ENSC 412/612

Week 9

Readings for this week

- Text Chapters 19, 20
- Millar, G.M, T. Abel, J. Allen, P. Barn, M. Noullett, J. Spagnol, P.L. Jackson, 2010: Evaluating human exposure to fine particulate matter Part II: Modeling. *Geography Compass*, **7,** 731-749**.** DOI 10.1111/j.1749-8198.2010.00344.x

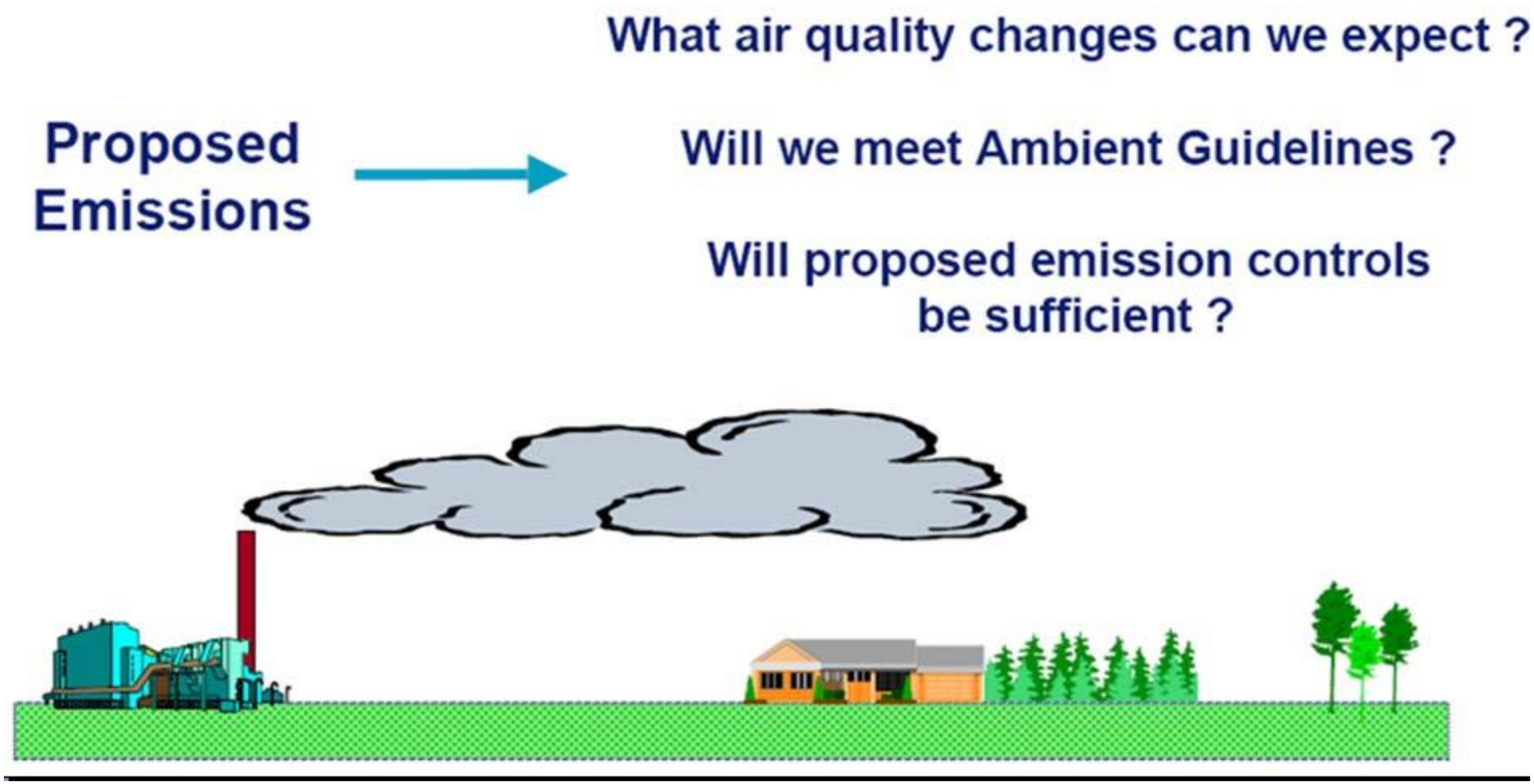
Modelling and Dispersion

- This week we will review Gaussian Plume model, expand on use of mesoscale models, and then show results of a mesoscale/AQ modelling study and preliminary results from a Calpuff modelling study for PG…

Why model Air Quality?

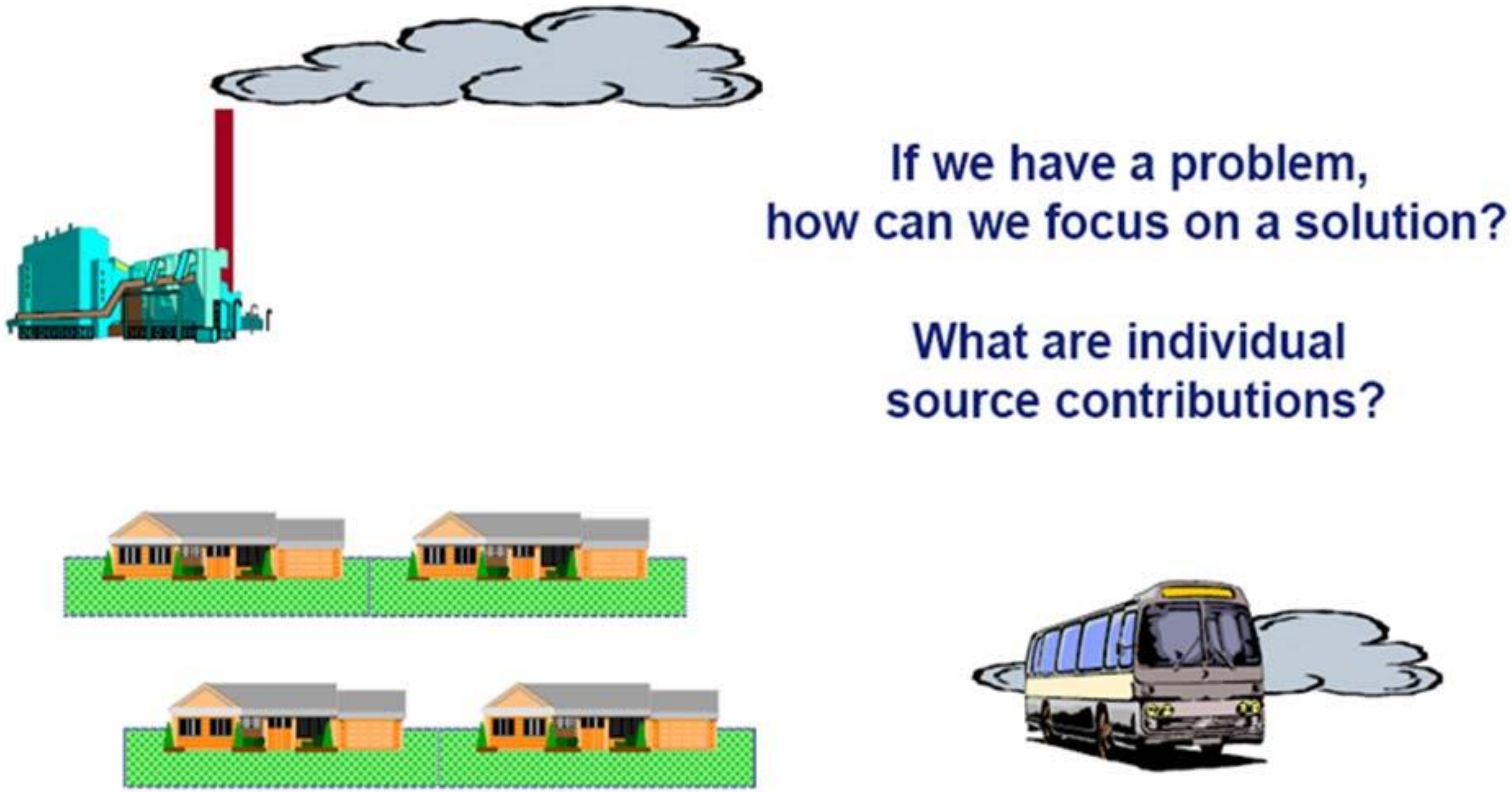
1. To assess the impact of existing or proposed new sources on ambient AQ
2. To discriminate sources in terms of their contribution to ambient levels
3. To evaluate control strategies
4. To complement ambient monitoring
5. To evaluate accidental releases
6. To forecast future levels

Assess impact of existing or new sources on ambient AQ



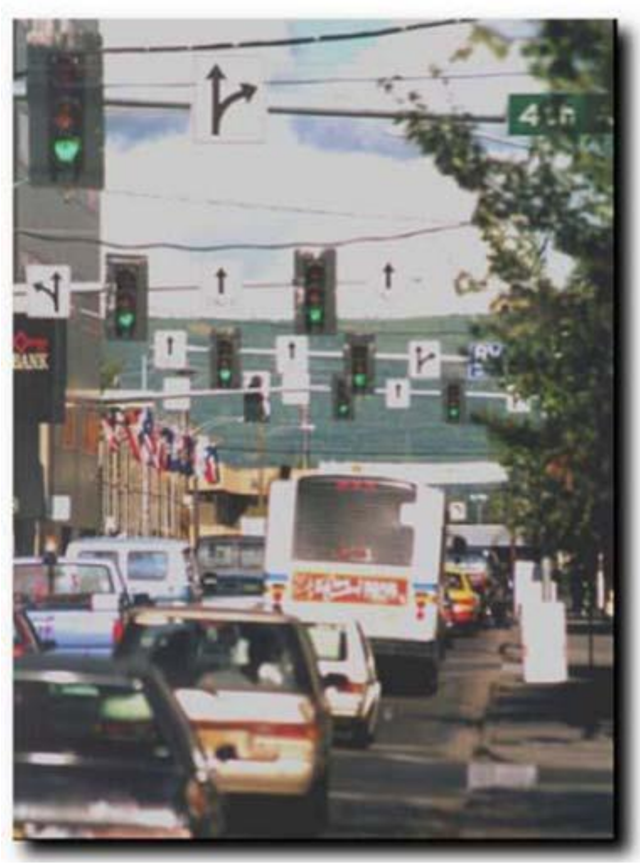
Source: Xiaoqin Yan

Assess contribution of individual sources



Source: Xiaoqin Yan

To evaluate control strategies



Where can we get the most benefit ?

