Evaluation of the Atmospheric Transport Model in the MACCS2 Code and its Impact on Decision Making at Department of Energy Sites

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June 5, 2012

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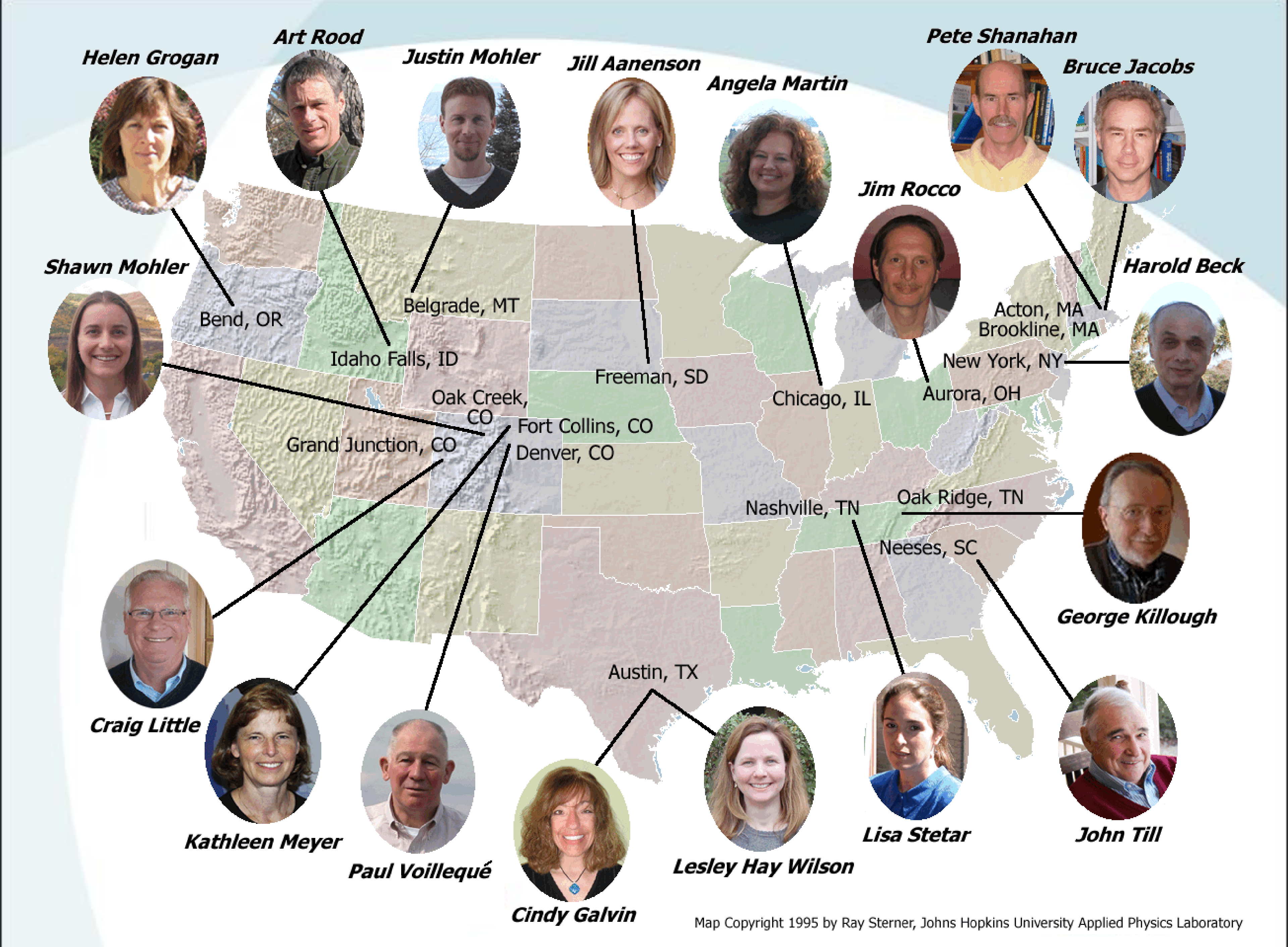

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RAC Historical Dose Reconstruction Projects

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Environmental Risk Assessment

"Understanding and communicating the movement of radionuclides and chemicals released to the environment, resulting exposure to humans, and the subsequent dose or risk from exposure."

Types of Dose/Risk

- Medical
- Occupational
- Public

Dose/Risk Can Be Estimated for

- Real people
- Hypothetical people

Purpose of Assessments

- Compliance
- Decision making
- Epidemiology
- Emergency response

Approaches to Estimating Risk

- In certain situations, and depending upon the decisions to be made, if the results of relatively conservative screening assessments demonstrate that doses are well below the dose criteria (e.g., a factor of three or more), there may be no need for further detailed assessment
- The deterministic approach multiplies single values for parameters chosen to be deliberately conservative to take account of uncertainty
- The probabilistic approach incorporates distributions for parameter values
- Combination of deterministic and probabilistic

Types of Dose Assessment in Different Exposure Situations

Situation	Type of Assessment		
	Retrospective	**Current**	**Prospective**
Normal	Past operation	Present operation	Design of new facility
Existing	Earlier exposures	Present exposure	Future prolonged exposures (e.g., after remediation)
Emergency	Actual impacts after emergency	Actual emergency	Emergency planning

Risk Assessment

$$\text{Risk} = (S \cdot T \cdot E \cdot D \cdot R)_{uvcp}$$

where

S = source term

T = environmental transport

E = exposure

D = dose coefficient

R = risk coefficient

u = uncertainty

v = validation

c = communication of results

p = participation of stakeholders

RAC Dose Assessment for MACCS2 Evaluation

$$\text{Dose} = (S \bullet \partial T \bullet E \bullet D)_{vcp}$$

where

S = source term (deterministic)

∂T = environmental transport (partial transport limited to atmospheric dispersion — deterministic but based on distribution of meteorological data)

E = exposure (deterministic)

D = dose coefficient (deterministic)

v = validation

c = communication of results

p = participation of stakeholders

MACCS2 Was Designed to Have Built-In Conservatism

DOE-EH-4.2.1.4-MACCS2-Code Guidance

MACCS2 Computer Code Application Guidance for Documented Safety Analysis

Final Report

Qualitative Effect of the Codes on Safety Analysis

The gross effect of the use of computer codes can be evaluated by examining their effect on the final MOI dose values calculated as part of the accident analysis. The values chosen or calculated for each parameter in the dose equation are near the conservative tail of any distribution that would be assigned to the individual parameter. Therefore, when each parameter is multiplied using the five-factor formula to obtain the dose, the conservatism in the calculation grows. If applied consistently in each phase of the process and in a reasonably bounding manner, this large conservatism in the calculation has always provided the DOE safety analysis process with sufficient margin when the doses are used to make decisions regarding safety. Even if a single value in the dose calculation were off by an order of magnitude, the resulting value would still not approach the mean value of dose if a cumulative distribution of dose also were calculated.

MACCS2

- **Built-in conservatisms in the model and methodology**
  - Straight-line Gaussian Plume Model
  - Conservative Source term
  - Meteorology (e.g., no buoyancy, no plume meander, no wet deposition, 95th percentile concentration from 1 year of data)
  - Exposure scenario (e.g., boundary exposure, duration of the accident)

Assessment Question

Does the predicted dose from MACCS2 code as prescribed in the DOE Guidance Manual (DOE-EH-4.2.1.4-MACCS2-Code Guidance) meet the target dose criteria?

Comparison of the Atmospheric Transport Model in MACCS with Lagrangian Puff Models

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Evaluation of (T) in MACCS2 Model

- Compare the MACCS2 dispersion model with state-of-the-art Lagrangian Puff Dispersion models, CALPUFF and RATCHET
- CALPUFF is EPA approved complex terrain model
- RATCHET was developed for the Hanford Environmental Dose Reconstruction Project and is incorporated into the GENII and RASCAL dose assessment models

Objective

- Review Gaussian plume and Lagrangian puff atmospheric dispersion models as implemented in MACCS, CALPUFF and RATCHET models
- Provide a comparison of model results for the WTP accident analysis at Hanford

Types of Air Dispersion Models

- **Classic Gaussian Plume Model**
  - Relatively simple analytical model for temporally and spatially constant wind field and steady-state release that forms the basis of most old-generation regulatory compliance modeling
- **Augmented Gaussian Plume Model**
  - Based on the classic Gaussian Plume model, but includes mixing lid reflection and dry and wet deposition processes. (MACCS2)

Types of Air Dispersion Models (continued)

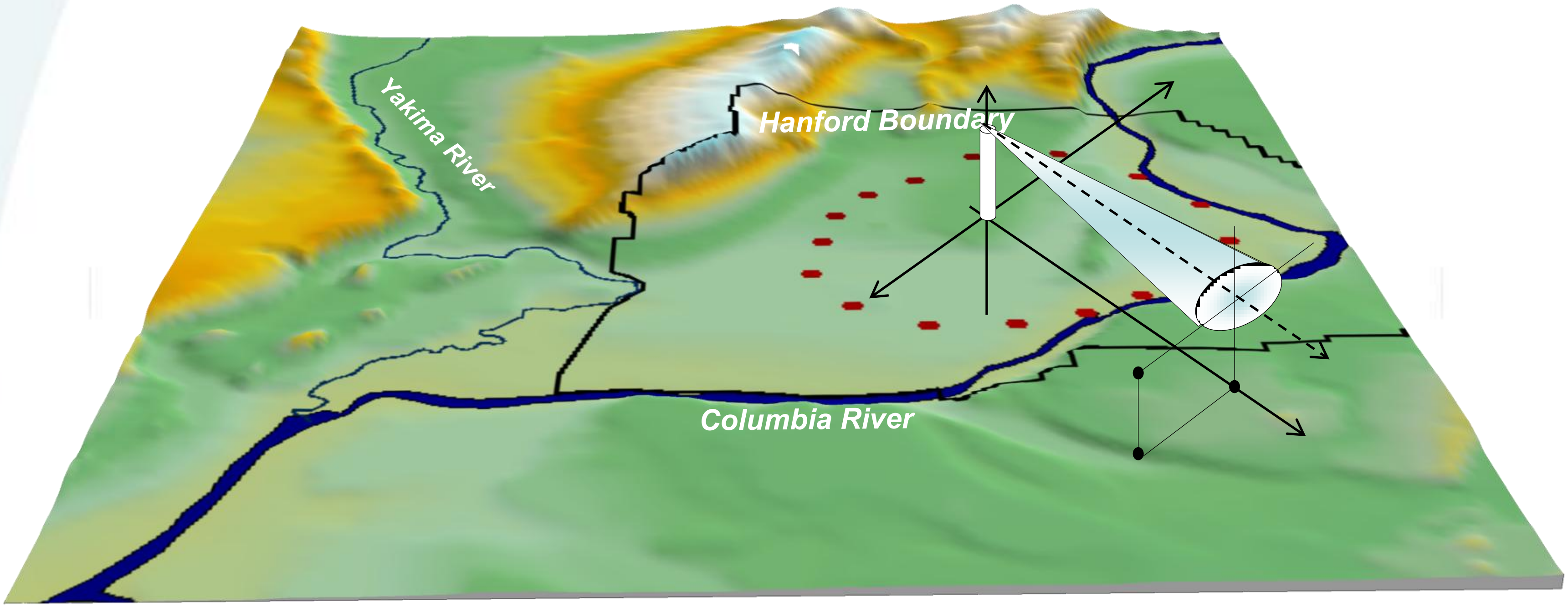
- **Steady-State Plume Model**
  - Similar to Augmented Gaussian Plume model, but incorporates recent understanding of the stable and convective boundary layer, vertical inhomogeneity, and terrain effects (AERMOD)
- **Puff (Lagrangian) Dispersion Model**
  - More complex model for evaluation of non-steady-state releases in temporally and spatially variable wind fields (CALPUFF, RATCHET)

