



SCIPUFF

AN OVERVIEW

Biswanath Chowdhury
Sage Management - an Xator Company

Description

- ▶ Second-order Closure Integrated Puff Model
- ▶ Gaussian puff atmospheric dispersion model
- ▶ Overlapping 3D puffs represent concentration field
- ▶ Solve ODE's for Puff moments

History

- ▶ 1984 - Development of Hierarchy of Improved Plume Models (EPRI funded)
- ▶ 1991 - Nuclear Cloud Rise (DOD funded)
- ▶ 1995 - Hazard Prediction and Assessment Capability (HPAC) (DOD funded)
- ▶ 1998 - SCIPUFF approved as alternative model (Appendix W)
- ▶ 2000 - SCICHEM 1.0 (EPRI funded)
- ▶ 2001 - Urban Wind Field model (DOD funded)

History (cont.)

- ▶ 2001 - Models-3/CMAQ-APT (EPRI funded)
- ▶ 2003 - Cryogenic pool model (DOD funded)
- ▶ 2004 - PRIME model in SCICHEM (EPRI funded)
- ▶ 2006 - Native coordinate support (DOD funded)
- ▶ 2009 - Source Estimation (DOD funded)
- ▶ 2011 - WRF and RAMS support (DOD funded)
- ▶ 2012-2015 - CB05 Gas Phase Chemistry, AERO5 Aerosol Chemistry (SCICHEM 3.0) (EPRI funded)

Development Team

- ▶ **Dr. Ian Sykes** - Environmental Sciences Group Manager
Overall model development, turbulence closure modeling of dispersion and concentration fluctuation intensity.
- ▶ **Dr. Stephen Parker** - Senior Engineer
Graphical output, user interfaces, general code architecture.
- ▶ **Douglas Henn** - Senior Engineer
Meteorological processing, boundary layer modeling.
- ▶ **Dr. Biswanath Chowdhury** - Senior Engineer
Thermodynamic modeling of liquid droplets and pools, model validation, SCICHEM development and source estimation.



Model Capabilities

Capabilities

- ▶ Transports gases, liquids and particles
- ▶ Includes primary and secondary evaporation for liquids
- ▶ Dynamics
- ▶ Variety of release types

Release Types

- ▶ Instantaneous
- ▶ Continuous
- ▶ Moving
- ▶ Pool
- ▶ Jet
- ▶ Stack (point)
- ▶ Area
- ▶ Volume

Unique Characteristics

- ▶ Carries variance as well as mean concentration
- ▶ Adaptive time stepping
- ▶ Adaptive grid resolution
- ▶ Efficient splitting/merging algorithm
- ▶ Laboratory scale to global scale

Model Validation

- ▶ PGT curves for short range, surface releases
- ▶ Instantaneous dispersion data (Weil et al., Mikkelsen et al., Hogstrom)
- ▶ Laboratory dispersion and fluctuation data (Fackrell and Robins, Deardorff and Willis)
- ▶ Continental-scale ANATEX field experiment
- ▶ EPRI PMV&D tall-stack emissions experiment

Model Validation (cont.)

- ▶ CONFLUX experiments (short range, fluctuations)
- ▶ Dugway chem/bio field tests
- ▶ Dense gas Model Data Archive (MDA)
- ▶ ATMES European tracer experiment (ETEX)
- ▶ Independent V&V studies
- ▶ Performs favorably compared to other LRT models