Emission reduction ?

Which sector ?

Fuel switching ?

Land use planning ?

What are the costs ?

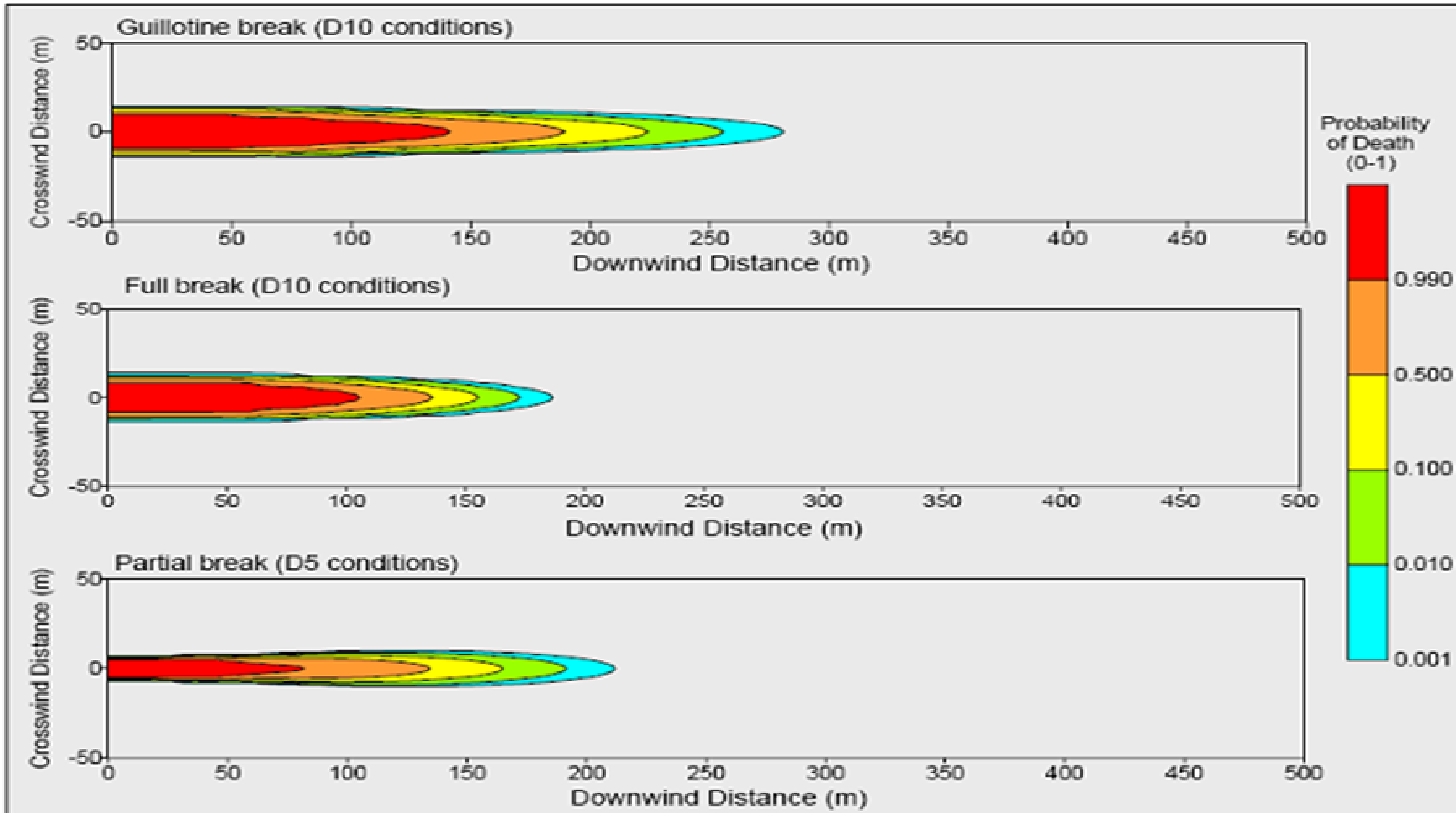
What are the improvements ?

Source: Xiaoqin Yan

Complement ambient monitoring

Source: Xiaoqin Yan

Evaluate accidental releases



Source: Xiaoqin Yan

Forecast future AQ levels

Other locations

Air Quality Health Index

Prince George

1	2	3	4	5	6	7	8	9	10	+

Risk: **Low (1 - 3)** **Moderate (4 - 6)** **High (7 - 10)** **Very High (Above 10)**

Current

Observed at 10:00 AM PDT Tuesday 15 March 2011

4
Moderate Risk

At-Risk Population:

- Consider reducing or rescheduling strenuous activities outdoors if you are experiencing symptoms.
- Find out if you are at risk

General Population:

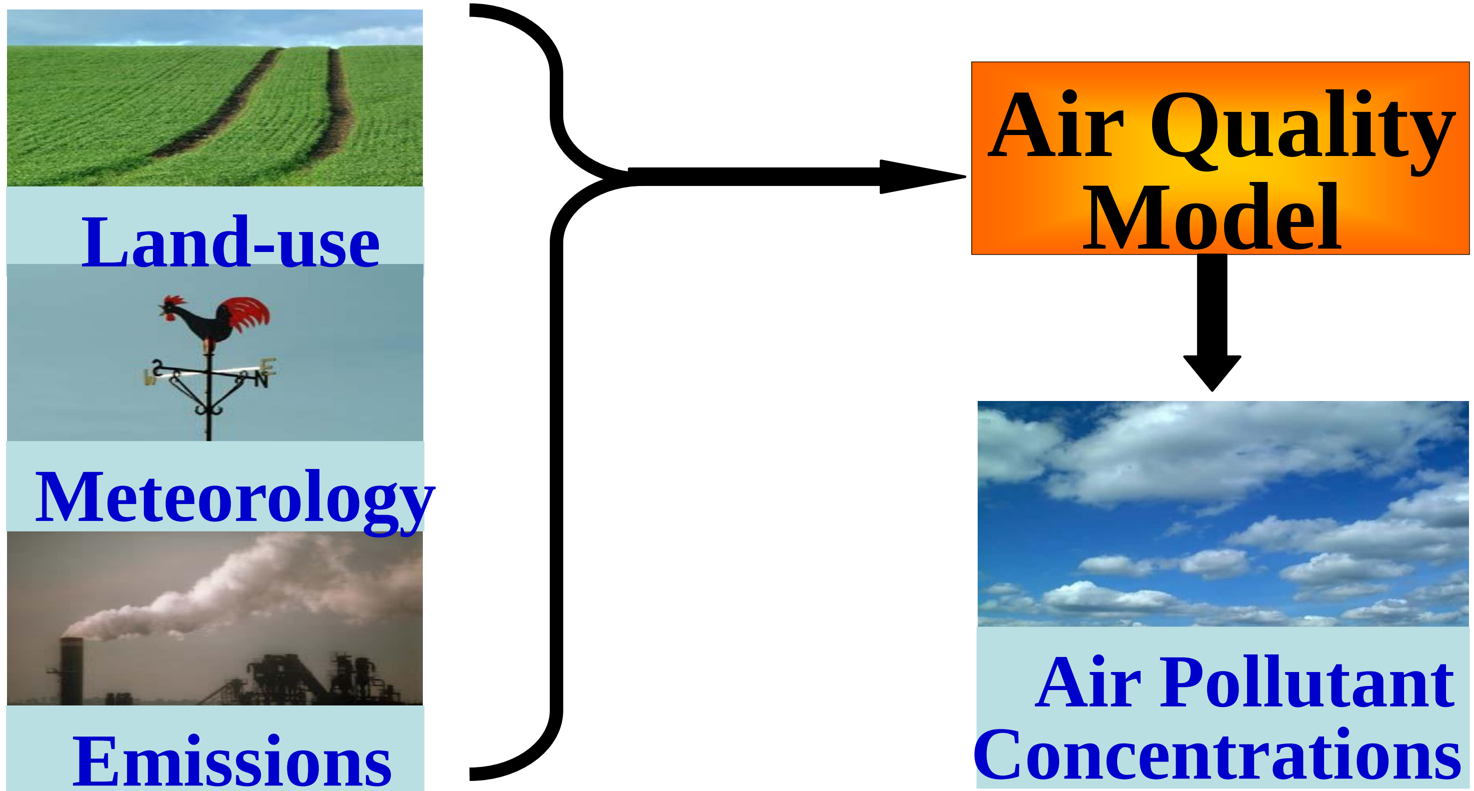
- No need to modify your usual outdoor activities unless you experience symptoms such as coughing and throat irritation.

