Developed and Presented By: Drew Michanowicz, MPH

Doctoral Student, GSPH

Department of Environmental and Occupational Health

Course Director: onrad aniel olz, r,

cdv pitt.edu

ssistant rofessor, nvironmental and ccupational ealth, niversity of ittsburgh, raduate chool of ublic ealth

http://www.pitt.edu/~cdv/

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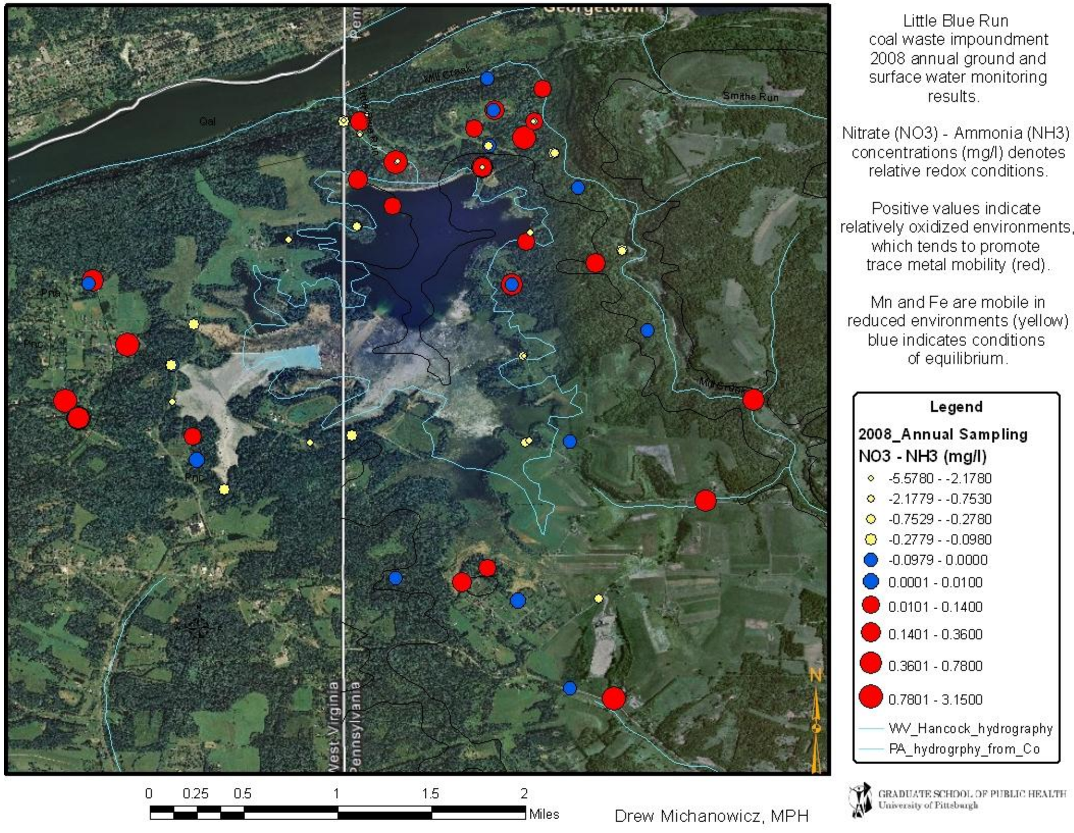
What is a Model?

- Simplified, conceptualizing, abstract view of complex phenomena
  - Abstract: degree of uncertainty or interpretability
- A model represents objects, mechanisms, and physical processes in a logical or empirical manner



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Why Model?

- Amplify thought processes – common sense rule
- Decision making - prioritization
- As a substitute for unknown data and much may be unknown

  -direct measurement and surveillance
- Cost
- Time
- Provides a means for deducing and extrapolating information
- Feasibility
  - Cant measure exposures for everyone in all populations
- Simulation
- Visualization
- Manipulation of parameters
- Estimation of exposure or dose

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Modeling is a Tool

- Thinking is the 1st step - CSM
  - Looking to make decision not find a "truth"
  - Complex v. simple
    - Threshold effect – Information by benefits??
  - I.e. Policy based, health care
- Computer as a thinking, hypothesis generating tool
  - Epistemic – hypothesis testing
- Forcastic – predicting conditions
- Hindcastic – retrodictive
  - Reliability to recreate historic contamination
  - Always will be seen as a "win-win"
- We can benefit by telling the public what we can and can't do as modeling can be a very powerful tool
- Disclaimer - Modeling has very ostentatious public perception

