Beltsville PBL Air Quality Modeling Atmospheric Chemistry
Atmospheric Chemistry / Air Quality 1-D models
(William Stockwell/Rosa Fitzgerald)

Objective: Students will modify their chemical box model developed in the previous assignment to read in simulated changes from a mixing-layer model and use the model to perform simulations of the effects of a rising boundary height on chemical concentrations.

Figure 1 shows a simple scheme for the mixed layer developed by Driedonks (1982). The left plot shows the variation in potential temperature (defined below) from the surface until the top of the layer (inversion height). The very thin warm surface layer heats the air in the mixing layer. It is assumed that adiabatic conditions apply to the mixing layer so while the potential temperature remains constant the real temperature decreases with altitude (adiabatic cooling). Also, this means that the layer is not stable and therefore well mixed. At the top of the mixing layer (at altitude H in the figure) it is assumed that there is a temperature increase (temperature inversion) that stabilizes the mixing layer and no further mixing occurs above the altitude H.

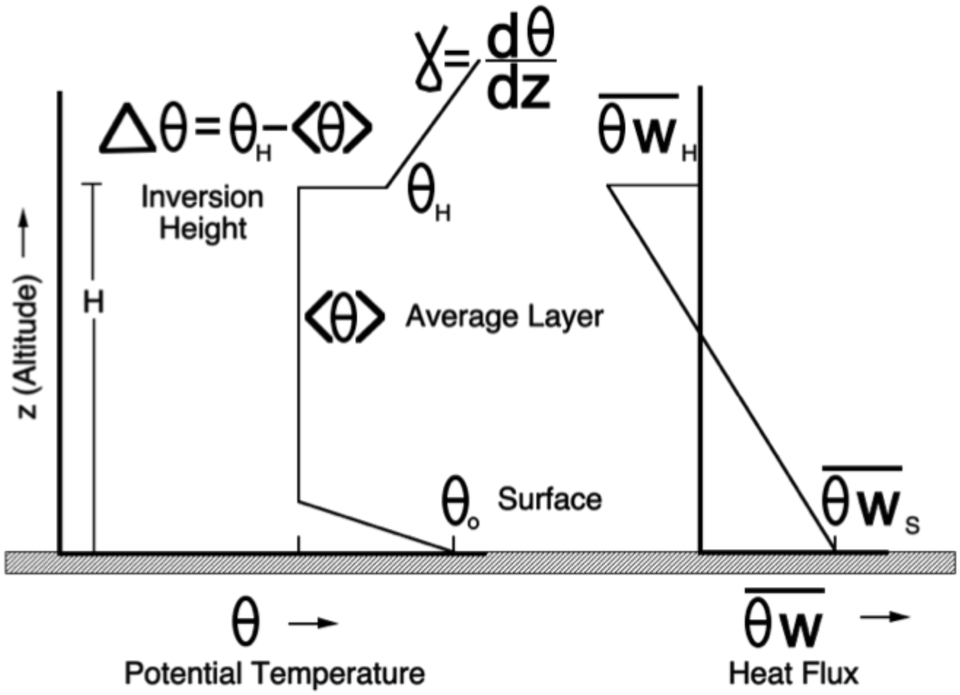

Figure 1. The figure shows profiles of potential temperature and heat flux in a mixed layer the Driedonks model (1982).

Potential Temperature

Potential temperature is the temperature a volume of air would have if it were adiabatically transported from its current temperature and pressure to an altitude with a standard pressure, usually taken as 1000 millibar. It can be calculated by Poisson's equation.

$$\theta = T \times \left(\frac{1000}{P}\right)^{R_d/C_p}$$

In Poisson's equation θ is potential temperature, T is the current temperature of the layer, P is the current temperature of the layer, R_d is the gas constant for dry air and C_p is the heat capacity of air at constant pressure.

$$R_d = 1000 \frac{g}{kg} \frac{R}{M_d}$$

In this equation R is the ideal gas constant and equal to R = 8.315 J K^{-1} mol^{-1}. M_d is the effective molecular weight of air and equal to 28.97 g mol^{-1}. Therefore, R_d is equal to 287.0 J K^{-1} kg^{-1}. The heat capacity of air per kilogram at constant pressure is 1004 J K^{-1} kg^{-1} and R_d/c_p is 0.2859.