Overview of MACCS CALPUFF/RATCHET

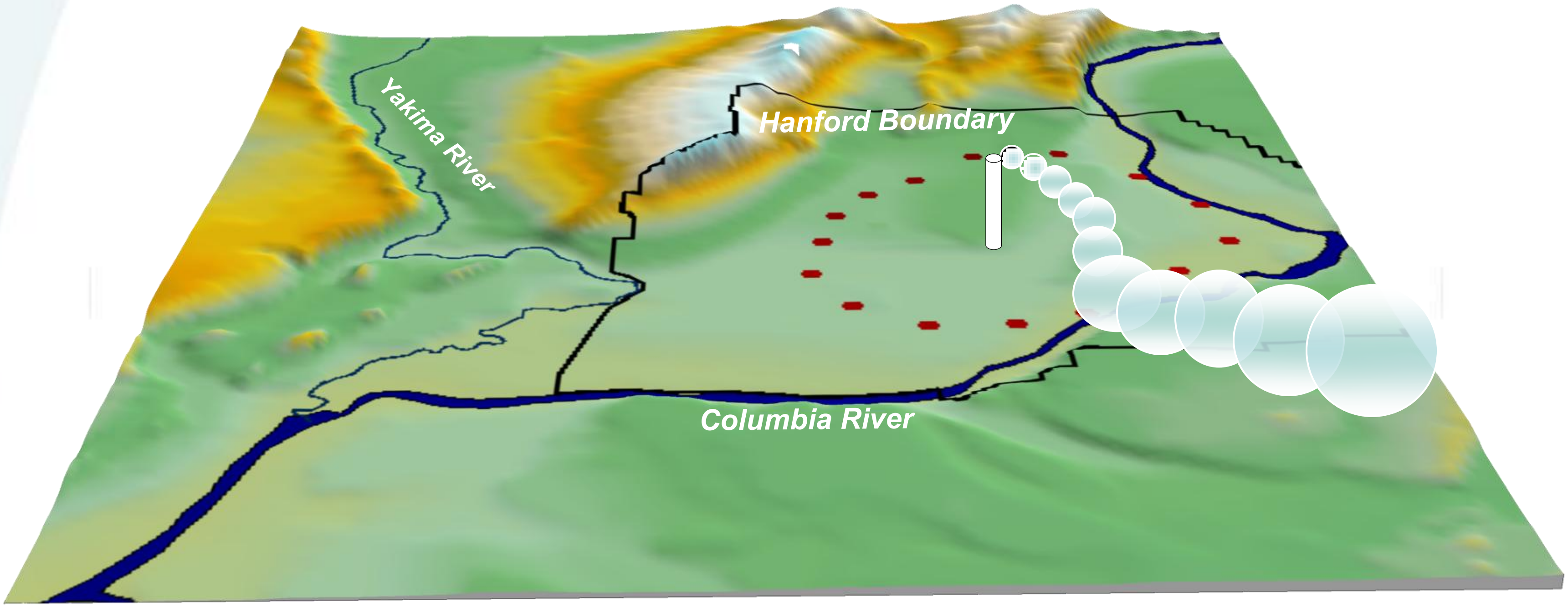
- **MACCS**
- Augmented Gaussian plume model
- Diffusion coefficients a function of downwind distance and stability class
- Fixed deposition velocity

- **RATCHET/CALPUFF**
- Lagrangian puff model
- Turbulence-based /similarity theory diffusion coefficients
- Calculated deposition velocity
- Terrain effects (CALPUFF)

Gaussian Plume Model



Lagrangian Puff Model



Turbulence Characterization – Atmospheric Stability

- **Classical GP models use a classification scheme for atmospheric stability**
- **Six classes (termed Pasquill-Gifford Stability Categories) are generally recognized**
  - Stability Class A (extremely unstable)
  - Stability Class B (moderately unstable)
  - Stability Class C (slightly unstable)
  - Stability Class D (neutral)
  - Stability Class E (slightly stable)
  - Stability Class F (moderately stable)
  - Stability Class G (extremely stable) OPTIONAL

State-of-the-Art Schemes for Characterizing Turbulence

- **Direct measurements of turbulence (σ_v and σ_w)**
  - Not very practical – airports do not routinely measure turbulence directly
    - σ_v – standard deviation of the horizontal cross wind component of the wind (m/s)
    - σ_w – standard deviation of the vertical component of the wind (m/s)
- **Estimate σ_v and σ_w from micrometeorological parameters (Hanna et al. 1982; Scire et al. 2000)**
  - u* – friction velocity
  - w* – convective velocity scale
  - h – mixing height
  - L – Monin-Obukhov Length

Micrometeorological Parameters

- **The micrometeorological parameters (u*, w*, L, and h) can be estimated from**
  - Routine meteorological data collected at airports (temperature, cloud cover, ceiling height, surface pressure, relative humidity, wind speed and direction)
  - Estimates of the surface roughness height (z_o)
  - Time-of-day and solar elevation angle
  - Land use (i.e., urban, rural, desert, forest, etc.)

Representative Equations for Micrometeorological Parameters

- **Friction velocity for neutral and unstable conditions (Scire et al. 2000)**
  - k = von Karman constant (0.4)
  - z_o = roughness height (m)
  - ψ_m = stability correction factor
  - u = wind speed (m/s)

$$u* = \frac{k\,u}{\ln\left(\frac{z}{z_o}\right) - \psi_m\left(\frac{z}{L}\right) + \psi_m\left(\frac{z_o}{L}\right)}$$

- **Convective velocity scale (Scire et al. 2000)**
  - Q_h = sensible heat flux (W/m2)
  - c_p = specific heat of air (996 m^2/s^2 K)
  - T = air temperature
  - h = convective mixing height

$$w* = \left(\frac{q Q_h h}{T \rho c_p}\right)^{1/3}$$

Representative Equations for Micrometeorological Parameters

- **Monin-Obukhov Length (Scire et al. 2000)**
  - Positive for stable conditions
  - Negative for unstable conditions
  - Infinite for neutral conditions
  - The absolute value of L can be thought of as the depth of the mechanically mixed layer near the surface
  - u* and L are calculated by iteration

$$L = \frac{\rho\, c_p\, T\, u_*^3}{k\, g\, Q_h}$$

- **Mixing height for neutral and unstable conditions (Ramsdell et al. 1994)**
  - β = constant, f = coriolis parameter ($\sim 10^{-4}\ s^{-1}$)

$$h = \frac{\beta\, u_*}{f}$$

Relationship between Monin-Obukhov Length and Stability Class

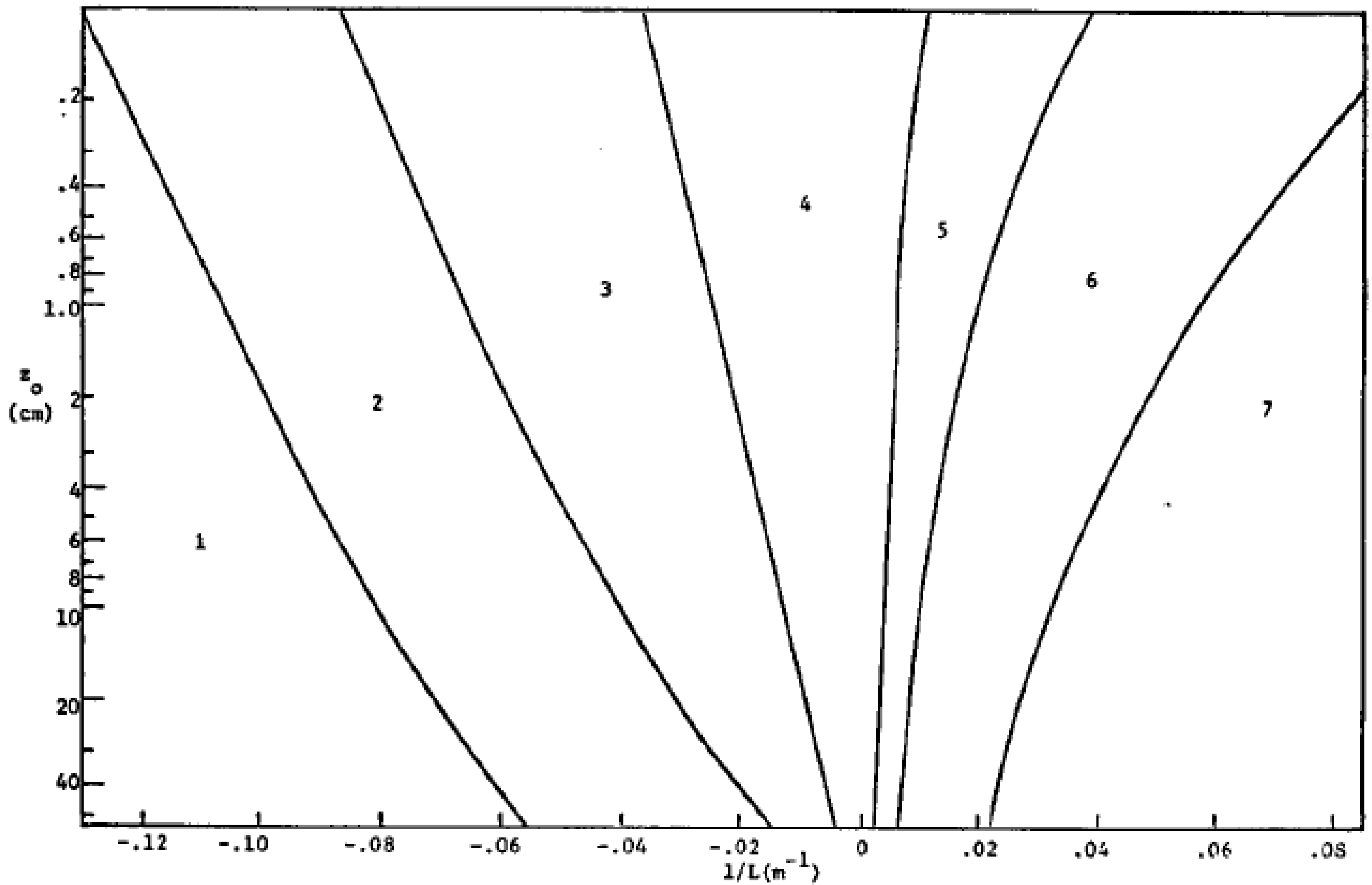


Fig. 5. $1/L$ as a function of Turner classes and z_0.