Types of Models

- Quantitative
- Qualitative
- Deterministic
- Statistical
  - (black box)
- Mechanistic
- Empirical
- Partionioning
- Dynamic
- Static
- Mixed
- Conceptual
- Predictive
- Retrodictive
- Stochastic

USAEPA acknowledges and has in use hundreds of environmental models in its standards and policy based decision making processes
See: http://www.epa.gov/epahome/models.htm

Modeling for Exposure

- Usually predictive models, but also hindcastic modeling is performed for E.A.
- 3 Types: Deterministic, Statistical, Mixed

Data Collection → Predictive Models → Exposure & Dose Estimates

- Data Collection: Direct measurement, monitoring, emission inventories
- Predictive Models: Transport and fate, human activity pattern, human exposure models, stochastic
- Exposure & Dose Estimates: Defined by the population or health endpoint

Exposure v. Dose

Table 2. Mathematical expressions for some important exposure-related and dose-related events

Exposure

$$E = \int_{t_1}^{t_1} C(t)\,\mathrm{d}t$$

Potential dose for intake processes

$$D_{\text{applied}} = \alpha \int_{t_1}^{t_1} C(t)\,IR(t)\,\mathrm{d}t$$

Applied dose

$$D_{\text{potential}} = \int_{t_1}^{t_2} C(t)\,IR(t)\,\mathrm{d}t$$

Internal dose

$$D_{\text{internal}} = D_{\text{applied}} \int_{t_1}^{t_2} f(t)\,\mathrm{d}t$$

E, magnitude of exposure; t_2 t_1, exposure duration; α, availability factor; C(t), exposure concentration as a function of time; IR, ingestion or inhalation rate; f(t), nonlinear absorption function (Sexton et al., 1995a)

