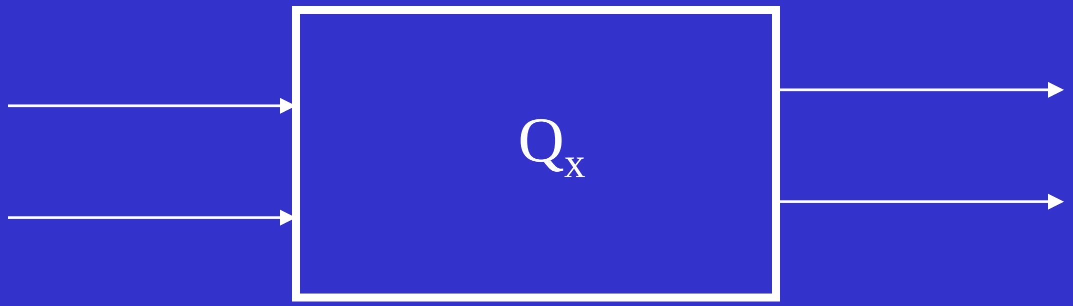
ATOC 3500
Tuesday, March 16, 2010
On Box Models

This is based on a past lecture that was on indoor air quality. We may return to some of the details of this topic, but for now, it is useful to illustrate some of the basics of box models that are used frequently in the field of atmospheric chemistry and air quality modeling. Many problems can be treated as a simple 'box' or reservoir where the amount of a particular substance X is often labeled as Q_x, and the arrows into and out of box represent fluxes of the substance X into and out of the box, respectively.

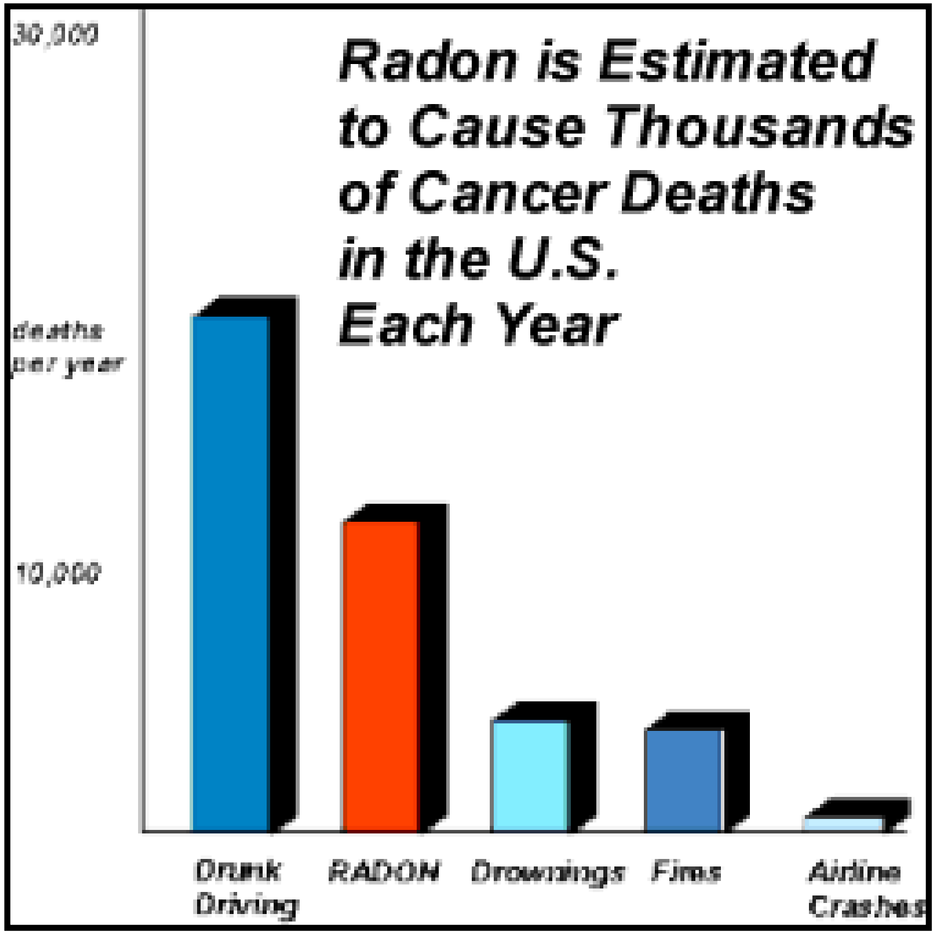


Risks from Radon (Rn) Exposure

Main health effect: lung cancer

- Among non-smokers, 10-20 cases/1000 people
- Add Rn at 1 pCi/L, 13-33 cases/1000 people
- Smokers' risk is about 15 times that of non-smokers'; due largely to the affinity of Rn and its daughters for smoke particles
- Comparison to risks from other sources

Note – a pCi/L is a unit called "picocurie per L". You can guess that it was named after Marie Curie, someone who studied radioactive elements.