Representative Equations for σ_v and σ_w

- **Stable** $$\sigma_v = c_1 u_* \left(1 - \frac{z}{H}\right), \quad \sigma_w = c_2 u_* \left(1 - \frac{z}{H}\right)$$
  - c_1 ~2, c_2 = 1.3, z = puff transport height
- **Neutral** $$\sigma_v = c_1 u_* \exp\left(\frac{-2f}{u_*}\right), \quad \sigma_w = c_2 u_* \exp\left(\frac{-2f}{u_*}\right)$$
  - f = coriolis parameter (~10^{-4} s^{-1})
- **Unstable** $$\sigma_v = u_* \left(12 - \frac{H}{2L}\right)^{1/3}, \quad \sigma_w = 1.3 u_* \left(1 - \frac{3z}{L}\right)^{1/3}$$

(from Hanna et al., 1982, Ramsdell et al., 1994)

Turbulence-Based σ's

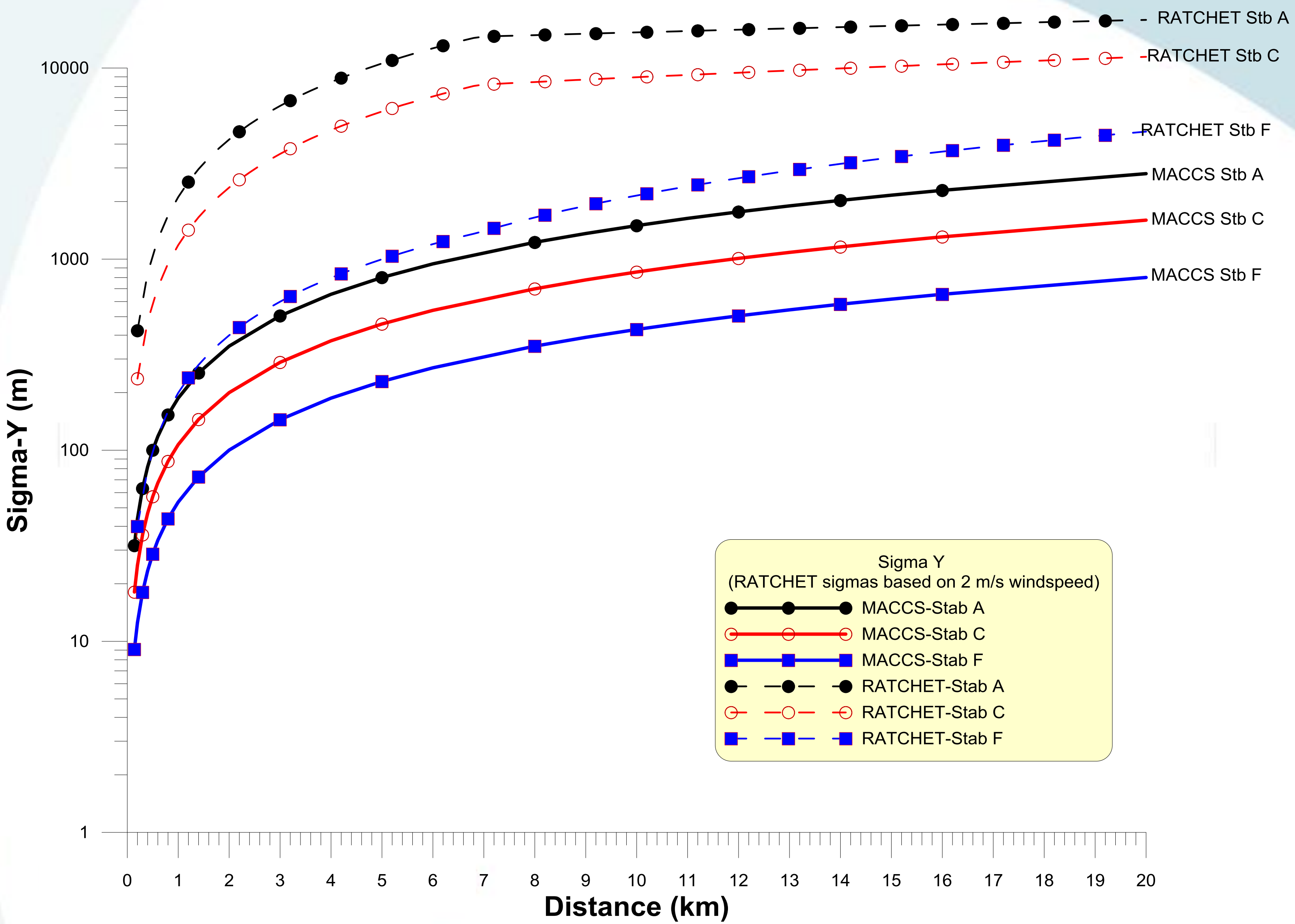
- **Plume growth is proportional to**
  - Travel time (t)
  - The horizontal and vertical components of the standard deviation of the wind vector (σ_w and σ_v)
  - The functions f_y and f_z
- **The functional form of f_y and f_z depends on the Monin Obukhov Length**

$$\sigma_{yt} = \sigma_v t \ f_y(t / t_{ly}) \qquad \sigma_{zt} = \sigma_w t \ f_z(t / t_{lz})$$

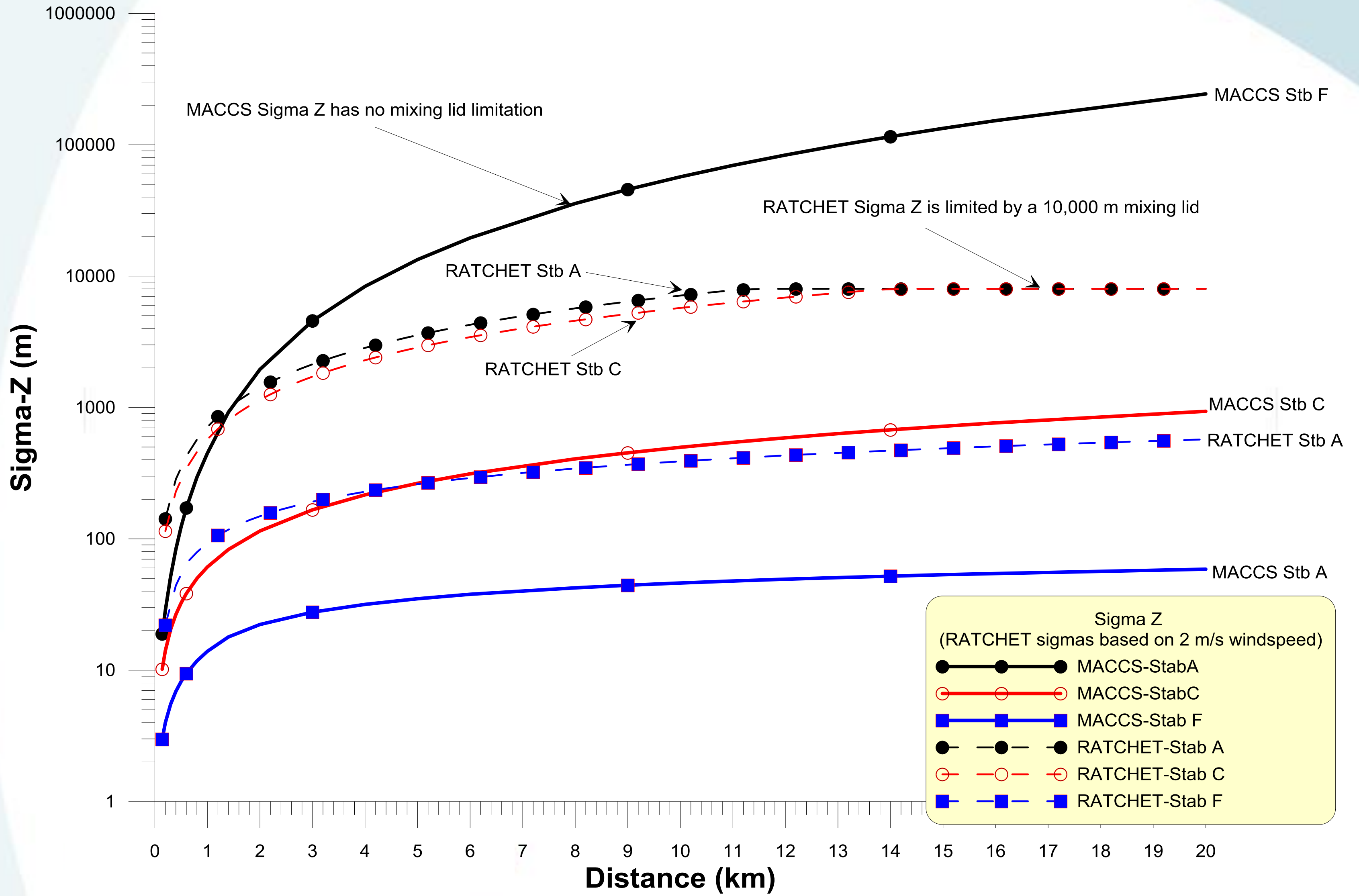
Diffusion Coefficients

- MACCS2 diffusion coefficients (σ_y and σ_z) use the P-G stability classes where diffusion coefficients are based on *downwind distance* for a steady-state plume
- Turbulence-based diffusion coefficients use similarity theory are based on *travel time.* These diffusion coefficients are used in the RATCHET and CALPUFF models
- In general, the turbulence-based σ_y and σ_z are higher than P-G σ_y and σ_z , but depend on the wind speed which in turn affects travel time

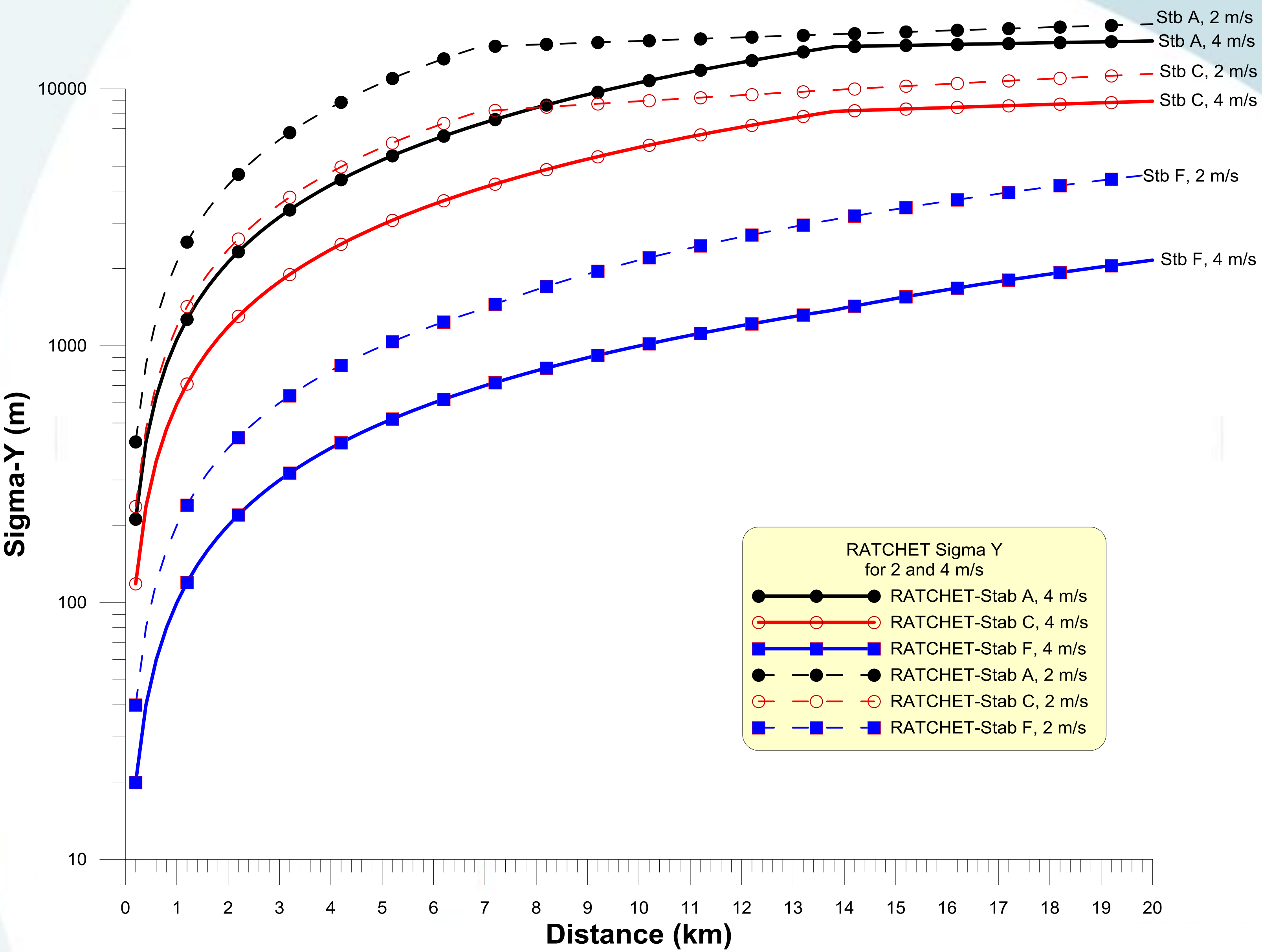
Comparison of Diffusion Coefficients (σ_y)



