JOINT REGIONAL CLIMATE AND HYDROLOGY MODELLING

Water and Energy Fluxes at the Land Surface and in the Atmosphere

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Dr. Harald Kunstmann Institute for Meteorology and Climate Research (IMK-IFU) Karlsruhe Institute of Technology KIT Kreuzeckbahnstraße 19 D-82467 Garmisch-Partenkirchen Email: harald.kunstmann@kit.edu Phone: +49 (0)8821 183208, Fax: +49 (0)8821 183243 http://www.imk-ifu.kit.edu

Part I: Land Surface

- Basic Aspects of Global Climate
- Global Energy and Water Fluxes
- Water in Soils
- Physics of Sensible and Latent Heat Fluxes
- Soil-Vegetation-Atmosphere-Transfer Modeling
- Concepts of Upscaling of Land Surface Parameters

Basic Aspects of Global Climate

Energy budget of the Earth

The sun radiates energy approximately as a blackbody with a temperature of 6000 *K*. its radiation spectrum extends from the ultraviolet to the infrared with a maximum in the visible range. However, gases in the earth's atmosphere are strong absorbers of energy at selected wavelengths in this range, so the radiation striking the earth's surface is depleted in portions of the spectrum.



Figure: Spectra of energy (a) emitted by a blackbody at 6000 K; (b) received at the Earth's surface (global average); (c) emitted by a blackbody at 290 K; (d) emitted to space by the earth-atmosphere system (global average). Upper graph shows absorption spectrum for principal absorbing gases in the atmosphere (Dingman, 1994)



Figure: Average global energy balance of the earth-atmosphere system. Numbers indicate relative energy fluxes; 100 units equals the solar constant, 1367Wm⁻².(Dingman, 1994)

Energy balance of the atmosphere:

- 11 of the 15 units radiated by the surface are absorbed to heat the atmosphere.
- the net effect of the exchange of radiant energy between the surface and the atmosphere is the upward transfer of 15 units of energy of which 4 are directly radiated to outer space.
- Transfer of latent heat via evaporation (mostly from oceans) adds another 24 units; this is the largest source of atmospheric energy. Sensible heat transfer (conduction/convection) contributes another 7 units because the surface is, on average, warmer than the overlying air.
- energy in atmosphere: (20 +4) +(11 +7 +24)= 66 units
- coming from land surface: 11+7+24 = 42 units $\Rightarrow 42/66 = 64\%$
- absorbed directly from solar radiation \Rightarrow 24/66=36%
- energy due to absorption of of longwave radiation via greenhouse gases:
 ⇒ 11/66=17%; without the greenhouse effect the earth surface would be around -18°C



Figure: Spectra of incoming solar and outgoing terrestrial radiation.

Stefan-Boltzmann law:

All matter at a temperature above absolute zero radiates energy in the form of electromagnetic waves that travel at the speed of light:

$$Q = \varepsilon \sigma T^4$$

- Q: rate of energy emission per unit area per unit time [Wm⁻²]
- σ : universal constant: 5.6710-8 Wm⁻²K⁻⁴ (**Stefan-Boltzmann constant**)
- ε: emissivity of surface [.]
- T: absolute temperature [K]

Surface	Conditions	Emissivity, a	
Clouds	Dense	0.99	
Liquid water		0.95	
Ice	At 0°C	0.97	
Sand	Dry	0.95	
	Wet	0.98	
Peat	Dry	0.97	
	Wet	0.98	
Rock	Light sandstone	0,98	
	Limestone, gravel	0.92	
Grass	Typical fields	0.95	
	Lawn	0.97	
Crops	Corn, beans	0.94	
-	Cotton, tobacco	0.96	
	Sugar cane	0.99	
Cactus		0.98	
Trees	Deciduous forest	0.95	
	Coniferous forest	0.97	

Table: Emissivity values for different vegetations

Basics of Energy Balance



(K: net shortwave radiation input; L: net longwave radiation input)

: Radiation balance at the earth's surface

α: albedo

Surface	Conditions	Albedo, d
Clouds	Low overcast: 100 m thick	0.40
	200 m thick	0.50
	500 m thick	0.70
Liquid water	Smooth; solar angle 60°	0.05
	30°	0.10
	20°	0.15
	10°	0.35
	5°	0.60
	Wavy; solar angle 60°	0.10
Solid water	Fresh snow; low density	0.85
	high density	0.65
	Old snow; clean	0.55
	dirty	0.45
	Glacier ice; clean	0.35
	dirty	0.25
Sand	Dry, light; high sun	0.35
	low sun	0.60
	Gray; wet	0.10
	dry	0.20
	White; wet	0.25
	dry	0.35
Soil	Organic; dark	0.10
	Clay	0.20
	Sandy; light	0.30
Grass	Typical fields	0.20
	Dead; wet	0.20
	dry	0.30
Tundra, heather		0.15
Crops	Cereals, tobacco	0.25
	Cotton, potato, tomato	0.20
	Sugar cane	0.15
Trees	Rain forest	0.15
	Eucalyptus	0.20
	Red pine forest	0.10
	Mixed hardwoods in leaf	0.18

Visible-Range Reflectance (albedo) of Various Forms of Water and Various Earth Materials

 Table:
 Typical values for reflectances (albedos)



Figure: Components of energy balance for a volume extending from just below the surface to the height at which the net radiation balance is determined

- R_n : net incoming radiation
- λE : outgoing energy as evaporation
- *H*: outgoing sensible heat flux
- *G*: outgoing heat conduction into the soil
- *P*: energy absorbed by biochemical processes in the plants, typically a taken as 2% of net radiation
- A_d : loss of energy associated with horizontal air movement; significant in an "oasis" situation but generally neglected otherwise.

all in [W/m²] e.g.

