ATSC 595D

Atmospheric Dispersion Modeling

Synthesis and Summary

R. Stull
Spring 2024
UBC

https://carbonfund.org/how-do-greenhouse-gases-contribute-to-global-warming/

Course Goals

https://www.eoas.ubc.ca/courses/atsc507/ADM/home/LearningGoals_ADM.html

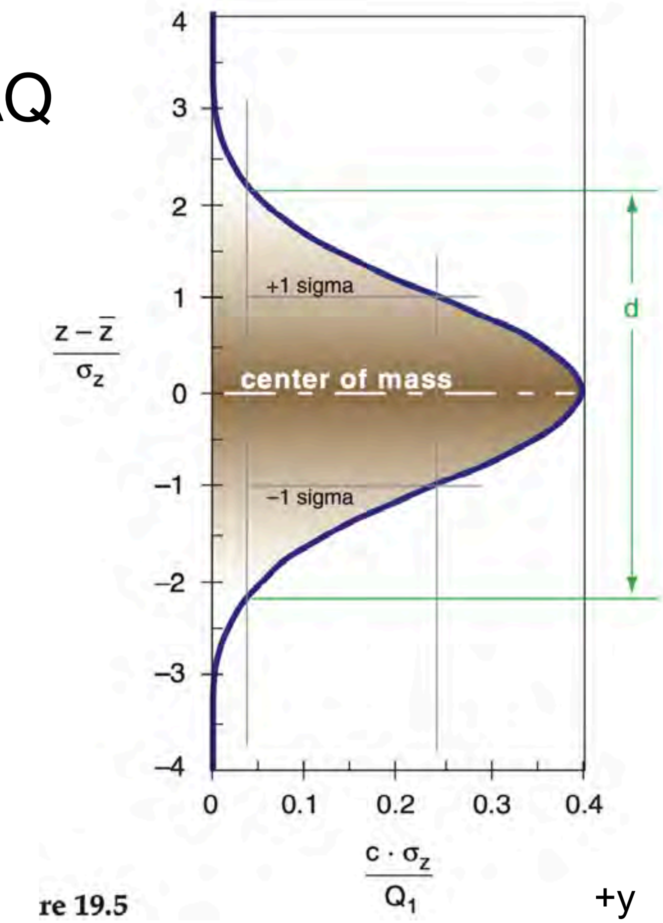
By the end of this course, you will be able to:

1. Independently install and run the following air-pollution dispersion models:
    - AERMOD
    - HYSPLIT
    - CALPUFF
    - CMAQ
2. Explain the physics, assumptions and limitations of those models (so they are NOT "black boxes").
3. Acquire appropriate input data for meteorology, pollutant source specs, etc. to run the models.
4. Visualize meteorological and air-quality fields using Panoply and Vapor.
5. Present and interpret the output from those models for clients and colleagues.

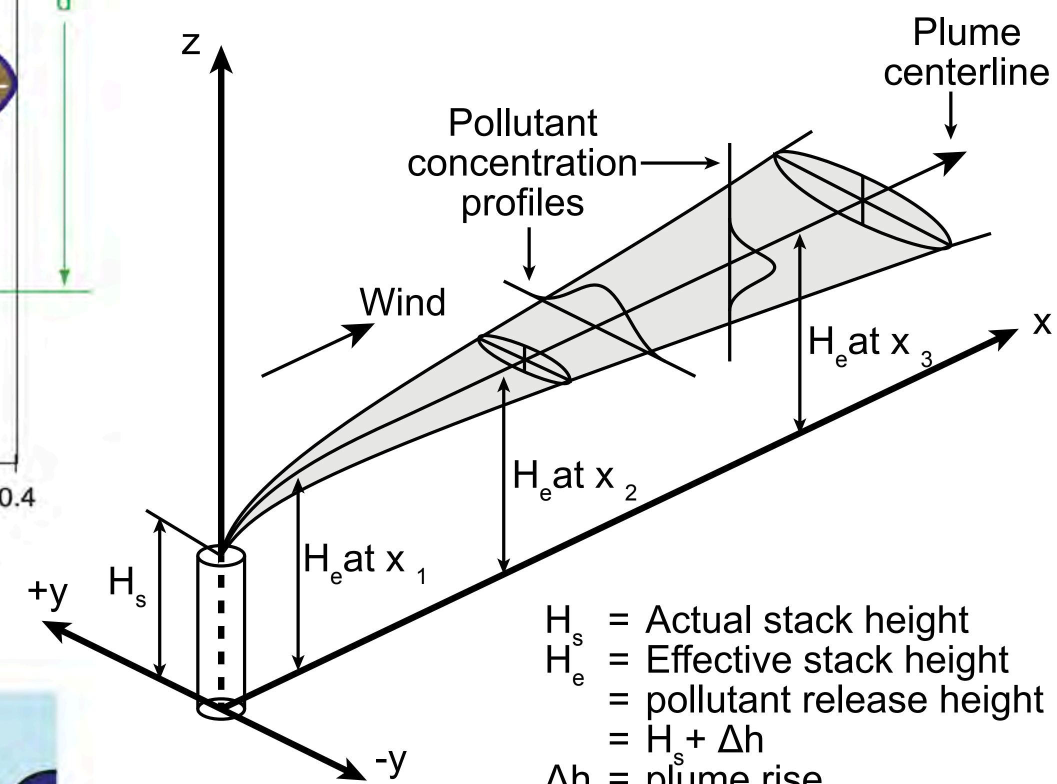
Theories & Derivations

See various ScanSets at: https://www.eoas.ubc.ca/courses/atsc507/ADM/intro/index.html

- Statistical (time-avg) nature of AQ standards & turbulence

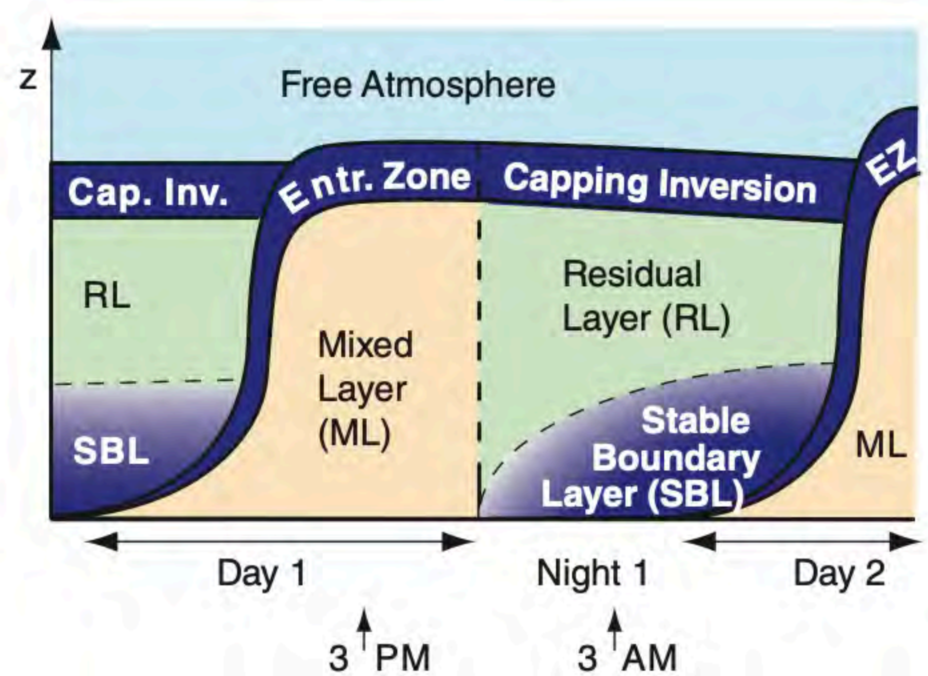


re 19.5



- Gaussian Plume Dispersion

- Planetary Boundary Layer similarity theory



Theories & Derivations

See various ScanSets at: https://www.eoas.ubc.ca/courses/atsc507/ADM/intro/index.html

- Turbulence theories (K-theory, TKE budget, Pasquill-Gifford)