Comparison of Diffusion Coefficients (σ_z)



Comparison of Diffusion Coefficients (σ_y), 2 m/s and 4 m/s



Assumptions Specific to the Gaussian Plume Model

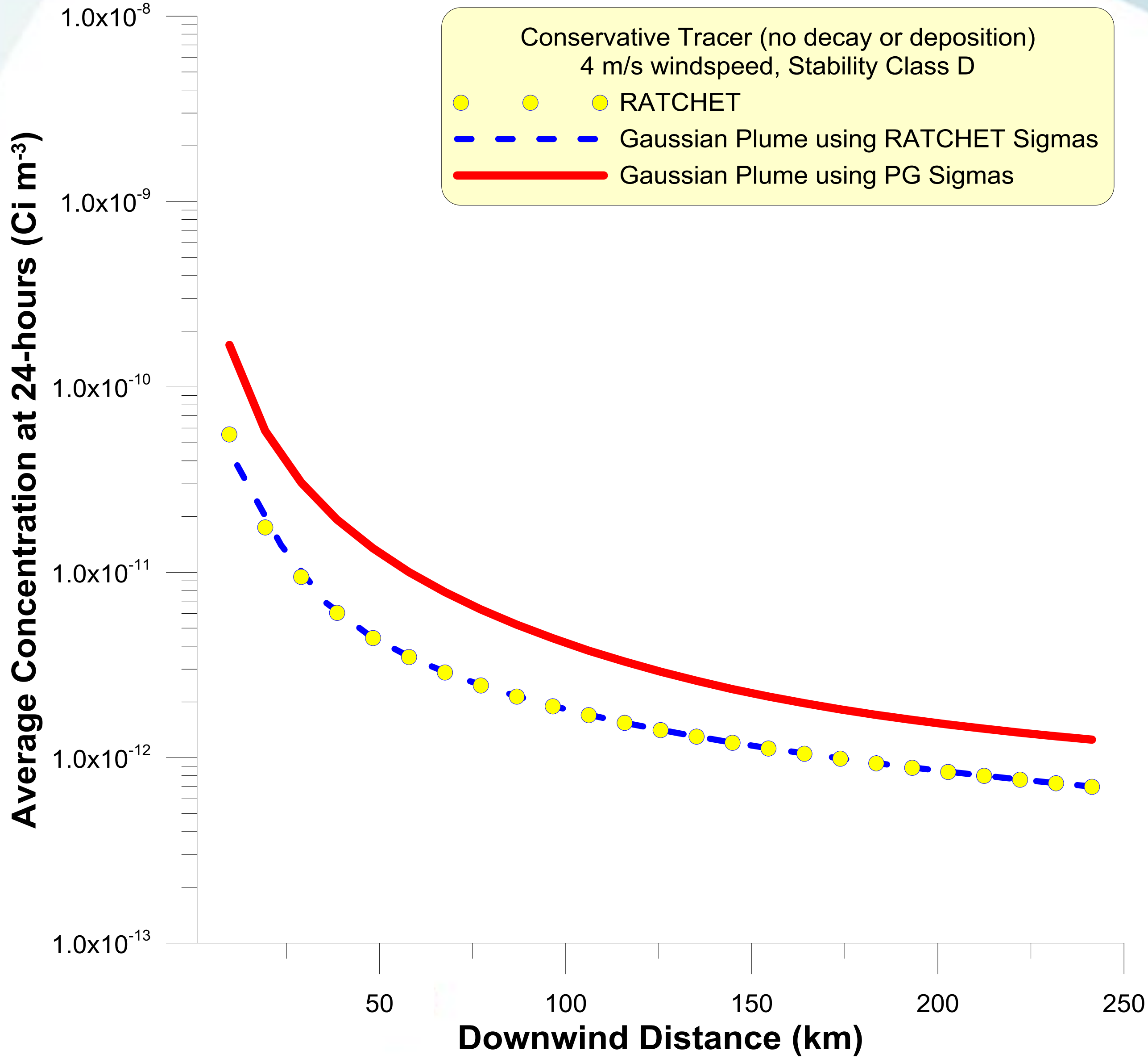
- Homogeneity of turbulence
- Stationary turbulence conditions and steady-state pollutant release
- Sufficiently long diffusion times (averaging times)
- Spatially constant, non-zero wind speed
- Material continuity (no sources or sinks) while being transported
- Total reflection of the plume on the ground

Puff Dispersion Models

- **Typically composed of two modules**
  - Wind field interpolation module
  - Pollutant transport model
- **Allows variable/curved plume trajectories[1]**
- **Spatially-variable meteorological conditions[1]**
- **Non steady-state releases**
- **Retains spatial distribution of concentrations from the previous meteorological sampling period**

[1]Not all puff dispersion models incorporate this feature

Benchmark – RATCHET Gaussian Plume,



Deposition Velocity

- **In MACCS, deposition velocity is specified by the user**
- **Modern atmospheric transport models (CALPUFF, AERMOD, RATCHET) calculate deposition velocity based on**
  - wind speed
  - friction velocity (turbulence level, roughness height)
  - Brownian diffusion (CALPUFF and AERMOD)
  - gravitational settling

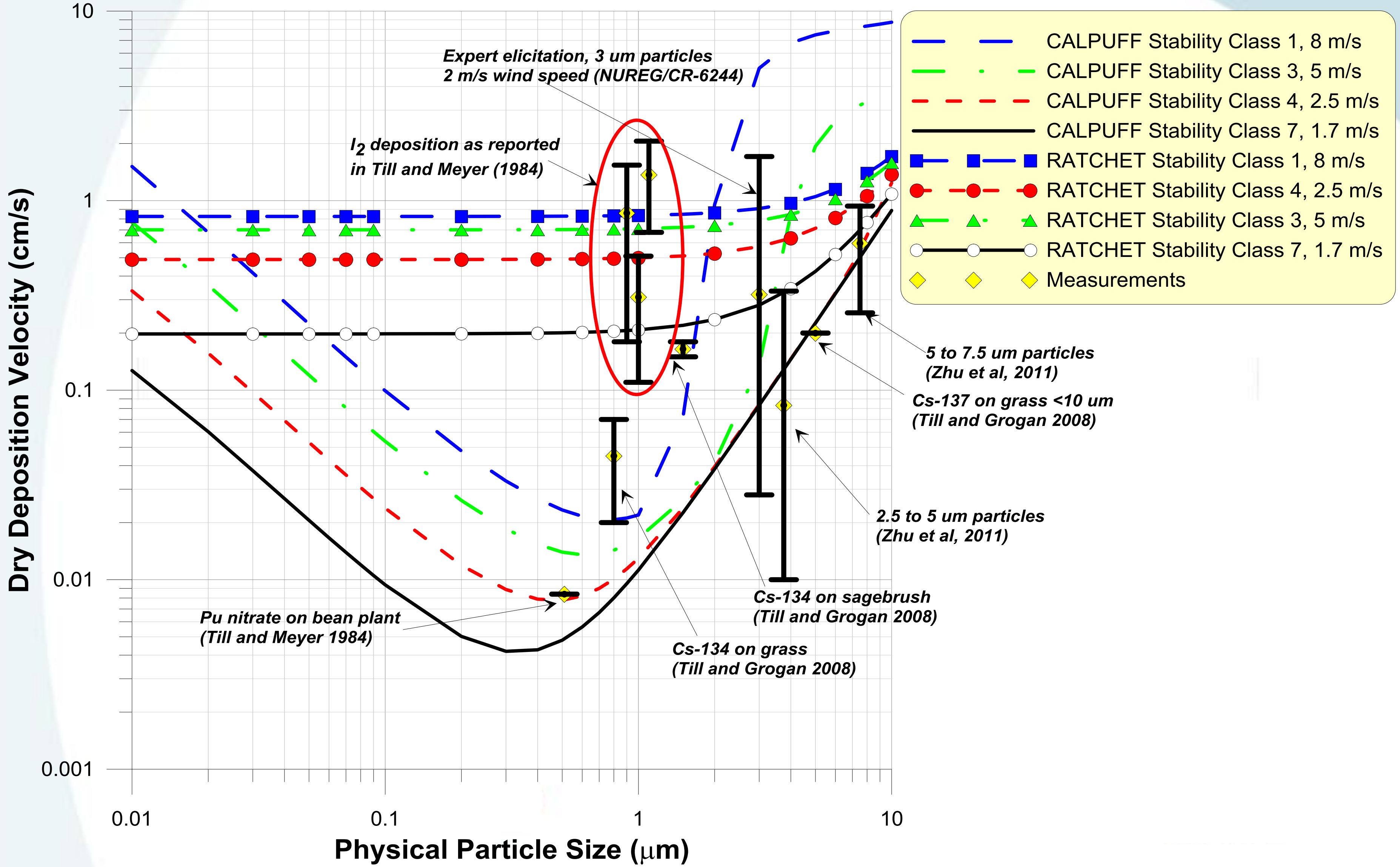
Deposition Velocity Models

- **Resistance model for particles** $$v_d = \frac{1}{r_a + r_d + r_a r_d v_g} + v_g$$
- **Resistance model for gases** $$v_d = \frac{1}{r_a + r_d + r_c}$$

  r_a = aerodynamic resistance (s/m)
  r_d = deposition layer resistance (s/m)
  r_c = canopy layer resistance (s/m)
  vg =gravitational settling (m/s)

- **Deposition velocity is a function of the friction velocity, viscosity of air, Brownian diffusivity, particle density and diameter, roughness length, and vegetation type**

Deposition Velocity as a Function of Particle Size for two Different Resistance Models



Measured Deposition Velocity (v_d) Values

Effluent	Value (cm/s)	Reference
Reactive gases	1	Brenk et al. 1983
Reactive gases	0.73	Geometric mean of measured values given in Hoffman et al 1984
Aerosols (1 μm in diameter)	0.1	Brenk et al. 1983
Particulates	0.33	Geometric mean of measured values given in Hoffman et al 1984
Un-reactive gases	0.01	Brenk et al. 1983

How does RATCHET Compare with Measurements at Hanford?