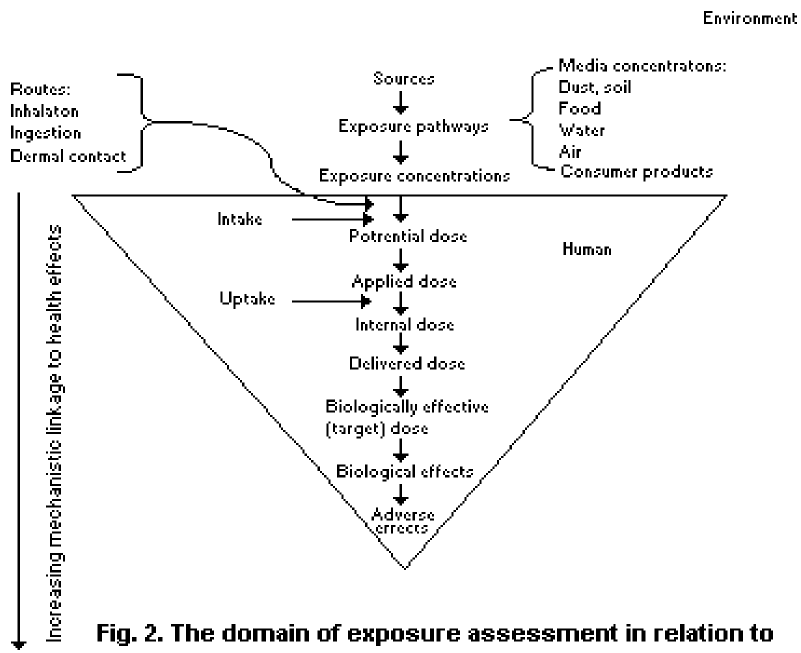
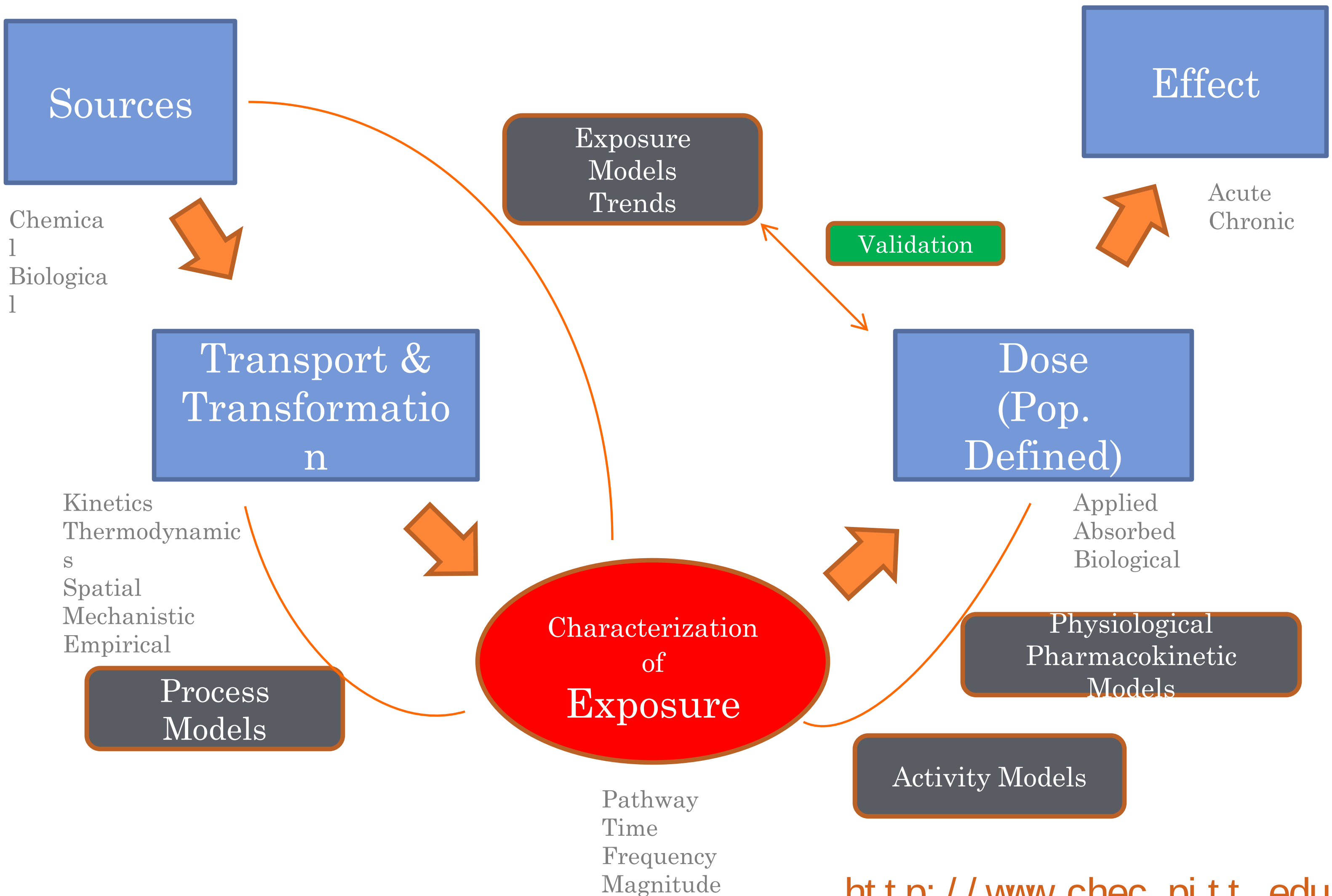


Fig. 2. The domain of exposure assessment in relation to an environmental health paradigm (adapted from IPCS, 1993; Sexton et al., 1995a)

What is the data source units to be modeled for exposure?

– concentration over time? Ie. ug/m^3 SO_2 over a 24 hour period

Models as Means for Assessments



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Exposure Assessment Assumptions

- EA rely implicitly on the assumption that exposure can be linked to ambient concentrations in air, water, soil, etc.
- Assessment requires the determination of how much of a contaminant crosses the route of exposure boundary to the receptor
- Complexity increases immensely
- Reasoning that most of the transport models are single media models, ie air, groundwater, surface water, soils

MENTOR

- Georgopoulos and Lioy (2006) presented a theoretical framework for exposure analysis, including multiple levels of empirical and mechanistic information while reducing uncertainties
- Mechanistic source-to-dose framework:
  - Modeling Environment for Total Risks (MENTOR)
- Person Orient Modeling (POM)
- USEPA's SHEDS (Stochastic Human Exposure and Dose Simulation

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MENTOR
Provides a good process framework

1) Characterizing background levels by combining model predictions and measurement studies
2) Characterizing multimedia levels over time in varying environments and populations
3) Selecting sample populations that statistically reproduce demographics of relevant population units
4) Develops human activity models that match USEPA's CHAD
5) Calculate intake rates for sample members
6) Combining intake rates from multiple routs to assess exposure
7) Estimate target tissue doses with physiologically based toxicokinetic modeling (Georgopoulos and Lioy 2006)

Exposure Factors

- Must define parameters and categories of environments encompassing activity models
  - Exposure duration
  - Averaging time
  - Time-activity patterns
  - Human factors ie. Weight
- Variability – true heterogeneity across people, places or time
- Uncertainty – represents lack of knowledge

Dose Model

- Magnitude of dose is the amount of constituent available at the human exchange boundaries over a specified period of time
- Once concentration is assumed constant over time, population averaged-potential dose can be expressed as an average daily dose
- Physiological based pharmacokinetic models
  - Distribution of contaminants that enter the body and distribute to locations within the body
  - Metabolism, excretion mechanisms etc.