30,000
Radon is Estimated to Cause Thousands of Cancer Deaths in the U.S. Each Year
deaths per year
10,000
Drunk Driving
RADON
Drownings
Fires
Airline Crashes

Estimating Exposure

Epidemiologists search for patterns in disease or illness that can reveal relationships to exposure to contaminants. One tool that modelers use to assess exposure to pollutants is the “box model”

The Box Model

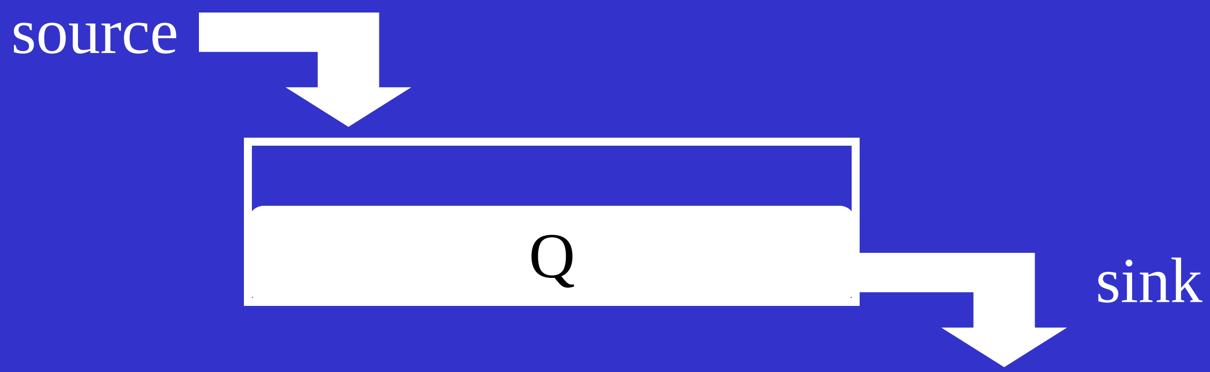
A simple tool for describing a situation or problem

Three basic elements: reservoir (box); sources; sinks

A simple example - the bathtub model:

“Source” = spigot
“Sink” = drain
“Reservoir” = tub

We often call Q the ‘burden’, since it represents a total mass of stuff, the more stuff there is, the more of a burden it is to move it around or remove it altogether.



How much water is in the tub? We express the total amount as Q

Q depends on relative sizes of source and sink; i.e., how much water is flowing from spigot and through drain. Usually, as the amount in the ‘tub’ or reservoir increases, the rate at which it drains (the “sink” term) increases proportionately.

What is the "residence time" of water in the tub? We express this as τ (the Greek letter “tau”)

τ depends on amount of water in tub and loss rate as follows:

$$\tau = Q/\text{sink}$$

The Steady-State Concept

This allows us to set up an equation that we can solve for one of the variables…either the source, or the sink, or the amount in the reservoir.

- A simplifying assumption: Q, the amount of material in the reservoir, is constant (i.e., $dQ/dt = 0$)

- As a consequence, the amount of material entering the reservoir must equal the amount leaving; that is, the source, S (sometimes called P for 'production rate') must equal the sink, which is typically called L. So steady state is often referred to as the condition when $P = L$ ("P equals L")

- Then the residence time is $\tau = Q/L$ or Q/P

Let's check our units:

$Q/P = \tau$, or $Q = P \times \tau$

so Burden = Production x Residence Time
kg = (kg seconds^{-1}) x seconds

For air pollution, it's usually more convenient to work with the concentration of a species X, than it is to work with the mass burden Q of species X (written as Q^X)

$$Q^X / \text{Volume} = [X]$$

$$[X] \times V = P\tau$$

(concentration) x (volume) = (production) x (residence time)
(mass/volume) x volume = (mass/time) x time

$$(\mu g\ m^{-3}) \times (m^3) = (g\ s^{-1}) \times (s)$$

Recall that our goal here is to try to estimate exposure to some pollutant based on things we can measure, such as the amount of the pollutant present, how quickly air enters or leaves a room, etc.