Forecast Maximums

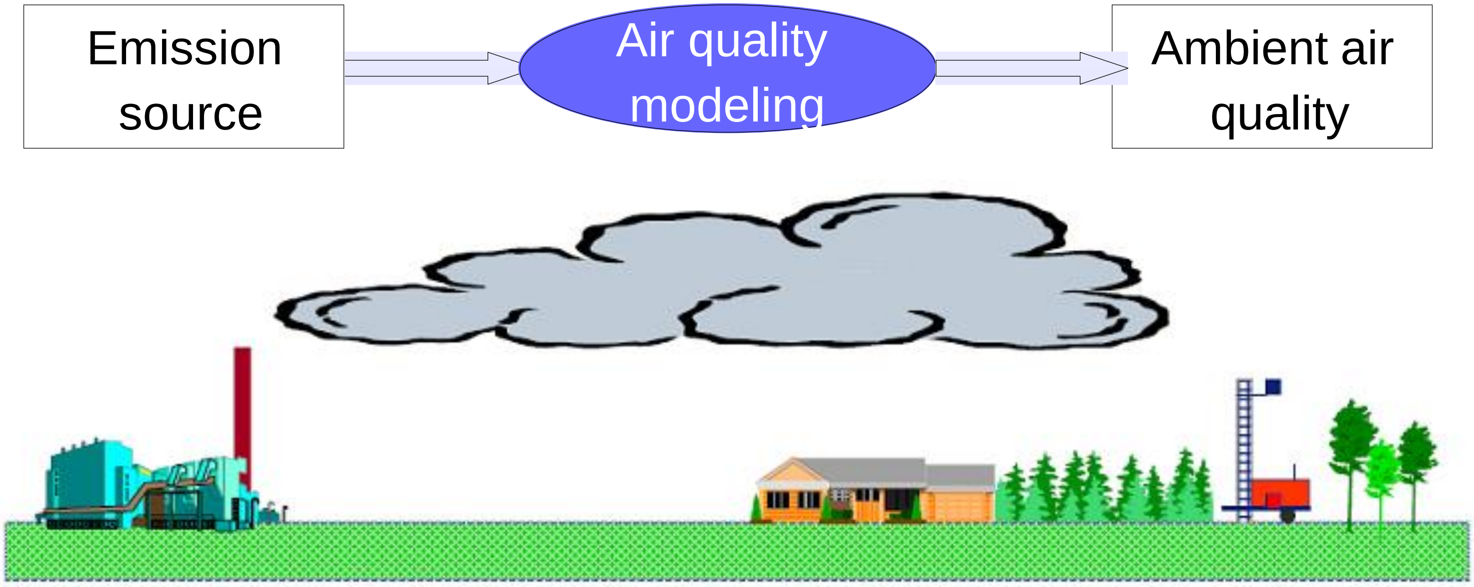
Issued at 6:00 AM PDT Tuesday 15 March 2011

Tuesday	Tuesday night	Wednesday
3 Low Risk	3 Low Risk	3 Low Risk
Health Message	Health Message	Health Message

Main Components of an AQ model



Source: Xiaoqin Yan



Source: Xiaoqin Yan

Equations that are in the model

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (u c_s)}{\partial x} - \frac{\partial (v c_s)}{\partial y}$$ hor. transport

$$+ \frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right)$$ hor. diffusion

$$-(k_{1s} + k_{2s})c_s$$ deposition

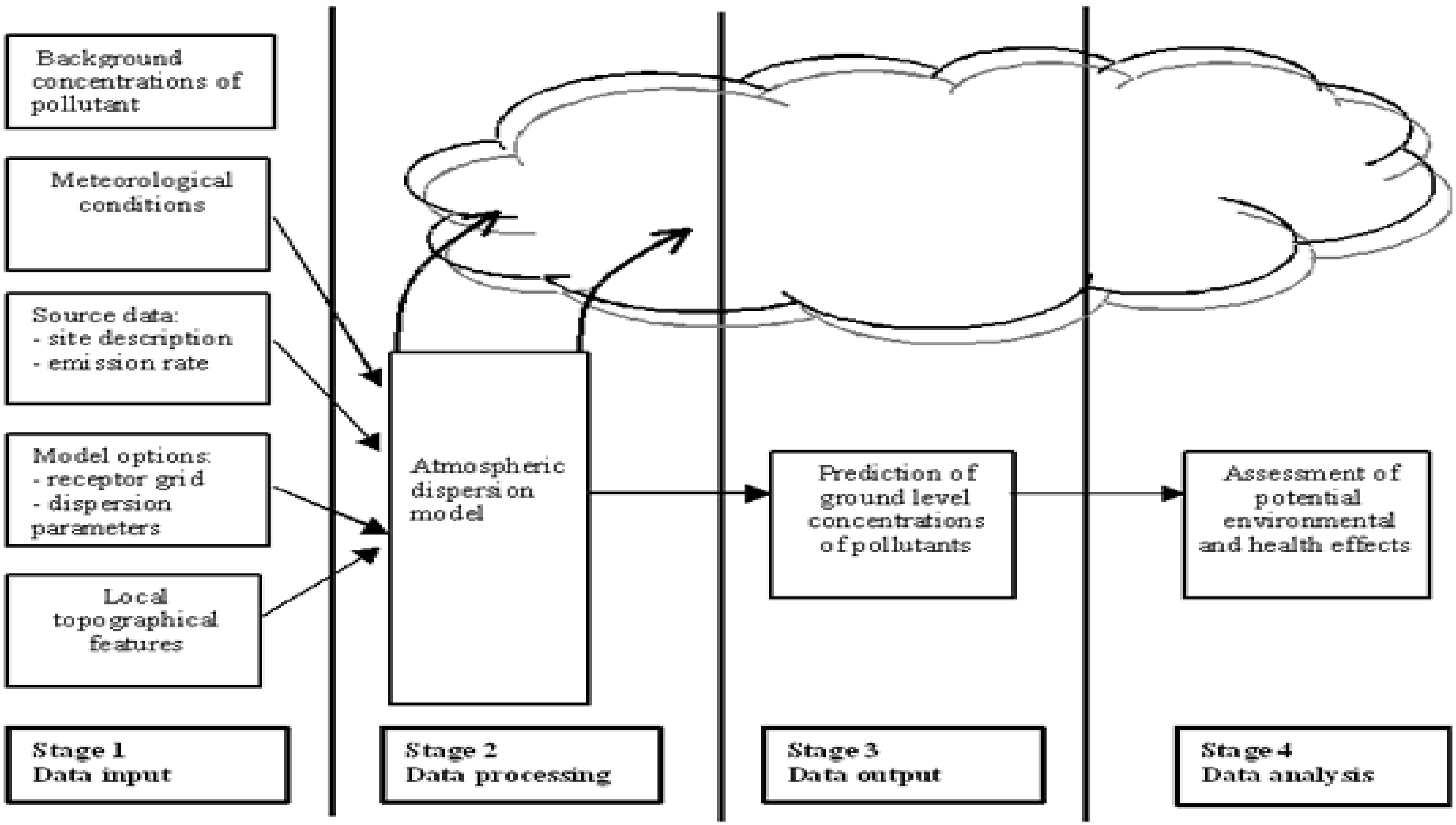
$$+ E_s + Q_s(c_1, c_2, \ldots, c_q)$$ chem. + emis.

$$-\frac{\partial (w c_s)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s}{\partial z}\right)$$ vert. transport

$$s = 1, 2, \ldots, q$$

Source: Xiaoqin Yan

Schematic of an AQ model



Source: Xiaoqin Yan

Scales and models

- ***Microscale***(10 to 100 m) and ***Middle-scale*** (100 to 500 m) –odors, dust, traffic, hazardous pollutants.

- ***Neighborhood scale***(500 m to 4 km) –vehicle exhaust, residential heating and burning, primary industrial emissions.

- ***Urban scale***(4 to 100 km) –ozone, secondary sulfates and nitrates, forest fires, regional haze.

- ***Continental scale***(1,000 to 10,000 km) –Asian and Saharan dust, large scale fires.

- ***Global scale***(> 10,000 km) –greenhouse gases, halocarbons, black carbon.

A hierarchy of AQ models

1. Gaussian Diffusion Models (plume and puff)
2. Box Models
3. Lagrangian particle models
4. 3D Eulerian Grid models (e.g. UAM)

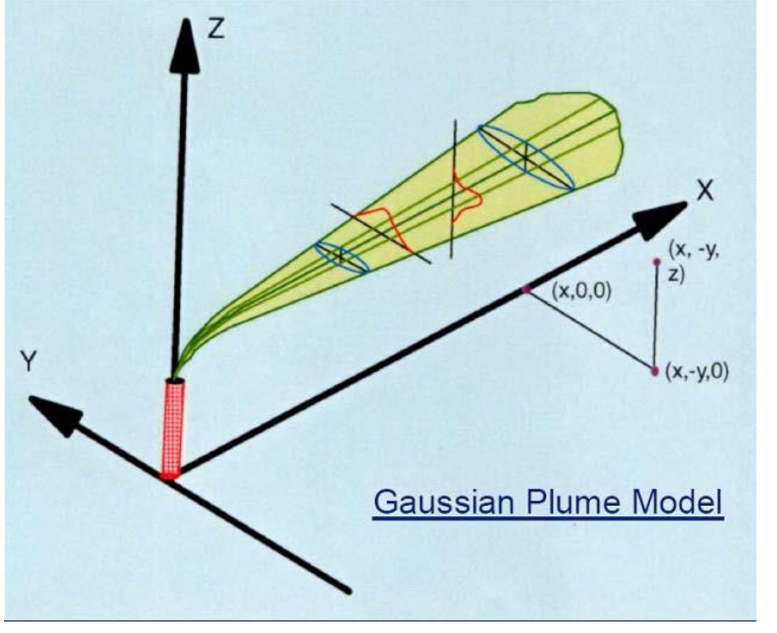
- Regional / Mesoscale AQ Models (e.g RADM / MM4, Models-3/MM5, MM5/CMAQ, MM5/Calmet/Calpuff RAMS/HYPACT, RAMS/Calmet/Calpuff)

Gaussian models

Assumptions:

1 Pollutants are transported in a straight line instantly to receptors that may be several hours or more in transport time away from the source.