Differential Equations for the Driedonks Model

The model shown in Figure 1 is described by the following set of coupled differential equations.

Average Potential Temperature of the Mixed Layer

$$\frac{d\langle\theta\rangle}{dt} = (1+k)\frac{C_T V_o(\theta_o - \langle\theta\rangle)}{H}$$

Mixing Height

$$\frac{dH}{dt} = w + \frac{kC_T V_o(\theta_o - \langle\theta\rangle)}{\Delta\theta}$$

T-Jump

$$\frac{d\langle\Delta\theta\rangle}{dt} = \gamma \times \left(\frac{dH}{dt} + w\right) - \frac{d\langle\theta\rangle}{dt}$$

Symbol	**Quantity:**
$\langle\theta\rangle$	Mixed-layer average potential temperature, K
k	Empirical Constant – Absolute value of ratio of upper to lower heat flux (Deardorf, Willis and Lilly = 2.0 × 10^{-1})
C_T	Dimensionless transfer coefficient with a maximum overland value of 1.5 × 10^{-2}
θ_o	Surface potential temperature
V_o	Horizontal surface wind-speed (m s^{-1})
H	Mixed layer height (m)
w	Vertical wind velocity (m s^{-1})
$\Delta\theta$	Temperature difference between mixed layer average potential temperature and potential temperature of layer above
γ	Constant equal to 2.6 × 10^{-3}

The difference between the surface potential temperature and average potential temperature of the mixed layer is a driving force for the change in the average potential temperature of the mixed layer and the change rate of the mixed layer height. The change rate of the average potential temperature of the mixed layer and the change rate of the mixed layer height are proportional to the horizontal surface wind velocity and some constants. The rate of change of the average potential temperature of the mixed layer is inversely proportional to the mixed layer height while the rate of change of the mixed layer height is inversely proportional to the temperature difference between mixed layer average potential temperature and potential temperature of the layer above (temperature inversion). This temperature difference can be regarded at the strength of the inversion so a greater positive temperature difference would strengthen the stability at the top of the boundary layer. The rate of change in the mixed layer height is proportional to the vertical wind speed.

The third equation characterizes the rate of change in the temperature difference between mixed layer average potential temperature and potential temperature of layer above, which is effectively the strength of the temperature inversion depends on the vertical wind speed and the rates of change in the mixed layer height minus the rate of change of the mixed-layer average potential temperature

The Driedonks model was applied to make a simulation for the following set of initial conditions.

Initial Conditions Used for Simulations

Condition	**Value**
Initial Simulation Time	360 min
End Simulation Time	1080 min
Surface Pressure	1035 millibars
Surface Temperature	300 K
Initial Mixing Layer Temperature	298 K
Initial T-Jump (Delta)	2 K
Surface Windspeed	2 m/s
Vertical Windspeed	0.5 m/s
Initial Mixing-Layer Height	150 m

Figure 1 shows that the temperature increased slightly over the course of one day. Figure 1 shows that the boundary layer height increased by a factor of about 3.3. This change in mixing height will cause dilution of trace gases in the layer and have a strong effect on the chemical change. Figure 3 shows that the strength of the inversion weakens slightly as the day progresses.