Radon sources and sinks:

- Seepage; typically 0.01 – 10 pCi L^{-1} hr^{-1}
- Ventilation; exchange time varies from 0.5 – 4 hr
- Radioactive decay; τ_{Rn} = 3.8 day = 91 hr

Assume steady-state**:**

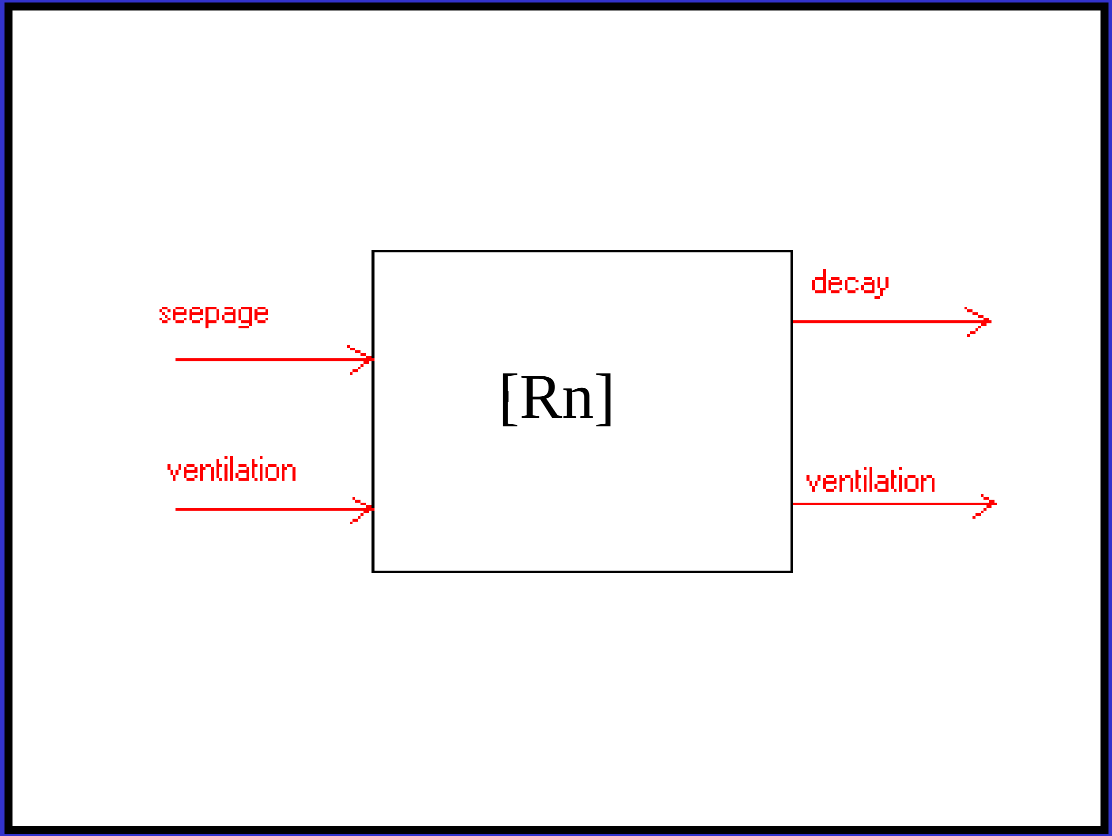
At steady-state, production equals loss, so

$$\Sigma_k P_k = \Sigma_j L_j$$

Derive steady-state concentration of indoor Rn:

Since Rn sources are given as pCi L^{-1}, we'll use the term "S" instead of "P"