2 The atmosphere is uniform across the entire modeling domain, and that transport and dispersion conditions exist unchanged long enough for the material to reach the receptor.



Application:

1 Relatively flat terrain

2 Input weather, terrain, and site information data are scarce

3 Evaluating concentrations near a source

Gaussian Plume Model Equation

$$\chi(x,y,z,H) = \frac{X}{2\pi\sigma_y\sigma_z\overline{u}} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \times \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right]$$

TERM: **1** **2** **3**

- where X is the rate of emission from the source (kg s^{-1}),
- σ_y, σ_z are the horizontal and vertical standard deviations of the pollutant distribution in the y and z directions (m),
- u is the mean horizontal wind speed through the depth of the plume direction (m s^{-1}),
- and H is the effective stack height (m) taking the actual stack height as well as plume rise into account.
- X is the pollutant concentration (kg m^{-3}), and is a function of space and the nature of turbulence.

- Term 1 in the equation denotes dilution due to horizontal stretching by the mean wind
- Term 2 denotes dispersion in the cross-wind direction
- Term 3 represents dispersion in the vertical (including reflection)
- If only the ground level concentrations are required, this equation simplifies somewhat:

$$\chi(x, y, 0, H) = \frac{X}{\pi \sigma_y \sigma_z \overline{u}} \exp\left[-\left(\frac{y^2}{2\sigma_y^2} + \frac{H^2}{2\sigma_z^2}\right)\right]$$

- The equation must be further modified to handle inversions, topography, local circulations, and different source configurations.
- The chief difficulty is in accurately finding the σ's
- Several approaches have been tried, from empirical ones based on qualitative evaluations of stability and roughness, to quantitative ones based on measurements of stability and turbulence.

- Values of σ's, will depend on the state of atmospheric turbulence: surface roughness, wind speed (mechanical) and stability (free convection).

- GPMs, despite severe limitations, have the advantage of being conceptually simple and easy to formulate, meaning that they can be run for multi-year simulations.
- Nearly all regulatory models used by government and industry are based on this kind of formulation.
- The only difficulty lies in the measurement or estimation of σ_y, σ_z that will depend on the state of turbulence $\rightarrow$ size and vigour of eddies.
- This can be done by direct measurement or by estimation based on the amount of sunshine by day, amount of clouds by night, wind speed, surface roughness.

Pasquill-Gifford Stability Classes

Table: Note: **A**, extremely unstable; **B**, moderately unstable; **C**, slightly unstable; **D**, neutral (heavy overcast day or night); **E**, slightly stable; **F**, moderately stable.

Surface wind m s^{-1}	Daytime solar radiation			Nighttime conditions	
	Strong	**Moderate**	**Slight**	$\geq$ **4/8 clouds**	$\leq$ **3/8 clouds**
< 2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-4	B	B-C	C	D	E
4-6	C	C-D	D	D	D
> 6	C	D	D	D	D

Briggs' sigma formulae

Stability Class	σ_y (m)	σ_z (m)
Open country conditions		
A	$0.22x(1 + 0.0001x)^{-.5}$	$.20x$
B	$0.16x(1 + 0.0001x)^{-.5}$	$.12x$
C	$0.11x(1 + 0.0001x)^{-.5}$	$.08x(1 + 0.0002x)^{-.5}$
D	$0.08x(1 + 0.0001x)^{-.5}$	$.06x(1 + 0.0015x)^{-.5}$
E	$0.06x(1 + 0.0001x)^{-.5}$	$.03x(1 + 0.0003x)^{-1}$
F	$0.04x(1 + 0.0001x)^{-.5}$	$.016x(1 + 0.0003x)^{-1}$
Urban conditions		
A-B	$0.32x(1 + 0.0004x)^{-.5}$	$.24x(1 + 0.001x)^{.5}$
C	$0.22x(1 + 0.0004x)^{-.5}$	$.20x$
D	$0.16x(1 + 0.0004x)^{-.5}$	$.14x(1 + .0003x)^{-.5}$
E-F	$0.11x(1 + 0.0004x)^{-.5}$	$.08x(1 + .00015x)^{-.5}$

Limitations

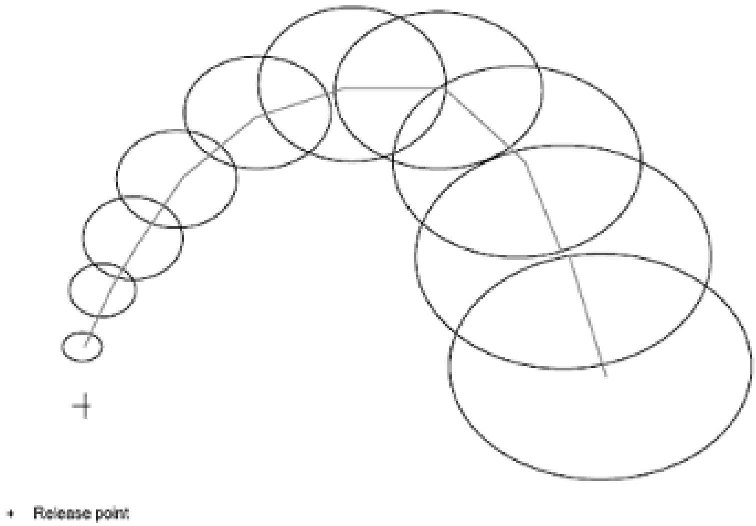
- Continuous emissions from a point source (can be modified to relax this)
- Inert weightless pollutants (< 20 μm or gases - can be modified to give deposition)
- Time periods > 10 min
- Distances of 100 m to 10 km form source
- Topography - need to allow plumes to rise over higher terrain
- Inversions/elevated stable layers
- Local circulations, especially in mountain or valley environments
- Modern implementations have parameterizations to remedy these shortcomings
- US EPA maintains several GPMs – ISC, RTDM, etc
- More advanced models have been developed…

Gaussian Puff model

Assumption:

1 Pollutant releases can be represented by a series of puffs of material which are transported by the model winds.

2 Each puff represents a discrete amount of pollution, whose volume increases due to turbulent mixing.



Application:

1 Complex terrain

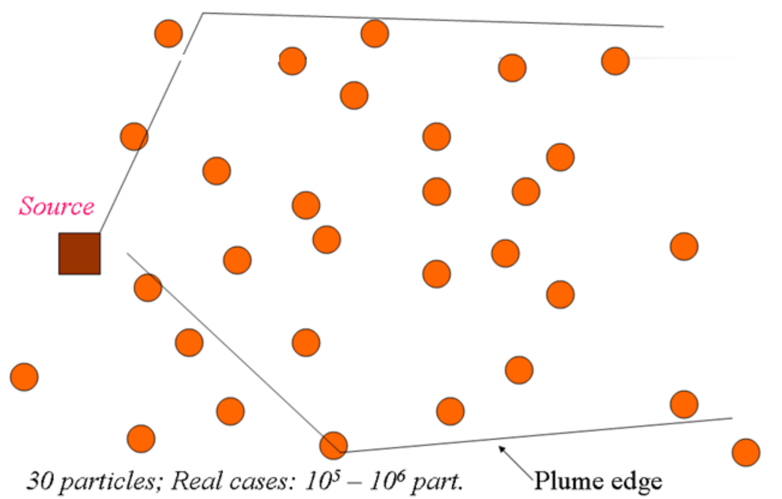
2 Variable weather is expected

3 Long-range transport

Lagrangian particle dispersion model

Assumption:

- Pollutant releases are represented by a stream of particles (even if the pollutant is a gas), which are transported by the model winds and diffuse randomly according to the model turbulence.



Application:

1 Complex terrain

2 Variable weather is expected

3 Long-range transport

4 Need trajectory information

5 Research applications

Box models

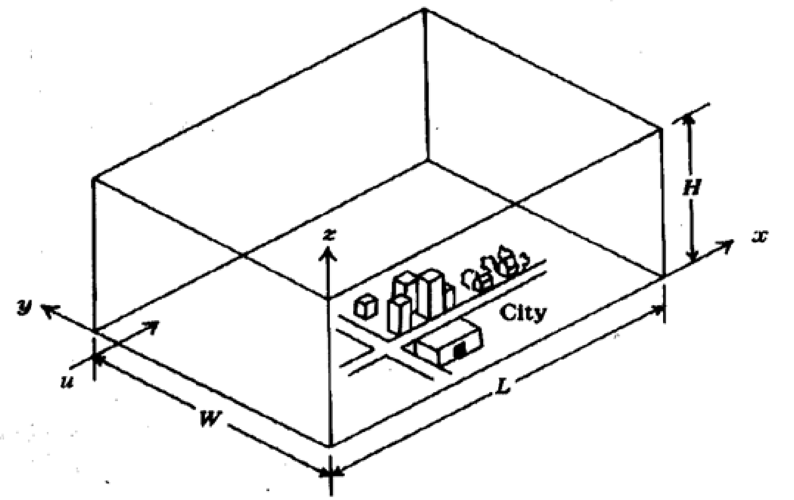
Assumptions:

1 Uniform mixing throughout the volume of a three dimensional box

2 Conservation of mass principle applied to relatively large scale systems such as an urban airshed.

3 ACCUMULATION =

INPUT -OUTPUT + GENERATION - CONSUMPTION



Mesoscale AQ Models

- Mesoscale Models (MM) solve full set of atmospheric equations for evolution of wind, temperature, etc.
- Can represent **3D fields** including **terrain effects**

