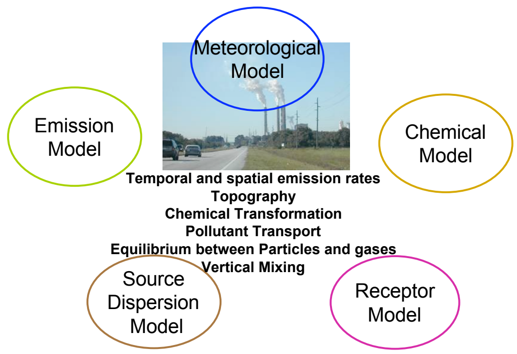
Introduction to Air Quality Models



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Q: What is the level of my exposure to these emissions? Is my family safe? Where is safe? How about the adverse impact on the environment (plants, animals, buildings)?

Q: Any other real examples?

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Q: What are the factors that affect the exposure to the emissions?

- **Temporal and spatial emission rates**
- **Terrain**
- **Chemical transformation**
- **Equilibrium between particles and gases**
- **Pollutant transport**
- **Vertical Mixing**

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- **Emission Model**
  - estimates temporal and spatial emission rates based on activity level, emission rate per unit of activity and meteorology
- **Meteorological Model**
  - Describes transport, dispersion, vertical mixing and moisture in time and space
- **Chemical Model**
  - Describes transformation of directly emitted particles and gases to secondary particles and gases; also estimates the equilibrium between gas and particles for volatile species

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- **Source Dispersion Model**
  - Uses the outputs from the previous models to estimate concentrations measured at receptors; includes mathematical simulations of transport, dispersion, vertical mixing, deposition and chemical models to represent transformation. Gaussian Plume, Puff and Grid Models.
- **Receptor Model**
  - Infers contributions from different primary source emissions or precursors from multivariate measurements taken at one or more receptor sites. Chemical Mass Balance (CMB), UNMIX, Positive Matrix Factorization(PMF)

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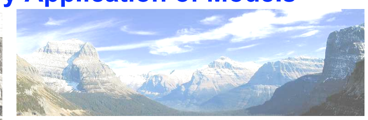
Regulatory Application of Models



- **PSD**: Prevention of Significant Deterioration of Air Quality in relatively clean areas (e.g. National parks)
- **SIP**: State Implementation Plan revisions for *existing sources* and to *New Source Reviews* (NSR)

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Guideline on Air Quality Models

- 40 CFR Pt 51, App. W. – effective *May 15, 2003* (http://www.epa.gov/ttn/scram/guidance/guide/appw_03.pdf)
  - Overview of Model Use
  - Recommended Air Quality Models – Preferred and Alternative
  - Traditional Stationary Source Models
  - Model use in Complex Terrain
  - Models for O_3, PM, CO and NO_2
  - Other Model Requirements
  - General Modeling Considerations
  - Model Input Data
  - Accuracy and Uncertainty of Models
  - Regulatory Application of Models

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Suitability of Models

- The meteorological and topographical complexities of the area
- The level of detail and accuracy need for the analysis
- The technical competence of those undertaking such simulation modeling
- The resources available
- The detail and accuracy of the data base; i.e. emission inventory, meteorological data and air quality data

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Levels of Sophistication of Models

- ***Screening***: simple estimation techniques use preset, worst-case meteorological conditions to provide conservative estimates.
- ***Refined***: Analytical techniques that provide more detailed treatment of physical and chemical atmospheric processes, require more detailed and precise input data and provide more specialized concentration estimates.

Screening Models

- Available at www.epa.gov/scram001/tt22.htm#screen
- **AERSCREEN is the screening model for AERMOD. The model will produce estimates of regulatory design concentrations without the need for meteorological data and is designed to produce concentration that are equal to or greater than the estimates produced by AERMOD with a fully developed set of meteorological and terrain data.**
- **COMPLEX1 is a multiple point source screening technique with terrain adjustment that incorporates the plume impaction algorithm of the VALLEY model.**
- **CTSCREEN is a Gaussian plume dispersion model designed as a screening technique for regulatory application to plume impaction assessments in complex terrain. CTSCREEN is a screening version of the CTDMPLUS model.**
- **VALLEY is a steady-state, complex terrain, univariate Gaussian plume dispersion algorithm designed for estimating either 24-hour or annual concentrations resulting from emissions from up to 50 (total) point and area sources.**

Recommended Air Quality Models

- **Preferred Modeling Techniques**
  - A single model found to outperform others
  - Selected on the basis of other factors such as past use, public familiarity, cost or resource requirements and availability
  - No further evaluation of a preferred model is required