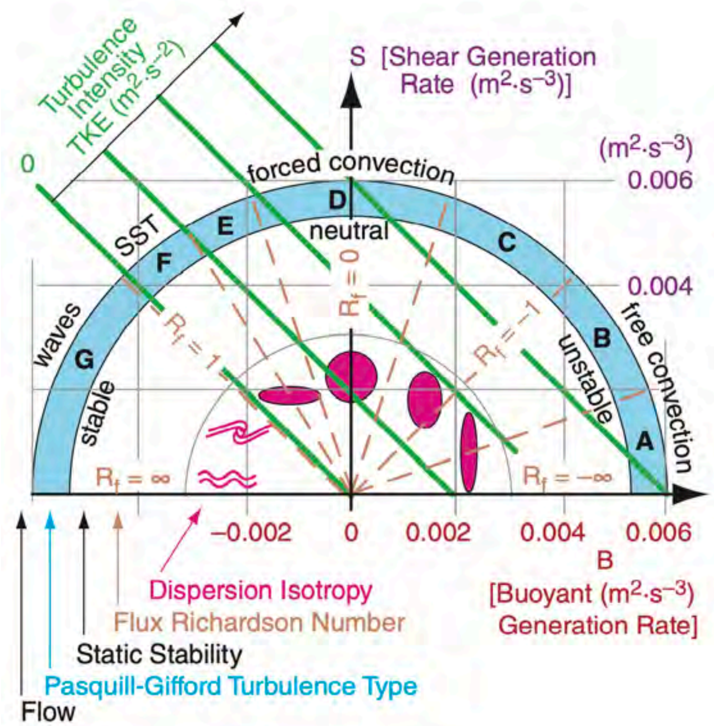


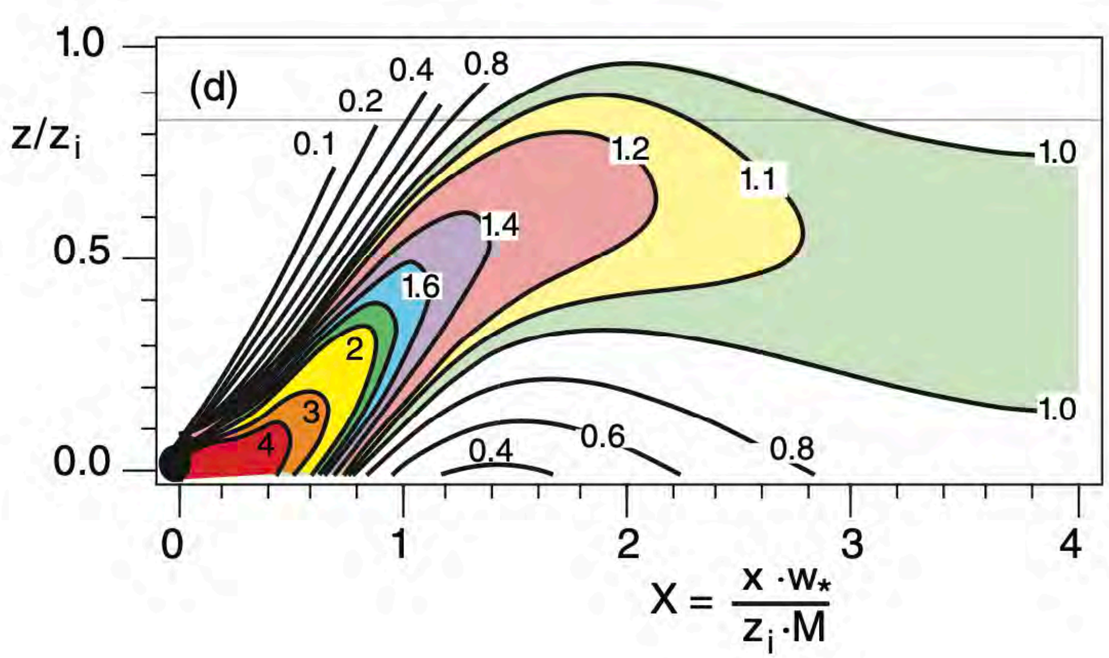
Table 19-2a. Pasquill-Gifford turbulence types for **Daytime**. M is wind speed at $z = 10$ m.

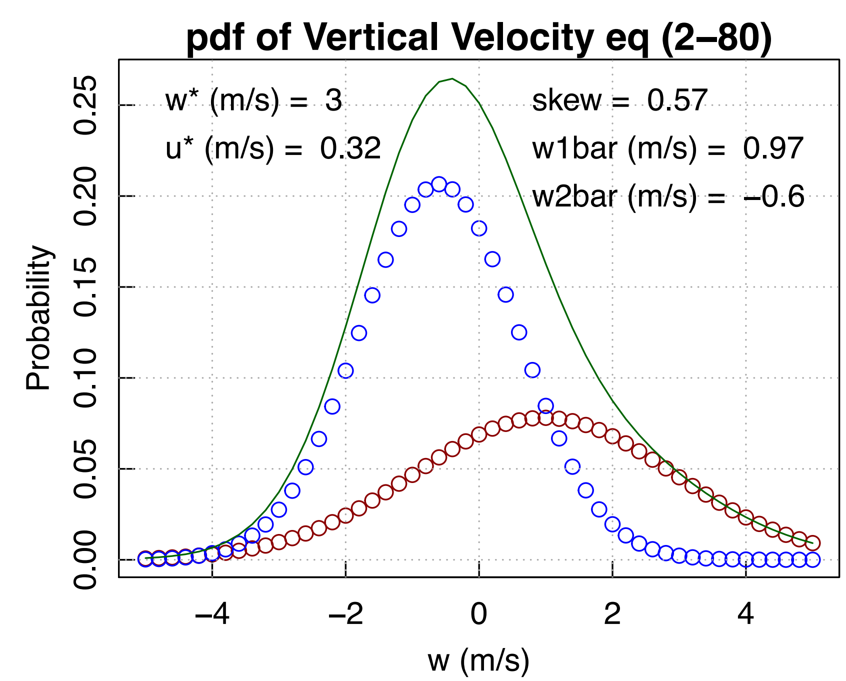
M (m s^{-1})	Insolation (incoming solar radiation) Strong	Moderate	Weak
< 2	A	A to B	B
2 to 3	A to B	B	C
3 to 4	B	B to C	C
4 to 6	C	C to D	D
> 6	C	D	D

Table 19-2b. Pasquill-Gifford turbulence types for **Nighttime**. M is wind speed at $z = 10$ m.

M (m s^{-1})	Cloud Coverage ≥ 4/8 low cloud or thin overcast	≤ 3/8
< 2	G	G
2 to 3	E	F
3 to 4	D	E
4 to 6	D	D
> 6	D	D

- Dispersion in Convective PBL (Deardorff). Stull eqs vs. Weil eqs (prob. distr. for up & downdrafts)

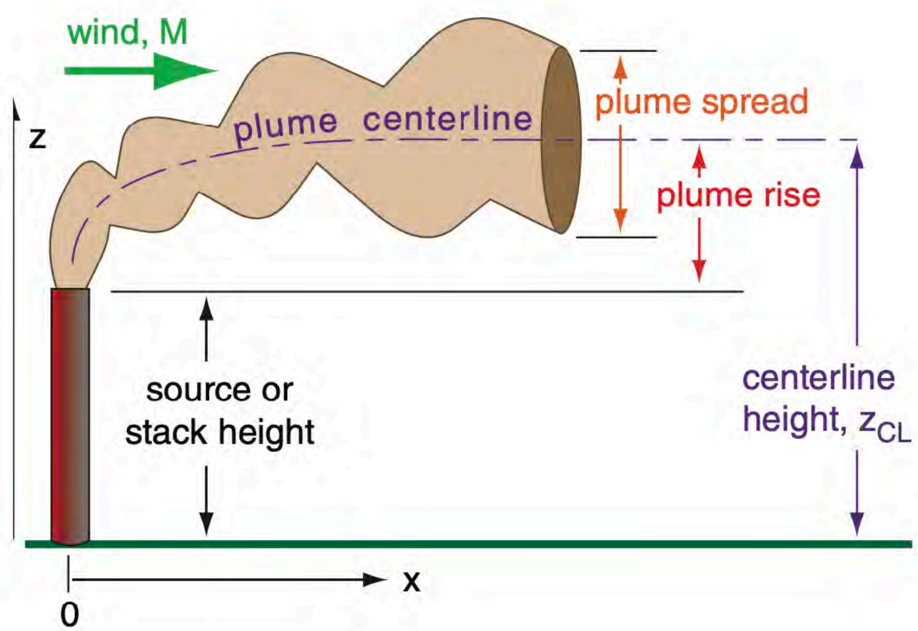




Theories & Derivations

See various ScanSets at: https://www.eoas.ubc.ca/courses/atsc507/ADM/intro/index.html