(II)
$$\begin{array}{l} R_n = \lambda E + H + G + P + A_d \approx \\ \approx \lambda E + H + G \end{array}$$

$$\mathbf{I+II} \ \boxed{(1-\alpha)SW_{in} + LW_{in} - \sigma \varepsilon T_{sfc}^{4} \approx \lambda E + H + G}$$

:Energy balance at land surface

Exercise: Energy-Balance of Global Radiational Temperature

I. Long term average rate of input to earth-atmosphere system

$$i = S(1 - a_p)$$

II. Boltzmann Law: average rate at which system radiates energy to outer space:

$$q = \sigma T_p^4 A$$
I.=II. $\Rightarrow \qquad \left[T_p = \left[\frac{S (1 - a_p)}{\sigma A} \right]^{1/4} \right]$

$$\begin{split} S &= 1.74 \ 10^{17} \ W \\ \sigma &= 5.78 \ 10^{-8} \ W \ m^{-2} \ K^{-4} \\ A &= 4 \ \pi \ R_{\text{Earth}}^2 = 5.1 \ 10^{14} \ m^2 \end{split}$$

a_p=0.3

 \Rightarrow T_p=253.6 K

Many naturally occurring and human induced gases strongly absorb long wave radiation (11 out of 15 units are absorbed to heat the atmosphere \Rightarrow greenhouse effect)

Most important greenhouse gases are 1) water vapour (accounts for 65% of the absorption), 2) carbon dioxide (33%) and methane, nitrous oxide, ozone and chlorinated fluorocarbons (2% combined).

Exercise: Energy-Balance Model of Earth-Surface Temperature

Simplified two layer atmosphere:

lower layer (roughly till 1.8 km) with temperature T_i: 20% of air and 50% of water vapour (main absorber of terrestrial radiation)

upper layer with temperature T_u: 80% of air and 50% of water vapour

I. Total system: $S + W = a_p S + \sigma T_u^{4} A + (1 - f)\sigma T_s^{4} A$

II. Upper atmosphere: $k_u S + \sigma T_l^4 A + 0.5Q_e = 2\sigma T_u^4 A$

III. Lower atmosphere: $k_l S + \sigma T_u^4 A + f\sigma T_s^4 A + 0.5Q_e + Q_h + W = 2\sigma T_l^4 A$

all energy terms expressed as long term fluxes in [E T⁻¹]

$$T_{s} = \left[\frac{(3 - 3a_{p} - 2k_{u} - k_{l})S - 1.5Q_{e} - Q_{h} + 2W}{(3 - 2f)\sigma A}\right]$$

$S = 1.74 \ 10^{17} \ W$ $Q_e = 4.08 \ 10^{16} \ W$ $Q_h = 8.67 \ 10^{15} \ W$ $W = 1.07 \ 10^{13} \ W$	solar flux latent heat flux from surface sensible heat flux from surface heat generated from fossil and nuclear fuels
$a_p = 0.3$ $k_u = 0.18$: $k_l = 0.075$: f = 0.95	planetary albedo fraction of solar radiation absorbed in upper layer fraction of solar radiation absorbed in lower layer fraction of thermal radiation from surface that is absorbed in atmosphere

 \Rightarrow T_s=290.4 K

Latitudinal energy transfer

The geometric relations of the earth's orbit cause seasonal and latitudinal variations in the receipt of solar energy.

Solar energy flux is spread out over large areas at high latitudes because the earth is a sphere. This strictly latitudinal effect is modified seasonally because the earth's axis of rotation is tilted at an angle of 23.5° to the orbital from the sun.



Figure: Variations of solar radiation intensity $[E L^{-2} T^{-1}]$ with angel of incidence. At higher angles (higher latitudes) a given energy flux is spread over a larger area (Dingman, 2002).



Figure: Revolution of the Earth around the sun, showing that the occurrence of summer and winter in the Northern and Southern Hemispheres is determined by the 23.5° tilt of the rotational axis toward or away from the sun (Dingman, 2002)

General circulation

The unequal latitudinal distribution of radiation and the requirements for conservation of angular momentum on the rotating earth give rise to a system of three circulation cells in the latitude bands from 0° - 30° , 30° to 60° , and 60° to 90° in each hemisphere.



Figure: The general circulation of the atmosphere. "H" indicates Hadley cells. Double headed arrows in cross section indicate that the wind has a component from the east.



Distribution of temperature

Figure: Distribution of mean temperature (°C) in a) January and b) July

Distribution of precipitation



Average precipitation over the globe

- Regions characterized by rising air tend to have relatively high average precipitation, those of descending air have low precipitation
- The general circulation produces belts of relatively high precipitation near the equator and 60° latitude and low precipitation near 30° (where most of the world's greats deserts occur).
- Intertropical convergence zone (ITCZ)
- Precipitation rates influences by topography, air temperatures, frontal activities, wind directions in relation to moisture sources

Significant deviations from general latitudinal distributions due to mountain ranges.



Figure: Latitudinal distribution of average precipitation.



Temporal distribution of precipitation

Figure: Generalized map of **seasonal precipitation** regimes. Heavy dashed line encloses the monsoon region of Asia and Africa.

The reversal of circulation associated with the winter high pressure and summer low pressure over the huge landmass of Asia interacts with the topography and the migration of the ITCZ to produce a particularly strong seasonality of precipitation in much of Asia and Africa: this is the **monsoon**.

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Distribution of snow cover

Snow has important climatic effects helping to maintain colder temperatures by reflecting much of the incoming solar energy, and, in melting, by absorbing energy that would otherwise contribute to warming the near surface environment.

During the ice ages, the reflection of solar radiation by ice and snow was an important feedback that contributed to creating and maintaining a colder climate.

Snow also acts as an insulating blanket that helps to retain heat in the soil, which is important hydrologically as well as biologically: if soil is prevented from freezing, its ability to accept infiltrating water is generally enhanced.



The principal hydrologic effect of snow is to delay the input of precipitated water into the land phase of the hydrologic cycle and thus to affect the seasonal distribution of runoff.

Distribution of evapotranspiration

As expected there is a general correlation between mean annual temperature and mean annual evapotranspiration. In the oceans, the basic latitudinal patterns are distorted largely by the effects of surface currents (e.g. Gulf stream and equator ward cold currents off western South America and North America). The highest continental values are in the tropical rain forests of South America, Africa and southeast Asia While the lowest are in the Sahara desert, Antarctica, arctic North America and central Asia.



Figure: Oceanic and continental evapotranspiration in [cm yr⁻¹]. Shaded areas: mountain zones where no data are available.

Distribution of runoff

is mostly the difference between precipitation and runoff for the continents. Virtually all the zones with the highest runoff also have the highest precipitation.



