SUMMARY OF UPDATES TO SCICHEM-2012 MODEL AND COMPARISION OF RESULTS WITH OBSERVATIONS AND PREVIOUS VERSION RESULTS

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1. INTRODUCTION

Air quality models, are instrumental in providing valuable insights into the processes involved in the transport, dispersion and chemical transformation of pollutants in the atmosphere. The typical grid resolution in Eulerian models in air quality applications, are in the order of km, which can result in artificial diffusion of sources. Lagrangian models have an inherent advantage because they allow accurate treatment of wide range of length scales without any artificial diffusion problems.

Second-order Closure Integrated puff model, SCIPUFF (Sykes et al., 1993, Sykes and Henn, 1995), is a Lagrangian model in which a collection of three dimensional Gaussian puffs are used to represent a time-dependant concentration field. The SCICHEM (Karamchandani et al. 2000) model was developed for EPRI to include complete gas phase, aqueous phase and aerosol chemistry in SCIPUFF. It has been used as a stand alone model and also as a part of Plume-In-Grid model in the CMAQ-APT (Karamchandani et al. 2006), for multiple studies. The SCICHEM model was branched from the SCIPUFF model more than a decade ago. There have been significant advances in the core transport dispersion model in SCIPUFF since the SCICHEM model was branched from it more than a decade ago. In the current work we present some of the details of the enhancements and changes that have being implemented in the SCICHEM-2012 model.

2. MODEL DESCRIPTION

a. Puff dispersion model

The concentration field in SCIPUFF is described using the sum of contributions from a collection of three-dimensional puffs

$$c(\boldsymbol{x}) = \sum_{\alpha} c^{(\alpha)}(\boldsymbol{x}) = \sum_{\alpha} Q^{(\alpha)} G^{(\alpha)}(\boldsymbol{x}) \qquad (2.1)$$

Where, the Gaussian function for puff α is given by

$$G^{(\alpha)}(\boldsymbol{x}) = \frac{1}{V}\exp\left[-\frac{1}{2}\left(\sigma_{ij}^{(\alpha)}\right)^{-1}\left(x_i - \overline{x}_i^{(\alpha)}\right)\left(x_j - \overline{x}_j^{(\alpha)}\right)\right] \qquad (2.2)$$

and puff volume V, is

$$V = (2\pi)^{3/2}\left\|\sigma^{(\alpha)}\right\|^{1/2}$$

The spatial moments in Equations (2.1) and (2.2) are given by the integral over all space as

Zeroth moment- mass

$$Q^{(\alpha)} = \int_v c^{(\alpha)}\, dV$$

First moment- centroid

$$Q^{(\alpha)}\overline{x}_i^{(\alpha)} = \int_v c^{(\alpha)} x_i\, dV$$

Second moment- spread

$$Q^{(\alpha)}\sigma_{ij}^{(\alpha)} = \int_v c^{(\alpha)}(x_i - \overline{x}_i^{(\alpha)})(x_j - \overline{x}_j^{(\alpha)})\, dV$$

The model is advanced in time by solving ordinary differential equations for the puff moments (Sykes et al. 1993)

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b. Reactive chemistry

The chemical reaction processes are described in SCIPUFF by using the concept of multi-component material. The tracer or non-reactive contaminant is associated with a set of species concentrations, $\{s_i: i=1,n\}$. It is assumed that the associated species are transported and diffused in the same way as the conserved tracer material. We define the effective species-A concentration perturbation for puff-α as

$$\hat{\mathrm{A}}_\alpha = \sum_\beta \mathrm{I}_{\alpha\beta} \langle A \rangle_\beta$$

where, $\mathrm{I}_{\alpha\beta}$, the interaction coefficient is given by

$$\mathrm{I}_{\alpha\beta} = \int_v G^{(\alpha)}(\boldsymbol{x}) G^{(\beta)}(\boldsymbol{x}) dV$$

The reactions in SCICHEM are generalized in the form

$$A + \zeta B \xrightarrow{k} \sum \gamma_i P_i$$

A, B, P_i represent individual species, k is the reaction rate and ζ and γ_i are the stoichiometric coefficients. If ζ is non-zero, the reaction is assumed first order in A, and first order in B and the overall reaction is considered as second order. Note that the coefficient ζ is a multiplicative factor and does not imply higher-order reactions. If ζ is zero, the reaction is first order decay of A. The species perturbation concentrations are advanced using the equation.

$$\frac{d\hat{A}_\alpha}{dt} = -k(\hat{A}_\alpha \hat{B}_\alpha + \hat{A}_\alpha B_0 + A_0 \hat{B}_\alpha)$$

Here, A_0 and B_0 are the ambient concentrations of species A and B respectively. The background reaction rate $-k(A_0 B_0)$ is excluded in the equation.