- Briggs plume-rise model



- Taylor's statistical theory

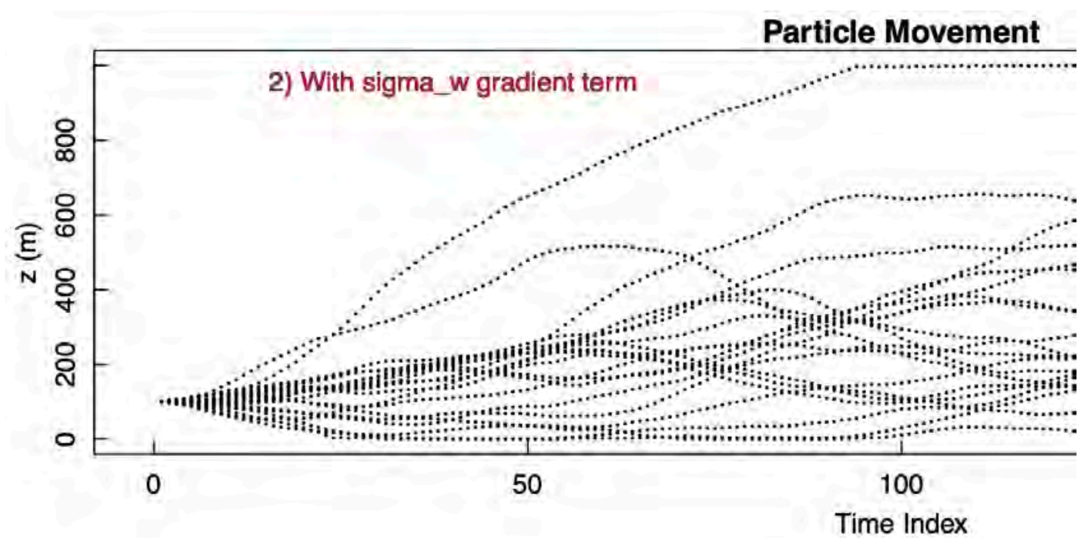
•(19.13a)

$$\sigma_y{}^2 = 2 \cdot \sigma_v{}^2 \cdot t_L{}^2 \cdot \left[\frac{x}{M \cdot t_L} - 1 + \exp\left(-\frac{x}{M \cdot t_L} \right) \right]$$

•(19.13b)

$$\sigma_z{}^2 = 2 \cdot \sigma_w{}^2 \cdot t_L{}^2 \cdot \left[\frac{x}{M \cdot t_L} - 1 + \exp\left(-\frac{x}{M \cdot t_L} \right) \right]$$

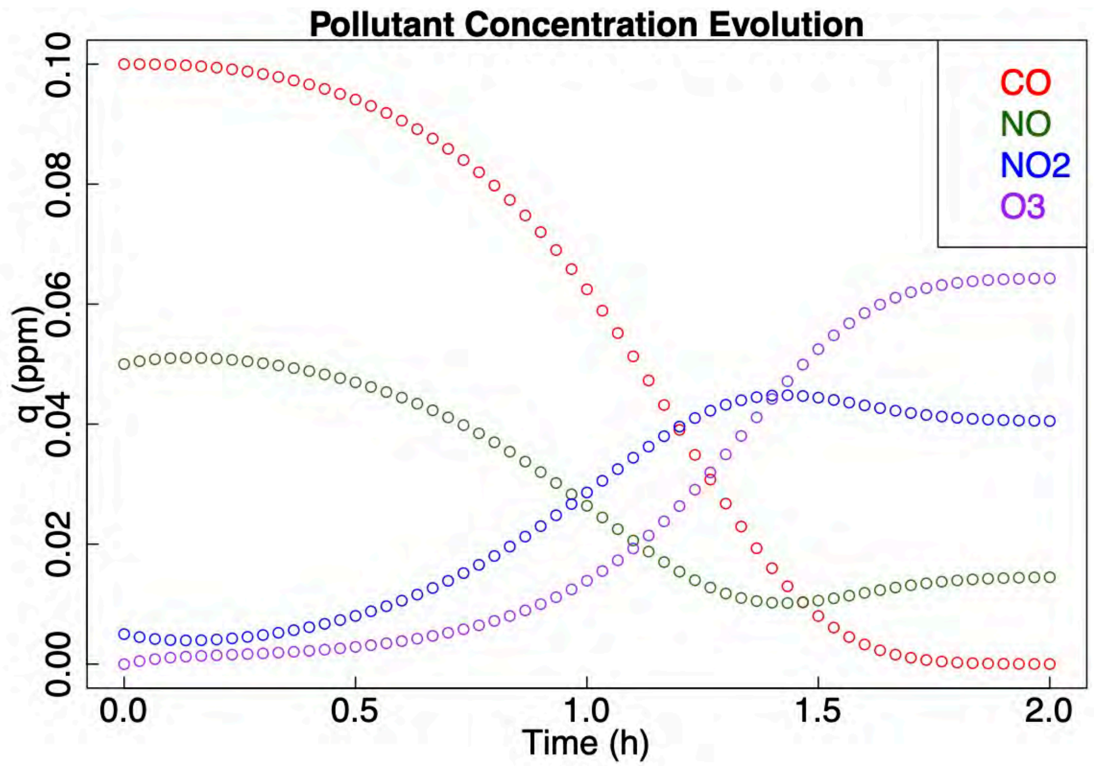
- Langevine theory



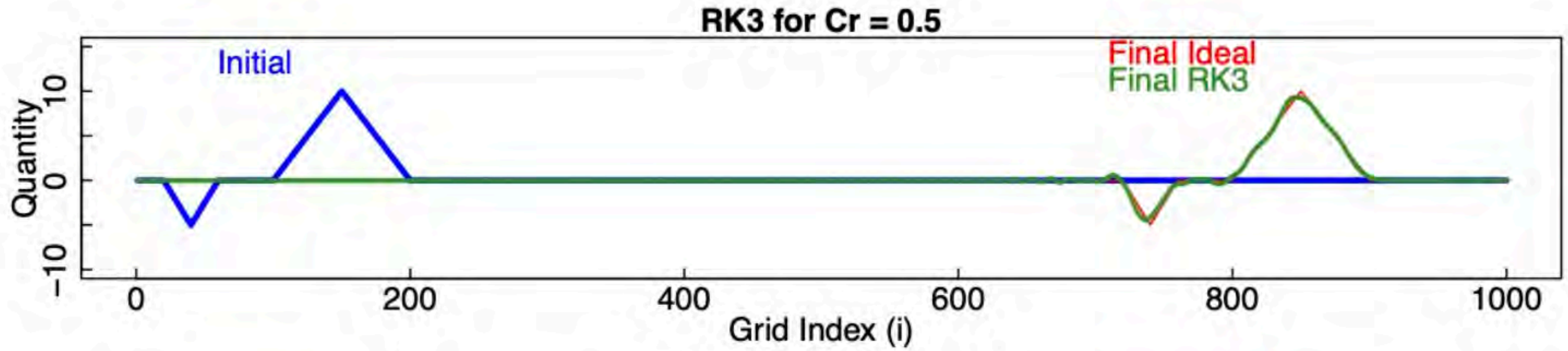
Theories & Derivations

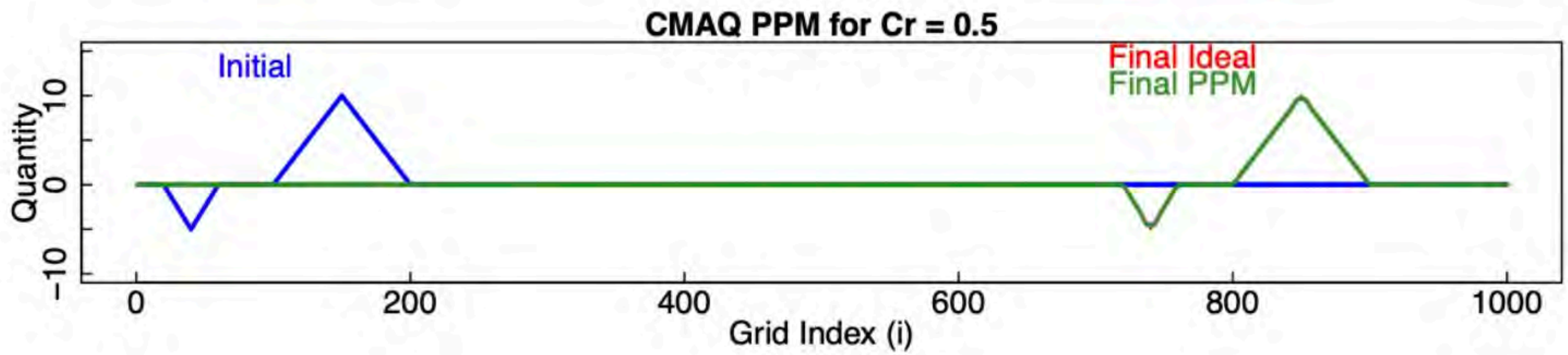
See various ScanSets at: https://www.eoas.ubc.ca/courses/atsc507/ADM/intro/index.html

- Photochemistry rate eqs.



- RK3 and PPM advection eqs that are (nearly) conservative.