Seasonal runoff regimes

In most regions that have seasonal snow cover, maximum runoff occurs in the melt season: summer in arctic and subarctic, and alpine regions, and spring at lower latitudes. A summer maximum also occurs in regions with monsoonal climates such as India and southeast Asia. Fall and winter runoff maxima are also directly related to concurrent rainfall maxima.



The Global Hydrologic Cycle

Stocks and fluxes in the global cycle

TABLE 3-1 Stocks in the Global Hydrologic Cycle^a

			Share of World	d Reserves (%)	
Form of Water	Area Covered (km²)	Volume (km ³)	Of Total Water Reserves	Of Fresh-Water Reserves	
World oceans	361,300,000	1,338,000,000	96.5		
Ground waters	134,800,000	23,400,000	1.7		
Fresh ground water		10,530,000	0.76	30.1	
Soil moisture	82,000,000	16,500	0.001	0.05	
Glaciers and permanent	16,227,500	24,064,100	1.74	68.7	
snowpack:					
Antarctica	13,980,000	21,600,000	1.56	61.7	
Greenland	1,802,400	2,340,000	0.17	6.68	
Arctic islands	226,100	83,500	0.006	0.24	
Mountain areas	224,000	40,600	0.003	0.12	
Ground ice in zone of	21,000,000	300,000	0.022	0.86	
permafrost strata					
Water reserves in lakes:	2,058,700	176,400	0.013		
fresh-water lakes	1,236,400	91,000	0.007	0.26	
saltwater lakes	822,300	85,400	0.006		
Marsh water	2,682,600	11,470	0.0008	0.03	
Water in rivers	148,800,000	2,120	0.0002	0.006	
Biologic water	510,000,000	1,120	0.0001	0.003	
Atmospheric water	510,000,000	12,900	0.001	0.04	
Total water reserves	510,000,000	1,385,984,610	100		
Fresh water	148,800,000	35,029,210	2.53	100	

	Aroo	Precipitation		Evapotranspiration		Runoff	
Continent	(10^6 km^2)	(km ³ yr ⁻¹)	(mm yr ⁻¹)	$(km^3 yr^{-1})$	(mm yr ⁻¹)	$(\mathrm{km}^3 \mathrm{yr}^{-1})$	(mm yr ⁻¹)
Europe	10.0	6,600	657	3,800	375	2,800	282
Asia	44.1	30,700	696	18,500	420	12,200	276
Africa	29.8	20,700	695	17,300	582	3,400	114
Australia ^a	7.6	3,400	447	3,200	420	200	27
North America	24.1	15,600	645	9,700	403	5,900	242
South America	17.9	28,000	1,564	16,900	946	11,100	618
Antarctica	14.1	2,400	169	400	28	2,000	141
Total land ^b	148.9	$111,100^{\circ}$	746	71,400	480	39,700°	266

^b Including New Zealand and adjacent islands.
 ^c Estimate differs from that of Table 3-2.

Data from Baumgartner and Reichel (1975)

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Stock	Volume	Percentage of All Water	Sources	Input Flux	Sinks	Output Flux
Oceans	1338	96.5	Pptn:	458	Evap:	505
A 4			Runoff:	47	_ · · · F ·	
Atmosphere	0.013	0.001	Land evap:	72	Pptn:	577
Law 1			Ocean evap:	505	1	
Land	48	3.46	Pptn:	119	Evap:	72
					Runoff:	47
Total	1386	100				.,

Table: Global stocks and fluxes of Water



*Fresh water only †Includes permafrost

Table: Schematic diagram of stocks (km³) and annual fluxes (km³ yr⁻¹) in the global hydrologic cycle. Inflows and outflows nay not balance for all compartments (Dingman, 1994)

Residence Times

TStock	
$I_r = \frac{1}{Flux}$	

 $\Rightarrow T_{Atmosphere} \cong 12{,}900 \; km^3 {\prime} \; 577{,}000 \; km^3 {\prime} year \cong 8 days$

 \Rightarrow T_{Rivers} \cong 2,120 km³/ 44,700 km³/year \cong 17.3 days

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	Drainage	Drainage Area Discharge			rge		Dunoff
River	(10 ³ km ²)	%o ^a	$(m^3 s^{-1})$	$(\mathrm{km^3 yr^{-1}})$	$(mm yr^{-1})$	<i>%</i> ь	Ratio
1. Amazon	7,180	4.8	190,000	6,000	835	13.0	0.47
2. Congo	3,822	2.6	42,000	1,330	340	2.9	0.25
3. Yangtzekiang	1,970	1.3	35,000	1,100	560	2.4	0.50
4. Orinoco	1,086	0.7	29,000	915	845	2.0	0.46
5. Brahmaputra	589	0.4	20,000	630	1,070	1.4	0.65
6. La Plata	2,650	1.8	19,500	615	235	1.3	0.20
7. Yenesei	2,599	1.7	17,800	565	215	1.2	0.42
8. Mississippi	3,224	2.2	17,700	560	175	1.2	0.21
9. Lena	2,430	1.6	16,300	515	210	1.1	0.46
0. Mekong	795	0.8	15,900	500	630	1.1	0.43
1. Ganges	1,073	0.7	15,500	490	455	1.1	0.42
2. Irrawaddy	431	0.3	14,000	440	1,020	1.0	0.60
3. Ob	2,950	2.0	12,500	395	135	0.9	0.24
4. Sikiang	435	0.3	11,500	365	840	0.8	
5. Amur	1,843	1.2	11,000	350	190	0.8	0.32
6. Saint Lawrence	1,030	0.7	10,400	330	310	0.7	0.33
otals	34,107	22.9	478,100	15.100		32.8	

^b Percent of total runoff to oceans (46 \times 10³ km³ yr⁻¹).

Ratio of long-term average discharge to long-term average precipitation (w in the model in Box 3-3).