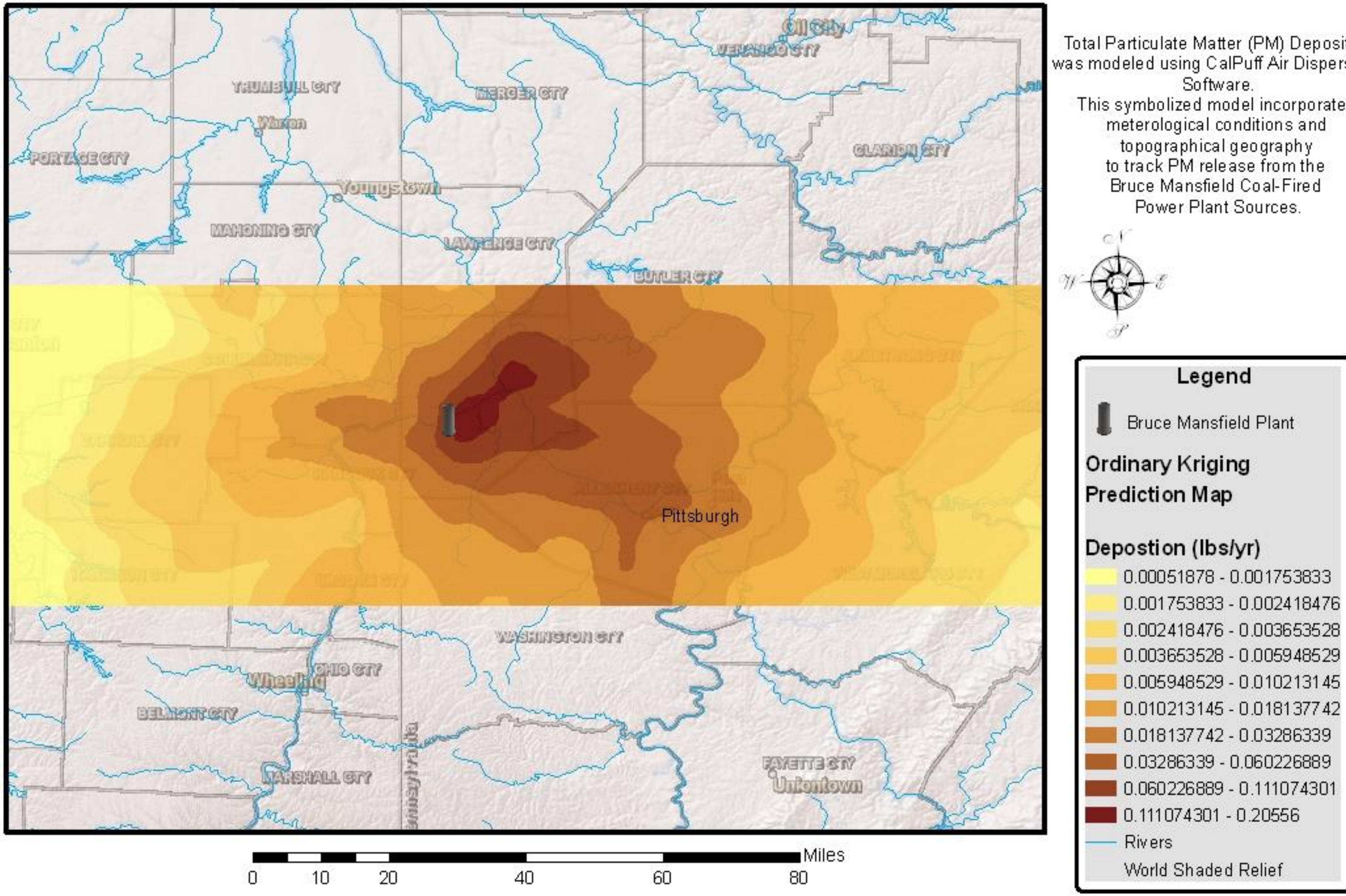
Validation

- Remember abstractions of reality..
- Must examine results to make sure the model is capable of providing useful information
- Comparing predicted values to values in the field is best in validating
- Can also compare within the model or to other models which is not as powerful
- Statistically, no validation is needed if sample size is appropriate, except when extrapolating to other populations