Monitoring Location	Monitoring Period	Number of Samples	Median P/O Ratios: Full Meteorological Data	Median P/O Ratios: Limited Meteorological Data
300 Area trench	1983–1987	42	1.12	2.06
300 Area trench	1983–1987	25	1.24	1.82
Fir Road	1984–1987	34	1.28	2.44
Prosser barricade	1984–1987	28	1.62	1.43
Ringold	1983–1987	41	2.31	2.36
Sagehill	1984–1987	32	1.72	1.59
Pasco	1986–1987	22	1.16	1.23
Eltopia	1986–1987	15	1.62	3.31
Sunnyside	1984–1987	41	1.09	0.82
Yakima	1986–1987	18	1.13	0.89
All stations	1983–1987	316	1.45	1.85

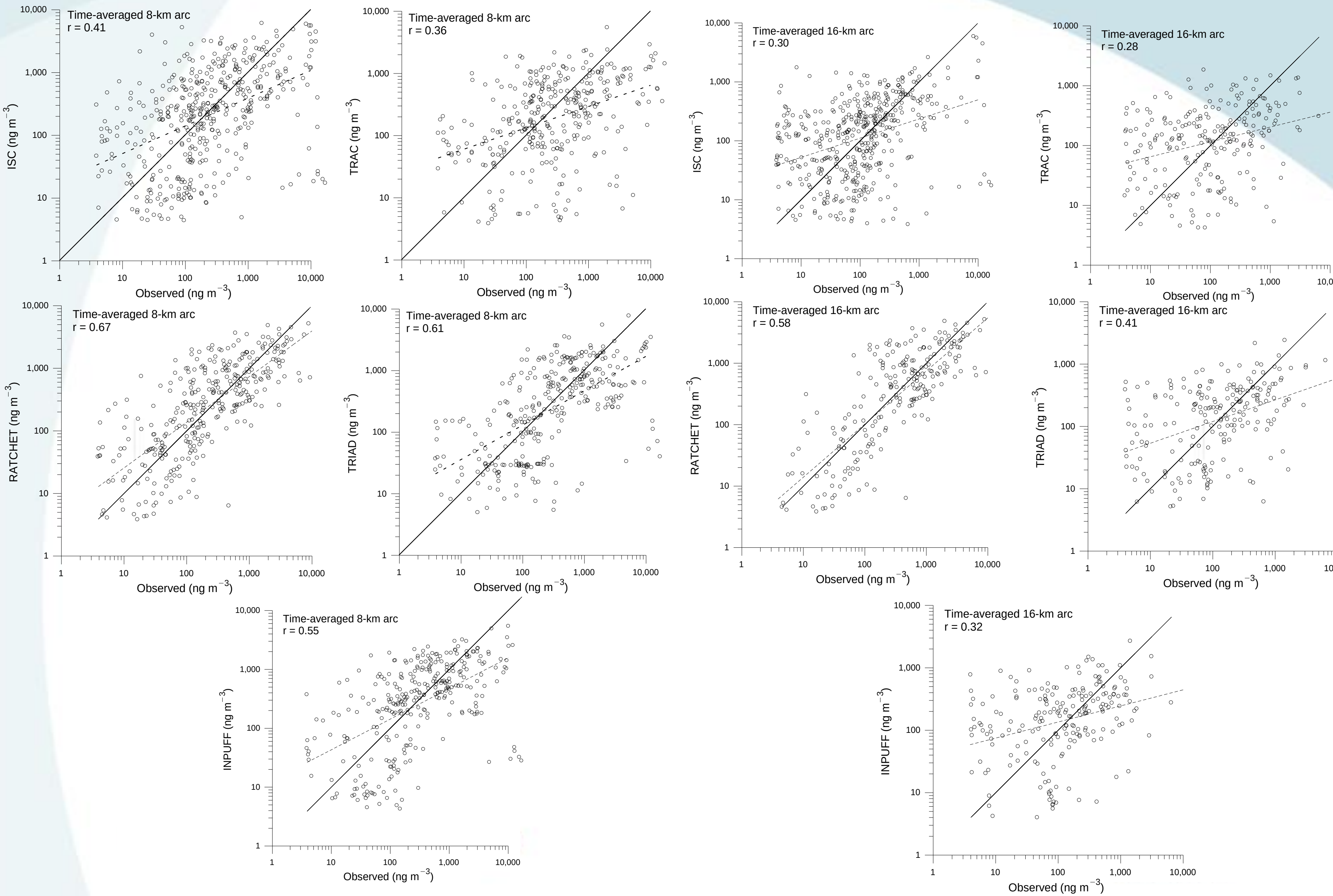
Overall RACTHET <u>over predicts</u> Kr-85 concentrations at Hanford by about a factor of 1.45 using full meteorology and 1.85 using limited meteorology

Ramsdell et al. 1994

How Does the Gaussian Plume and Lagrangian Puff Model Compare with Measurements?

	Gaussian Plume	Lagrangian Puff Models			
	ISC	TRAC	RATCHET	TRIAD	INPUFF2
8 km data					
Geometric Mean P/O ratio	1.9	1.0	0.91	1.2	1.0
Geometric Std P/O ratio	2.2	2.3	2.7	2.0	1.9
16 km data					
Geometric Mean P/O ratio	2.7	1.9	0.93	1.6	1.7
Geometric Std P/O ratio	2.2	3.9	2.5	2.5	2.2

From Rood 1999, Rood et al, 1999, 1-hr maximum concentration in 8-hr period

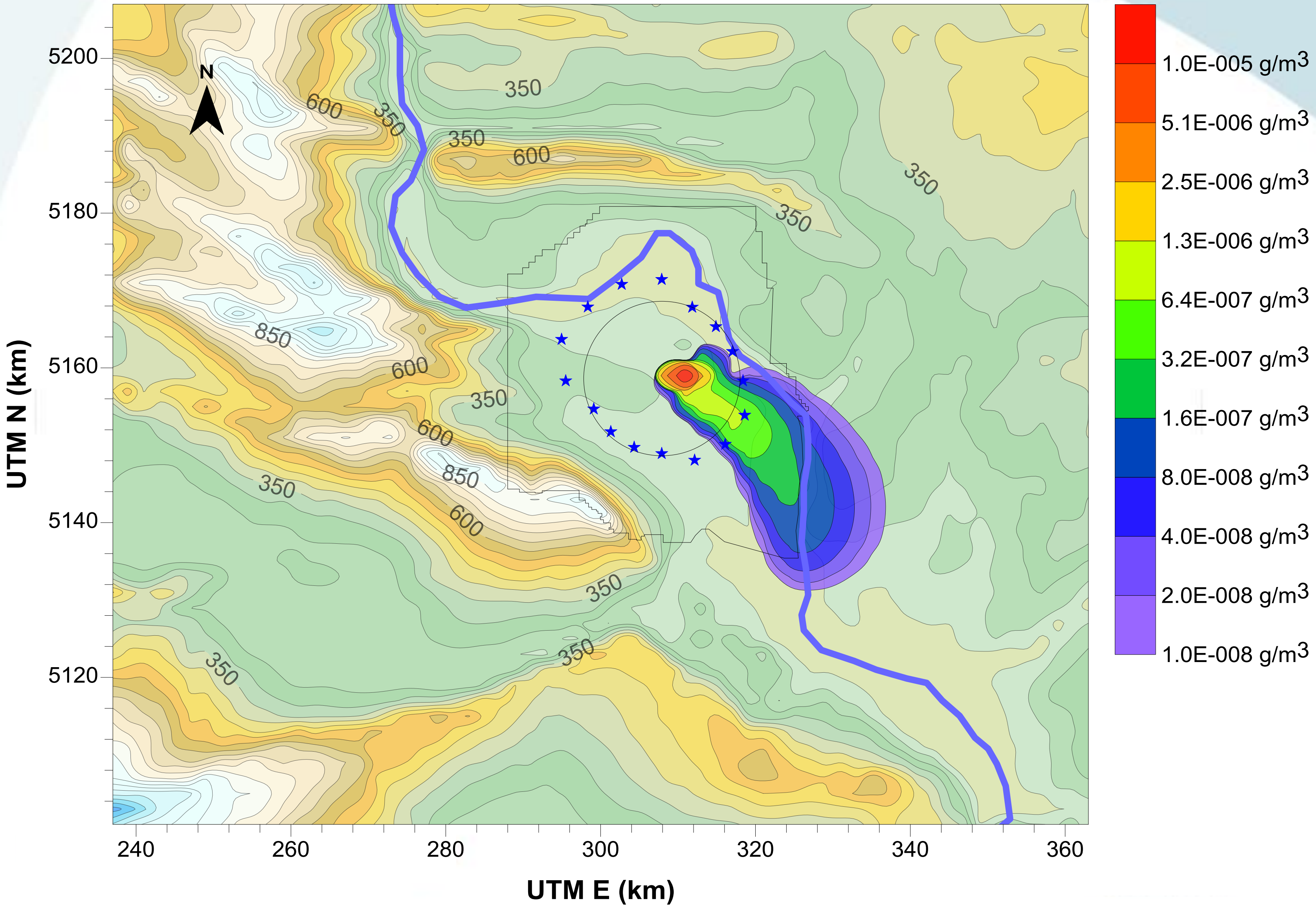


Time-averaged 8-km arc
r = 0.41
ISC (ng m−3)
Observed (ng m−3)
Time-averaged 8-km arc
r = 0.36
TRAC (ng m−3)
Observed (ng m−3)
Time-averaged 16-km arc
r = 0.30
ISC (ng m−3)
Observed (ng m−3)
Time-averaged 16-km arc
r = 0.28
TRAC (ng m−3)
Observed (ng m−3)
Time-averaged 8-km arc
r = 0.67
RATCHET (ng m−3)
Observed (ng m−3)
Time-averaged 8-km arc
r = 0.61
TRIAD (ng m−3)
Observed (ng m−3)
Time-averaged 16-km arc
r = 0.58
RATCHET (ng m−3)
Observed (ng m−3)
Time-averaged 16-km arc
r = 0.41
TRIAD (ng m−3)
Observed (ng m−3)
Time-averaged 8-km arc
r = 0.55
INPUFF (ng m−3)
Observed (ng m−3)
Time-averaged 16-km arc
r = 0.32
INPUFF (ng m−3)
Observed (ng m−3)
1
10
100
1,000
10,000