- **Requirements for consideration to be a preferred model**
  - Functioning in a common computer code suitable for use in a variety of computer systems
  - Documented in a user's guide which identifies the mathematics of the model, data requirements and program operating characteristics at a level of detail comparable to that available for currently recommended models.
  - Useful for typical users
  - Include a comparison with air quality data or with other well established analytical techniques
  - Developers be willing to make the model available to users at reasonable cost or make it available for public access

Preferred/Recommended Models

- Available at http://www.epa.gov/scram001/dispersion_prefrec.htm
- **AERMOD Modeling System - A steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.**
- **CALPUFF Modeling System - A non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation, and removal. CALPUFF can be applied for long-range transport and for complex terrain.**
- **Other Models - Other dispersion models including BPL, CALINE3, CTDMPLUS, and OCD.**
  - BLP (***Bouyant Line and Point Source Model*** **):** a Gaussian plume dispersion model designed to handle unique modeling problems associated with aluminum reduction plants, and other industrial sources where plume rise and downwash effects from stationary line sources are important.
  - CALINE3**:** a steady-state Gaussian dispersion model designed to determine air pollution concentrations at receptor locations downwind of "at-grade," "fill," "bridge," and "cut section" highways located in relatively uncomplicated terrain.
- EPA Guidance on what to use
- http://www.epa.gov/scram001/guidance/guide/appw_05.pdf

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AEROMOD

- The American Meteorological Society/EPA Regulatory Model Improvement Committee (AERMIC) was formed to introduce state-of-the-art modeling concepts into the EPA's air quality models. The AERMOD modeling system was developed that incorporated air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.
- AERMOD has two input data processors for the regulatory components of the system: AERMET, a meteorological data preprocessor that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, and AERMAP, a terrain data preprocessor that incorporates complex terrain using USGS Digital Elevation Data. Other non-regulatory components of this system include: AERSCREEN, a screening version of AERMOD; AERSURFACE, a surface characteristics preprocessor, and BPIPPRIME, a multi-building dimensions program incorporating the GEP technical procedures for PRIME applications.
- As of December 9, 2006, AERMOD is fully promulgated to replace ISC3

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- **CALPUFF**: a multi-layer, multi-species non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation and removal. CALPUFF can be applied on scales of tens to hundreds of kilometers. It includes algorithms for subgrid scale effects (such as terrain impingement), as well as, longer range effects (such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, and visibility effects of particulate matter concentrations).
- **OCD** (Offshore and Coastal Dispersion Model) a straight line Gaussian model developed to determine the impact of offshore emissions from point, area or line sources on the air quality of coastal regions. OCD incorporates overwater plume transport and dispersion as well as changes that occur as the plume crosses the shoreline. Hourly meteorological data are needed from both offshore and onshore locations.

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- **CTDMPLUS** (Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations): a refined point source Gaussian air quality model for use in all stability conditions for complex terrain. The model contains, in its entirety, the technology of CTDM for stable and neutral conditions.
- **ISC3** (Industrial Source Complex Model): a steady-state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial complex. This model can account for the following: settling and dry deposition of particles; downwash; point, area, line, and volume sources; plume rise as a function of downwind distance; separation of point sources; and limited terrain adjustment. ISC3 operates in both long-term and short-term modes.

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Alternative Models

- Falls under a Regional Office's responsibility
- Need to be evaluated from both a theoretical and a performance perspective before use
  - The model produces concentration estimates equivalent to those obtained using a preferred model
  - Statistical performance evaluation are conducted using measured air quality data and the results indicate the alternative model performs better for the given application than a comparable preferred model
- Used when the preferred model is less appropriate for the specific application or there is no preferred model
- Available at http://www.epa.gov/scram001/tt22.htm#alt