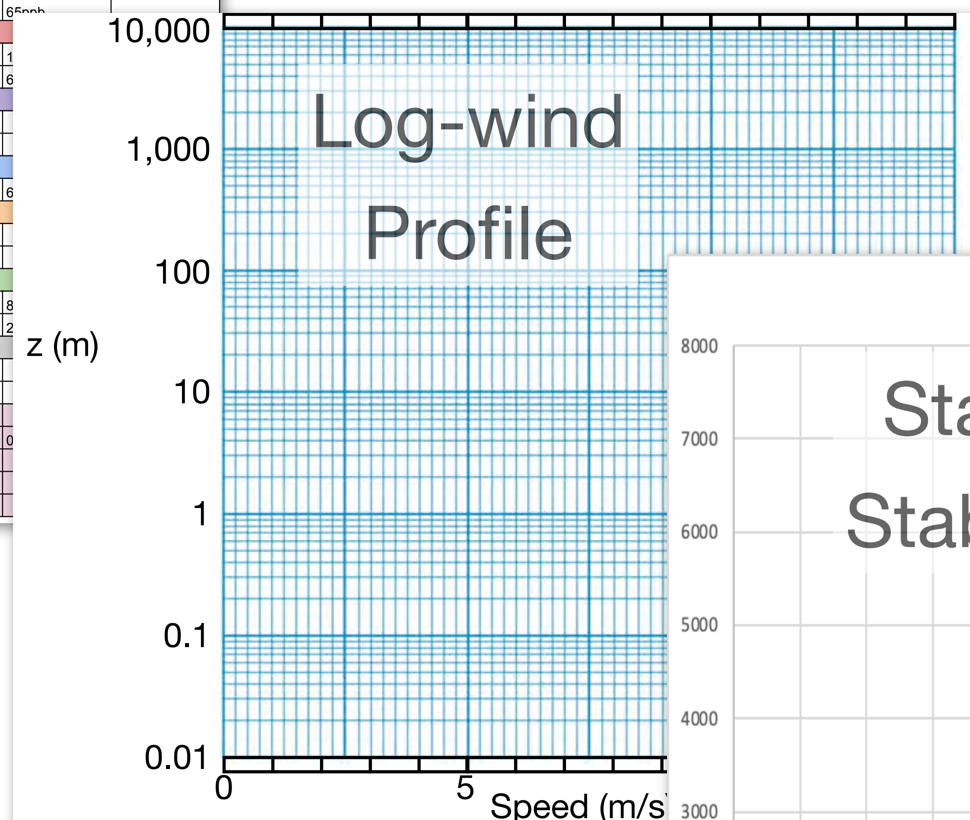


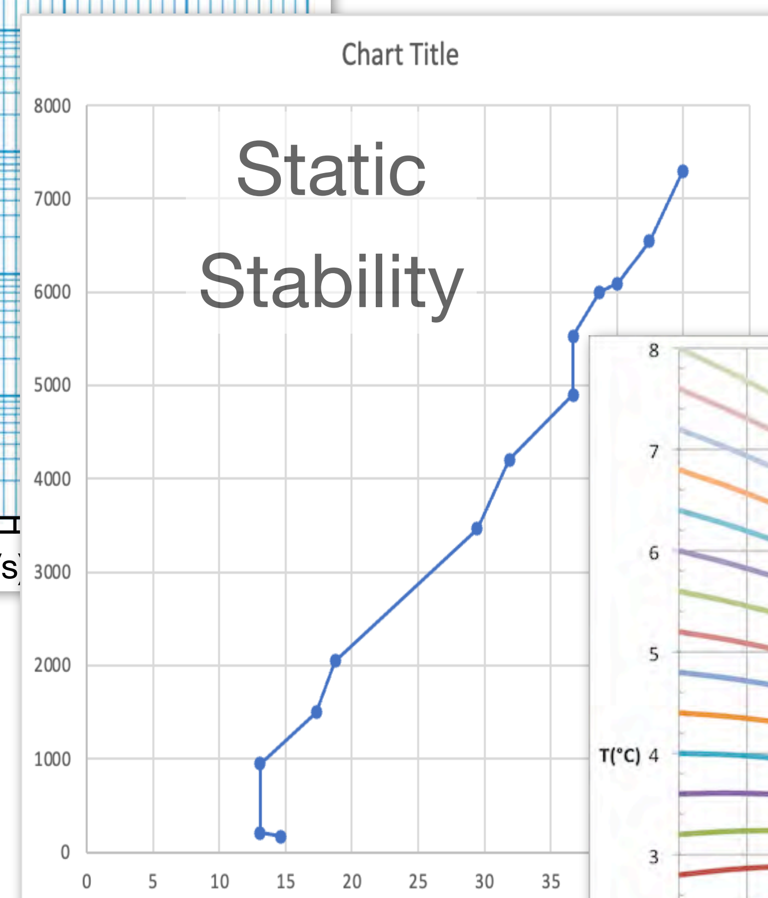
In-class Group Exercises

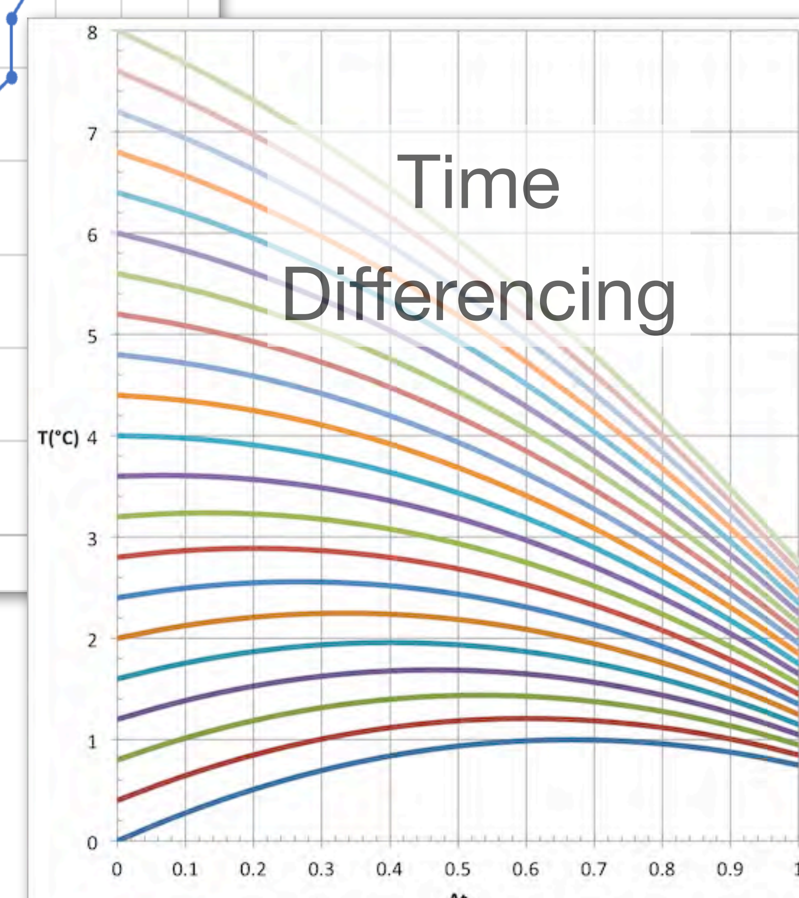
Air Quality concentration standards, as of Jan 2024

Averaging Time	US	Canada	EU	BC	AB	World Health Organization
Sulfur Dioxide (SO2)						
1 yr		5 ppb - > 4 ppb	N/A	5ppb -> 4ppb	4ppb	
1 day			125 ug/m^3			40 µg/m3
3 h	0.5 ppm		N/A			
1 h	75 ppb	70 ppb -> 65 ppb	350 ug/m^3	70 ppb -> 65 ppb	65ppb	
Nitrogen Dioxide (NO2)						
1 yr	53 ppb	17 ppb -> 12 ppb	40ug/m^3	17ppb -> 12ppb	1	
1 h	100 ppb	60 ppb - > 42 ppb	200ug/m^3	60ppb -> 42ppb	6	
Carbon Monoxide (CO)						
8 h	9 ppm		10mg/m^3	5000ppb		
1 h	35 ppm	25 ppm (indoor, CEP	N/A	13000ppb		
Ozone (O3)						
8 h	0.07 ppm	62 ppb -> 60 ppb	120ug/m3	62ppb -> 60ppb	6	
PM10						
1 yr			40ug/m3			
1 day	150 µg/m3		50ug/m3	50µg/m3		
PM2.5						
1 yr	12 µg/m3	8.8 ug/m3	20	8.8µg/m3	8	
1 day	35 µg/m3	27 ug/m3	N/A	27µg/m3	2	
Lead						
1 yr			0.5ug/m^3	N/A		
3 mo	0.15 µg/m3			N/A		
Benzene-1yr			5ug/m3			
Arsenic-1yr			6ng/m3		0	
Cadmium-1yr			5ng/m3			
Nickel-1yr			20ng/m3			
PAH-1yr			1ng/m3			

https://docs.google.com/spreadsheets/d/1sTfOCTUpOy8ajhCT7GxwUSByVnzxr5AjT0vzhf9eZuA/edit#gid=284499998







Overview of AQ Models

Most Dispersion Models have similar components.