3. ENHANCEMENTS

Some of the major enhancements that are part of the SCICHEM-2012 model are listed below:

- Allocatable Arrays
- Nested meteorology grid
- Skew Turbulence
- CB-05 chemical mechanism
- CMAQ 4.7 AE5 aerosol aqueous module
- Dense gas effects
- AERMOD type input file
- Area and Volume sources
- AERMET input file
- Same code for parallel runs
- Multiple PRIME sources
- New sampler capabilities

3.1 Allocatable arrays

The maximum number of puffs and maximum size of the meteorological grid were set using parameters in the previous SCICHEM model. SCICHEM-2012 uses allocatable arrays and pointers. The array sizes are set based on values from the SCIPUFF initialization file. Therefore, the code no longer needs recompilation when the maximum grid size or maximum number of puffs is changed.

3.2 Nested meteorology grid

The meteorological field description in SCIPUFF has been generalized to allow multiple fields to be specified. Nested domains can be used for cases where detailed description of smaller sub-domains are required. Each meteorological field contains a complete description of the spatial grid, surface terrain and all dynamic, thermodynamic and boundary layer field variables.

3.2 Skew turbulence

The probability density function of the vertical velocity in the convective boundary layer is non Gaussian. Under convective condition the updrafts are usually confined to narrow regions with high velocity and downdrafts occupy wider regions with lower velocity. The skew PDF can be well represented by using the sum of two Gaussian distributions. This is implemented in SCIPUFF by releasing two puffs, an up and a down puff. The appropriate w-statistics ($w_{d,u}$ and $\sigma_{d,u}$) are used to advect and diffuse the puffs.

3.3 CB-05 Chemical Mechanism

Carbon Bond (CB-05) mechanism (Yarwood et al. 2005) is used for stepping the gas phase chemistry in SCICHEM-2012. This mechanism consists of 156 reactions and 52 species.

3.5 CMAQ 4.7 AE5 aqueous aerosol module

CMAQ 4.7 AE5 aqueous aerosol module is used for stepping the aqueous aerosol species in SCICHEM-2012. AE5 uses the modal aerosol treatment with three modes viz. Aitken, Accumulation and Coarse. The total number of species needed is 80 for the aerosol module and 67 for the aqueous chemistry module.

3.6 Dense gas effects

Dense gas dynamics which account for the interaction of puffs with solid ground surface have been added. The dense gas dynamics cause lateral spreading as a dense cloud collapses and suppresses the vertical diffusion due to the stable buoyancy distribution.

3.7 AERMOD type input file

In addition to the standard SCICHEM namelist input files, SCICHEM-2012 can read inputs from AERMOD type files. The AERMOD type input files use pathways such as source pathways “SO”, control pathways “CO”, etc

3.8 Area and volume sources

New source types namely, area and volume can be specified using the AERMOD type input files.

3.7 AERMET input file

The meteorology input file format has been extended for SCICHEM-2012 to read AERMET surface and profile files.

3.8 Same code for single or multiple processor runs

In SCICHEM-2012, the single processor and multi processor code have been merged into a single version. The version can be set based on a logical from the SCIPUFF initialization file.

3.9 Multiple PRIME sources

Plume rise and building downwash effects are implemented in SCICHEM-2012 using the PRIME model (Schulman et al. 1997). Multiple PRIME sources can be specified using the AERMOD type input format.

3.10 New sampler capabilities

New sampler output capabilities such as Line of sight sampler, time averaged concentration, time integrated concentration and meteorological samplers have been added to SCICHEM-2012.

4. RESULTS AND DISCUSSION

4.1 Copenhagen Experiment

The Copenhagen Experiment consisted of ten continuous releases of SF_6 in Gladsaxe, Copenhagen in 1978 and 1979. The tracers were released from a TV tower 115m above ground level. Seven of the releases, were under convective boundary layer conditions and 3 were under neutral boundary layer conditions. The samplers were placed in arcs between 2 and 6 km from the source. The average surface concentrations for 20 minute intervals were measured for three successive periods. Using the standard model, the maximum arc concentrations were greatly under-predicted. When the skew turbulence model was applied, it resulted in a significant improvement over the standard model as seen in Fig. 1.