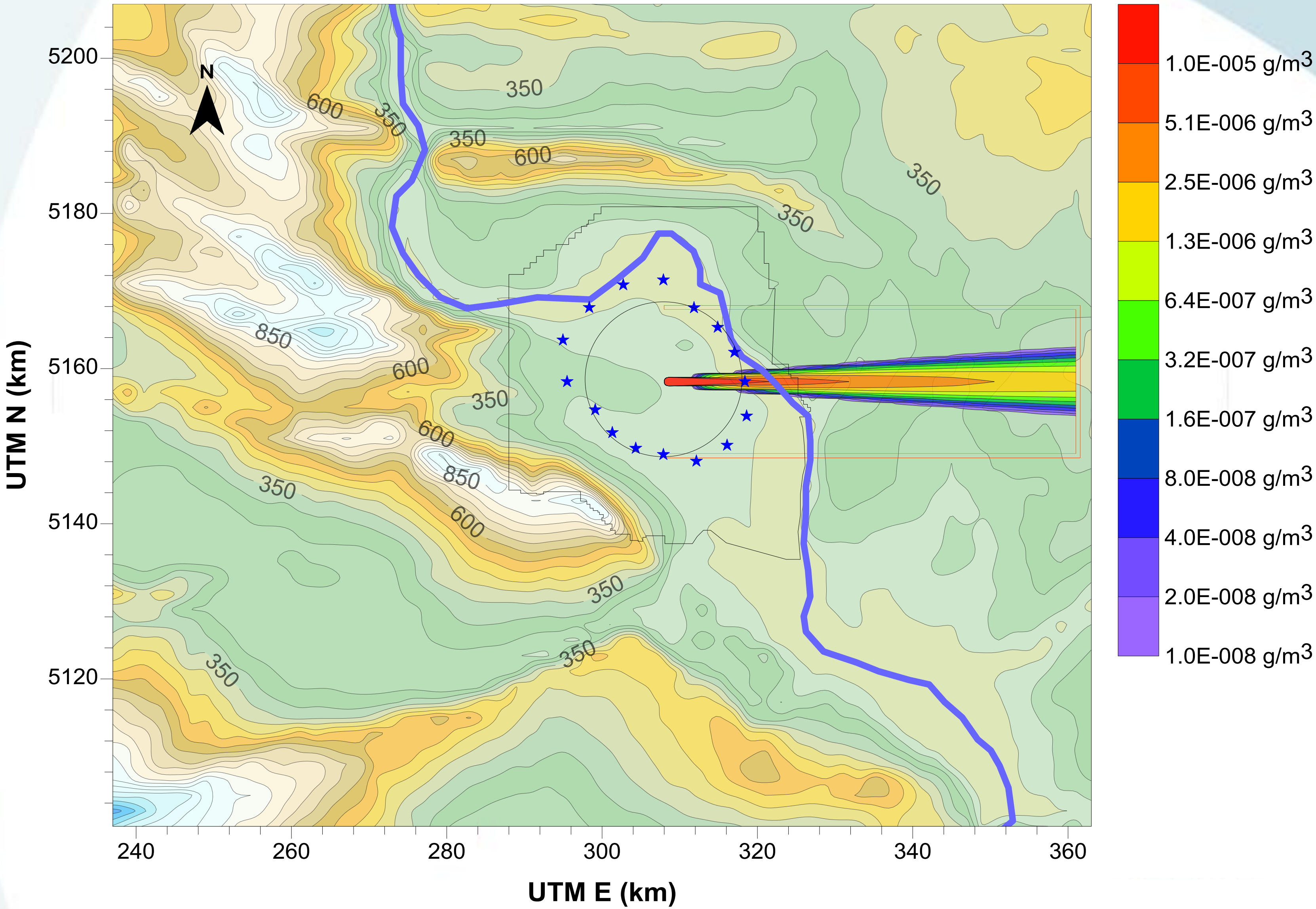
Model Comparison of MACCS, CALPUFF, and RATCHET for Hanford WTS

- Compare overall dispersion patterns
- 1-year of meteorological data (1994)
- V_d of 0, 0.1, 0.3, and 1.0 applied for MACCS
- V_d internally calculated for CALPUFF and RATCHET
- Compared the 95% highest X/Q at various distances

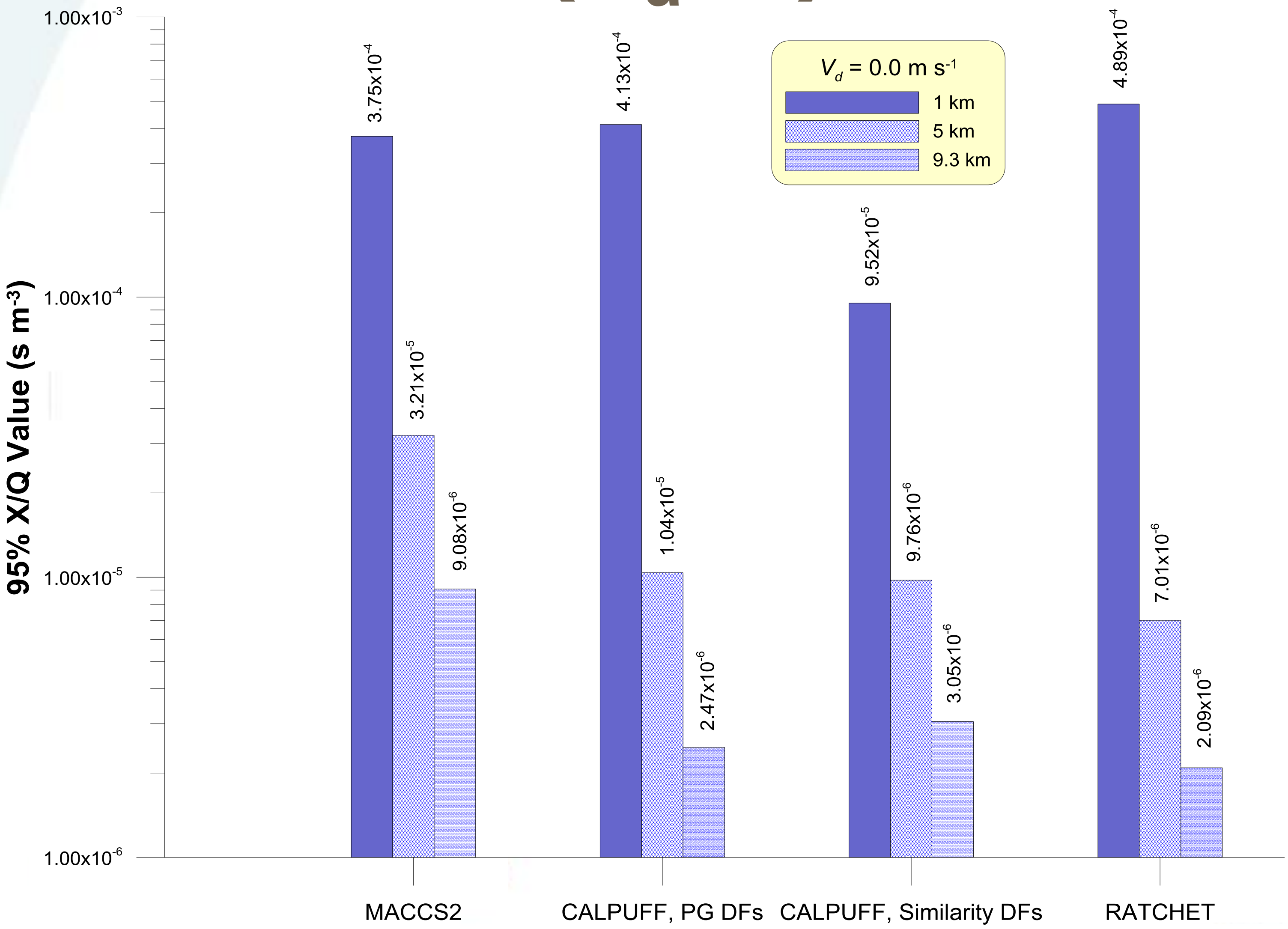
Hour 3 of a 14-hour Simulation using CALPUFF



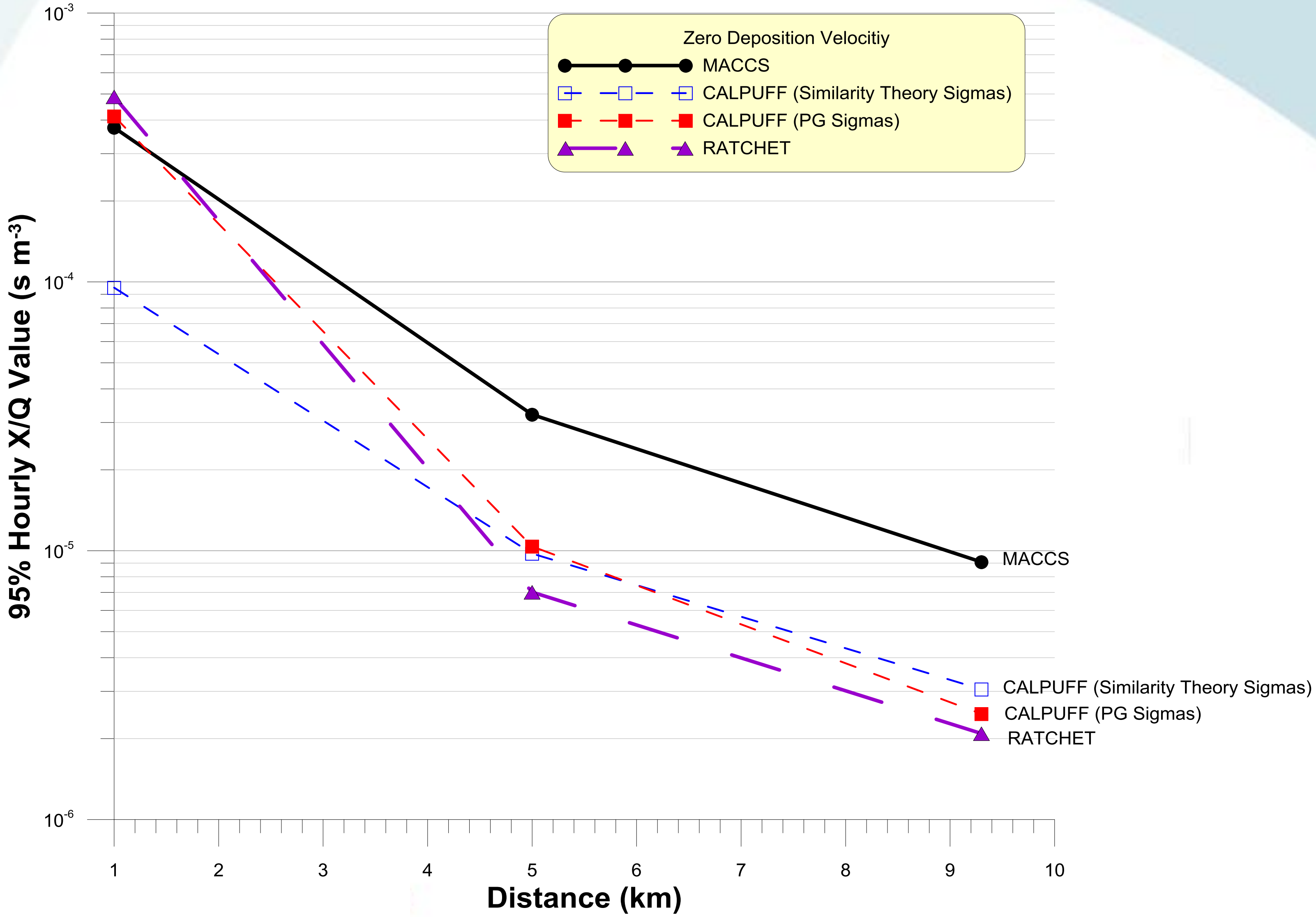
Hour 3 of a 14 hour Simulation using Gaussian Plume Model



95% X/Q, No Deposition (V_d=0)