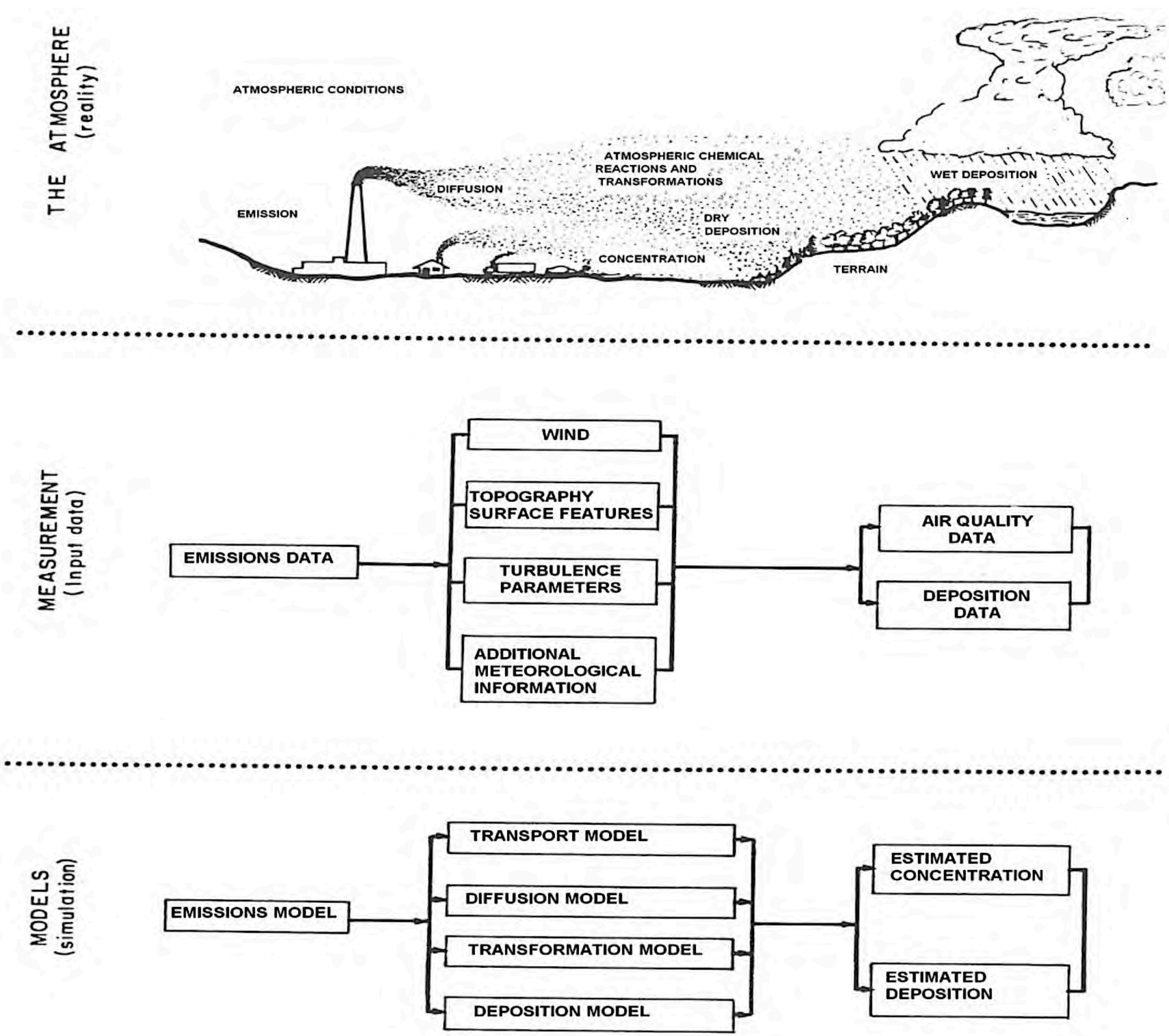


Figure 1. Dispersion in the Atmosphere and the Corresponding Dispersion Model Components

Source: primer_bc_dispersion_modelling_guideline_2021.pdf

Question for Discussion

Why do all the models require many years of hourly weather inputs?

Question for Discussion

What are some of the common outputs from most of the models we used?

Fundamentally Different Approaches

Analytical

- Known: c(x, y, z, t) directly from a Gaussian eq.
- Uses mean wind to define coord. system.
- Uses Taylor's stat theory: σ_y = fnt (σ_v)

-- AERMOD

Lagrangian (pure)

- Known: each particle represents m grams of pollutant p.
- Unknown: need to solve for position (x, y, z) of each particle vs time, under influence of transport (by mean wind) and dispersion (random walk with inertia is function of σ_v).
- Disadvantage, needs thousands of particles to get a good statistic.
- Disadvantage: need to convert from Lagrangian to Eulerian for output.

-- HYSPLIT

Fundamentally Different Approaches

Lagrangian (hybrid) - Puffs or Slugs

- Known: each puff/slug represents m grams of pollutant p.
- Unknown: need to solve for position of each puff center vs. time, under influence of transport (by mean wind).
  & need to solve for puff spread: Gaussian/Taylors theories: σ_y = fnt (σ_v).
- Advantage: needs hundreds of particles to get a good statistic.
- Disadvantage: need to convert from Lagrangian to Eulerian for output.

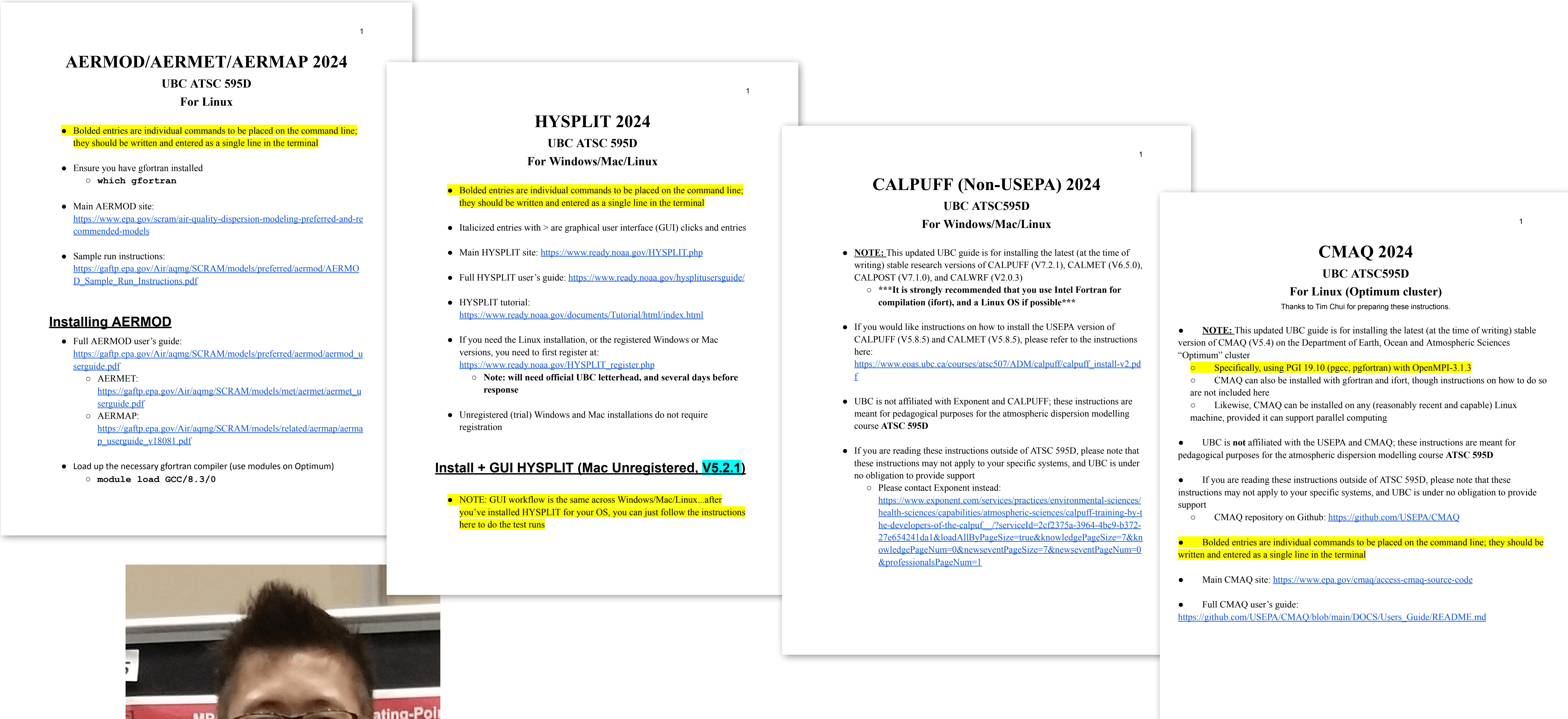
-- HYSPLIT & CALPUFF

Eulerian

- Known: Fixed grid cells locations.
- Unknown: Need to forecast average c in each cell.
- Uses mean wind to advect pollutant from each cell to neighboring cells.
- Needs to compute dispersion between neighboring cells: K-theory (σ_v).
- Enables modeling of chemical transformations among constituents.