Outdoor Air

- Transported from sources by advection and dispersion
- Assumptions: concentrations are proportional to emissions outputs (TRI) and inversely proportional to dispersion
- Meteorological effects: wind direction, velocity, turbulence, precipitation, and stability of substituent
- Many models use Gaussian dispersion model

2006 Total Particulate Matter Deposition
Bruce Mansfield Power Plant



Total Particulate Matter (PM) Deposition was modeled using CalPuff Air Disperstion Software.
This symbolized model incorporates meterological conditions and topographical geography to track PM release from the Bruce Mansfield Coal-Fired Power Plant Sources.

World Imagery layer obtained from ESRI ArcGIS Online Standard Services, 2009.
EPA, AP 42, 5th ed. Complilation of Air Pollutant Emission Factors, Volume 1: Stationary Point and Area Sources. http://www.epa.gov/ttnchie1/ap42/

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WATER

- Exposure by ingestion, dermal, inhalation
- Transport of contaminants in surface water are assumed to move by physical transport and transformation (mechanistic)
- Many surface water models incorporate a water balance models:
  - Mass balance equation
  - $P = Q + E + \Delta S$

  P = precipitation, Q = runoff, E = Evapotranporation, S = storage capacity (saturation)
- Ground water models can be 1-D or 3-D and can incorporate solute movement by hydraulic gradient, advective and dispersion and also retardation factors, ie. Adsorption
- Darcy's Flow models

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Surface Water

- Topographic index is a simple example of hydrological modeling first developed by Kirby and Weyman (1974) (Beven, 1997)
- K = a/tan Beta
  - Where K = the soil-topographic index
  - Where a = area draining through a point from upstream
  - Tan Beta = local slope angle
  - All values of same index are assumed to act the same so looking to calculate differences
  - A high index indicates high area draining through a point, a low slope angle and a higher degree of saturation
  - Simple and easily visualizing
  - TOPMODEL

Deterministic and Statistical Models

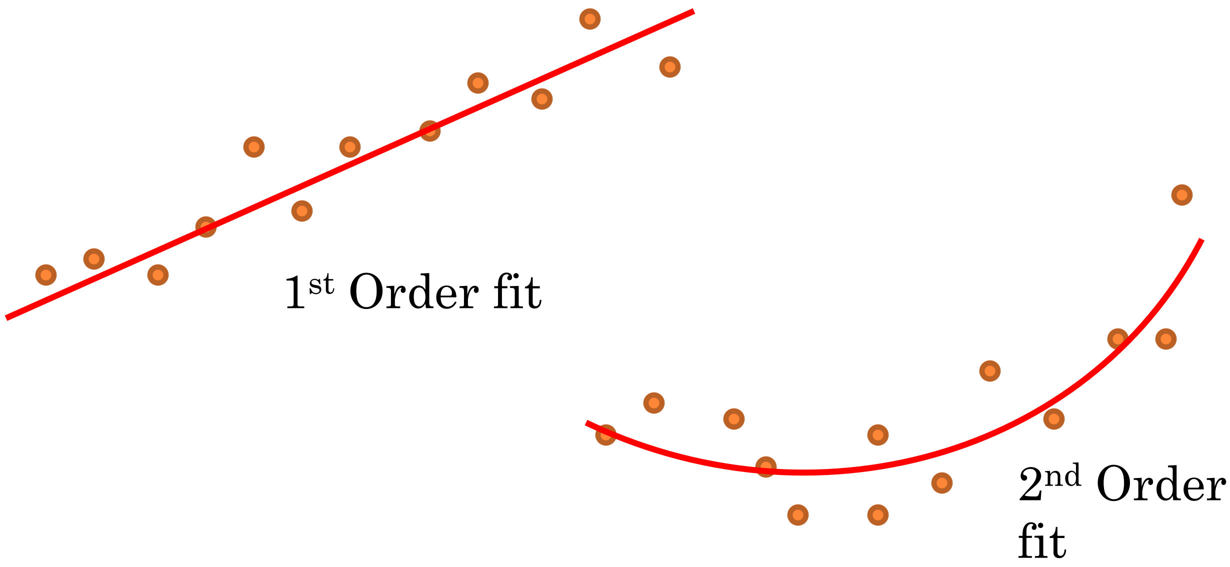
- Majority of environmental modeling is regression analysis
  - Dependent and Independent variables
  - Effect on dependent by changing independents
  - What is the relationship?
- Interpolations
  - Takes known sample points at different locations and creates a continuous surface (prediction model)
  - Relies on the theory of similarity of nearby points (Tobler's First Law)
    - Raining in S. Side, greater probability its raining Downtown