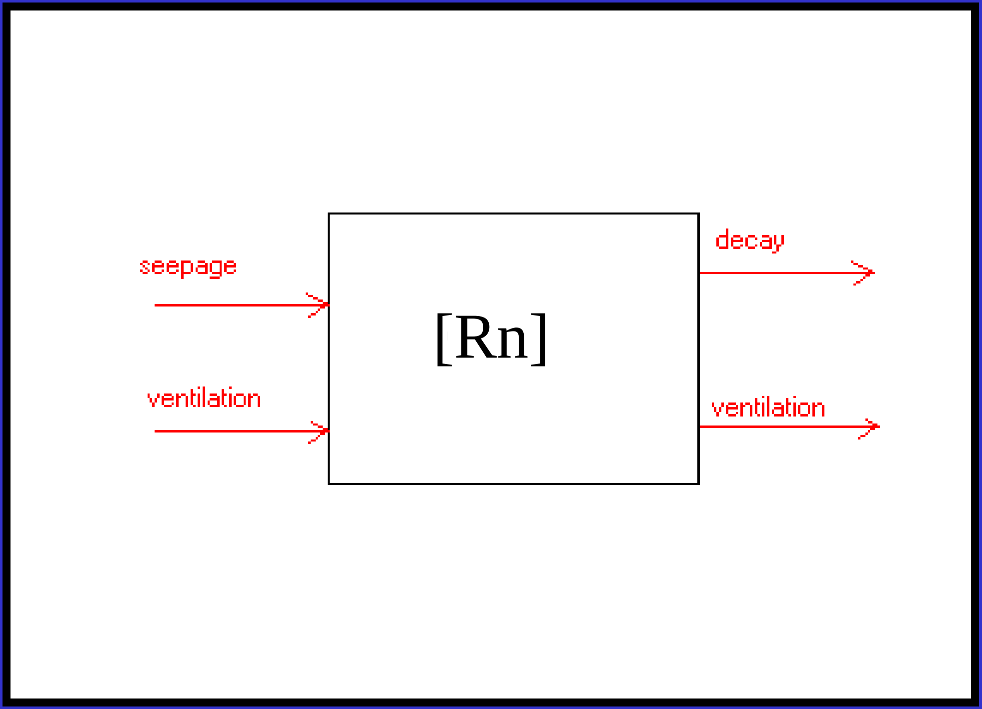
Schematically, we combine these terms into a figure



The seepage source is denoted S_{Rn} and is given in units of pCi L^{-1} hr^{-1}.

The ventilation source is denoted S_v and is equivalent to the concentration of Rn in ambient air ($[Rn]_o$) divided by the ventilation time, τ_v. The units on S_v are pCi L^{-1} hr^{-1}.

The decay loss is denoted L_d, and is given by the indoor concentration of Rn ([Rn]) divided by the decay time or half-life, τ_d.



The ventilation sink is denoted L_v. Analogous to the ventilation source, $L_v = q^{Rn}/\tau_v$. Assuming steady-state, the sum of the sources is equal to the sum of the sinks:

$$S_{Rn} + S_v = L_d + L_v$$
$$S_{Rn} + ([Rn]_o/\tau_v) = ([Rn]/\tau_d) + ([Rn]/\tau_v)$$

Multiplying through by τ_v:

$$S_{Rn}\tau_v + [Rn]_o = [Rn]\ [(\tau_v/\tau_d) + 1]$$

Rearranging:

$$\boxed{[Rn] = ([Rn]_o + S_{Rn}\tau_v)/\ [(\tau_v/\tau_d) + 1]}$$

There are some special cases to consider that can simplify this formulation: If the ventilation time is much shorter than the decay time ($\tau_v << \tau_d$), then the denominator of the above expression is about 1. Therefore, $[Rn] \sim [Rn]_o + S_{Rn}\tau_v$

Under these conditions ("well ventilated"), the indoor radon will be equal to the outdoor value plus a contribution from the seepage source that is proportional to the ventilation time. If ventilation is slow, the indoor concentration will be higher than if the ventilation is rapid.

The other limiting case will occur if the ventilation time is very long, in which case $\tau_v/\tau_d >> 1$ and $[Rn]_o + S_{Rn}\tau_v \sim S_{Rn}\tau_v$.