- Dispersion Models (DM) traditionally had uniform winds, uniform stability, etc. → poor representation of meteorology especially in complex terrain

- MM meteorological outputs are combined with a dispersion model, combined with a chemical model to calculate pollutant concentrations across space and through time
- Traditional DM treat concentration across a plume as a gaussian distribution whose standard deviation depends on downwind distance and atmospheric turbulence
- Recently developed DM (e.g. Calmet/Calpuff) are more of a hybrid to approach MM in realism
- They are still limited to essentially physically constrained interpolation of observations onto a 3D grid → still not fully physically based

Issues with MM AQ models

- MM are computationally much more expensive than DM, especially when high spatial resolution is required
- For EIA / scenario planning this can be problematic as typically a five year simulation is a minimum to represent the range of meteorological variability
- MM are not trivial to run → require capable hardware, and highly qualified operator → they are just leaving the research realm

- Sub-grid scale parameterization schemes (e.g for turbulence, cloud physics, etc.) for MM models have been developed at coarse resolution (typically > 10 km), but are increasingly being applied at much higher resolution
- MM have many more options / settings → it is unlikely that two different operators would choose exactly the same settings limiting repeatability

- MM need accurate, high spatial and temporal resolution initial and boundary conditions to successfully simulate the atmosphere
- MM can only be as good as the coarser resolution model used for IC/BCs → errors in synoptic scale forecasts will degrade MM
- 2.5 degree NCEP fields on standard levels not always sufficient, especially to initialize and nudge the boundary layer which is critical for dispersion

- If one wants to get close to the “right” answer, MM offer usually the best chance of that, almost certainly for forecasts, and probably for hindcasts
- If one wants to “understand” the answer, be able to hindcast long time periods quickly, and with less operator training, and have (more) repeatable results, DM will continue to have a role even though the “answer” they give is almost certainly incorrect

Toward Resolving Issues

- MM have been shown successful in case studies and in forecast mode for real-time AQ assessments
- Traditional DM still have a place for regulatory purposes as they are standardized, repeatable, computationally efficient and can be used more easily by practitioners

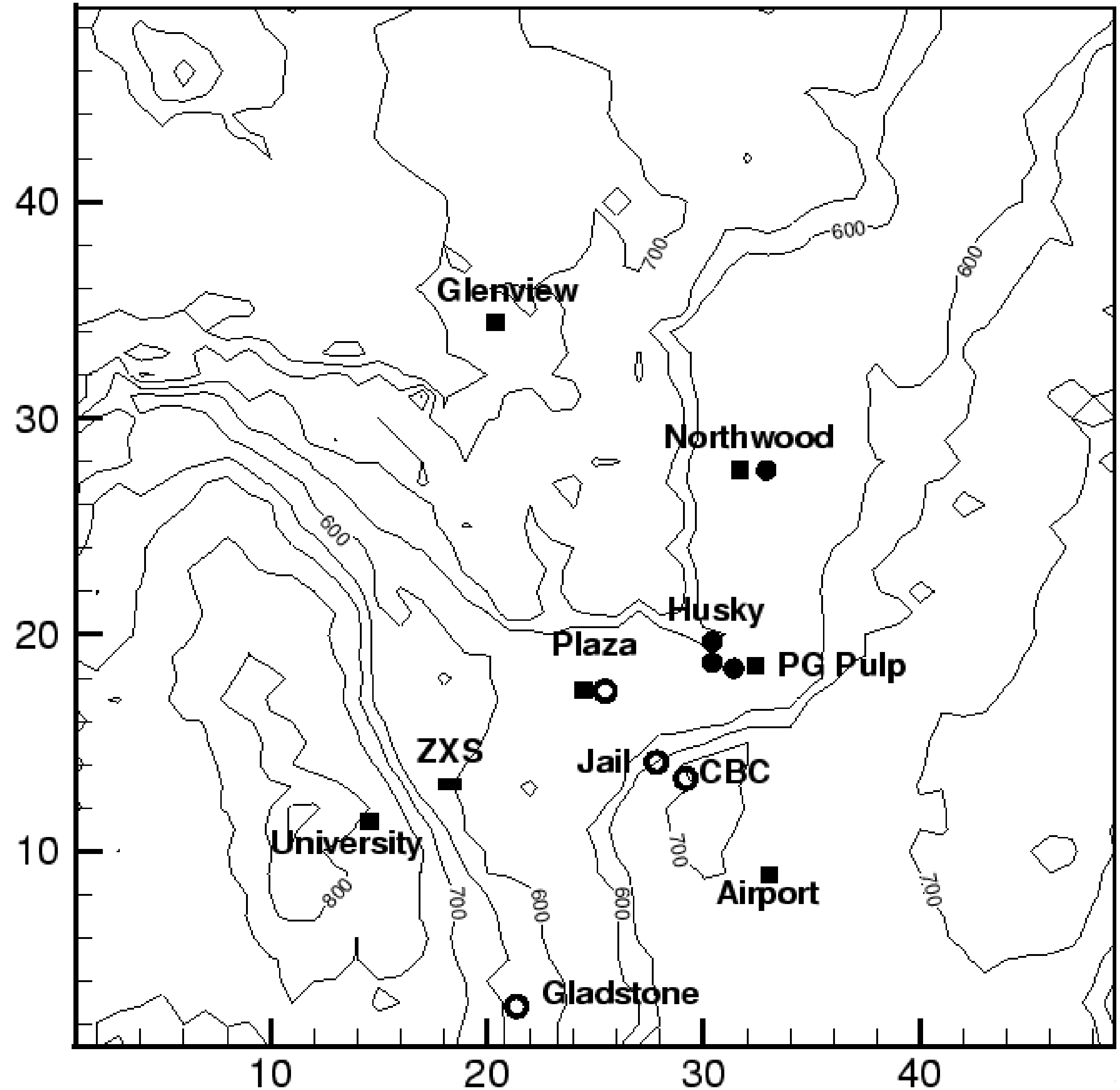
- For MM to enter regulatory realm, things either need to be standardized:
  - Production of high-resolution, validated, gridded datasets for IC/BCs (these may be able to be utilized directly by a dispersion/chemical model) to be used in hindcasts
  - Designation of a “frozen” model and settings
- **Or** ensemble approaches in which variation in models, settings, IC/BCs can be used to drive the suite of models (e.g. Warner et al 2002, *Mon. Wea. Rev.* 488-504.)

Example of application of MM

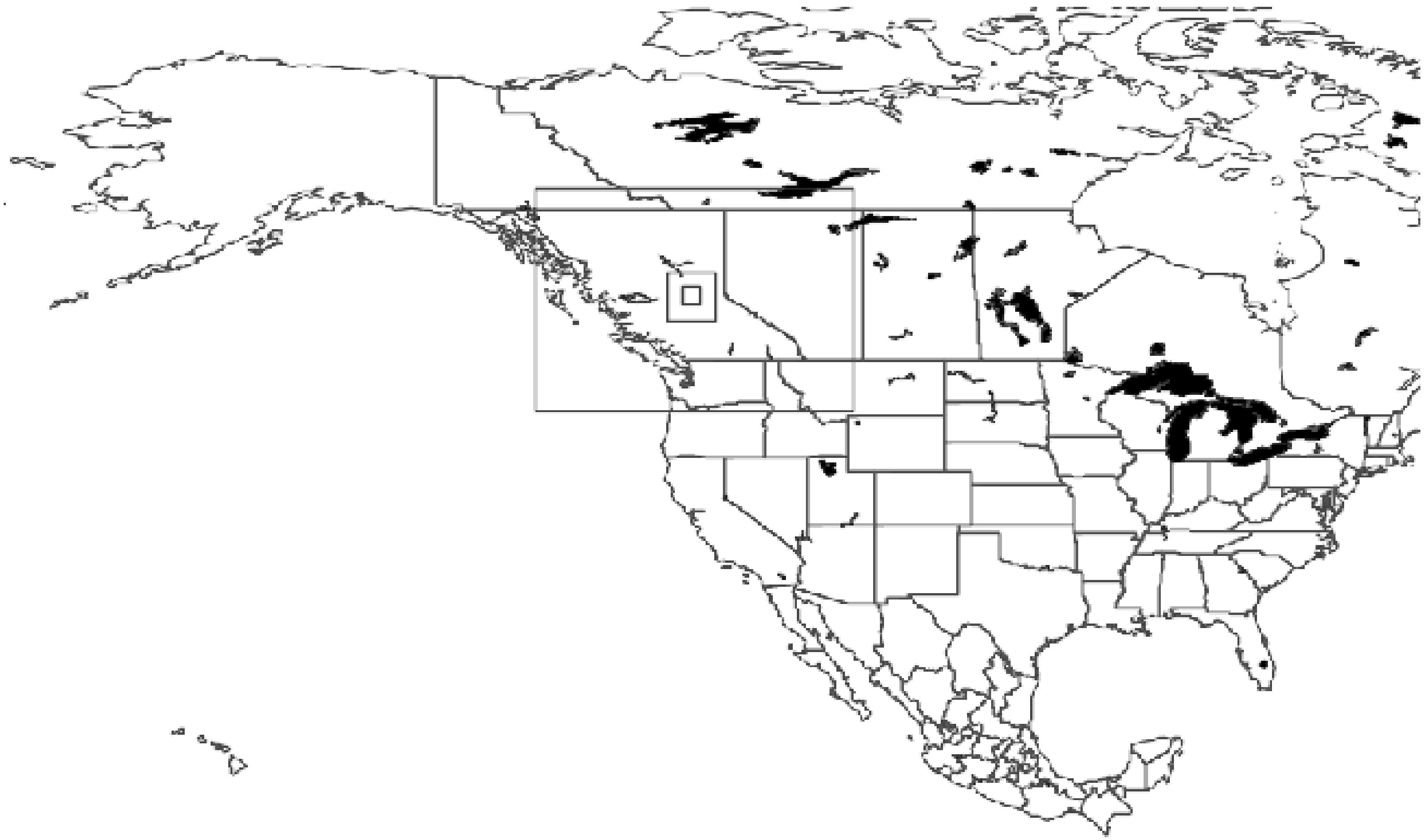
Application of High Resolution Mesoscale Model Fields with the Calpuff Dispersion Modelling System in Prince George