Deterministic Methods

- Use only mathematical functions for interpolation or logical expression of physical environment
- Amount and distribution of sample points depends on the character of the data
  - Trends, variability
- Inverse distance weighting accounts for weights of data points in relation to distance
  - Closer points to prediction point carry more weight

DETERMINISTIC

- Goal is to minimize error of prediction points
- By fitting a plane (polynomial) between sample points
- Subtracting each measured point from predicted value on plane, squaring it, and adding results together gives error value (least-squares regression fit)



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Statistical Models

- Statistical is critical to all stages of exposure assessment
  - Data collection to determine sample
  - Determine characteristics of exposure
  - Hypothesis testing
  - Relationships between ideal measurements
  - Generalize results to other populations
  - Quality assurance
- Many exposure measurements are lognormally distributed (right skewed)

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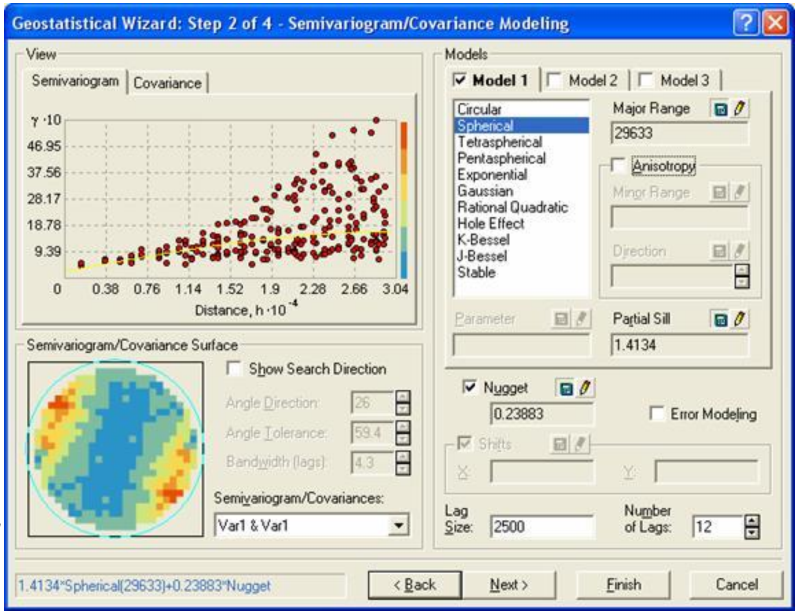
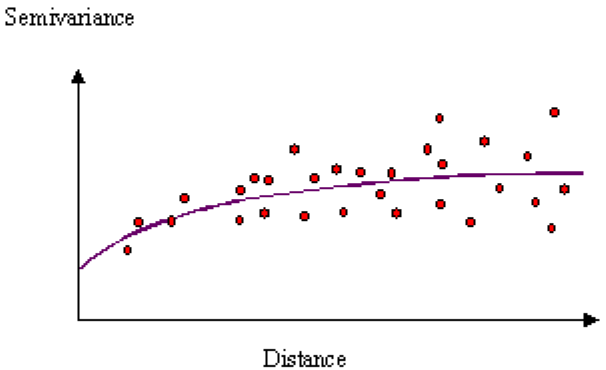
GEOSTATISTICAL