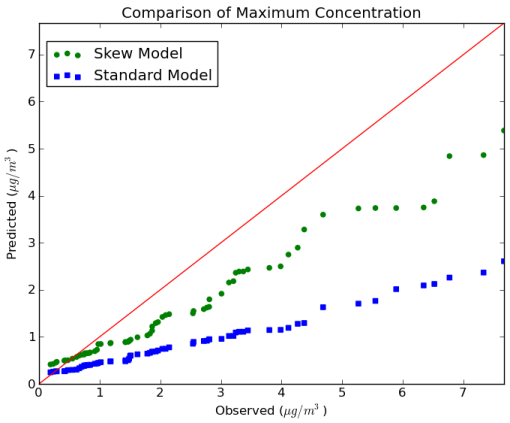

Fig.1. Maximum ordered concentration for Copenhagen data

4.2 AERMOD test cases

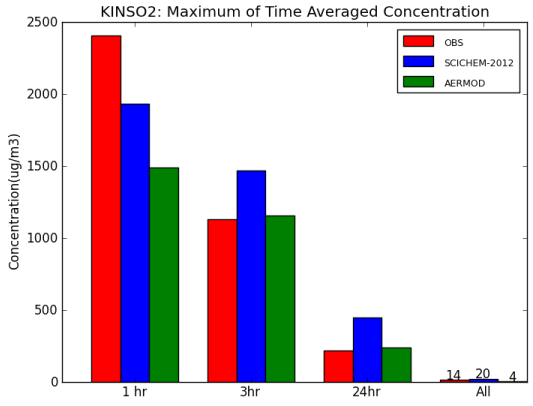

Fig. 2. Comparison of AERMOD and SCICHEM-2012 predicted maximum concentration values Kincaid(SO_2) field study

The results for Kincaid (SO_2) power plant field study (Liu and Moore 1984; Bowne et al. 1983) are presented in Fig. 2. This study included 30 SO_2 monitoring stations at downwind distance of 2 to 20 km. The source was a buoyant continuous release from a 187 m stack. SCICHEM-2012 model predicted values for 1-hr average and average over all time periods are closer to the observed value. The predicted to observed ratios were 0.8 and 1.4, compared to AERMOD ratios of 0.6 and 0.3. However, AERMOD model is more accurate in predicting the 3-hr and 24-hr highest concentration values (ratios of 1.0 and 1.1) when compared to SCICHEM-2012 (ratios of 1.3 and 2.1).

Using AERMOD type input files SCICHEM-2012 was also run for the Baldwin Power Plant study (Hanna and Chang, 1993). This study included three 184 m stacks with horizontal spacing of 100m between them. There were 10 SO_2 monitors at distance from 2 km to 10 kms. Fig. 3 shows the comparison of results from SCICHEM-2012 and AERMOD model for the Baldwin power plant field study. SCICHEM-2012 over-predicts the values for the maximum predicted average concentration over 1-hr, 3 hr, 24 hr and all time periods but the values are within 20% of the observed values with ratios of 1.1, 1.1, 1.2 and 1.1 respectively.

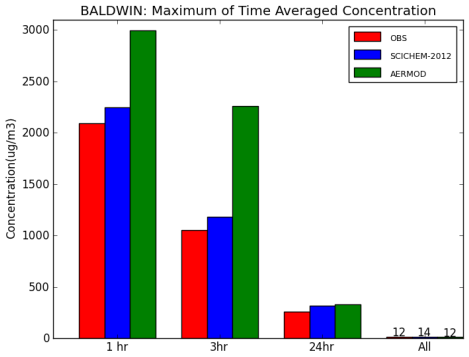

Fig. 3. Comparison of AERMOD and SCICHEM-2012 for Baldwin field study

4.3 Cumberland power plant cases

The SCICHEM-2012 model is used to simulate the results of the Cumberland Plume study conducted by TVA. On August 25th 1998 and July 15th 1999, the TVA helicopter made multiple traverses of the Cumberland plume at various downwind distances. The comparison of the SCICHEM-2012 model results with observed plume measurements and SCICHEM-01 model simulation results for a few traverses are presented here. There are significant deviations in the plume centerlines for observed and modeled measurements. The plume centerlines have been aligned with each other in order to compare them.