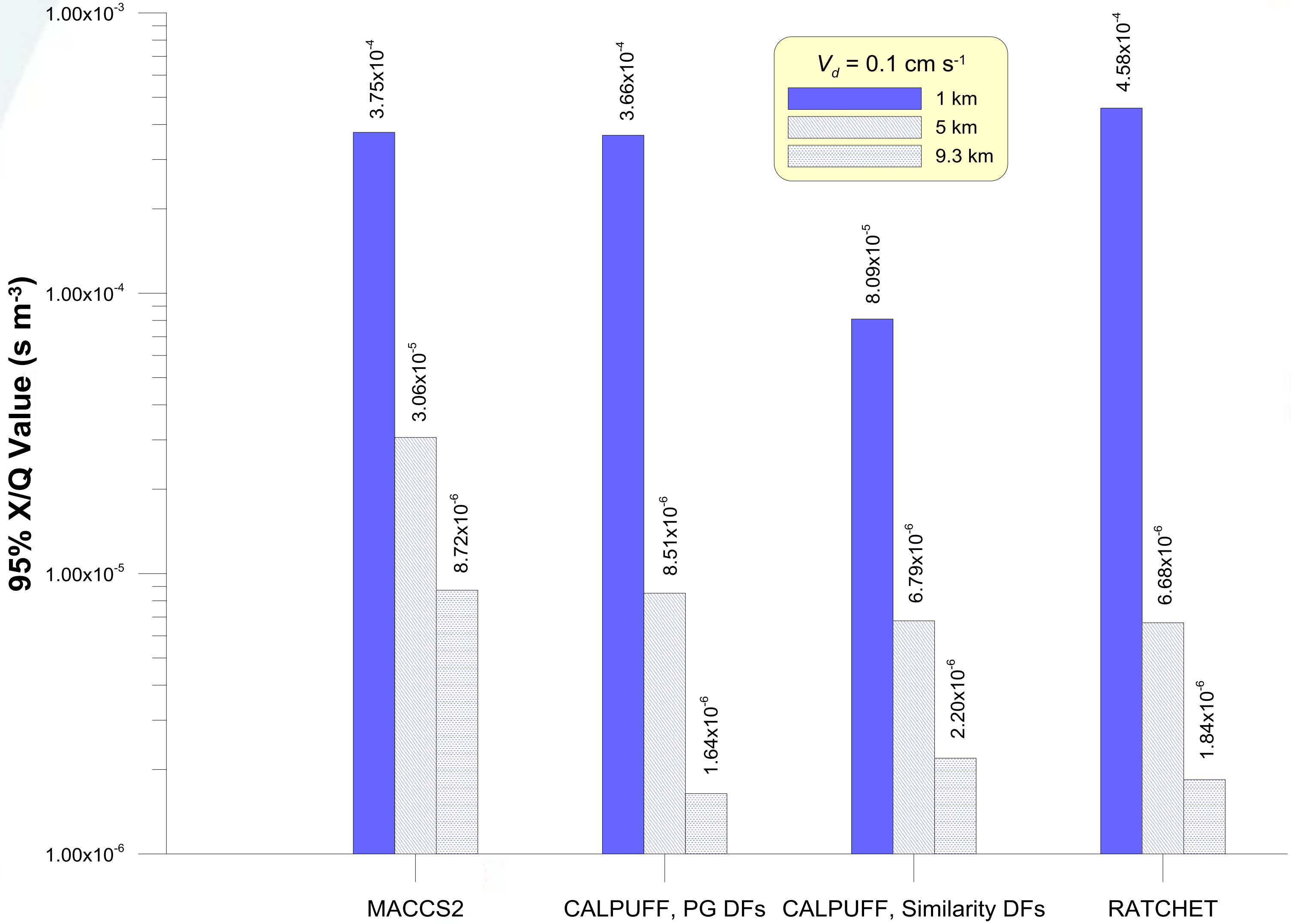


95% X/Q, No Deposition (V_d=0)