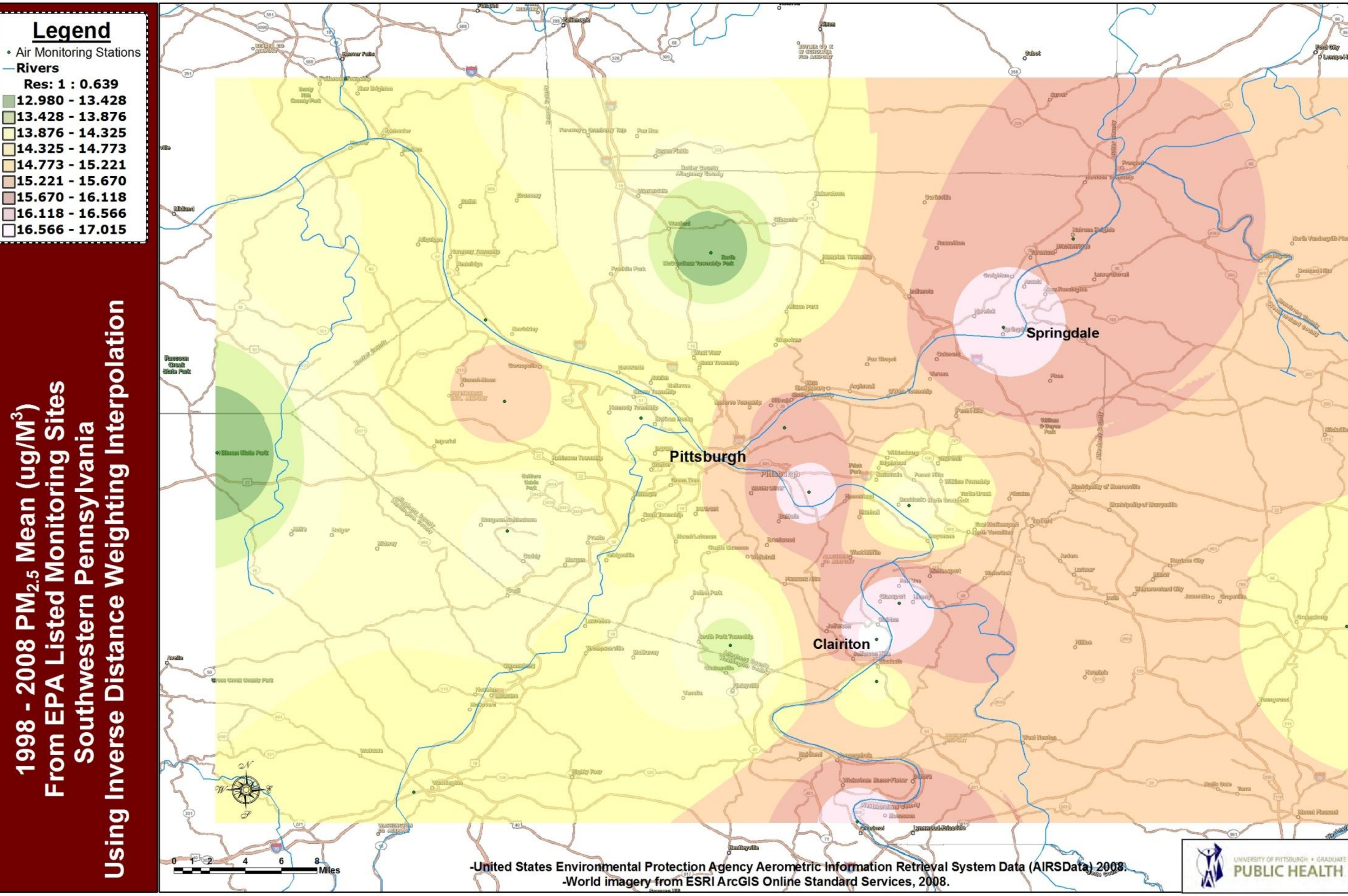
- Statistical models of spatial autocorrelation
- Provide not only predictions but certainty or accuracy of predictions and tools to manipulate
- Kriging is a linear least-squares algorithm
  - Weights points like IDW but also on the overall spatial arrangement (autocorrelation)
  - Semivariogram – means to explore relationship of distance and measurement difference





