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Evaluation of Urban Atmospheric Transport and Dispersion Models Using Data from the Joint Urban 2003 Field Experiment

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Sponsors:

U.S. Defense Threat Reduction Agency / Joint Science and Technology Office (DTRA / JSTO) Joint Program Manager for Information Systems / Joint Effects Model (JPM-IS / JEM)



- Past studies have compared urban modes within HPAC (DTRA)
 - Allows for better understanding of T&D modeling in urban areas
 - Permits an objective comparison of different modeling capabilities

• Urban HPAC modes

- Urban Canopy parameterization (UC)
- Urban Dispersion Model (UDM)
- Urban Windfield Module (UWM)
- Combination of UDM and UWM
- Micro-SWIFT/SPRAY (MSS)
- Studies were supported by comparisons to urban field experiments
 - Urban 2000 Salt Lake City
 - Mock Urban Setting Test (MUST) Dugway Proving Ground
 - Joint Urban 2003 (JU03) Oklahoma Čity
- Our most recent work has involved Urban HPAC comparisons to Joint Urban 2003 data
- This study extends our model comparisons to MESO/RUSTIC (ITT) and QUIC-URB/QUIC-PLUME (LANL), generalizing the results beyond HPAC



- Urban HPAC* / Urban Canopy
 - "Urban canopy" parameterization for SCIPUFF T&D calculations
- Urban HPAC* / UDM [UK Dstl]
 - Empirically-parameterized entrainment of puffs by urban obstacles
- Urban HPAC* / UWM [Titan]
 - Averaged RANS CFD urban wind flow model w/ turbulence & drag

• Urban HPAC* / MSS [ARIA/SAIC]

- Micro-SWIFT: Röckle-based urban wind flow model
- Micro-SPRAY: Urbanized Lagrangian particle T&D model
- MESO/RUSTIC [ITT]
 - RUSTIC: Reduced RANS-CFD urban wind flow model w/ turbulence
 - MESO: Urbanized Lagrangian particle T&D model
- QUIC-URB/QUIC-PLUME [Los Alamos NL]
 - QUIC-URB: Röckle-based urban wind flow model
 - QUIC-PLUME: Urbanized Lagrangian particle T&D model

These models incorporate different degrees and types of atmospheric physics

* HPAC uses SWIFT or MC-SCIPUFF (non-urban wind field models) for meteorological pre-processing and SCIPUFF for T&D in open (non-urban) terrain



Overview of Joint Urban 2003

- Large, multi-agency SF6 tracer release experiment conducted in Oklahoma City (OKC) in June and July of 2003
- Urban releases in 10 intensive operating periods (IOPs)
 - Combined puff and 30-minute continuous releases of SF₆ in each IOP
 - Our focus is on the 29 30-minute continuous releases, which were monitored for 2 hours following the start of each release
 - Each IOP used one of 3 downtown tracer release sites
 - Day continuous releases (09:00 15:30 CDT): IOPs 1-6, 17 releases
 - Night continuous releases (21:00-03:30 CDT): IOPs 7-10, 12 releases
- Meteorology; Heavily instrumented experiment
 - Data taken outside and within Oklahoma City urban domain
 - Multiple met sensors
 - » Surface and rooftop met stations (PWIDs)
 - » SODARs, Radiosondes, Tethersondes
 - » Lidars, Sonic anemometers, Ceilometer
 - » Radar, Airborne sensors
 - Oklahoma Mesonet data
- SF6 sensors
 - Fast-response tracer analyzers
 - Bag samplers: Programmable Integrating Gas Samplers (PIGS)
 - Sampler coverage in OKC Central Business District (CBD) and downwind sampler arcs



Surface Samplers Used in Comparison (OKC Central Business District)