-- CMAQ

You got a "taste" of running each model



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AERMOD/AERMET/AERMAP 2024

UBC ATSC 595D

For Linux

- Bolded entries are individual commands to be placed on the command line; they should be written and entered as a single line in the terminal
- Ensure you have gfortran installed
  - **which gfortran**
- Main AERMOD site: https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models
- Sample run instructions: https://gaftp.epa.gov/Air/aqmg/SCRAM/models/preferred/aermod/AERMOD_Sample_Run_Instructions.pdf

Installing AERMOD

- Full AERMOD user's guide: https://gaftp.epa.gov/Air/aqmg/SCRAM/models/preferred/aermod/aermod_userguide.pdf
  - AERMET: https://gaftp.epa.gov/Air/aqmg/SCRAM/models/met/aermet/aermet_userguide.pdf
  - AERMAP: https://gaftp.epa.gov/Air/aqmg/SCRAM/models/related/aermap/aermap_userguide_v18081.pdf
- Load up the necessary gfortran compiler (use modules on Optimum)
  - **module load GCC/8.3/0**

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HYSPLIT 2024

UBC ATSC 595D

For Windows/Mac/Linux

- Bolded entries are individual commands to be placed on the command line; they should be written and entered as a single line in the terminal
- Italicized entries with > are graphical user interface (GUI) clicks and entries
- Main HYSPLIT site: https://www.ready.noaa.gov/HYSPLIT.php
- Full HYSPLIT user's guide: https://www.ready.noaa.gov/hysplitusersguide/
- HYSPLIT tutorial: https://www.ready.noaa.gov/documents/Tutorial/html/index.html
- If you need the Linux installation, or the registered Windows or Mac versions, you need to first register at: https://www.ready.noaa.gov/HYSPLIT_register.php
  - **Note: will need official UBC letterhead, and several days before response**
- Unregistered (trial) Windows and Mac installations do not require registration

Install + GUI HYSPLIT (Mac Unregistered, V5.2.1)

- NOTE: GUI workflow is the same across Windows/Mac/Linux...after you've installed HYSPLIT for your OS, you can just follow the instructions here to do the test runs

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CALPUFF (Non-USEPA) 2024

UBC ATSC595D

For Windows/Mac/Linux

- NOTE: This updated UBC guide is for installing the latest (at the time of writing) stable research versions of CALPUFF (V7.2.1), CALMET (V6.5.0), CALPOST (V7.1.0), and CALWRF (V2.0.3)
  - *****It is strongly recommended that you use Intel Fortran for compilation (ifort), and a Linux OS if possible*****
- If you would like instructions on how to install the USEPA version of CALPUFF (V5.8.5) and CALMET (V5.8.5), please refer to the instructions here: https://www.eoas.ubc.ca/courses/atsc507/ADM/calpuff/calpuff_install-v2.pdf
- UBC is not affiliated with Exponent and CALPUFF; these instructions are meant for pedagogical purposes for the atmospheric dispersion modelling course **ATSC 595D**
- If you are reading these instructions outside of ATSC 595D, please note that these instructions may not apply to your specific systems, and UBC is under no obligation to provide support
  - Please contact Exponent instead: https://www.exponent.com/services/practices/environmental-sciences/health-sciences/capabilities/atmospheric-sciences/calpuff-training-by-the-developers-of-the-calpuff__/?serviceId=2cf2375a-3964-4bc9-b372-27e654241da1&loadAllByPageSize=true&knowledgePageSize=7&knowledgePageNum=0&neweventPageSize=7&neweventPageNum=0&professionalsPageNum=1

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CMAQ 2024

UBC ATSC595D

For Linux (Optimum cluster)

Thanks to Tim Chui for preparing these instructions.

- NOTE: This updated UBC guide is for installing the latest (at the time of writing) stable version of CMAQ (V5.4) on the Department of Earth, Ocean and Atmospheric Sciences "Optimum" cluster
  - Specifically, using PGI 19.10 (pgcc, pgfortran) with OpenMPI-3.1.3
  - CMAQ can also be installed with gfortran and ifort, though instructions on how to do so are not included here
  - Likewise, CMAQ can be installed on any (reasonably recent and capable) Linux machine, provided it can support parallel computing
- UBC is **not** affiliated with the USEPA and CMAQ; these instructions are meant for pedagogical purposes for the atmospheric dispersion modelling course **ATSC 595D**
- If you are reading these instructions outside of ATSC 595D, please note that these instructions may not apply to your specific systems, and UBC is under no obligation to provide support
  - CMAQ repository on Github: https://github.com/USEPA/CMAQ
- Bolded entries are individual commands to be placed on the command line; they should be written and entered as a single line in the terminal
- Main CMAQ site: https://www.epa.gov/cmaq/access-cmaq-source-code
- Full CMAQ user's guide: https://github.com/USEPA/CMAQ/blob/main/DOCS/Users_Guide/README.md

Thanks, Tim.

You are not experts in these models, but hopefully you have a solid starting point to learn more on your own.

Question for Discussion

How would you select which model to use?

In-class Exercise

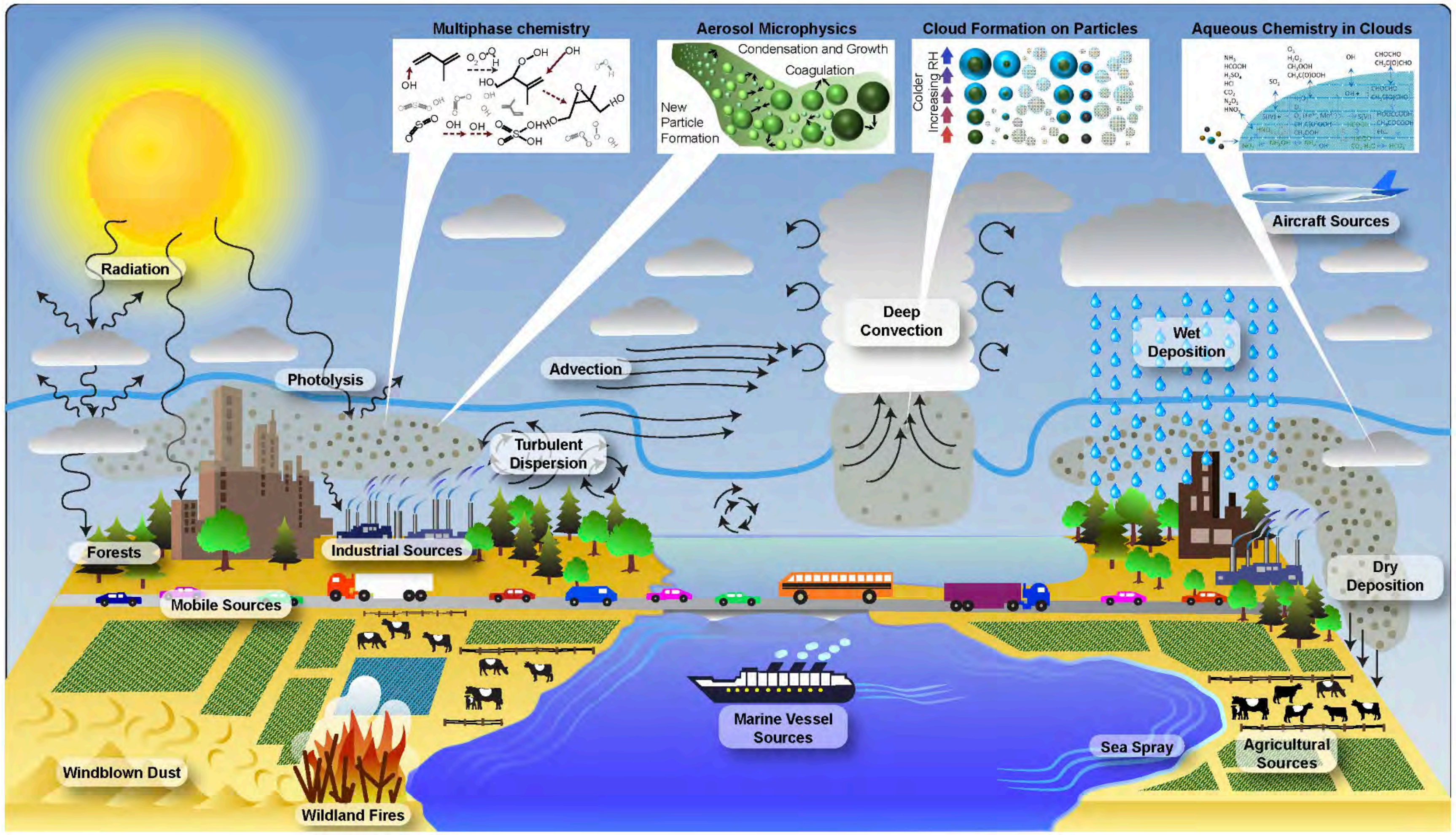
Consult the manuals to fill in the missing "?" cells in our model comparison spreadsheet.