Data from Baumgartner and Reichel (1975), Wigley and Jones (1985), and L'vovich (1974),

Outlook: Water Stress



Figure: Human appropriation of estimated accessible RFWS $_{land}$ (terrestrial renewable fresh water supply) is 30% and human appropriation of total RFWS $_{land}$ is 23% (Postel, 1996)

Exercise: Future climate change and water resources

- I. R = P ET
- II. ET = (1 w)P

runoff ratio $w \equiv \frac{R}{P}$

relative change of precipitation $p = \frac{P_{future}}{P_{max}}$

relative change of evapotranspiration $e = \frac{ET_{future}}{ET_{now}}$

Relative change in runoff as a function of the present runoff ratio and the relative changes in precipitation and evapotranspiration:



Example: Model for estimating effects of climatic changes on runoff

• Changes in runoff are everywhere more sensitive to changes in precipitation than to changes in evapotranspiration

$$\left(\frac{\partial r}{\partial p} > \frac{\partial r}{\partial e}\right)$$

- Relative change in runoff is always greater than relative change in precipitation (*r* > *p*)
- Runoff is most sensitive to climatic changes in arid and semiarid regions where the runoff ratio *w* is small

Water in Soils: Infiltration and Redistribution



Figure: Definitions of terms used to describe water movement in the unsaturated zone

Redistribution can involve

- exfiltration (evaporation from the upper layers of the soil),
- capillary rise (movement from the saturated zone upward into the unsaturated zone due to surface tension),
- recharge (movement of percolating water from the unsaturated zone to the subjacent saturated zone),
- interflow (flow that moves downslope) and
- uptake by plant roots (transpiration)



Material properties of soil

Figure: Grain size distribution curve for a soil formed on glacial till in southwestern New Hampshire. The boundaries between size classes designated clay, silt, sand and gravel are shown as vertical lines.



Figure: Soil texture triangle, showing the textural terms applied to soils with various fractions of sand, silt, and clay.

Definitions

Particle density	$ \rho_m = rac{M_m}{V_m} $
with M _m : mass of mineral grains V _m : Volume of mineral grains	
Bulk density	$\rho_b = \frac{M_m}{V_s} = \frac{M_m}{V_a + V_w + V_m}$
With V _s : total volume of soil sample V _a : volume of air V _w : volume of liquid water V _m : volume mineral components	
Porosity	$\phi = \frac{V_a + V_w}{V_s}$
Volumetric water content	$\theta = \frac{V_w}{V_s}$
Degree of saturation	$S = \frac{V_w}{V_a + V_w} = \frac{\theta}{\phi}$

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Figure: Ranges of porosities

In general, finer grained solids have higher porosities than coarser grained soils. This is in part due to the very open "House of cards" arrangement of clays, which is maintained by electrostatic forces between the roughly disk-shaped grains; In contrast, quasi-spherical sand and silt grains are in more closely packed grain-to grain architecture.



Figure: Schematic diagrams of structures of aggregates of (a) clay and (b) sand. The architecture of clay particles is maintained by intergrain electrostatic forces.

Soil water tension

The porous medium is made up of a matrix of particles. When the void spaces are only partially filled with water, the water is attracted to the particles surface through electrostatic forces between the water molecules' polar bounds and the particles surfaces. This surface adhesion draws the water up around the particles surfaces, leaving the air in the center of the voids. As more water is added to the porous medium, the air exits upwards and the area of free surfaces diminishes within the medium, until the medium is saturated.

The effect of soil suction can be seen if a column of dry soil is placed vertically with its bottom in a container of water – moisture will be drawn up into the dry soil to a height above the water surface at which the soil suction and gravity are equal. This height ranges from *mm* for a coarse sand to several *meters* for a clay soil.



Figure: Soil water pressure (tension) Ψ vs. degree of saturation S for soils of different textures.

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Explanation of surface tension

Molecules in the surface of liquid water are subjected to a net inward force due to hydrogen bonding with the molecules below the surface.

Surface tension, σ , is equal to the magnitude of that force divided by the distance over which it acts; thus its dimension are [F L⁻¹].



Figure: Intermolecular forces acting on typical surface (S) and nonsurface (B) molecules

Water has a surface tension higher than that of most other liquids; its value at 0°C is

 $\sigma = 0.0756 \ Nm^{-1}$

Surface tension decreases rapidly as temperature increases:

 $\sigma \approx 0.001 \cdot (20987 - 92.613 \cdot T)^{0.4348}$

where T is in °C and σ in Nm⁻¹.



Figure: Sketch of phenomenon of capillary rise in a circular tube of radius r, θ_c is the contact angle between the meniscus and the wall. P is atmospheric pressure.

When capillary rise has ceased, the column of water is suspended from the meniscus, which is in turn attached to the walls by hydrogen bounds. Thus the water is under tension. Because of the intermolecular hydrogen bonds, the entire mass of water within the tube will also be drawn upward until the adhesive force between the molecules of the tube and those of the water is balanced by the downward forces due to the weight of the water suspended within the tube.

Upward force:	$F_u = \sigma \cdot \cos(\theta_c) \cdot 2 \cdot \pi \cdot r$	[N]
Downward force:	$F_d = \gamma \cdot \pi \cdot r^2 \cdot h_{cr} \qquad [N]$	

The vertical extent of water rise in the tube can be approximately calculated by $(F_u = F_d)$

$$h_{cr} = \frac{2\sigma\cos\theta_c}{\gamma_w r}$$

with

h_{cr}: height of column $θ_c$: contact angle between water surface and tube r: radius of tube $γ_w$: weight density of water σ: surface tension (σ=0.0756 N m⁻¹ at 0°C) The pressure in the suspended water P_m is

$$P_m = -\gamma \ h_{cr} = -\frac{2 \ \sigma \cos(\theta_c)}{r}$$

Thus the pressure difference across a meniscus, like the height of capillary rise, is inversely proportional to the radius of a capillary opening.