48 of 55 near-ground (3 m AGL) CBD samplers used





Methodology



Model Parameters

- Urban HPAC Urban Canopy
 - HPAC default parameters
- Urban HPAC Urban Dispersion Model
 - HPAC default parameters, except used "higher fidelity" UDM mode
- Urban HPAC Micro-SWIFT/SPRAY
 - 1000 m × 1000 m grid (3 m horizontal resolution)
 - Model domain larger for SCIPUFF T&D
 - 100,000 Micro-SPRAY particles
- MESO/RUSTIC
 - 1200 m \times 1500 m \times 200 m grid (5-10 m variable resolution)
 - » RUSTIC ran near the 1 GB memory limit of some of our computers
 - 600,000 MESO tracers
 - Sensible heat flux values from Indiana U. sites (5-6 km upwind)
 - Surface roughness and displacement height from JU03 data
- QUIC-URB/QUIC-PLUME
 - 1180 m × 1110 m × 230 m grid (5 m × 5 m × 6 m resolution)
 - 400,000 QUIC-PLUME particles`

Study philosophy: operate each model according to the recommendations of its developers, rather than strive for perfect parity in model parameters



- Two sources of upwind wind velocity data ("MET")
 - <u>PNS:</u> 10- or 15-minute frequency vertical wind profile (30 500 m AGL) from PNNL SODAR (~1.5 km upwind of releases)
 - <u>PO7</u>: 15-minute central vector average of single-altitude 40 m AGL measurements from Post Office rooftop sonic (slightly upwind of releases)
- "Default" values of other meteorological parameters used for all models when possible
- PNS and PO7 meteorology was processed using MC-SCIPUFF and SWIFT, respectively, in Urban HPAC runs
 - In previous studies we observed HPAC performance differences that may be associated with the choice of meteorological pre-processor

RUSTIC-specific meteorology

- Four RUSTIC steady-state wind solutions (4 runs) were generated per release using 15-minute forward-in-time vector-averaged winds
 - » Other models use wind input as described above
- Upwind sensible heat flux values derived from Indiana U. towers
- Estimates of upwind surface roughness length and displacement height required for single-altitude (e.g., PO7) wind input
 - » Values of z0 = 0.5 m, d = 11.0 m derived by ITT from JU03 data



Overview of Comparison Methodology

- Considered only predictions that were common to all three modeling • suites

 - 48 (of 55) surface CBD samplers from NOAA ARL FRD
 » Limited by size of QUIC OKC building database and by MESO/RUSTIC runtimes and memory requirements
 - 1 hour of simulated transport and dispersion
 - » Limited by MESO/RUSTIC runtimes

Visual comparison of contour plots of observations and predictions ٠

- **Calculate Measures of Effectiveness (MOEs) and Statistics** ٠
 - Calculate 2D user-oriented MOEs and 13 statistics for different and various quantities of interest
 - » 48 surface CBD samplers
 - » 30-min and 1-hour average concentrations, both 30-minute intervals together
 - » For Statistics
 - Focus here on Normalized Absolute Difference, Fractional Bias
 - » For MOEs
 - "Summed" averaged concentration
 - Threshold Exceedance (25, 250, 2500 pptv) → "Hazard Areas"
 - Focus here on 30-minute average concentration MOEs
 - Predictions and observations are paired in time and space
- Non-parametric tests ("2-dimensional sign" & general permutation) to • check for significant statistical differences
 - Hypothesis tests on metrics paired by release



Run Times per Simulated Release

	Model	T&D	Grid size / Min. grid res.	Num. particles	Computer	Mean Run Time
Urban HPAC	UC	2 hr			Dell Xeon 3.8 GHz, 2 GB RAM	1.9 min [PO7]
	UDM	2 hr			Dell Xeon 3.8 GHz, 2 GB RAM	2.9 min [PO7]
	MSS	2 hr	1.00×1.00 / 3 m	100k	Dell Xeon 3.8 GHz, 2 GB RAM	61.8 min [PO7]
MESO/ RUSTIC	RUSTIC	1 hr	1.20×1.50×0.20 km / 5 m		Various Dell (≥2 GB RAM)	75 <u>hr</u> [PO7] [4 RUSTIC runs]
	MESO	1 hr	1.20×1.50×0.20 km / 5 m	600k	Various Dell (≥2 GB RAM)	2.5 <u>hr</u> [PO7]
QUIC	QUIC- URB	2 hr	1.18×1.11×0.23 km / 5 m		MacBook Pro (2.33 GHz, 2 GB RAM)	6.9 min [PO7+PNS]
	QUIC- PLUME	2 hr	1.18×1.11×0.23 km / 5 m	400k	MacBook Pro (2.33 GHz, 2 GB RAM)	29.1 min [PO7+PNS]