https://www.eoas.ubc.ca/courses/atsc507/ADM/intro/A595D-model-comparison-2024.xlsx

	A	B	C	D	E
1	**Comparison of Atmospheric Dispersion Models**			UBC-ATSC 595D	Feb 2024
2	Prof. Roland Stull				
3	**Characteristic**	**AERMOD**	**HYSPLIT**	**CALPUFF**	**CMAQ**
4	Model complexity	simple	simple to medium	medium to complex	very complex
5	For range from source	10 m to 50 km	5 km to ∞	10 m to ∞	multi-state
6	Framework	Eulerian	Lagrangian	Lagrangian	Eulerian
7	Advection	Analytical	Trajectory	Analytical & Trajectory	Piecewise Parabolic Method (PPM)
8	Dispersion	Gaussian with Deardorff ML	Langevin (random walk)	Gauss., Deard. & Langevin	?
9	Includes Deardorff convective mixed layer	Yes, using prob. dist. fncts. for up & downdrafts	No	Yes, using prob. dist. fncts. for up & downdrafts	?
10	Type	Plume	Puff or particles	Puff or Slug	Grid-cell avg.
11	Chemistry	none	none	simple thru complex	very complex, 100s of eqs., smog

Question for Discussion

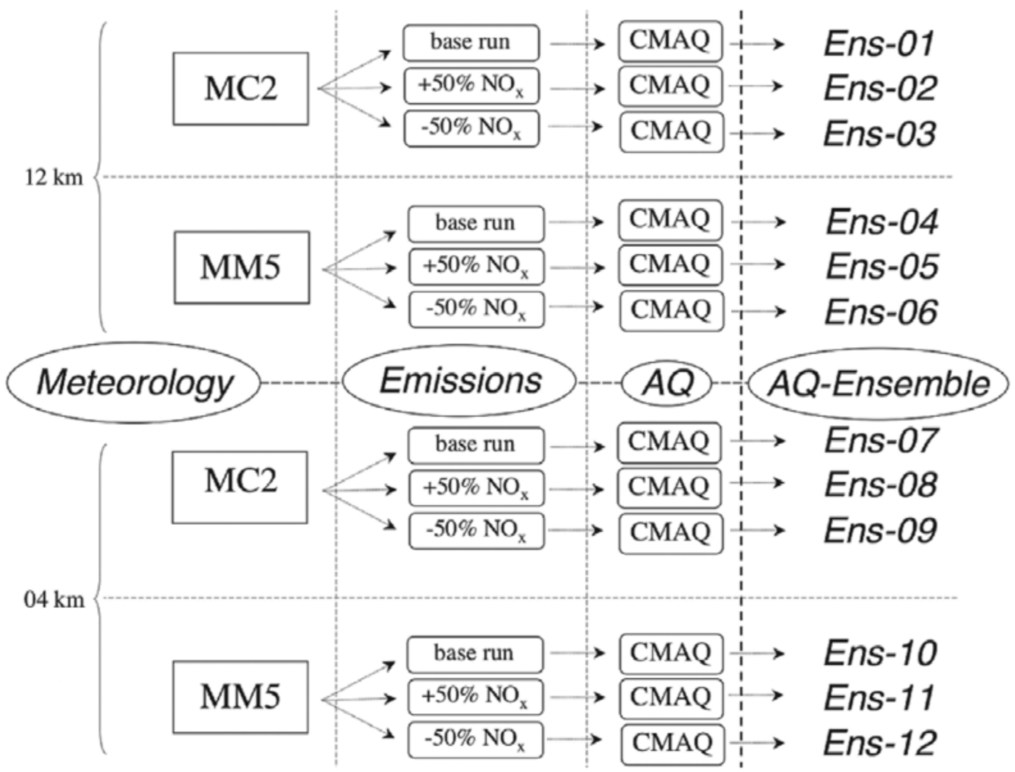
For which situations would you want to use CMAQ?



https://www.epa.gov/cmaq/overview-science-processes-cmaq

For which situations would you want to use CMAQ?

Luca Delle Monache used CMAQ in his dissertation



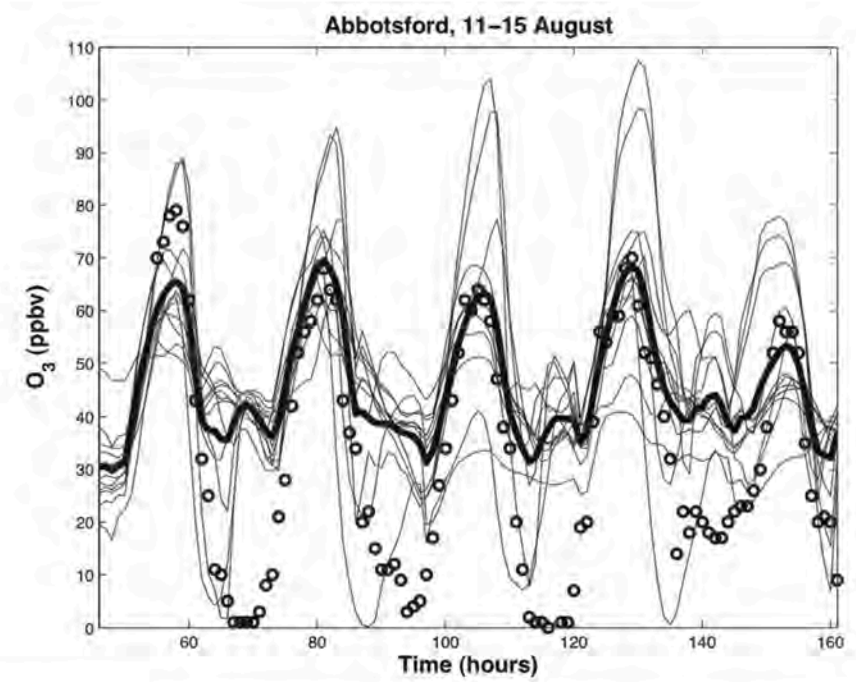
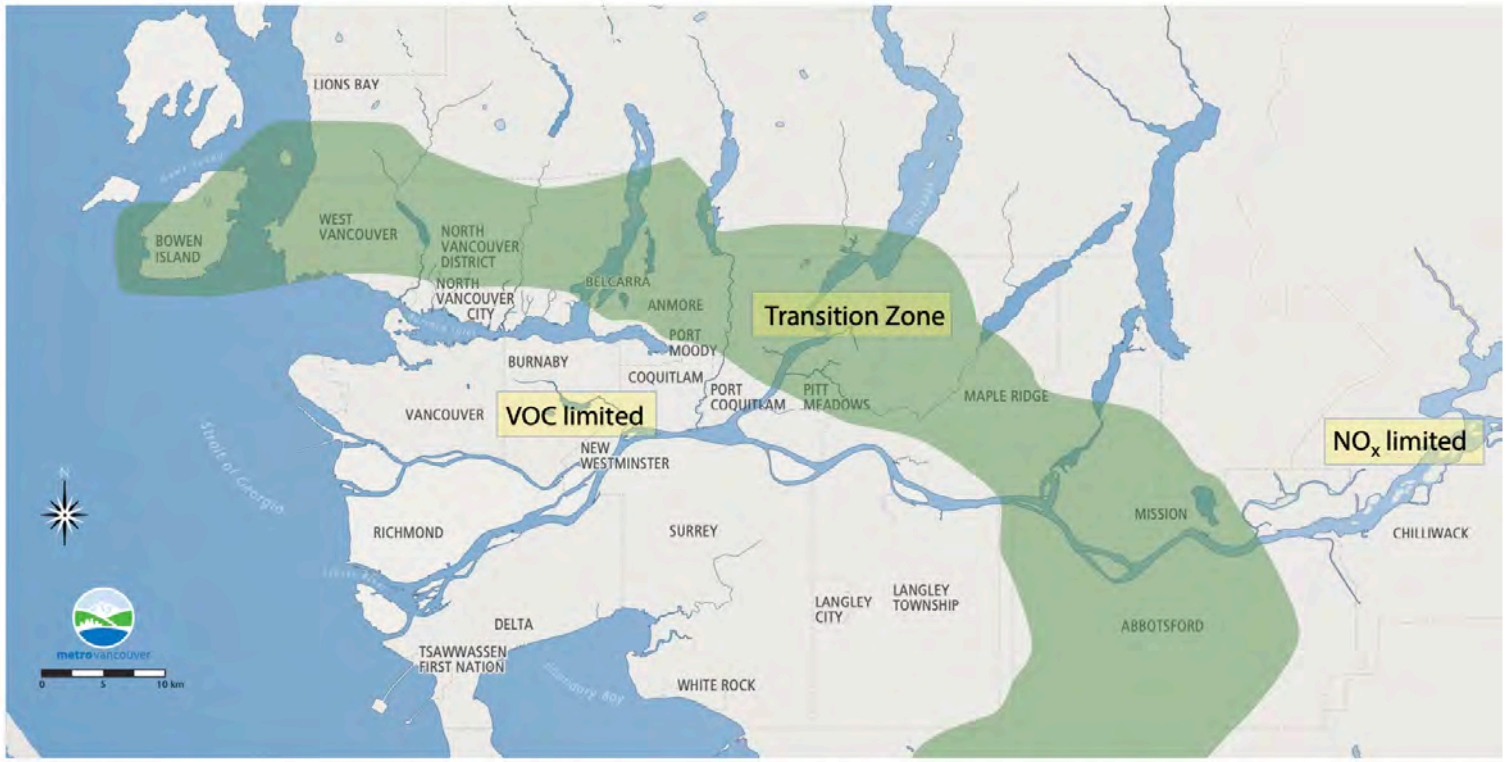


Figure 4. Twelve ensemble members (solid lines) and the ensemble mean (thick solid line) predictions along with the observations (circles), at Abbotsford, 11–15 August 2004.