Some Alternative Models

- **ADAM *(Air Force Dispersion Assessment Model)*: a modified box and Gaussian dispersion model which incorporates thermodynamics, chemistry, heat transfer, aerosol loading, and dense gas effects. Release scenarios include continuous and instantaneous, area and point, pressurized and unpressurized, and liquid/vapor/two-phased options.**
- **ADMS-3 *(Atmospheric Dispersion Modeling System)*: an advanced model for calculating concentrations of pollutants emitted both continuously from point, line, volume and area sources, or discretely from point sources. Includes algorithms for effects of buildings; complex terrain; wet deposition, gravitational settling and dry deposition; short term fluctuations in concentration; chemical reactions; radioactive decay and gamma-dose; plume rise as a function of distance; jets and directional releases; averaging time ranging from very short to annual; condensed plume visibility; meteorological preprocessor.**
- **OZIPR (A one-dimensional photochemical box model): an alternative version of the OZIP model that deals with toxic pollutants**
- **PAL-DS *(Point, Area, Line Source Algorithm with Deposition and Sedimentation)*: a method of estimating short-term dispersion using Gaussian-plume steady-state assumptions. The model can treat deposition of both gaseous and suspended particulate pollutants in the plume since gravitational settling and dry deposition of the particles are explicitly accounted for.**
- **PLUVUEII: a model used for estimating visual range reduction and atmospheric discoloration caused by plumes resulting from the emissions of particles, nitrogen oxides, and sulfur oxides from a single source. The model predicts the transport, dispersion, chemical reactions, optical effects and surface deposition of point or area source emissions.**

Simple Terrain Stationary Source Models

- Terrain features are all lower in elevation than the top of the stack of the source
- Criteria pollutants
- Average time of concentration estimates ranges from 1 hour to annual average
- SCREEN3 – urban or rural; worst case meteorological conditions
- ISC3; BLP, CALINE3, OCD and EDMS

Complex Terrain

- Terrain exceeding the height of the stack
- SO_2 and PM from stationary source
- CTSCREEN – 3-D nature of plume and terrain interaction; VALLEY, SHORTZ/LONGZ, COMPLEX I, RTDM

Placement of receptors?

- CTDMPLUS

Plume modeling

- Goal
  - Given emission rate of a pollutant, determine the concentration at specific locations
    - If I am standing 2 miles from a smelter, what concentration of smelter emissions am I breathing?
- Great for point sources, but can be used for line sources

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Eddy diffusion derivation

C = concentration of the pollutant in the environment
J = flux, with units of mass/area*time
r = removal

C = f(x,y,z,t)

$$\frac{\partial C}{\partial t} = -\frac{\partial \mathbf{J}}{\partial x} - \frac{\partial \mathbf{J}}{\partial y} - \frac{\partial \mathbf{J}}{\partial z} + r$$

$$J_x = UC - \varepsilon_x \frac{\partial C}{\partial x}$$

$$J_y = \varepsilon_y \frac{\partial C}{\partial y}$$

$$J_z = \varepsilon_z \frac{\partial C}{\partial z}$$

Often we encounter, advection and diffusion in 3-D from a continuous point source for a nonreactive pollutant.

$$U\frac{\partial C}{\partial x} - \varepsilon_y \frac{\partial^2 C}{\partial y^2} - \varepsilon_z \frac{\partial^2 C}{\partial z^2} = 0$$

ε replaced with σ

If we solve, we get the plume equation

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Gaussian "point source" plume model

$$C(x, y, z) = \frac{Q}{2\pi u \sigma_y \sigma_z}\left\{\exp\left(\frac{-(z-h)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+h)^2}{2\sigma_z^2}\right)\right\}\left\{\exp\left(\frac{-(y)^2}{2\sigma_y^2}\right)\right\}$$

- Pollutant concentration as a function of downwind position (x,y,z)
- Mass emission rate
- "Effective" stack height, including rise of the hot plume near the source
- Wind speed evaluated at "effective" release height
- Corresponds to disk area in simple model (values depend upon downwind distance, x)
- Distribution of mass in vertical dimension (z) at a given downwind distance, x (includes the effect of surface reflection)
- Distribution of mass in cross-wind dimension (y) at a given downwind distance, x

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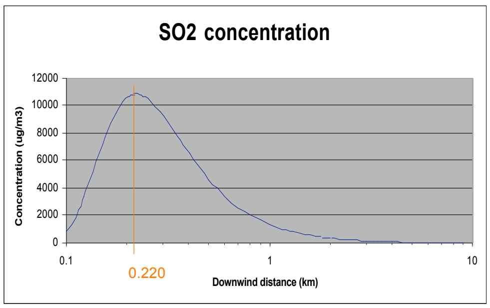
Example: Exhaust from coal-fired power plant

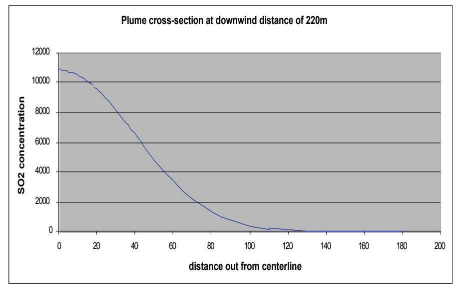
Using Gaussian Plume Model and the given information:
(a) Plot the ground-level SO2 concentration vs distance downwind.
(b) Where does the maximum concentration occur?
(c) At this distance, plot the cross-sectional concentration of SO2.
(d) If the US standard for SO2 is 365 ug/m3, where are the problems?