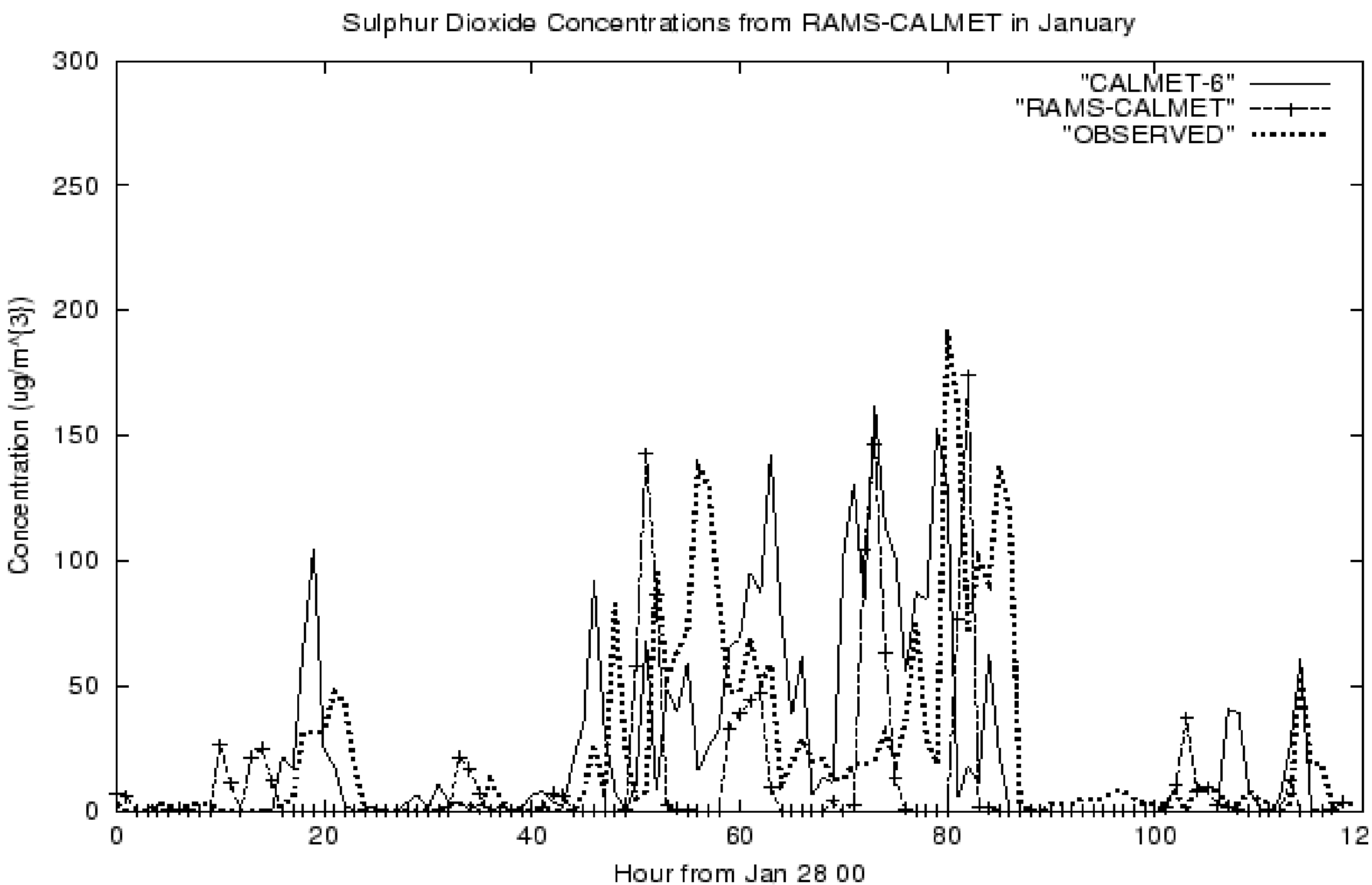
Bryan McEwen, MSc. Thesis 2002

- Thesis project is to see if using RAMS as input to Calmet/Calpuff can “add value” to predictions compared with Calmet/Calpuff driven by observations alone.
- Three 5 day periods in 1999 with elevated SO_2 at some locations were modelled
- RAMS windfields were inserted into Calmet, and Calpuff was used to find ambient SO_2
- Calmet was also run without RAMS, using observations from 1, 3, and 6 surface stations



Glenview
Northwood
Husky
Plaza
PG Pulp
ZXS
Jail
CBC
University
Airport
Gladstone
600
700
800
10
20
30
40




Sulphur Dioxide Concentrations from RAMS-CALMET in January
"CALMET-6"
"RAMS-CALMET"
"OBSERVED"
Concentration (ug/m^(3))
Hour from Jan 28 00
0
50
100
150
200
250
300
0
20
40
60
80
100
120

Calmet-6	RAMS-Calmet	Calmet-1	Calmet-3
61%	67%	99%	98%

Mean Relative Error scores for 24 Hour SO2 during January case

Calmet-6	RAMS-Calmet	Calmet-1	Calmet-3
71%	68%	97%	97%

Mean Relative Error scores for 24 Hour SO2 during April case

Calmet-6	RAMS-Calmet	Calmet-1	Calmet-3
83%	84%	79%	97%

Mean Relative Error scores for 24 Hour SO2 during June case

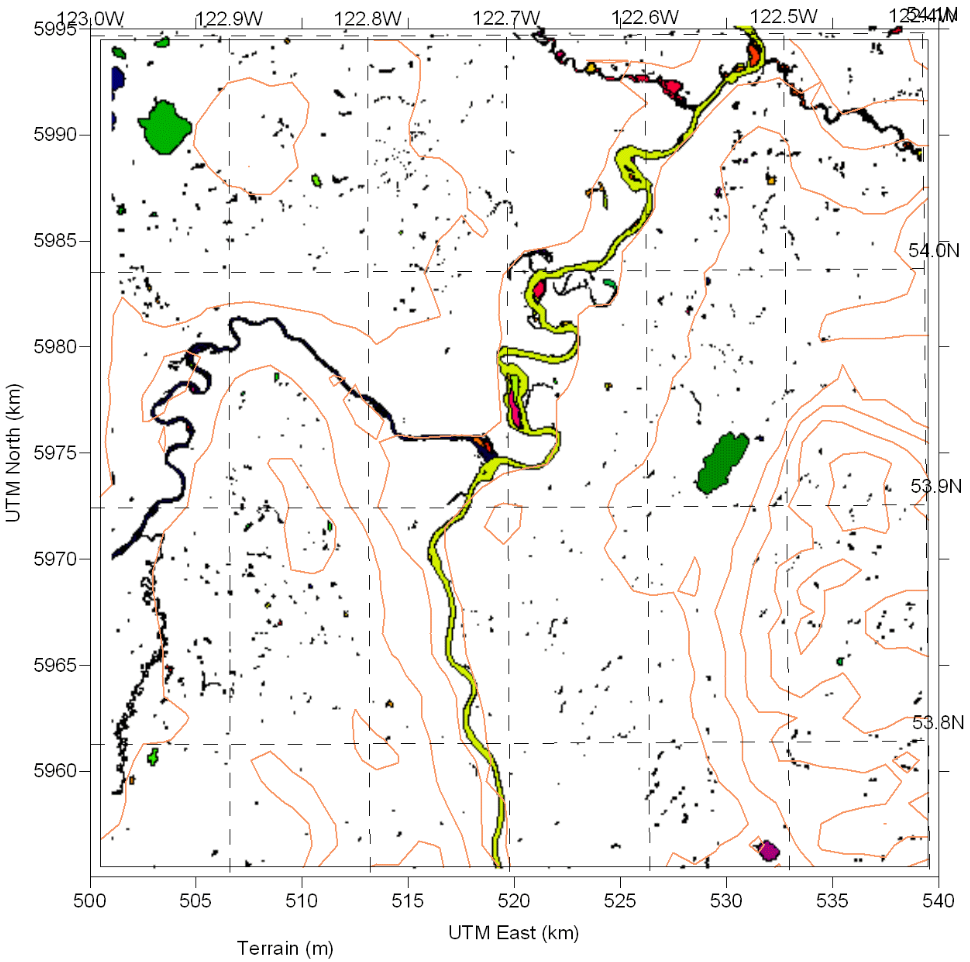
Conclusions

- Considerable variability from all model systems
- RAMS generally better than Calmet 1, 3; not consistently better when Calmet has more obs
- RAMS over predicts at the higher elevation stations and under predicts at lower elevations → related to poor resolution of inversion
- RAMS run with only NCEP 2.5 degree fields → no observations or soundings – a harsh test of the strategy
- Need to run system over a longer test period to fully evaluate

Acknowledgments for RAMS/Calpuff study

- This is Bryan McEwen's work!
- BC Oil & Gas Commission Environmental Fund funded it
- Computations made on the UNBC HPC SGI 28 processor Origin 3400
- BC Ministry of Water, Land and Air Protection