JGR, VOL. 111, D05307, doi:10.1029/2005JD006310, 2006

BCMoE & MetroVan used it to determine regional emission policies.

https://www.eoas.ubc.ca/courses/atsc507/ADM/cmaq/Vancouver-ozone-strategy-2014.pdf



Question for Discussion

Which model(s) are recommended by:

- BC (as of 2022)

  https://www2.gov.bc.ca/assets/download/9960E7796D6E43249D2A768E3AC20B66

- AB (as of 2021)

  https://open.alberta.ca/publications/air-quality-model-guideline-2021

You can find a link to these gov't guidelines from our course:

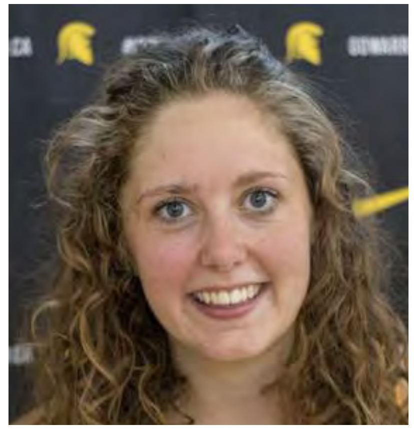
https://www.eoas.ubc.ca/courses/atsc507/ADM/aermod/index.html

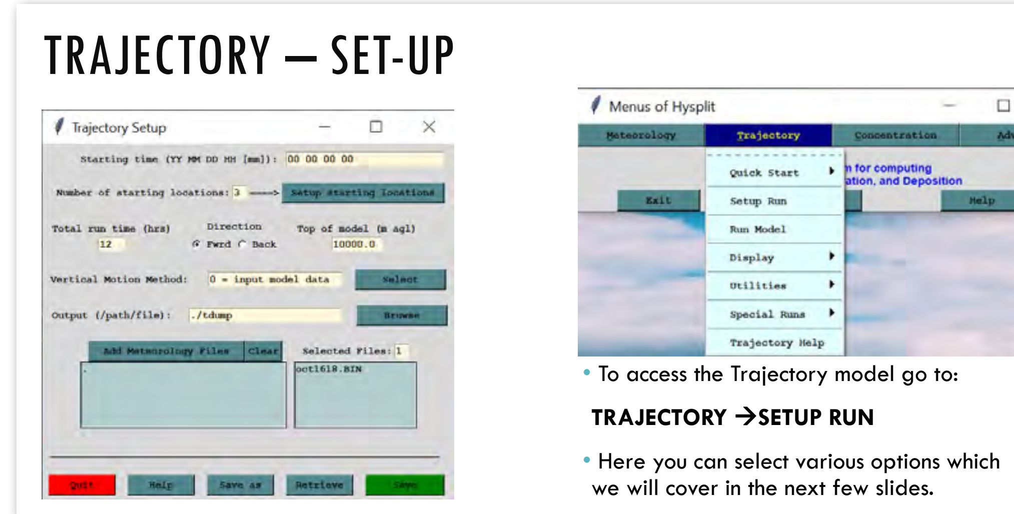
Compare Recommendations - in class exercise

Topic	BC	AB
Bowen Ratio for coniferous forest		
Roughness Length for large city		
Albedo for grassland in summer		
Background NO_2/NO_x ratio		
Fugitive source methods		
Receptor grid resolution (Cartesian)		

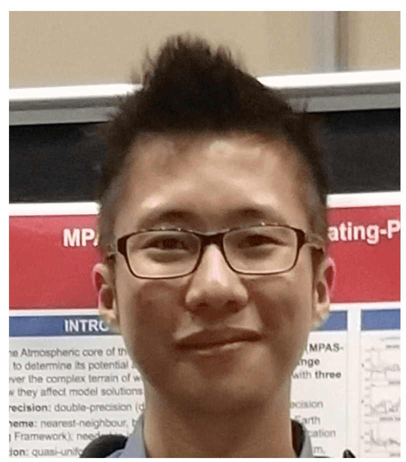
Tutorials by Guest Speakers

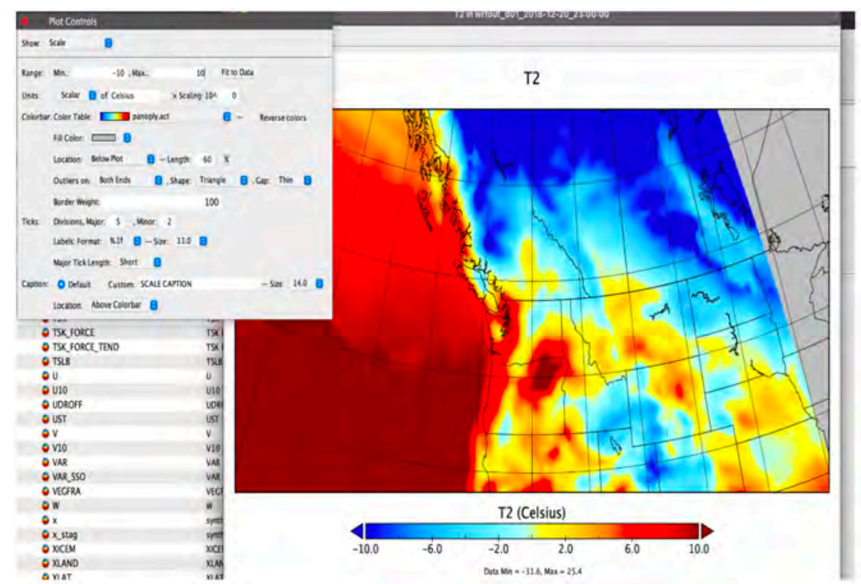
Hysplit, by
Reagan McKinney



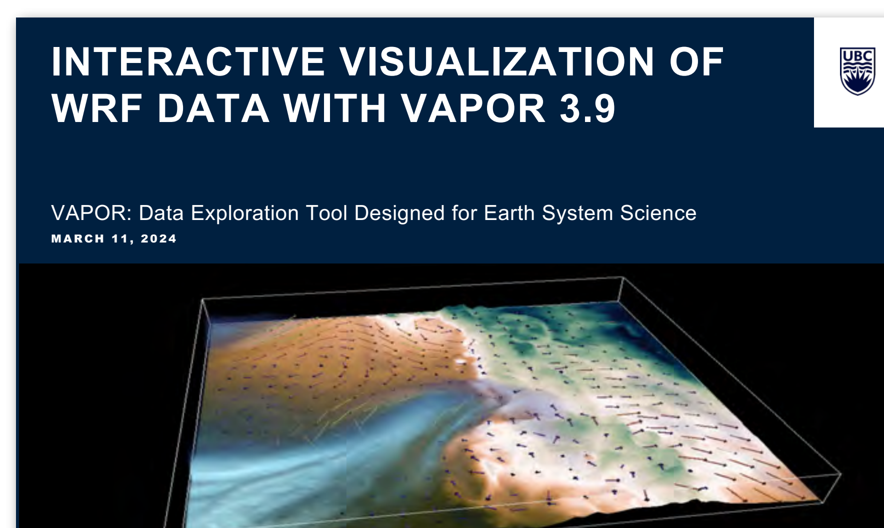


Panoply, by
Tim Chui





Vapor, by
Nadya Moisseeva



You also improved your skills in

- Teamwork / Group work
- Computer programming (python or R)
- Producing well documented code
- Producing publication-ready graphs

The End

ATSC 595D - Atmospheric Dispersion Modeling


https://carbonfund.org/how-do-greenhouse-gases-contribute-to-global-warming/

Any Questions?