Hydraulic Properties of Soils

Infiltration and redistribution are unsaturated flows in porous media (soils) that are described by

Darcy's law
$$V_x = \frac{Q}{A_x} = -K_h \frac{d(z + p/\gamma_w)}{dx} = -K_h \frac{dh}{dx}$$

Q: volumetric flow rate [L³/T] e.g. [m³/s]]

 V_x : specific discharge in x-direction [L/T] e.g. [m³/m²/s]] z: water table elevation above arbitrary datum [L] e.g. [m] (-> gravitational head)

 γ_w : weight density of water $(\gamma_w = \frac{M}{V}g = \rho_w g)$ e.g. [N/m³]

p: water pressure [F/L²] e.g. [N/m²]

(i.e. gage pressure: difference between actual pressure and atmospheric pressure) K_h: **hydraulic conductivity** [L/T e.g. [m/s]]

h: total hydraulic head [L] ($h = z + \frac{p}{\gamma_w}$)

Pressure head	$\Psi = \frac{p}{m}$ in [L] e.g. [m]	
	γ_w	

Darcy's law
$$V_x = -K_h \frac{d(z + \Psi(\theta))}{dx}$$

It is conventional to measure pressure relative to atmospheric pressure:

p > 0 and $\psi > 0$: saturated flows p < 0 and $\psi < 0$: unsaturated flows

Negative pressure is called tension or suction.

 Ψ is called **tension head** when p<0. The water table is the surface at which p=0.



Infiltration: focus is on flows in vertical (z) direction.

$$q_{z} = -K_{h}(\theta) \frac{d(z + \Psi(\theta))}{dz} = -K_{h}(\theta) \left[1 + \frac{d \Psi(\theta)}{dz}\right]$$

The relations between pressure and water content $[\psi(\theta)]$ and between hydraulic conductivity $[K_h((\theta)]$ are crucial determinants of unsaturated flow in soils.
Hysteresis

In real soils, the value of tension at given water content is not unique, but depends on the soil's history of wetting and drying. While this hysteresis can have significant influence on soil-moisture movement, it is difficult to model mathematically and is therefore not commonly incorporated in hydrologic models.



Figure: Hysteresis in the $\Psi(\theta) - \theta$ relation for Rubicon sandy loam. The paths with arrows trace the relation as the soil undergoes successive cycles of wetting (arrows pointing to right) and drying (arrows pointing to left).

Analytic approximations of soil hydraulic properties

Clapp and Hornberger, 1978

$$|\psi(S)| = |\Psi s| S^{-b}$$
, or $|\psi(\theta)| = |\Psi s| \phi^{b} \theta^{-b}$
 $K_{h}(S) = K_{h,sat} S^{c}$ or $K_{h}(\theta) = K_{h,sat} \phi^{-c} \theta^{c}$
 $c \approx 2b + 3$

 \Leftrightarrow Cosby et al, 1978

$$K_{h}(\theta) = K_{h,sat} \left(\frac{\theta}{\theta_{sat}}\right)^{2b+3}$$
$$\psi(\theta) = \Psi_{sat} \left(\frac{\theta}{\theta_{sat}}\right)^{-b}$$

Van Genuchten, 1980:

$$K_{h}(\theta) = K_{h,sat} \sqrt{\frac{\theta - \theta_{res}}{\phi - \theta_{res}}} \left[1 - \left(1 - \left(\frac{\theta - \theta_{res}}{\phi - \theta_{res}} \right)^{1/m} \right)^{m} \right]^{2}$$

Brooks and Corey, 1966

$$K_{h}(\theta) = K_{h,sat} \left(\frac{\theta - \theta_{res}}{\phi - \theta_{res}}\right)^{n}$$

Baver, Gardner, and Gardner, 1972

$$K_h(\psi) = \frac{a}{\psi}$$

Childs and Collis-George 1950

$$K_h(\psi) = \frac{K_{h,sat}}{b + \psi^n}$$



Water conditions in natural soils

Field capacity θ_{tc} : water that can be held against gravity

Plants cannot exert suctions stronger than -15,000 cm. when the water content is reduced to the point corresponding to that value on the moisture characteristic curve, transpiration ceases and plants wilt. This water content is called **Permanent wilting point** θ_{wa} :

Available water content for plant use: $\theta_a \equiv \theta_{fc} - \theta_{wp}$



Figure: Drainage of two soils (Schematic); the arrows indicate the values of field capacity



Figure: Soil-water status as a function of pressure (tension). Natrual soils do not have tensions exceeding about -31,000 cm

Hydrologic Horizons



Figure: Designation of hydrologic soil-profile horizons.

Ground water zone (sometimes called *phreatic zone*) is saturated and the pressure is positive. If there is no groundwater flow, the pressure will be hydrostatic – that is, increasingly linearly with depth according to

$$p(z) = \gamma_w(z - z_0)$$

with

p: gage pressure

 γ_w : weight density of water

z: measured distance vertically downward

 z_0 : value of z at the water table

Thus the water table is at atmospheric pressure; it is the level at which water would stand in a well

Tension-saturated zone (Capillary Fringe) or *vadose zone*: entire zone of negative water pressures above the water table. The lowest portion of this zone is a region that is saturated or nearly saturated as a result of capillary rise. The pore spaces in a porous medium act like a capillary tube and surface tension forces draw the water into the spaces above the water table.

Water in the tension-saturated zone is under tension; pressure remains hydrostatic and head is given by

 $\Psi = z - z_0$

with $z < z_0$ and $\Psi < 0$.

The pressure head at the top of this zone is the air-entry tension Ψ_{ae} , since at greater tensions the pores are partially filled with air. As noted, Ψ_{ae} , is equal to the height of capillary rise in the soil.

The height of the tension-saturated zone may range from negligible in coarse sands to several meters in clay soils.

Intermediate Zone Water enters the intermediate zone largely by as percolation from above and leaves by gravity drainage. Thus, water content in this zone may rise above field capacity when water from rain or snow passes through the root zone, after which it gradually returns to field capacity. Tensions in this zone are usually stronger than Ψ_{ae} and depend on soil texture and water content.

The intermediate zone may occupy much of the soil profile and, in arid regions, extend over many tens of meters. In other situations it may be absent at least seasonally.

Root zone The root zone (also called soil moisture zone) is the layer from which plant roots extract water during transpiration; its upper boundary is the soil surface, while its lower boundary is indefinite and irregular. Water enters by infiltration and leaves via transpiration and gravity drainage. The water content is usually above the permanent wilting point. There are many places in which the root zone extends to the water table.