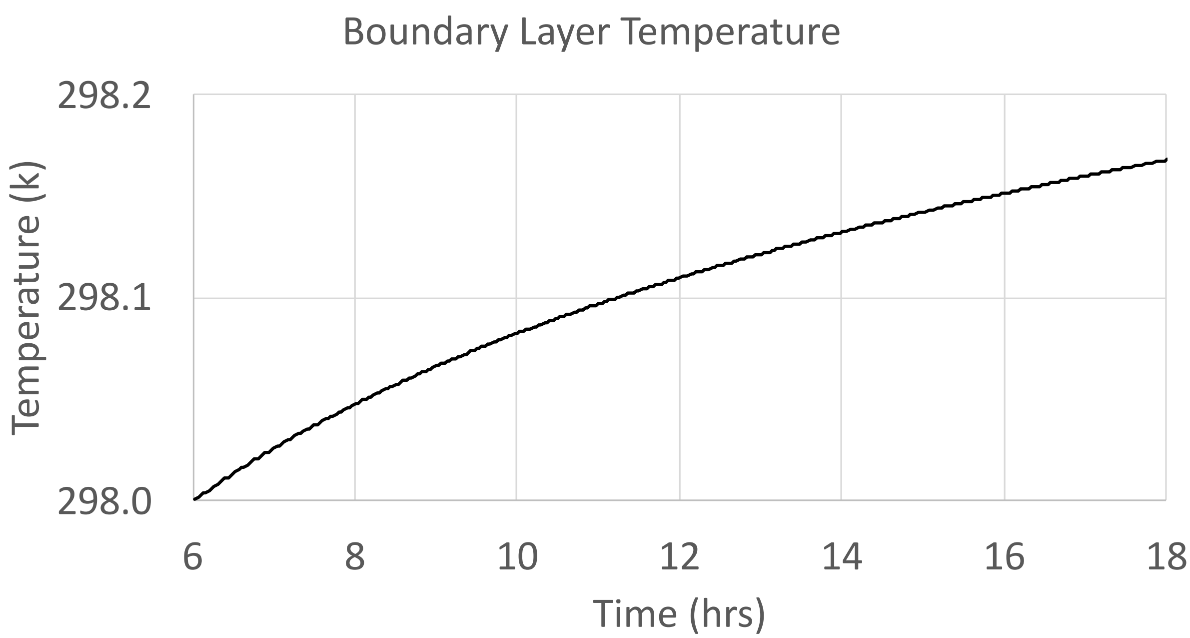

Figure 1. A plot of the average temperature of the mixed layer for the initial conditions given above. This is a plot of the absolute temperature and not potential temperature.

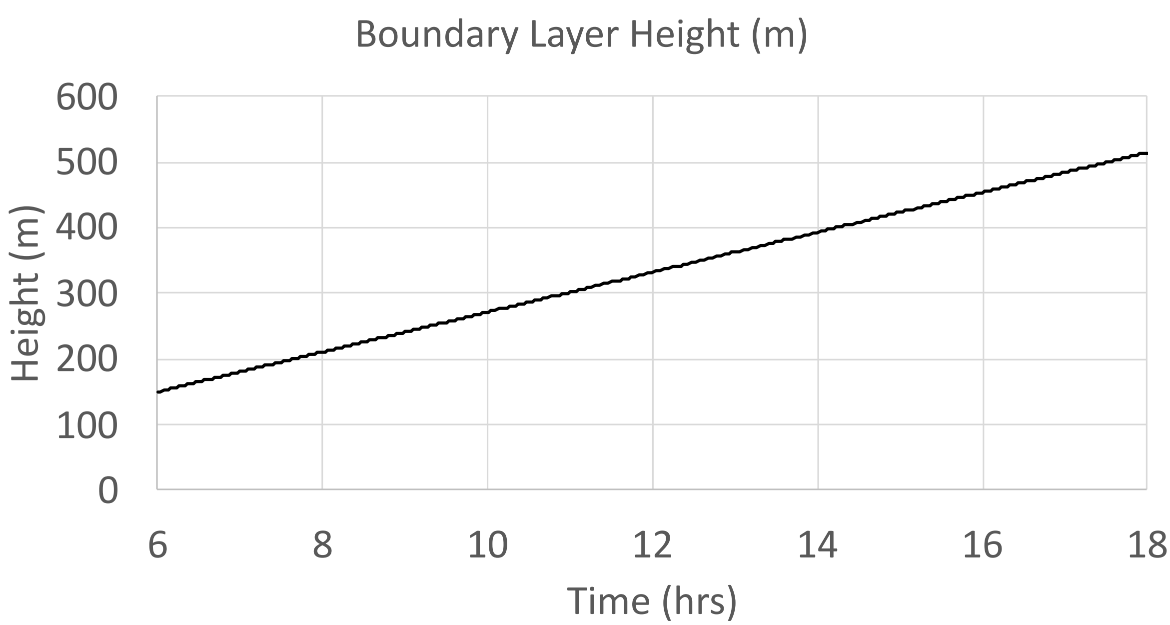

Figure 2. A plot of the height of the mixed layer for the initial conditions given above.