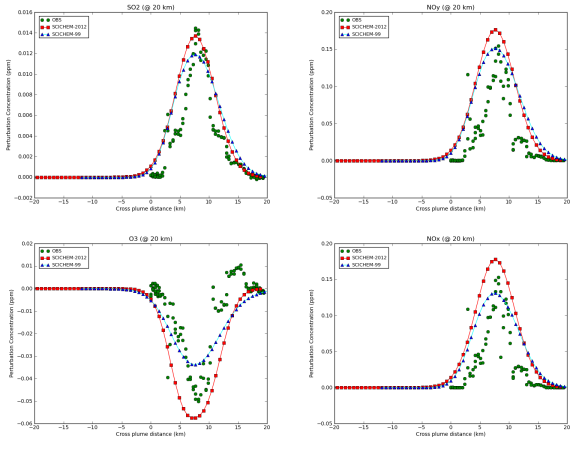

Fig. 4. Results from the TVA Cumberland plume traverse study at 20 Km on 08/25/98

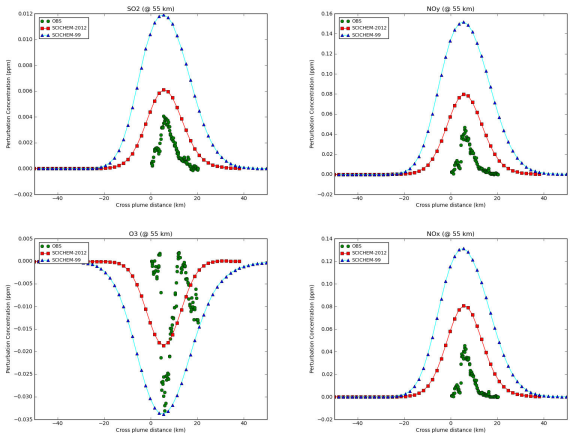

Fig. 5. Results from the TVA Cumberland plume traverse study at 55 Km on 08/25/98.

Fig. 4 and 5 shows the comparison of perturbed concentrations (difference from the background values) between the model results and observations for the plume traverse for 20 km and 55 km on Aug 25th 1998.

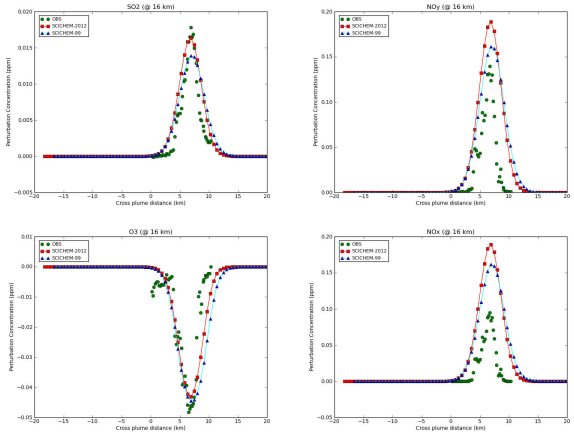

Fig. 6. Results from the TVA Cumberland plume traverse study at 16 km on 07/15/99

The results for 16 km and 62 km downwind distance on July 15th 1999 are given in Fig. 6 and Fig. 7 respectively. For close range (16 and 20km) traverses, the plume width as well as the concentration perturbation for the modeled results is in good agreement with the observed values for SO_2 and O_3. At medium range (55 and 62 km), SCICHEM-2012 over predicts the maximum concentrations and the plume width. However, it performs better than SCICHEM-99. In all cases, SCICHEM-2012 does a better job of predicting the SO_2 concentration when compared to SCICHEM-99.

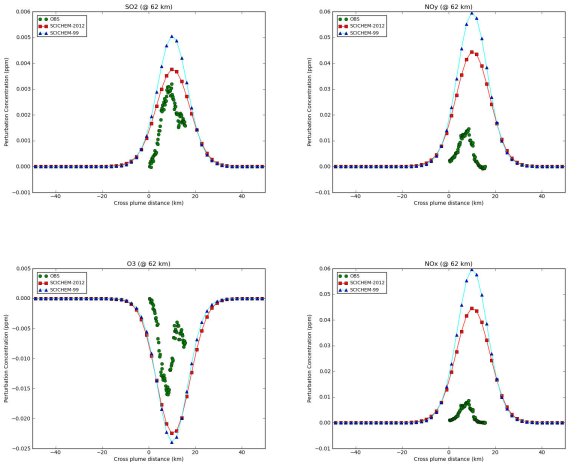

Fig. 7 Results from the TVA Cumberland plume traverse study at 62 km on 07/15/99.

5. SUMMARY AND CONCLUSION

The comparisons for the different SCICHEM versions show that tracer dispersion and transport has improved in majority of test cases. For AERMOD test cases we used the source and meteorological data at 1 hour intervals. However, it is recommended that higher frequency data be used if available and we will conduct further runs for some of the relevant cases.

In case of the TVA studies, the maximum SO_2 concentrations and the plume width from SCICHEM-2012 show improvements over SCICHEM-99. However, the NO_y concentrations are over predicted at distances less than or equal to 20 kms which might be related to uncertainties in NO_x emissions.

The preliminary results from SCICHEM-2012 (Beta) model are very promising. We will be conducting additional runs for further evaluation.

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