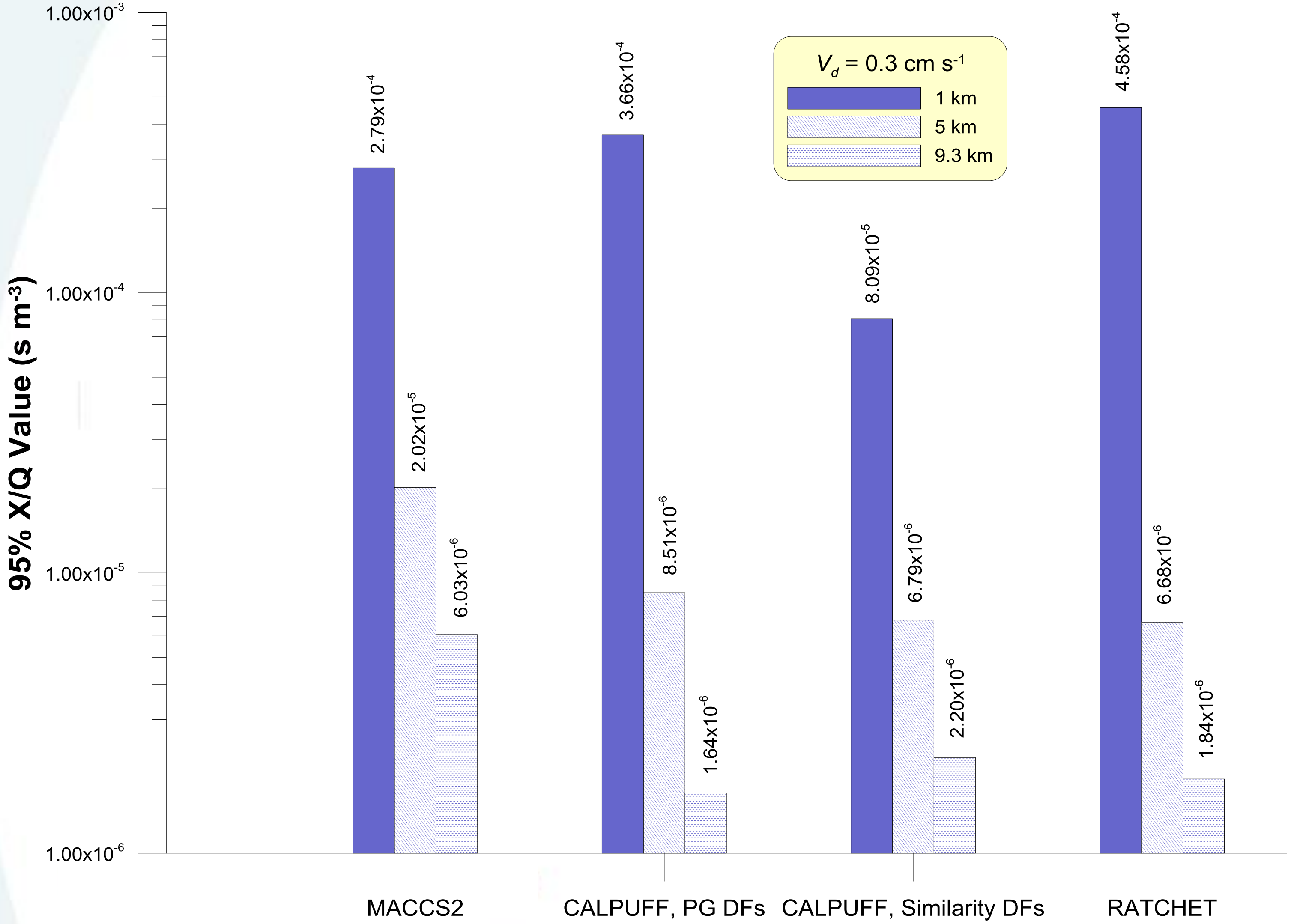
95% X/Q, MACCS V_d=0.1 cm/s

CALPUFF and RATCHET V_d calculated internally



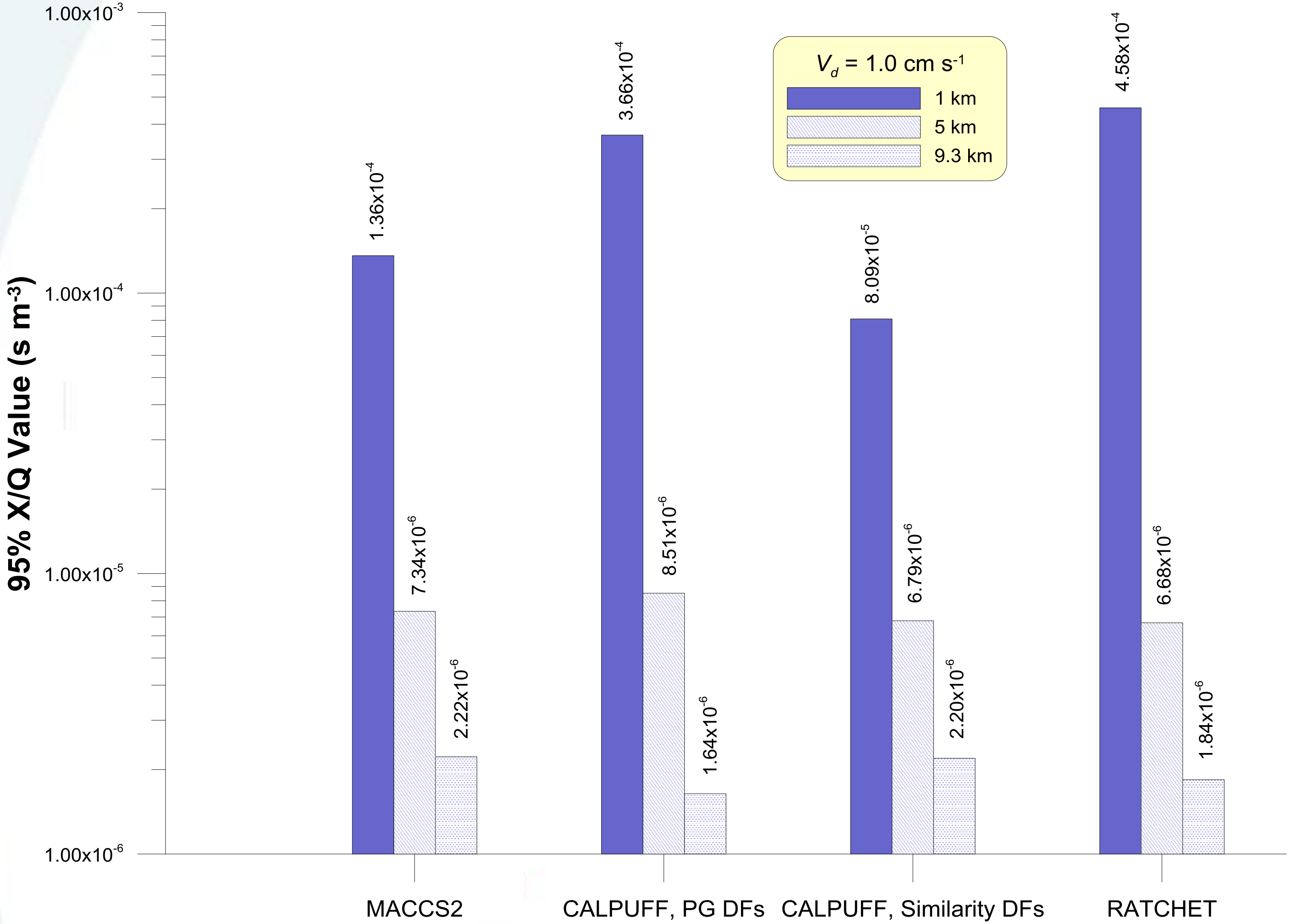
95% X/Q, MACCS V_d=0.3 cm/s

CALPUFF and RATCHET V_d calculated internally



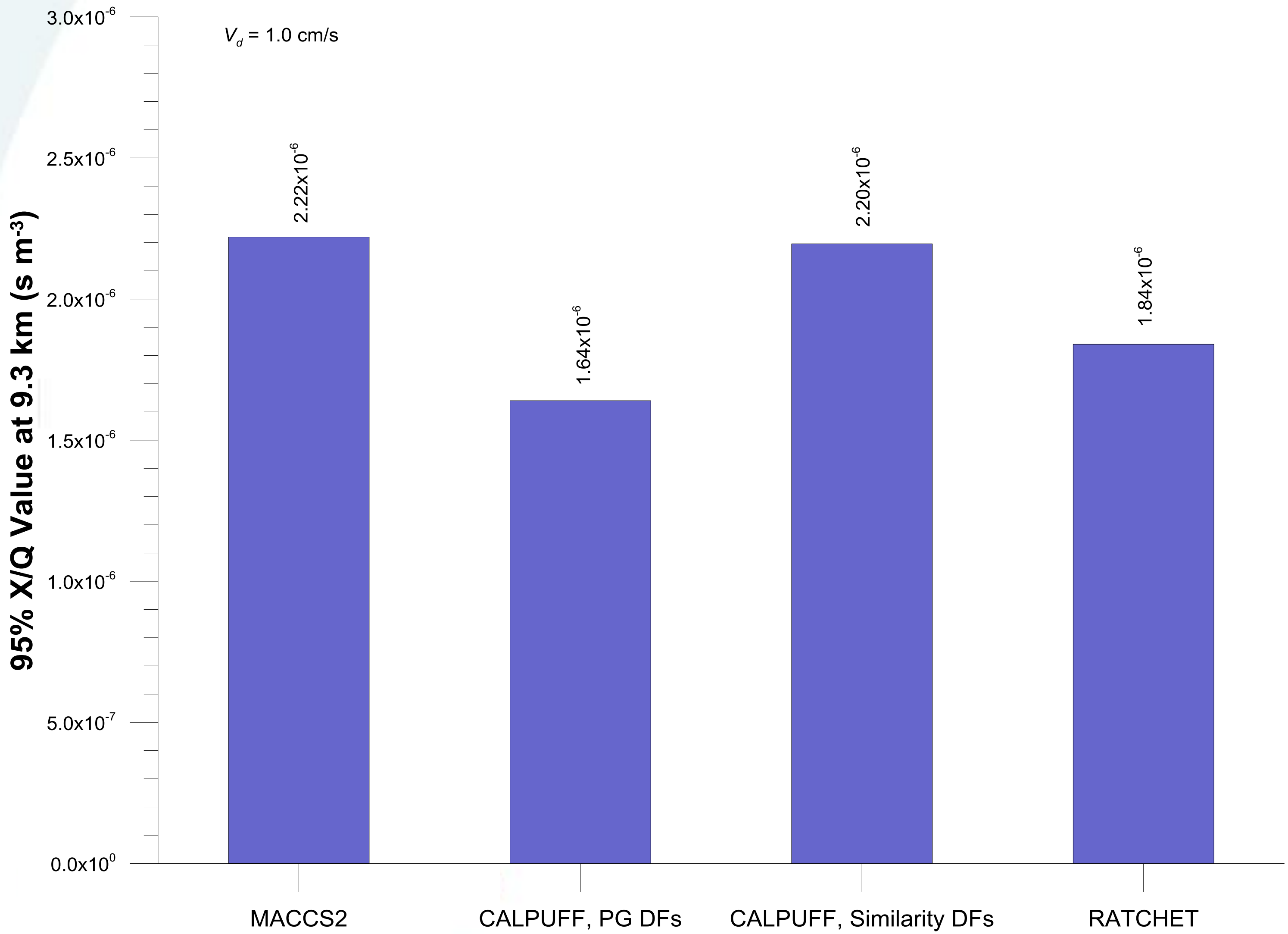
95% X/Q, MACCS V_d=1.0 cm/s

CALPUFF and RATCHET V_d calculated internally

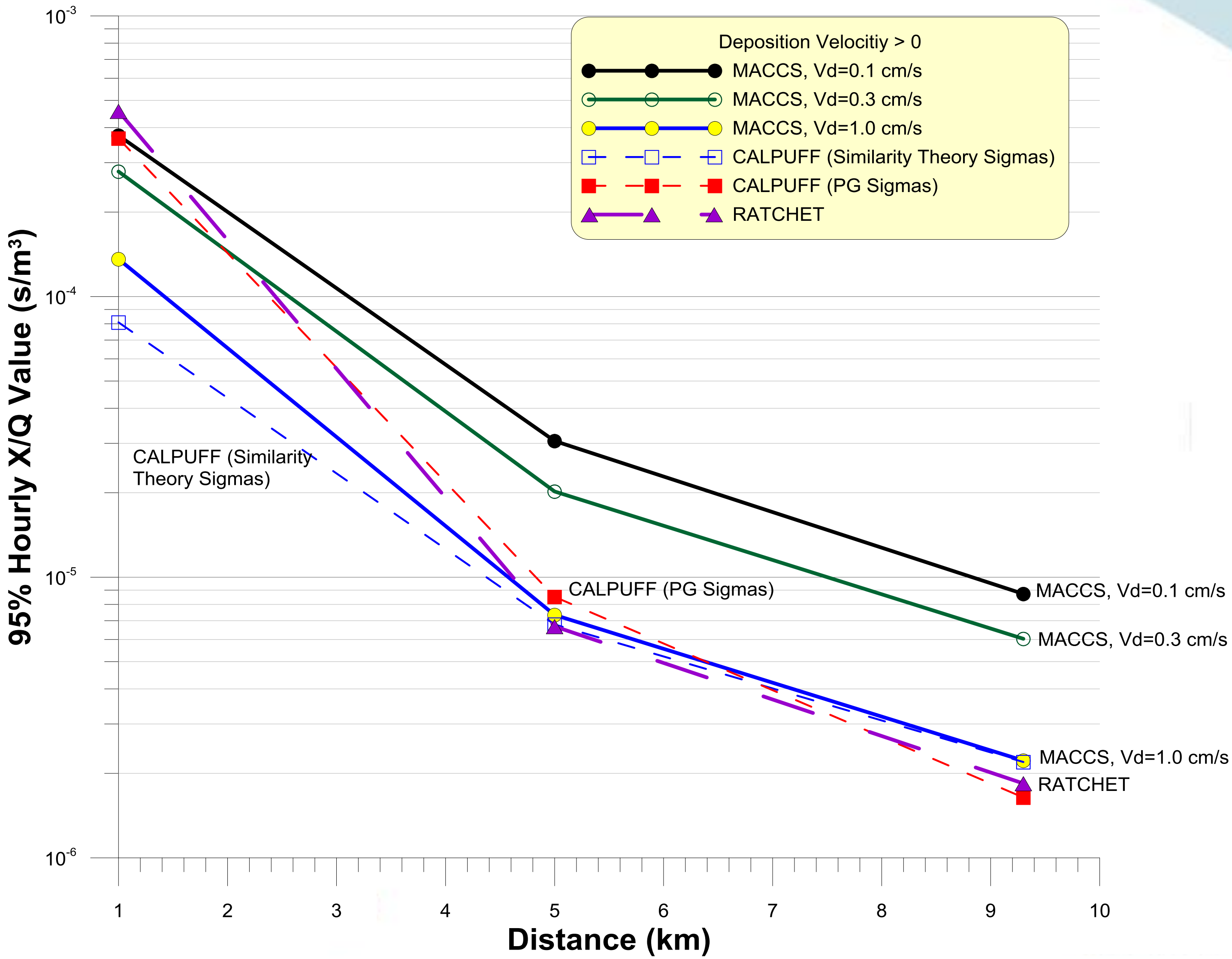


95% X/Q, MACCS V_d=1.0 cm/s

CALPUFF and RATCHET V_d calculated internally



95% X/Q vs Distance (Vd>0)



Conclusions

- **With No Deposition**
  - The Gaussian plume and Lagrangian puff models yield about the same 95% X/Q value at 1 km
  - The Gaussian plume and Lagrangian puff models 95% X/Q values diverge with increasing distance
  - At 9.3 km, the Gaussian plume model 95% X/Q is about 3 to 4 times <u>higher</u> than Lagrangian puff models

Conclusions (continued)

- **With Deposition**
  - At 9.3 km, the Gaussian plume model 95% X/Q using a deposition velocity of 1 cm/s is about the same as the Lagrangian puff models using internally calculated deposition velocity

Conclusions (continued)

- **Comparison of Gaussian plume and Lagrangian puff models at distances in the 8-16 km range reveal that the Gaussian plume model overpredicts concentrations for short-term (i.e. 1-hr) average concentrations.**

Conclusions (continued)

- **The reasons for difference results among the models are numerous and complex, but in general differences may be attributed to**
  - Conceptual differences in the Gaussian Plume and Lagrangian Puff Models
  - Differences in diffusion coefficients
  - Differences in deposition velocity

What Have We Learned?

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What We have Learned

- The MACCS2 as implemented in its documentation with a V_d of 1.0 cm s^{-1} results in approximately the same concentration of radionuclides at the point of exposure when compared to state of the art meteorological models using Hanford site-specific meteorological data and an internally calculated V_d
- The calculated V_d for WTP analyses using state of the art models and site specific meteorological conditions is in the range of 0.1-0.3 cm s^{-1}

What We have Learned

- Conservatisms in MACCS2, namely the use of a conservative source term, the straight-line Gaussian Plume model for short-duration events, and exposure occurring at the 9.3 km receptor distances, result in a highly conservative estimate of atmospheric concentrations regardless of the the use of a deposition velocity of 1 cm s^{-1}
- But how conservative?
- What level of conservatism is our goal?

Conclusions (1)

We recommend a target level of conservatism be established to be used in decision making related to nuclear safety.

Conclusions (2)

Ground rules must be established for decision making using agreed upon methods and the prescribed level of conservatism.

Conclusions (3)

We conclude that the MACCS2 code as designed for generic use at DOE sites provides a useful tool for screening calculations for decision making.

When the results of screening calculations show there is no significant chance of exceeding the target dose criteria, no further action should be taken related to the assessment of dose.

Conclusions (4)

When screening fails, we recommend the use of site specific environmental transport data, state of the art meteorological models, and a more comprehensive probabilistic approach to make decisions related to nuclear safety.

- A tiered approach to decision making should be considered, applying codes such as MACCS2 (v. 2.5) or GENII prior to implementing robust site-specific analyses that incorporate comprehensive probabilistic calculations.

Conclusions (5)

The comprehensive probabilistic methodology should consider the following deterministic and probabilistic components:

- Probabilistic source term with a 100% chance of occurring
- Probabilistic transport calculations including pathway analysis to clearly show key pathways of exposure
- Deterministic exposure scenario parameters using ICRP 101 guidelines
- Deterministic dose coefficients

THANK YOU!

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