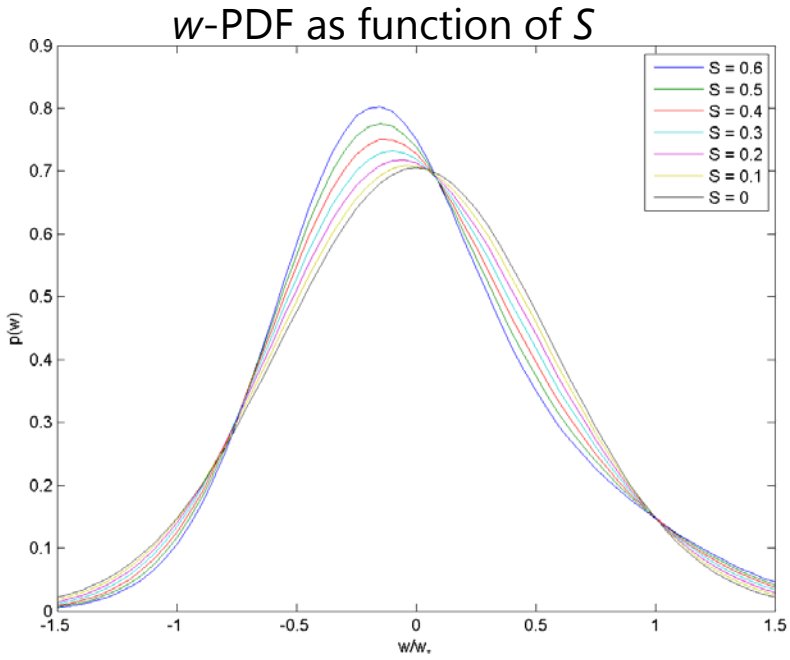
$$\sigma_d = \sigma_w \left(\frac{\lambda_u}{\lambda_d \left(1+m^2\right)} \right)^{1/2}, \qquad \sigma_u = \sigma_w \left(\frac{\lambda_d}{\lambda_u \left(1+m^2\right)} \right)^{1/2}$$

where $\lambda_d = 1-\lambda_u$, and $\lambda_u = \frac{1}{2}\left[1-\left(\frac{r}{4+r}\right)^{1/2}\right]$

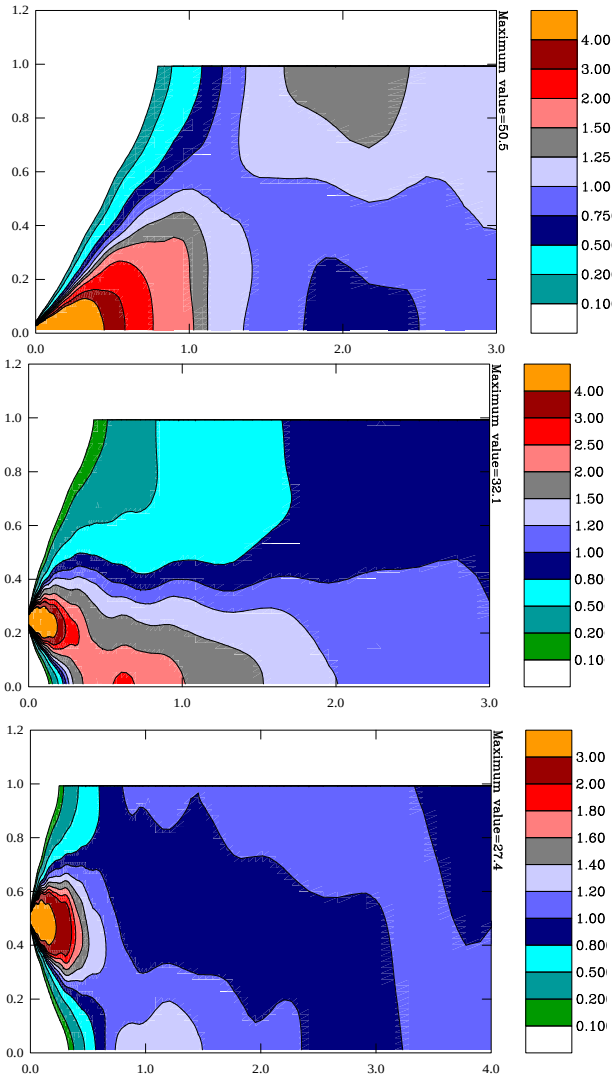
$$m = \frac{2}{3}S^{1/3} \qquad r = \frac{\left(1+m^2\right)^3 S^2}{m^2\left(3+m^2\right)^2}$$