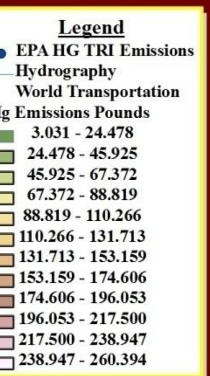
Semivariance = Slope * Distance

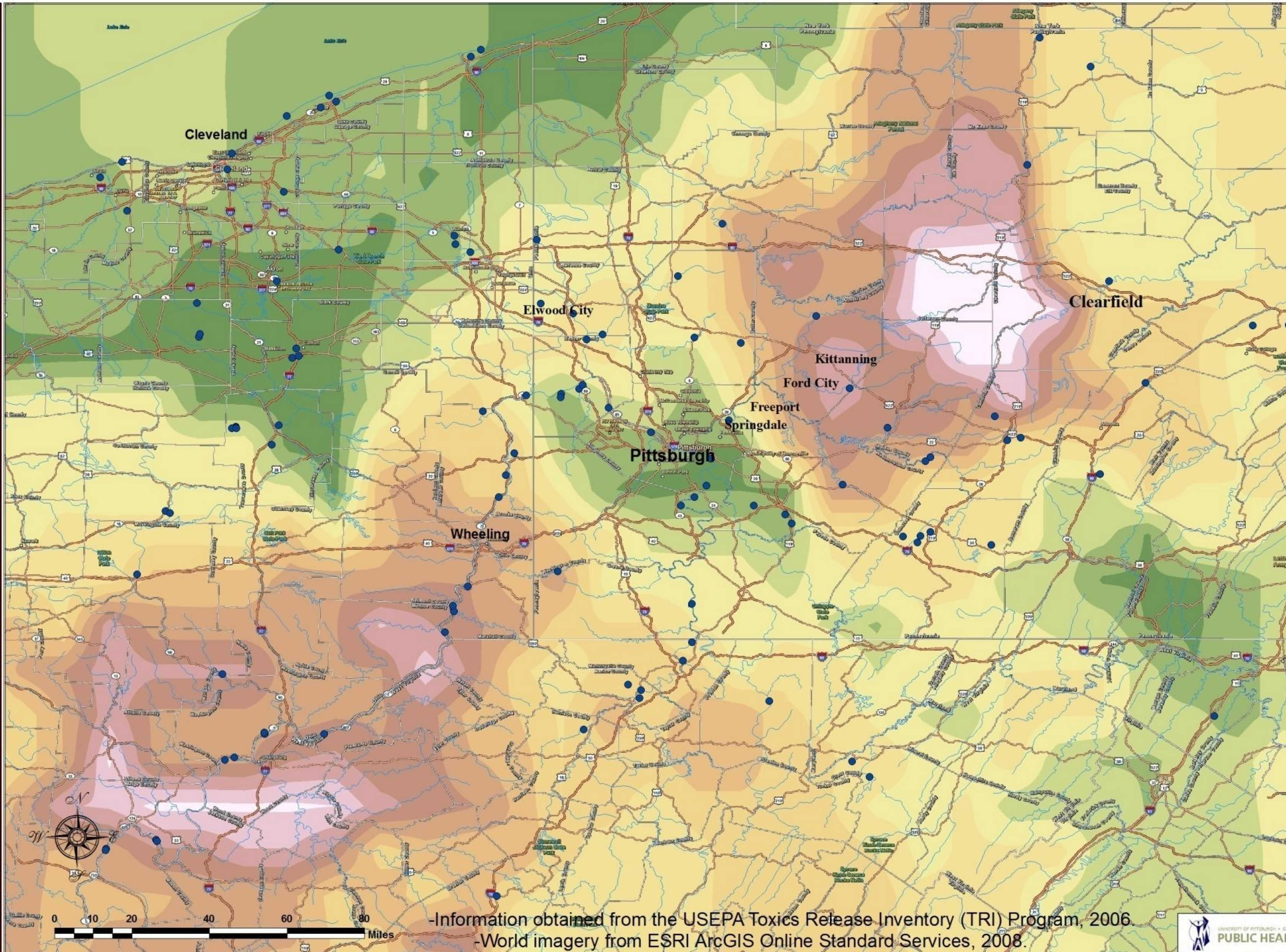
Quantify autocorrelation: pairs of locations that are close (far left x axis) should have a smaller variance (low on y axis)



1998 - 2008 PM2.5 Mean (ug/M3)
From EPA Listed Monitoring Sites
Southwestern Pennsylvania
Using Inverse Distance Weighting Interpolation
Legend
Air Monitoring Stations
Rivers
Res: 1 : 0.639
12.980 - 13.428
13.428 - 13.876
13.876 - 14.325
14.325 - 14.773
14.773 - 15.221
15.221 - 15.670
15.670 - 16.118
16.118 - 16.566
16.566 - 17.015
Pittsburgh
Springdale
Clairiton
0 1 2 4 6 8 Miles
-United States Environmental Protection Agency Aerometric Information Retrieval System Data (AIRSData) 2008.
-World imagery from ESRI ArcGIS Online Standard Services, 2008.
PUBLIC HEALTH

2006 All Mercury Emissions (Pounds)
From EPA Listed TRI Sites
Pennsylvania, W. Virgina, Ohio & Maryland
Kriging Spatial Interpolation





Conclusion

- Modeling should be approached in a thoughtful manner
- Assumptions of the models are key and should not be sacrificed
- Can provide a very powerful tool that the public seems to fancy
- Visual representations are extremely useful resources in decision making
- Modeling of exposure must take into account benefits v. cost

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