Hydraulic conductivity k [ms⁻¹]:

(Cosby et al., 1978)



$$k = k_{sat} \left(\frac{\theta}{\theta_{sat}}\right)^{2b+3}$$

 θ_{sat} : Volumetric water content at saturation

k_{sat}: Saturated hydraulic conductivity

b: slope Parameter

Mathematica exercise:



Soil water tension $\Psi(\theta)$ (Cosby et al., 1978)

$$\psi = \psi_{sat} \left(\frac{\theta_{sat}}{\theta}\right)^b$$

ignoring hysteresis!

Mathematica exercise:



Parameterizations

Soil - related parameters in the SVAT-model

- volumetric water content at saturation (θ_{sat}) (respectively porosity ϕ)
- saturation soil suction (Ψ_{sat})
- hydraulic conductivity at saturation (K_{sat})
- field capacity (θ_{ref}) , respectively (θ_{fc})
- wilting point (θ_w)
- b is an exponent in the function that relates soil water potential and water content.

Soil type	$\theta_{sat}(m^3m^{-3})$	$\Psi_{s}(m)$	$K_s(ms^{-1})$	b	$\Theta_{ref}(m^3m^{-3})$	$\Theta_w(m^3m^{-3})$
Sand	0.339	0.069	1.07*E-6	2.79	0.236	0.01
Loamy sand	0.421	0.036	1.41*E-5	4.26	0.283	0.028
Sandy loam	0.434	0.141	5.23*E-6	4.74	0.312	0.047
Silt loam	0.476	0.759	2.81*E-6	5.33	0.36	0.084
Silt loam	0.476	0.759	2.81*E-6	5.33	0.36	0.084
Loamy sand	0.439	0.355	3.38*E-6	5.25	0.329	0.066
Sandy clay loam	0.404	0.135	4.45*E-6	6.66	0.314	0.067
Silt clay loam	0.464	0.617	2.04*E-6	8.72	0.387	0.12
Clay loam	0.465	0.263	2.45*E-6	8.17	0.382	0.103
Sandy clay loam	0.406	0.098	7.22*E-6	10.73	0.338	0.1
Silty clay	0.468	0.324	1.34*E-6	10.39	0.404	0.126
Clay	0.468	0.468	9.74*E-7	11.55	0.412	0.138
Organic material	0.439	0.355	3.38*E-6	5.25	0.329	0.06
Water						
Bedrock	0.25	7.59	9.74*E-8	11.55	0.233	0.094
Other (land - ice)	0.421	0.036	1.34*E-6	11.55	0.283	0.028

Energy and Water Fluxes in Soils

Water content profiles



Figure: Soil moisture profiles in a light clay with ϕ =0.5 at various times during steady infiltration with no ponding. The number on the curve is the time since infiltration began in hours.

Water Fluxes: Partial Differential Equation for Soil Moisture

Derivation of Richard's-Equation



Figure: Definition sketch for terms used in deriving the Richard's equation

I. Darcy
$$q \equiv V_{z'} = -K_h \frac{d(z + \Psi(\theta))}{dz'}$$

II. Mass balance
$$-\frac{\partial V_{z'}}{\partial z'} = \frac{\partial \theta}{\partial t}$$

I and II together yield
$$\frac{\partial}{\partial z'} \left(K_h(\theta) \frac{\partial \Psi(\theta)}{\partial z'} \right) - \frac{\partial K_h(\theta)}{\partial z'} = \frac{\partial \theta}{\partial t}$$

Soil Water Diffusivity

$$\frac{\partial}{\partial z'} \left(K_h(\theta) \frac{\partial \Psi(\theta)}{\partial \theta} \frac{\partial \theta}{\partial z'} \right) - \frac{\partial K_h(\theta)}{\partial z'} = \frac{\partial \theta}{\partial t}$$
$$\Leftrightarrow \qquad \frac{\partial}{\partial z'} \left(D \frac{\partial \theta}{\partial z'} \right) - \frac{\partial K_h(\theta)}{\partial z'} = \frac{\partial \theta}{\partial t}$$

with $D = K_h(\theta) \frac{\partial \Psi(\theta)}{\partial \theta}$ soil water diffusivity [L²/T] e.g. [m²/s]

Mathematica exercise:

$$D = Abs \left[-\frac{b \cdot k_{sat} \cdot \left(\frac{\theta}{\theta_{sat}}\right)^{2+b} \cdot \psi_{sat}}{\theta_{sat}} \right]$$

with

 $\Psi_{\rm sat}$: saturated matrix potential (suction head)



Excel-Exercise: Computation of soil moisture fluxes (Deep Dean, Sussex, England) Average flux q_{12} between measurement points 1 and 2

$$q_{12} = -K\frac{h_1 - h_2}{z_1 - z_2}$$

Observations:

Week	Total head h1 at 0.8m (cm)	Total head h2 at 1.8m (cm)
1	-145	-230
2	-165	-235
3	-130	-240
4	-140	-240
5	-125	-240
6	-105	-230
7	-135	-215
8	-150	-230
ç	-165	-240
10	-190	-245
11	-220	-255
12	-230	-265
13	-255	-275
14	-280	-285



Assuming a=3 in *Baver et al. (1972)* parameterisation of $K(\Psi)$

Mathematica Exercise: Numerical Solution of Richards Equation

Discretisation into 4 layers with thicknesses 0.1, 0.3, 0.6, 1m.

The layer – integrated form the ith soil layer is:

$$d_{z_{1}} \frac{\partial \theta_{1}}{\partial t} = -D\left(\frac{\partial \theta}{\partial z}\right)_{z_{1}} - K_{z_{1}}$$

$$d_{z_{2}} \frac{\partial \theta_{2}}{\partial t} = D\left(\frac{\partial \theta}{\partial z}\right)_{z_{1}} - D\left(\frac{\partial \theta}{\partial z}\right)_{z_{2}} + K_{z_{1}} - K_{z_{2}}$$

$$d_{z_{3}} \frac{\partial \theta_{3}}{\partial t} = D\left(\frac{\partial \theta}{\partial z}\right)_{z_{3}} - D\left(\frac{\partial \theta}{\partial z}\right)_{z_{3}} + K_{z_{2}} - K_{z_{3}}$$

$$d_{z_{4}} \frac{\partial \theta_{4}}{\partial t} = D\left(\frac{\partial \theta}{\partial z}\right)_{z_{3}} + K_{z_{3}} - K_{z_{4}}$$

d_{zi}: thickness of layer i [m]