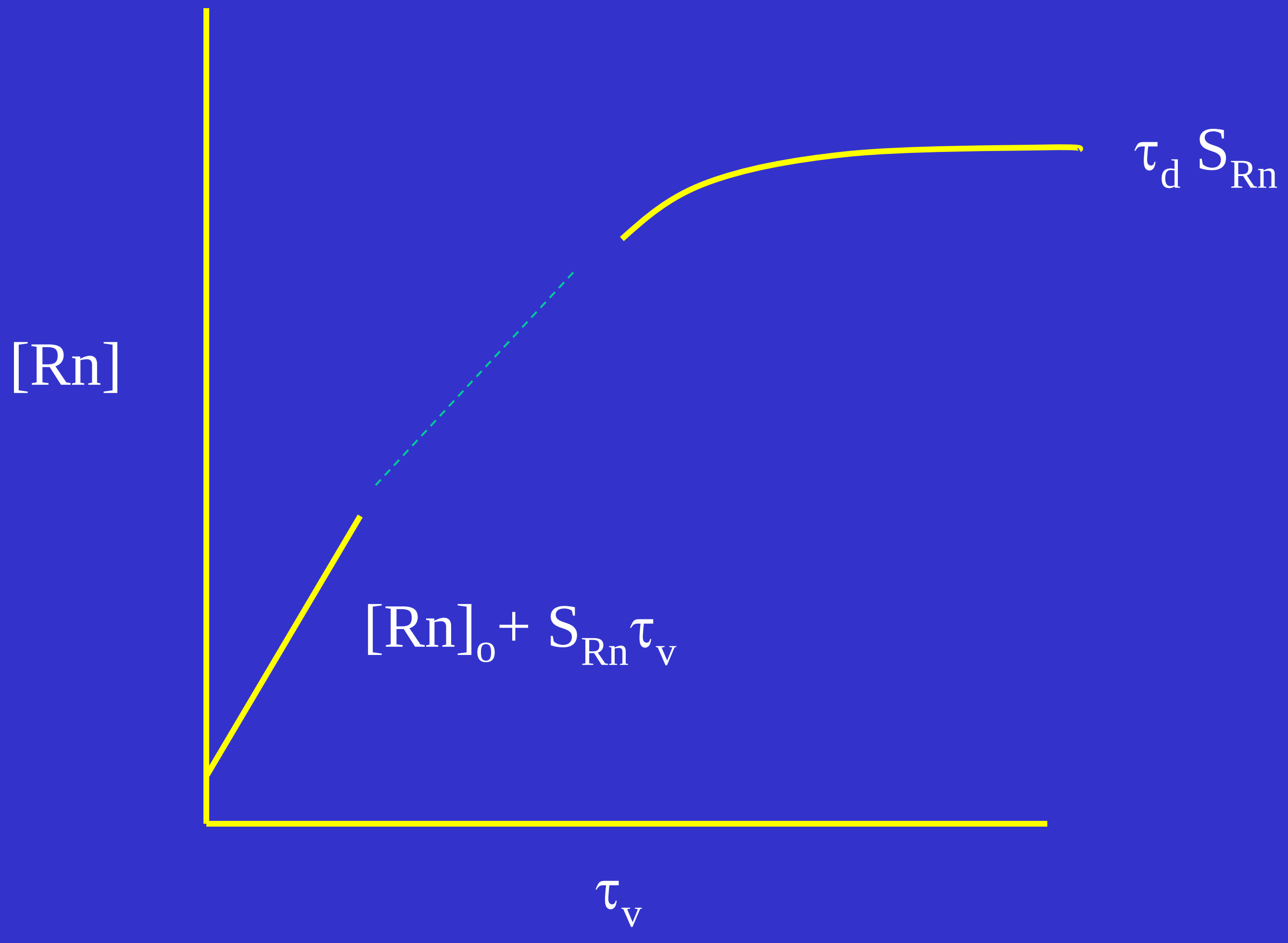
$$[Rn] \sim (S_{Rn}\tau_v)/(\tau_v/\tau_d)$$

$$= \tau_d S_{Rn}$$

Under these conditions, as $\tau_{v \text{ increases,}}$ the equation will asymptote to a value that is independent of the outdoor radon abundance, and one that is proportional to the seepage source strength of radon.

So we can now better understand why, when homes are tested for radon, the windows must be kept closed and ventilation kept to a minimum. This will provide the largest value possible. This might not be representative of actual living conditions, but at least it provides a uniform testing standard. Otherwise, all the test will reveal is what the ambient radon abundance is, which isn't very interesting!

We can summarize the equation graphically:



Given some average conditions:

S_{Rn} = 0.5 pCi L^{-1} hr^{-1}
τ_v = 1 hr
$[Rn]_o$ = 0.4 pCi L^{-1}

What is the indoor Rn concentration?

We can used the expression derived above: $[Rn] = [Rn]_o + S_{Rn}\tau_v$ because the 1 hour ventilation time is very much shorter than the 91 hour decay half-life of Rn. Substituting appropriate values, we obtain an indoor radon concentration of 0.9 pCi L^{-1}.

Note that our homework problems ozone stratospheric ozone were essentially box models without ventilation.

In this case, catalysts destroy ozone at rates that depend on the concentration of the catalysts:

$$d[O_3]/dt = 2k[O][ClO] + 2k[O][NO_2] + 2k[O][HO_2] + \ldots$$

For Homework Problem 16, we had a box model with no source, so in this case, we just saw ozone drop over time. This would be an example of transient behavior in the model – turning on or off a source or sink. The concentration of the reservoir would adjust to the new conditions, eventually reaching a new steady state where the new combination of sources and sinks balanced. In the case of the ozone hole, this new balance is close to zero ozone, because the only major source at high latitudes in springtime would be transport of ozone from the tropics, which is quite slow.