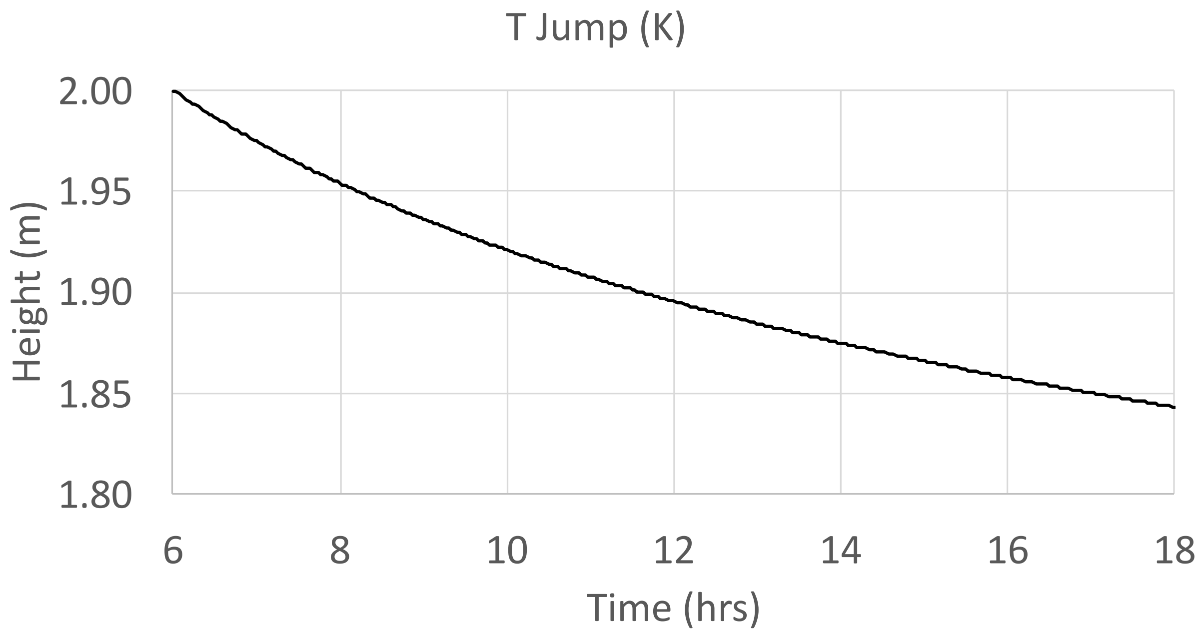

Figure 3. A plot of the temperature difference between mixed layer average potential temperature and potential temperature of the layer above (temperature inversion) for the initial conditions given above. This is a plot of the absolute temperature and not potential temperature.

Assignment

Data for simulation are provided as a separate file (provided in text and Excel formats). Modify the box model to read in the calculated absolute temperatures and mixing heights. Use the mixing heights to calculate dilution terms for each trace gas concentration. You might consider a time-splitting approach where you solve the chemistry equations, perform a dilution step and repeat. Or you could consider modifying the differential equations. We leave the decision and the details to the students.

Following modification of the box model repeat the simulations for the rising boundary layer values in the provided data file. Compare results for the original model (with a fixed boundary layer height) and your new model.

Reference

Driedonks, A.G.M. Sensitivity analysis of the equations for a convective mixed layer. *Boundary-Layer Meteorol 22*, 475–480 (1982). https://doi.org/10.1007/BF00124706