Given:
- Average wind speed (U) = 2 m/s
- Stack height (H) = 30 m
- Emission rate of SO2 = 150 g/s
- Atmospheric stability class = B

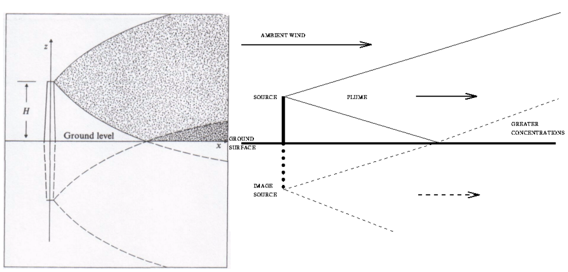
Ground-level SO_2



Crosswind concentration



Plume Reflection



- Real source (above ground) and image source (below ground). The total ambient concentration for the spatial region z > 0 is the same as it would be if the pollutant molecules were reflected upward as they struck the ground.

Atmospheric Stability

- According to the ideal gas law and the barometric equation, <u>the tempreature decreases approximately ~10ºC every 1 km</u> going upward in the atmosphere.
- We know that if a gas is lighter than its surroundings, it moves upward. In other words, a gas with more pressure (i.e. less density) than its surroundings will <u>move upward</u>
- The higher the temperature of a gas, the higher its pressure

Therefore…

- An emitted gas, which generally is <u>hotter</u> than the ambient air, will <u>move upward</u>
- As long as its surrounding is colder, it will continue the upward motion

Dry Adiabatic Lapse Rate (_)

- Consider an dry air parcel that is forced to move up or down from its original position.
- This process can be approximated as a adiabatic process (no heat transfer between the parcel and the environment)
- Using thermal dynamics, we can derive that temperature change of the air parcel with respect to height is ~ 9.8K/1000m (5.4F per 1000 ft)

c_p: heat capacity of air under constant pressure (J/kg·K)
g: gravitation acceleration constant (m/s²)

Atmospheric Stability

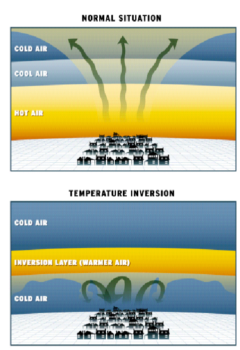
However…

- Sometimes, the previously mentioned vertical temperature profile may change (e.g. due to the very sudden cooling of the surface). In an extreme case, T may stay constant or increase with altitude
- If that happens, the emitted gas will soon stop its vertical upward motion since it will be colder than its surrounding.

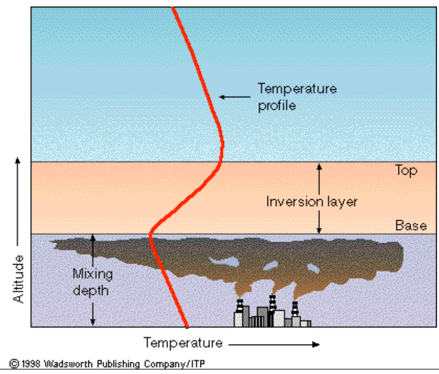
Atmospheric Stability

- Such an atmosphere is said to be **STABLE**, since the vertical motion is hindered
- An extreme stability condition is the **INVERSION**.
- During inversion, the pollutants can't be dispersed and they accumulate in the lower atmosphere, leading to a very big pollution problem

Normal vs. Inversion conditions



Inversion



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Atmospheric Stability

- When <u>vertical motion is enhanced</u>, the atmosphere is said to be **<u>UNSTABLE</u>**.
- Unstable atmospher is <u>desired</u>, since the pollutants can be <u>dispersed</u> very easily and <u>diluted</u>.