Energy Fluxes: Partial Differential Equation of Ground Heat Flux

Similarly to derivation of Richard's equation: Mass balance & gradient based heat flux yields PDE for ground heat flux...:



Figure: Schematic of heat transfer in a vertical column of soil below a flat, horizontal surface

Through solid media and still fluids, heat is transferred primarily through conduction, which involves molecular exchanges. The rate of heat transfer (or heat flux) in a given direction is proportional to the temperature gradient:

$$I. \ G = -K \frac{\partial T}{\partial z}$$

with G: ground heat flux [W m⁻²]

II.
$$\frac{\partial}{\partial t}(CT) = -\frac{\partial G}{\partial z}$$

(law of conservation of energy)

I. and II yield

$$C(\theta)\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[K(\theta)\frac{\partial T}{\partial z} \right]$$

C: volumetric heat capacity [J/m³/K]

K: thermal conductivity [W/m/K]

T: soil temperature [K]

 θ : soil moisture [.] (fraction of unit soil volume occupied by water)

assuming that C is not time dependent and that C and K depend on θ .

Material	Condition	Mass density ρ (kg m ⁻³ × 10 ³)	Specific heat c (J kg ⁻¹ K ⁻¹ × 10 ³)	Heat capacity C $(J m^{-3} K^{-1} \times 10^6)$	Thermal conductivity k (W m ⁻¹ K ⁻¹)	Thermal diffusivity α_1 (m ² s ⁻¹ × 10 ⁻⁶
Air	20°C, Still	0.0012	1.01	0.0012	0.025	20.5
Water	20°C, Still	1.00	4.18	4.18	0.57	0.14
lce	0°C, Pure	0.92	2.10	1.93	2.24	1.16
Snow	Fresh	0.10	2.09	0.21	0.08	0.38
Snow	Old	0.48	2.09	0.84	0.42	0.05
Sandy soil	Fresh	1.60	0.80	1.28	0.30	0.24
(40% pore space)	Saturated	2.00	1.48	2.96	2.20	0.74
Clay soil	Dry	1.60	0.89	1.42	0.25	0.18
(40% pore space)	Saturated	2.00	1.55	3.10	1.58	0.51
Peat soil	Dry	0.30	1.92	0.58	0.06	0.10
(80% pore space)	Saturated	1.10	3.65	4.02	0.50	0.12
Rock	Solid	2.70	0.75	2.02	2.90	1.43

Table: Molecular thermal properties of natural materials

Evapotranspiration

Classification of evapotranspiration processes

The general energy balance for an evapotranspiring body during a time can be written as

 $LE = K + L - G - H + A_w - \frac{\Delta Q}{\Delta t}$

LE: [E L⁻² T⁻¹] z.B. Wm⁻²

LE: evaporation

K: net shortwave radiation input

L: net longwave radiation input

G: net output via conduction to the ground

H: net output of sensible heat exchange with the atmosphere

A_w: net input associated with inflows and outflows o water (water advected energy)

 ΔQ : Change in amount of heat stored in the body per unit area between beginning and end of Δt

Evapotranspiration Type	Type of Surface	Availability of Water	Stored Energy Use	Water- Advected Energy Use	Air- Advected Energy Use
Free-water evaporation	Open water	Freely available to air	Negligible	Negligible	Negligible
Lake evaporation	Open water	Freely available to air	May be involved	May be involved	May be involved
Transpiration	Leaf or leaf canopy	May be limited to air; limited to leaf	Negligible	Negligible	May be involved
Interception loss	Leaf or leaf canopy	Freely available to air	Negligible	Negligible	May be involved
Potential evapotranspiration	Land area ^a	Freely available to leaves; limited to air	Negligible	Negligible	Negligible
Actual evapotranspiration	Land area ^a	May be limited to leaves; limited to air	Negligible	Negligible	May be involved

^a May include surface-water bodies and areas of bare soil.

Clausius-Clapeyron Equation

Condensation/evaporation and liquid-water (and also ice-particle) formation is dependent on the saturation vapour pressure. The saturation vapour pressure is the partial pressure of gas at a specific temperature when the gas is in equilibrium with a liquid or solid surface. In a gross sense, it is the maximum amount of vapour the air can hold without the vapour condensing as a liquid or depositing as ice on a surface.

The temperature variation of the saturation vapour pressure of water over a liquid surface $p_{v,s}$ [mb] is approximated with the Clausius-Clapeyron equation

$$\frac{dp_{v,s}}{dT} = \frac{\rho_{v,s}}{T} \lambda_e = \frac{\lambda_e p_{v,s}}{R_v T^2}$$

 L_e : latent heat of evaporation [Jkg-1], $\rho_{v,s}$ [kg m⁻³]

$$\rightarrow \frac{dp_{v,s}}{p_{v,s}} = \frac{1}{R_v} \left(\frac{A_h}{T^2} - \frac{B_h}{T}\right) dT$$

 $T = T_0 = 273.15 \ p_{v.s.0} = 6.112 \ mb$

$$p_{v,s} = 6.112 \exp\left[6816\left(\frac{1}{273.15} - \frac{1}{T}\right) + 5.1309 \ln\left(\frac{273.15}{T}\right)\right]$$

with T[K], $p_{v,s}[mb]$.



Figure: Saturation vapour pressure $p_{v,s}$ [*mb*] over liquid water

 p_v is often denoted as *e* and $p_{v,s}$ is denoted as e_{sat} .

Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere

Example T=253.15K (-20°C), p_{v,s} = 1.26mbar T=298.15K (25°C), p_{v,s} = 31.60mbar

Climate change:

T=288.15K (15°C), $p_{v,s}$ =17.03mbar T=289.15K (16°C), $p_{v,s}$ =18.16mbar Δ T=1°C -> Relative change of precipitable water by 5.5% -> impact on precipitation (e.g. intensity)



Figure: a) *condensation* occurs when the partial pressure of water vapour exceeds its saturation vapour pressure over liquid water, **b)** *evaporation* occurs when the saturation vapour pressure exceeds the partial pressure of water vapour (schematics not to scale).