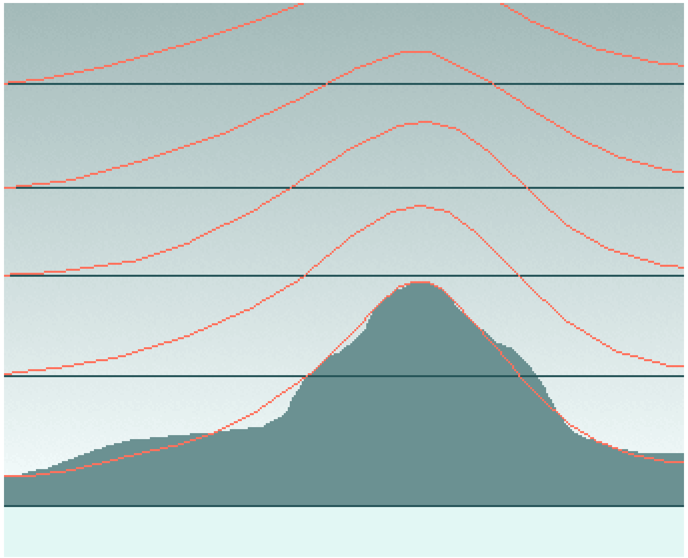
PGAQ Calmet/Calpuff Modelling Study



40 km x 40 km @ 1 km resolution

11 levels (10 layers) (metres)

0, 20, 50, 80, 100, 200, 400, 800, 1400, 2000, 3000

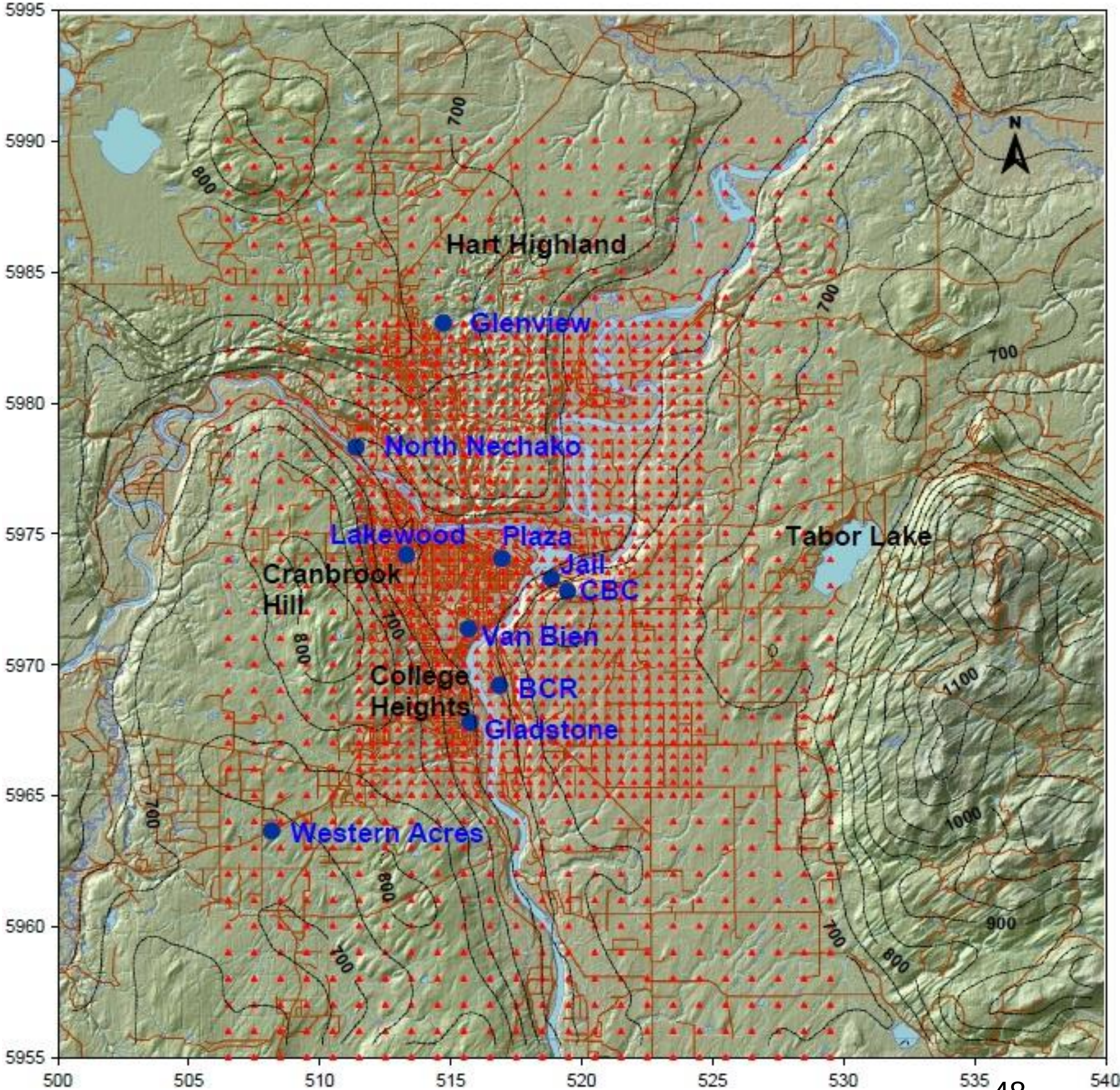


Results

- Strategy was to have emission inventory valid for year 2005, and to use this year for evaluating the model
- Years 2003-2005 were then simulated with the 2005 emissions, in order to understand range of conditions due to inter-annual variations in meteorology
- We found out in interim stages that there are some errors in the emission inventory that needed to be remodelled → rail locomotive emissions are too high; sawmill emissions are over-estimated; there are some “missing” sources…
- We are currently updating this study to be valid from 2014-2016 (sources and meteorology)

Model Domain

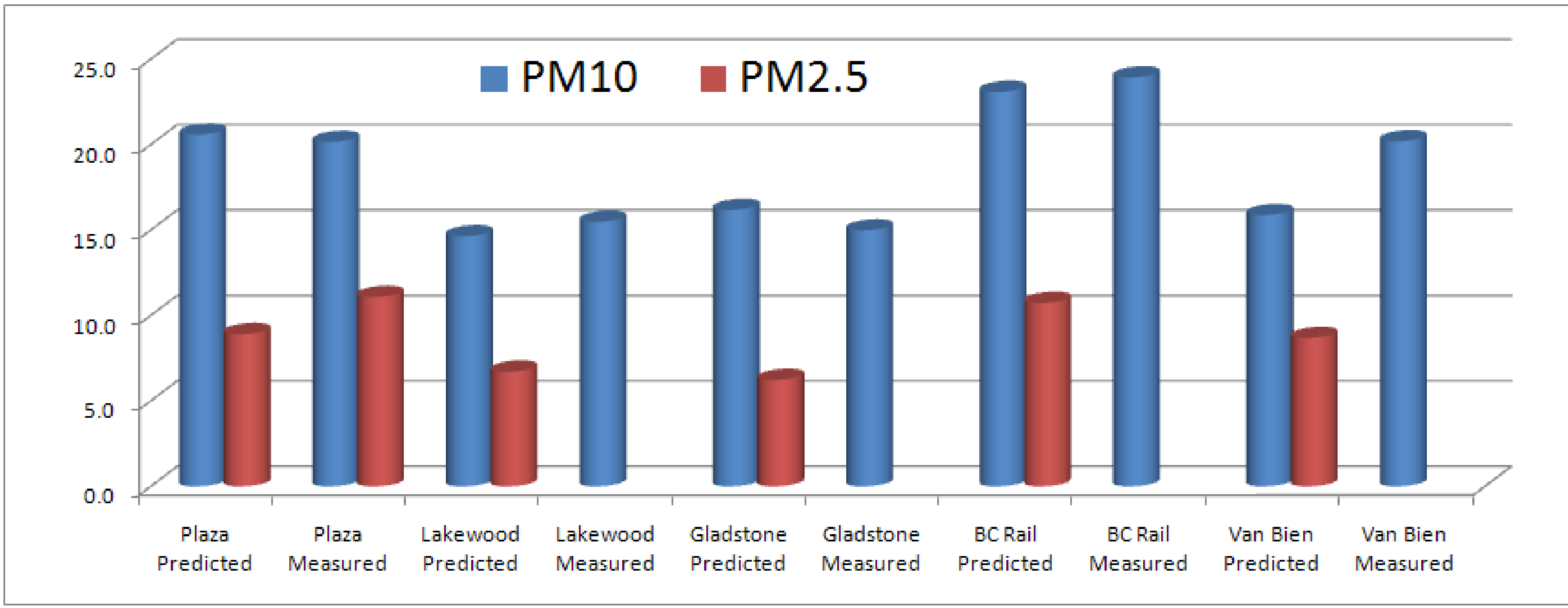
- There were 1883 receptors where ambient pollutant levels were calculated (red dots)
- Every hour between 2003-2005 was modelled
- About 1500 individual sources were modelled, as point, area or lines
- 33 permitted (industrial) sources with about 350 emitting units