Stable _ BAD

Unstable _ GOOD

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Stable Atmosphere

Unstable Atmosphere

Unstable Atmosphere

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Atmospheric Stability

Atmospheric stability depends on various meteorological conditions, the most important being

- Wind speed
- Solar radiation
- Cloud cover

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Mixing Height

- **Mixing Height** or Mixing Depth is used by meteorologists to quantify the **vertical height of mixing in the atmosphere**. It is the height at which vertical mixing takes place. Forecasting of mixing height is done with the aid of the vertical temperature profile.
- A radiosonde is sent aloft and temperatures at various altitudes are radioed back. The altitude at which the dry adiabatic line intersects the radiosonde measurements is taken as the maximum mixing depth

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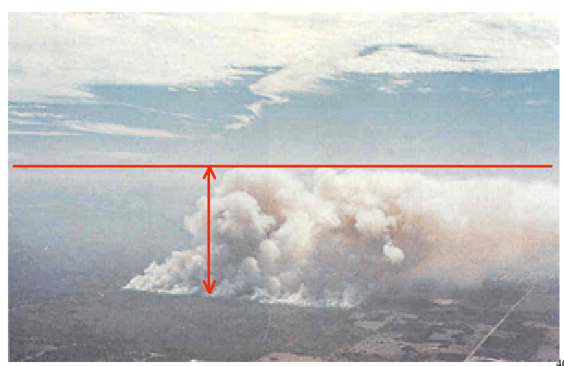
Mixing Height



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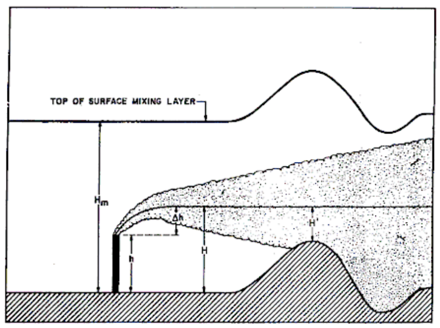
Mixing Height



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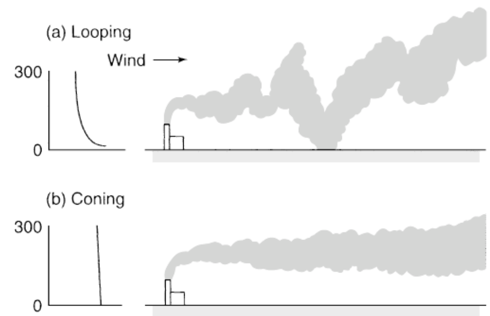
The relationship between plume dispersion and stability class



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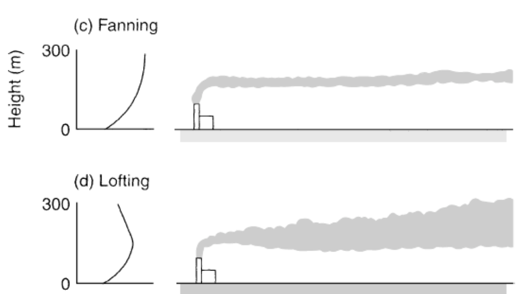
The relationship between plume dispersion and stability class



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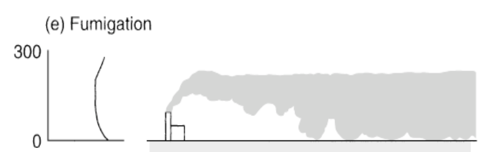
The relationship between plume dispersion and lapse rate



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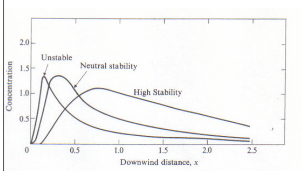
Maximum Ground Concentrations

- Patterns of ground-level concentrations shift with changing stability
  - As an example, the figure below illustrates the fact that a much more extensive length along the plume line will experience high concentrations during periods of high stability
  - However away from the plume line, the concentrations are much lower



Effect of atmospheric stability on the ground-level concentration under the plume line. The source is assumed to have a volume emission rate of Q_v = 4.7 liters/sec (10 ft^3/min) from a 30-m stack; and the wind speed is u= 0.5 m/sec (100 ft/min). The distance is in kilometers.

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The Pasquill Stability Classes

Stability class	Definition	Stability class	Definition
A	very unstable	D	neutral
B	unstable	E	slightly stable
C	slightly unstable	F	stable

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Meteorological Conditions Define the Pasquill Stability Classes

Surface wind speed		Daytime incoming solar radiation			Nighttime cloud cover	
m/s	mi/h	Strong	Moderate	Slight	> 50%	< 50%
< 2	< 5	A	A – B	B	E	F
2 – 3	5 – 7	A – B	B	C	E	F
3 – 5	7 – 11	B	B – C	C	D	E
5 – 6	11 – 13	C	C – D	D	D	D
> 6	> 13	C	D	D	D	D

Note: Class D applies to heavily overcast skies, at any wind speed day or night

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