- UC and UDM: ~ Minutes / Release
- MSS and QUIC: ~ Tens of minutes / Release
- MESO/RUSTIC: ~ Tens of hours / Release



Comparison of Previous and Current

Joint Urban 2003 Studies Scope of previous Urban HPAC JU03 evaluations

- 29 continuous 30-minute SF6 releases
- 110 near-surface samplers in OKC Central Business District (CBD) and on 1 km, 2 km, 4 km downwind sampler arcs
- 2 hours of simulated transport and dispersion per release
- 5 Urban HPAC modes: UC, UDM, UWM, UDM+UWM, MSS
- Many sources of wind input: upwind and downwind measurements, single-altitude and vertical profile, OKC MesoNet data, gridded numerical weather predictions
 - » Some pre-processed with SWIFT, some with MC-SCIPUFF

• Scope of current Urban HPAC – MESO/RUSTIC – QUIC comparison

- Scope scaled down in order to put all models on equal footing
- 29 continuous 30-minute SF6 releases
- 48 near-surface samplers in OKC CBD only
- 1 hour of simulated transport and dispersion per release
 - » Appropriate given the size of the modeling domain
- 3 Urban HPAC modes only: UC, UDM, MSS
- Added 2 more models (MESO/RUSTIC and QUIC)
- Two sources of wind input (upwind measurements)
 - » One single-altitude measurement, one vertical wind profile
 - » One pre-processed with SWIFT, one with MC-SCIPUFF



Urban HPAC – MESO/RUSTIC – QUIC Comparative Results: Normalized Absolute Difference and Fractional Bias (30-minute average concentrations in OKC CBD)



Normalized Absolute Difference 30 minute average concs. PNS [HPAC MC-SCIPUFF]





Normalized Absolute Difference 30 minute average concs. PO7 [HPAC SWIFT]





Fractional Bias 30 minute average concs. PNS [HPAC MC-SCIPUFF]





Fractional Bias 30 minute average concs. PO7 [HPAC SWIFT]





Urban HPAC – MESO/RUSTIC – QUIC Comparative Results: Two-Dimensional User-Oriented Measures of Effectiveness (MOEs) (30-minute average concentrations in OKC CBD)





Average Concentration MOE 30 minute average concs. PNS [HPAC MC-SCIPUFF]





Average Concentration MOE 30 minute average concs. PO7 [HPAC SWIFT]



Summary of Results: Urban HPAC vs. MESO/RUSTIC vs. QUIC

- Day-night performance discrepancy (particularly bias metrics)
 - UC and DM tend to under-predict at day and over-predict at night
 - MSS and QUIC do not seem to have this bias discrepancy, with a small overall over-prediction bias
 - MESO/RUSTIC also appears to have little day-night discrepancy (somewhat larger with PNS MET than with PO7 MET), perhaps also with a small overall over-prediction bias
 - » Some substantial MESO/RUSTIC under-predictions at night using PNS MET

• Relative model performance – Day

- By scatter metrics, no model has clear advantage
 Bossible exception: MESO/DUSTIC with DNS MET
 - » Possible exception: MESO/RUSTIC with PNS MET
- By bias metrics, MSS, MESO/RUSTIC, and QUIC are closer to zero prediction bias than UC or UDM, which under-predict

• Relative model performance – Night

- Most models tend to outperform UC at night, particularly for PO7 (HPAC SWIFTpreprocessed) MET
- QUIC is one of the best performers at night for PO7 MET, but one of the worst for PNS MET
 - » Problem with handling low-altitude nighttime winds?
- Runtime considerations
 - UC, UDM < MSS, QUIC < MESO/RUSTIC



- Heat flux inputs for HPAC UC, UDM, MSS for PO7 and PNS MET
 - Adding heat fluxes to HPAC causes some performance differences among UDM and UC during the day in the CBD, but does not affect relative model ranking
 - Results available in backup slides
- Investigation of effects of low altitude winds at night in Joint Urban 2003
 - Including mini-SODAR wind data below ~70-100 m AGL (e.g., in PNS MET) degrades both Urban HPAC and QUIC performance
 - MESO/RUSTIC investigation underway
- Investigations of model performance at low grid resolution or low particle number (with decreased run times)
 - Significant decreases in run times correspond to significant decreases in performance