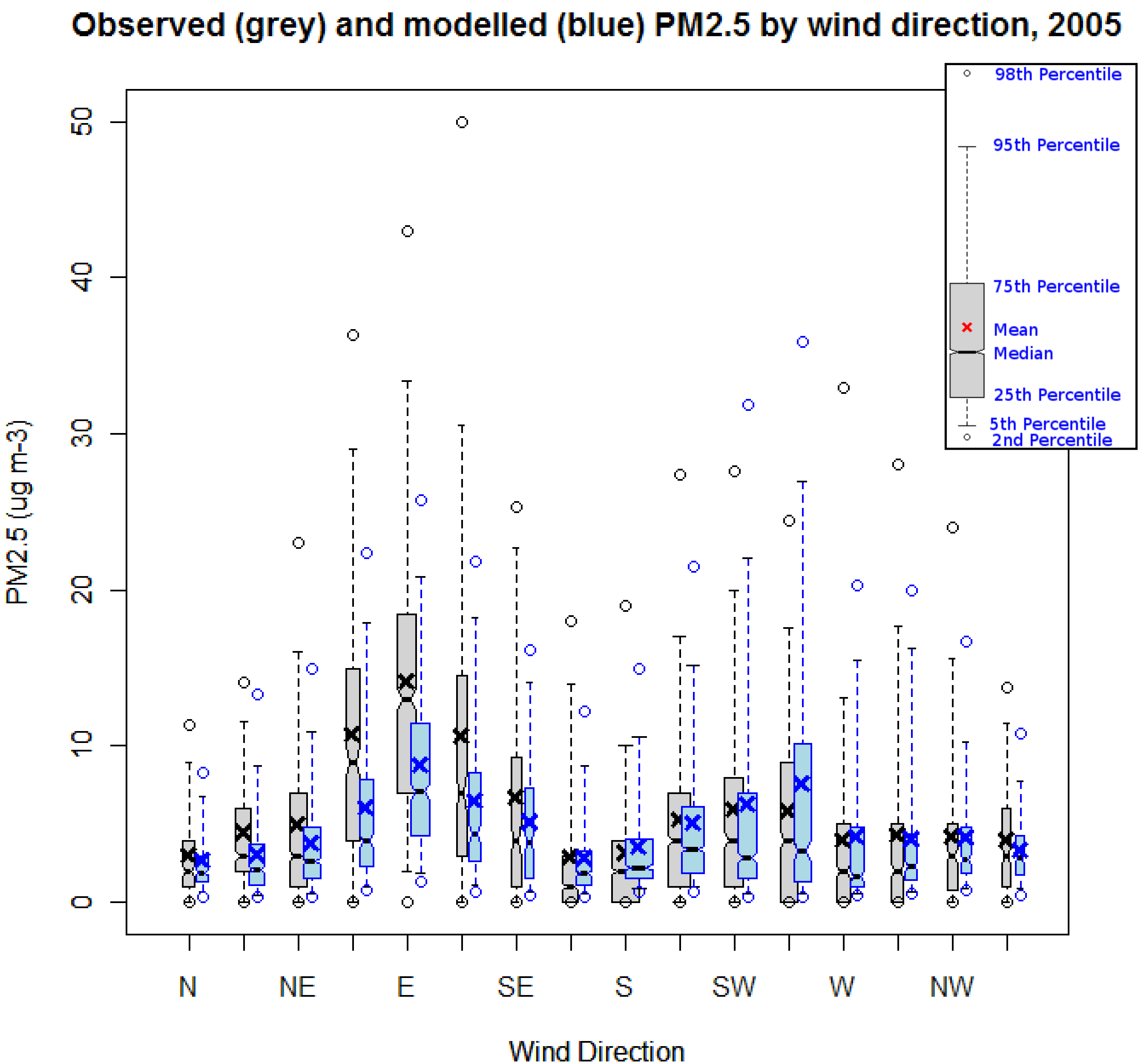
Source: Stantec (2010)

Model Performance

- 2003-2005 Average Predicted vs Measured PM_{10} & $PM_{2.5}$
- The mean is reasonably well predicted at most locations



Source: Stantec (2010)



Plaza **observed** and **modelled** $PM_{2.5}$

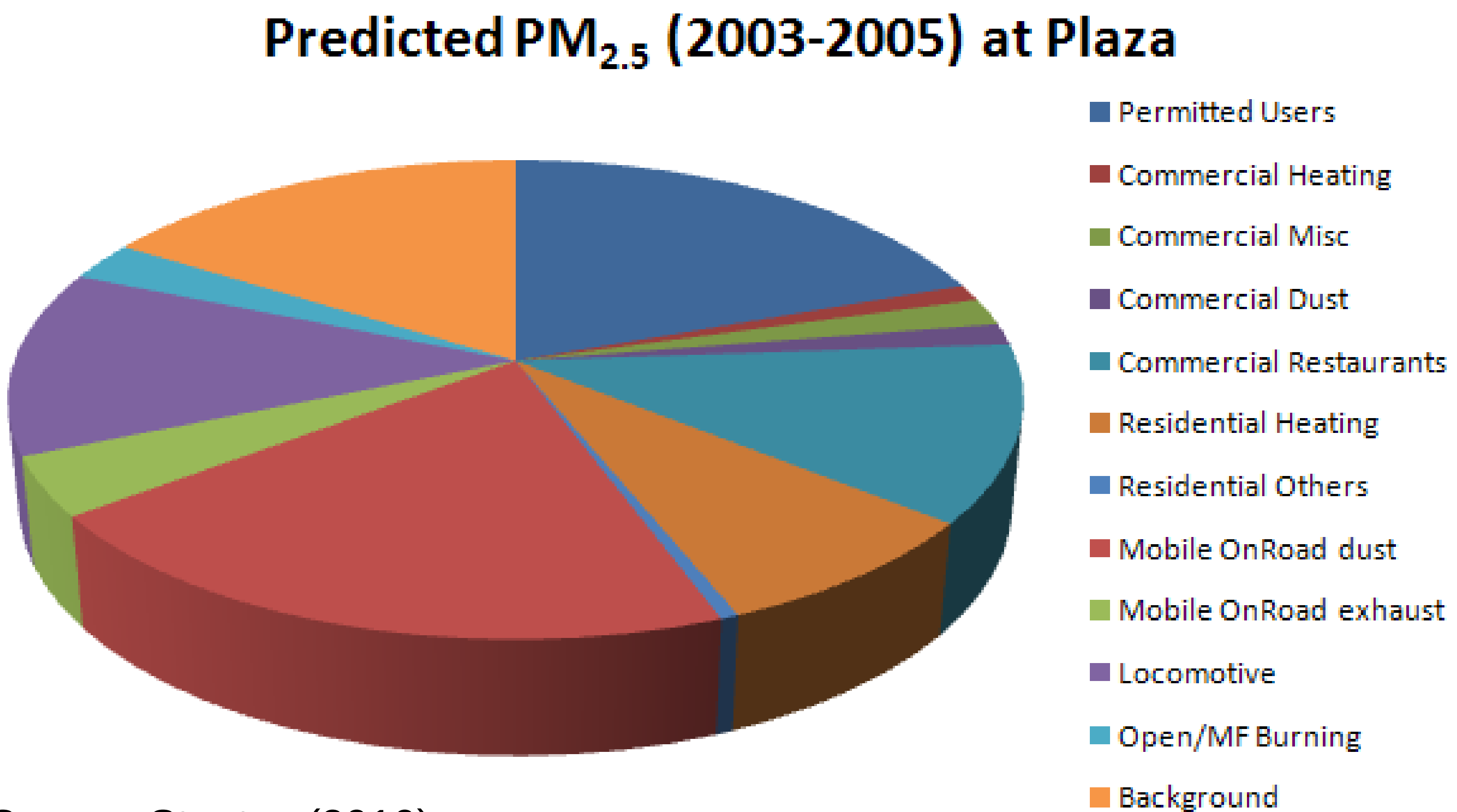
- Model under-predicts from the easterly quadrant
- We think this is a model windfield issue
- Could also be underestimating the sources in the industrial sector (e.g. condensable PM, secondary PM, fugitive dust)

Model Performance

- These results show that the model is generally performing well, at times over predicting but usually under predicting.
- There appears to be an under-predicting bias downtown with winds from the east and northeast
- Some uncertainty results from use of background values derived from measurements taken some 300 km to the east of Prince George, and in different years.
- There is also uncertainty in the measured concentrations.

Monitoring Site Receptor Results

Predicted $PM_{2.5}$ Contributions by Source Category at the Plaza Site



Source: Stantec (2010)

Comparison between STI source apportionment of $PM_{2.5}$ and Calpuff dispersion modelling for Plaza 2005

STI categories	CMB STI (2008)	PMF STI (2008)	Calpuff Stantec (2010)	Stantec Categories
Pulp Mill	25 %	24%	21%	Permitted
Burning	26%	18%	25%	Restaurants Res. Heating Open Burning Res. Other
Carbon (HDDV, LDGV, OC)	24%	22%	22%	Locomotives, On-road mobile, Com. heating
Soil	5%	10%	30%	On-road dust Com. dust Background
Other	20%	26%	2%	Com. misc.

Calpuff Summary

- The predicted PM_{10} and to a lesser extent, $PM_{2.5}$ concentrations are heavily influenced by dust emission sources, especially on-road vehicles.
- For downtown, the predicted concentrations attributed to restaurants ranked higher than expected – Dennis Fudge has been re-evaluating the emission inventory (emissions could be two-times too large) and dispersion model settings (results mostly neutral so far).
- Permitted users emissions do not appear to dominate the predicted PM_{10} and $PM_{2.5}$ concentrations except near the facilities
  - However the model is under-predicting ambient levels at Plaza when winds are from the east, so there may be a bias
  - These conclusions may differ had *fugitive dust* emissions from industrial yards and storage piles been included in the dispersion modelling.
  - As well, *condensable PM* emissions were ignored, perhaps leading to an under prediction in permitted users emissions and secondary particulate matter formation.

Readings for next week

- Text Chapters 5, 26, 27
- Millar, G., 2007: Best Practices in Air Quality Management. Prince George Mayor's Air Quality Task Force. 43 pp.
- Longhurst et al, 2009: The development of effects-based air quality management regimes. Atmos. Env., 43, 64-78.