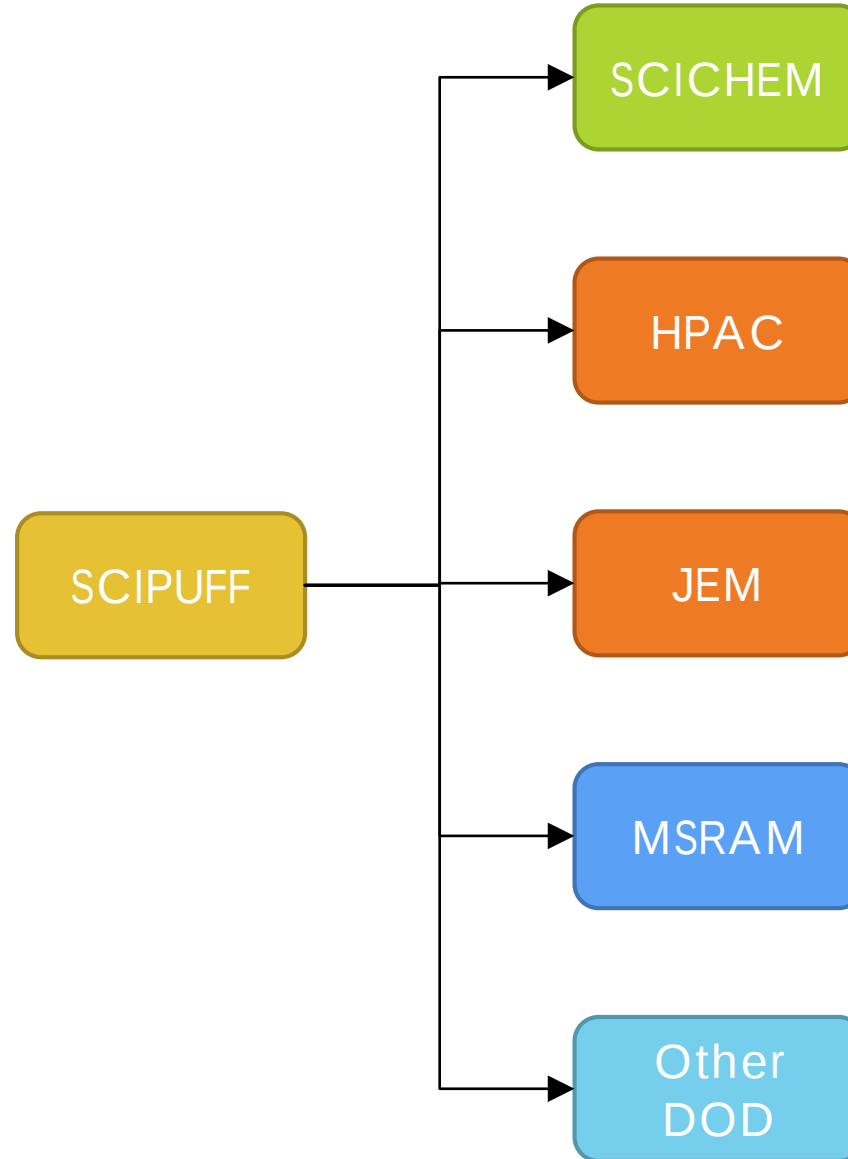
Research & Development

Collaboration

- ▶ LANL – Integration with QUIC-URB model
- ▶ ENSCO - Chemical deposition
- ▶ ARIA - Plume in grid with CHIMERE model
- ▶ ENVIRON - Gas, aerosol and aqueous phase chemistry
- ▶ PSU - Ensemble modeling
- ▶ AERODYNE - Source estimation
- ▶ NCAR - Source estimation

Systems using SCIPUFF

- **SCICHEM** – SCIPUFF with Chemistry
- **HPAC** - Hazard Prediction and Assessment Capability
- **JEM** - Joint Effects Model
- **MSRAM** - Maritime Security Risk Analysis Model
- Other Department of Defense systems



Current Research & Development

- ▶ OpenMP for parallel computations
- ▶ Integration with Los Alamos National Laboratory QUIC-URB model
- ▶ SCIPUFF as inline component of WRF-ARW simulations
- ▶ Source Attribution

R&D - Parallel SCIPUFF

- ▶ Speed increase of 1.7x - 3.4x on 4 core machines. Performance dependent on source characteristics, meteorology, sensors, etc.
- ▶ Virtually identical results between serial and parallel due to fixed list puff merging methodology.

Maximum difference*:

Concentration = 0% (identical)

Deposition = 0.00004%

Dosage = 0.000021%

* Intel Core i5, Linux OS, RAMS meteorology, continuous release, ~ 27 million data points(6,504 hours * 4,161 sensors)



R&D - QUIC-URB Integration

- ▶ Current effort to implement QUIC-URB as a nested model
- ▶ QUIC-URB represents building flow and dispersion in near-field
 - ▶ Lagrangian particle plus “Rockle” flow field
 - ▶ Multiple buildings, complex flow
- ▶ Aggregate particles into Gaussian puffs on nest boundary
- ▶ Hand over puffs to SCIPUFF for longer range dispersion
- ▶ Models run concurrently with continuous transfer
 - ▶ Seamless transition across boundary

R&D - WRF Integration

- ▶ Investigate embedding SCIPUFF inside WRF-ARW
- ▶ Run dispersion in sync with meteorology
- ▶ Direct access to full meteorological fields

R&D - Source Attribution

- ▶ Tracking of puff source origin and time of release
- ▶ Modified puff merging scheme with release time a mass-weighted quantity within puff
- ▶ Ability to query results for new sampler sets based on time(s) of release and release ID(s)



Conclusion

Summary

- ▶ SCIPUFF R&D ongoing and in managed environment
- ▶ Public domain source
- ▶ Sage works well with multiple contributors to advance capabilities
- ▶ Extensive model verification and validation
- ▶ Committed to regulatory air quality community

Applications

- ▶ Air Quality Permitting – Appendix W Alternative Model:
 - ▶ Long-range transport
- ▶ Emergency Response:
 - ▶ Department Homeland Security (DHS)
 - ▶ Department of Defense (DOD)
 - ▶ Coast Guard



Contact

Dr. Biswanath Chowdhury

biswanath.chowdhury@sage-mgt.net





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