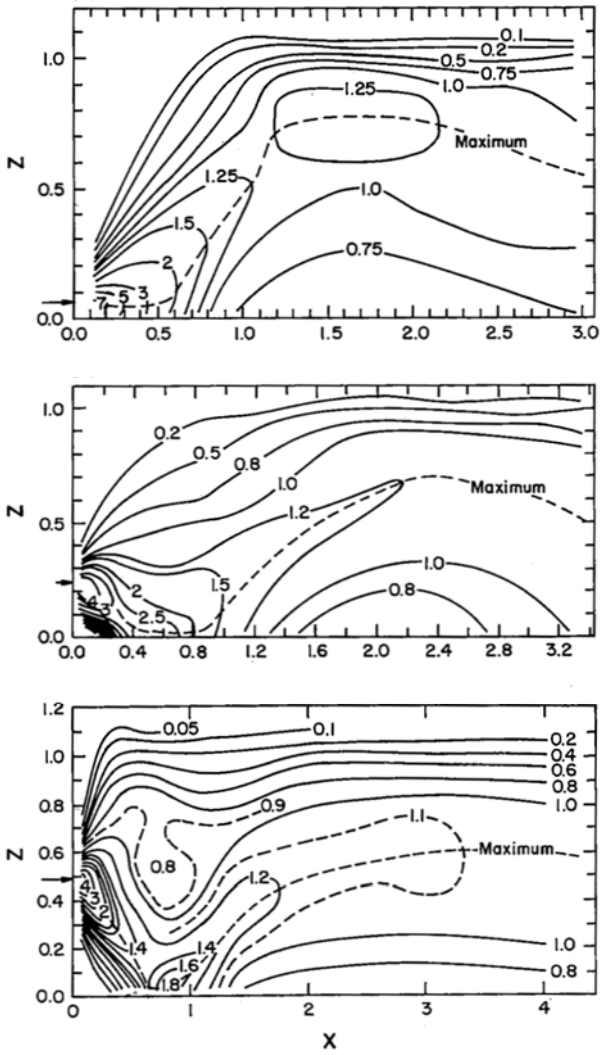
Puff Implementation

- Release 2 puffs ("u" and "d")
- Use appropriate *w*-statistics ($w_{d,u}$ and $\sigma_{d,u}$) to advect and diffuse
- Switch type on reflection at ground or inversion



Comparison with Deardorff and Willis

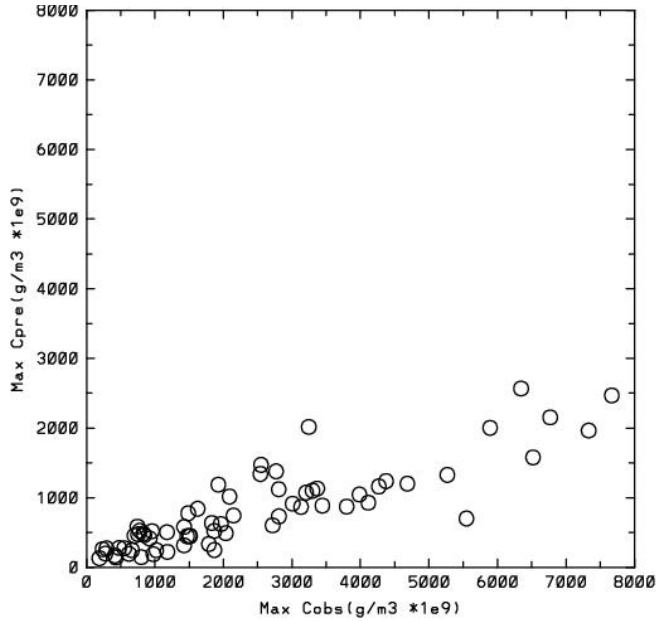




Improvement for Copenhagen Data

- Elevated release at 115m under convective conditions
- Surface concentration measurements
- Arc max comparisons

Standard Model



Skew Model