Backup



Summary of Runs

- Urban HPAC (v4.04 SP3)
 - UC: 20 runs (10 IOPs × 2 MET options)
 - UDM: 20 runs (10 IOPs × 2 MET options)
 - MSS: 58 runs (29 releases × 2 MET options)
 - » MSS run within HPAC 4.04 using developer-provided *.DLL files
 - − All of the above were run again using heat fluxes as input (for parity with MESO/RUSTIC) \rightarrow 196 Urban HPAC runs
 - Two hours of simulated T&D per release (CBD + Arc samplers)

• MESO/RUSTIC (Jan. 2007 version)

- RUSTIC: 229 runs (29 releases × 2 MET options × 4 wind updates per release, minus gaps in PO7 data)
- MESO: 58 runs (29 releases × 2 MET options)
 - » Post-processing: Gridded concentrations interpolated to sampler locations
- RUSTIC and MESO were run as DOS executables using *.BAT files
- One hour of simulated T&D per release (CBD samplers)
- QUIC (v4.7)
 - QUIC-URB: 58 runs (29 releases × 2 MET options)
 - QUIC-PLUME: 58 runs (29 releases × 2 MET options)
 - QUIC executables run from MATLAB programming environment
 - Two hours of simulated T&D per release (Partial CBD samplers)

For parity between modeling suites, we only <u>compared</u> 1 hour of simulated T&D over a reduced set of 48 OKC CBD samplers



Summary of <u>Previous</u> Urban HPAC Joint Urban 2003 Findings

- Performance of most Urban HPAC models (except MSS) differs between day and night
 - Under-prediction bias for daytime releases vs. over-prediction bias for nighttime releases
 - Degraded performance for nighttime predictions w/ SWIFT (vice MC-SCIPUFF) processed MET
- MSS performance differed from that of other Urban HPAC modes
 - Lack of significant performance difference between daytime and nighttime predictions
 - MSS tended to produce the least prediction bias of all the Urban HPAC modes
- Use of UWM within HPAC did not result in significant performance improvements
- MSS and UDM (and combined UDM+UWM) improved performance over baseline UC capability <u>for nighttime releases</u> when <u>SWIFT-</u> <u>processed MET</u> input was used
 - Relative performance of Urban HPAC modes for nighttime releases using MC-SCIPUFF processed MET input options was mixed and inconsistent
- Relative performance of Urban HPAC modes <u>for daytime releases</u> was <u>mixed and inconsistent</u> across MET input options



250 pptv Concentration Threshold MOE 30 minute average concs. PNS [HPAC MC-SCIPUFF]





250 pptv Concentration Threshold MOE 30 minute average concs. PO7 [HPAC SWIFT]





HPAC Heat Fluxes



Average Concentration MOE 30 minute average concs. PNS (no heat flux) vs. PSHM (heat flux)





250 pptv Concentration Threshold MOE30 minute average concs.PNS (no heat flux) vs. PSHM (heat flux)





Average Concentration MOE 30 minute average concs. PO7 (no heat flux) vs. PO7H (heat flux)





250 pptv Concentration Threshold MOE30 minute average concs.PO7 (no heat flux) vs. PO7H (heat flux)





- The addition of heat fluxes to Urban HPAC may have a nonnegligible effect in the OKC CBD:
 - UC and UDM (but not MSS)
 - Daytime (but not nighttime)
- If there is any change, heat fluxes tend to improve the results slightly
 - Bias seems to be improved more than scatter
- The addition of heat fluxes to Urban HPAC does not seem to affect the relative ranking of models (either within HPAC or against MESO/RUSTIC and QUIC)



MESO/RUSTIC Computational Grid

Variable-resolution computational grid is $1200 \text{ m} \times 1500 \text{ m} \times 200 \text{ m}$ ($190 \times 220 \times 33 = 1.38$ Million grid points, Resolution = 5-10 m)



Blue Rectangle = boundaries of 1200 m x 1500 m RUSTIC grid

Green Rectangle = boundaries of 1200 m x 1400 m buildings domain

Red Triangles = NOAA ARL FRD surface samplers in the CBD

Yellow Stars = tracer gas release sites

Prevailing winds are usually from the south