Physics of Evaporation



Figure: Schematic diagram of flux of water molecules over a water surface. The vapor pressure at the surface is $e_s(T_s)$; the vapor pressure of the overlying air is less than or equal to $e_s(T_a)$. The rate of evaporation is proportional to $e_{sat}(T_s) - e_a$

Dry air with a temperature of T_a lies above horizontal water surface with temperature T_s . The molecules at the surface are attracted to those in the body of the liquid by hydrogen bonds, but some of the surface molecules have sufficient energy to sever bonds and enter the air. The number of molecules with this "escape energy" increases as T_s increases.

At equilibrium rate of escape and reentry are equal and the vapor pressure in the molecular layer immediately above the temperature is the saturation vapor pressure $e_{sat}(T_s)$.

The **rate of evaporation** is the rate at which molecules move from the saturated surface layer into the air above and that rate is proportional to the difference between vapor pressure of the surface layer and the vapor pressure of the overlying air.

 $E \propto (e_s(T_s) - e_a)$

Note:

E rate of evaporation/condensation [Mass/Time] i.e. [kg/s]

 $\lambda E = \lambda_v \cdot E$: rate of latent heat transfer [Energy/Time] i.e.[J/s]

 λ_{v} : latent heat of evaporation [Energy/Mass], i.e. [J/kg] $\lambda_{v} \approx 2.501 \cdot 10^{6} - 2370 \cdot T_{c}$

If *E* is expressed in [Length³/Length²/Time] i.e. [m³/m²/s], [m/s]

 $\lambda E = \rho \cdot \lambda_v \cdot E$ [Energy/Length²/Time], i.e. [J/m²/s], [W/m²]

Evaporation is a diffusive process

$$E = K_E v_a (e_s - e_a)$$

E: evaporation rate [L T⁻¹]

 e_s , e_a vapour pressure of evaporating surface and air respectively [M L⁻¹ T⁻²] K_E: [L T² M⁻¹] exchange coefficient reflecting the efficiency of vertical transport of water vapour by turbulent eddies of wind

$$K_{E} \equiv \frac{D_{WV}}{D_{M}} \frac{0.622\rho_{a}}{p\rho_{w}} \frac{k^{2}}{\left[\ln\left(\frac{z_{m}-z_{d}}{z_{0}}\right)\right]^{2}}$$

 D_{WV} , D_M : diffusivities of water vapour and momentum [L² T⁻¹] ρ_a : air density [M L⁻³] p: atmospheric pressure [M T⁻² L⁻¹] k=0.4: von Kárman constant z_m : height at which air vapour pressure and wind speed are measured [L] (usually $z_m = 2m$) z_d : zero plane displacement [L]

z₀: roughness height [L]

 $\begin{array}{l} z_d \approx 0.7 \ z_{veg} \\ z_0 \approx 0.1 \ z_{veg} \end{array}$

Vapor pressure relations

$$e_s = e_{sat}(T_s)$$

 $e_{sat}(T) = 6.11 \exp\left(\frac{17.3T}{T + 237.3}\right)$

with T in °C and e in mbar.

Vapour pressure in the air depends on relative humidity, RH:

 $e_a = RH \ e_{sat}(T_a)$

Latent heat exchange

$$LE = \rho_{w}\lambda_{v}E = \rho_{w}\lambda_{v}K_{E}v_{a}(e_{s} - e_{a})$$

LE: rate of latent heat transfer [E $L^{-2} T^{-1}$] λ_{v} : latent heat of vaporization

Physics of sensible heat exchange

The upward rate of sensible heat exchange by turbulent transfer, H, is given by

$$H = K_H v_a (T_s - T_a)$$

H: sensible heat transfer [E $L^{-2} T^{-1}$]

T_s, T_a: Temperature of surface and air respectively [K] or [°C]

 K_{H} : [L T² M⁻¹] exchange coefficient

$$K_{H} \equiv \frac{D_{H}}{D_{M}} c_{a} \rho_{a} \frac{k^{2}}{\left[\ln \left(\frac{z_{m} - z_{d}}{z_{0}} \right) \right]^{2}}$$

 D_H : diffusivity of heat c_a : heat capacity of air (c_a =0.24 cal g⁻¹ °C⁻¹)

The ratio of diffusivities D_H/D_M depends on stability conditions in the air which are determined by vertical gradients of wind speed and temperature.

$$D_{H} \approx D_{WV}$$

The Bowen ratio and the psychrometric constant

$$B = \frac{H}{LE}$$

$$B = \frac{c_a p(T_s - T_a)}{0.622\lambda_v(e_s - e_a)}$$

Thus the Bowen ratio depends on the ratio of surface-air-temperature difference to surface-air vapour-pressure difference, multiplied by a factor γ

$$\gamma = \frac{c_a p}{0.622\lambda_v}$$

: psychrometric constant.

$$\Rightarrow K_{H} = \gamma \rho_{W} \lambda_{V} K_{E}$$

Derivation of the Penman Combination Equation

 $LE = \rho_w \lambda_v E = \rho_w \lambda_v K_E v_a (e_s - e_a)$

LE: [E L⁻² T⁻¹] z.B. Wm⁻²

$$LE = K + L - G - H + A_w - \frac{\Delta Q}{\Delta t}$$

Approximation:

$$E \approx \frac{K + L - H}{\rho_w \lambda_v}$$

Sensible heat transfer flux: $H = K_h v_a (T_s - T_a)$

Slope of saturation-vapor versus temperature curve at air temperature

$$s(T_a) \approx \frac{e_{sat}(T_s) - e_{sat}(T_a)}{T_s - T_a}$$
$$T_s - T_a \approx \frac{e_{sat}(T_s) - e_{sat}(T_a)}{s(T_a)}$$

 \Rightarrow

 \Rightarrow

$$H = \frac{K_h v_a}{s(T_a)} \left[e_{sat}(T_s) - e_{sat}(T_a) \right]$$
$$= \frac{K_h v_a}{s(T_a)} \left[e_{sat}(T_s) - e_a \right] - \frac{K_h v_a}{s(T_a)} \left[e_{sat}(T_a) - e_a \right]$$
$$e_{sat}(T_s) - e_a = \frac{E}{K_E v_a}$$

$$H = \frac{K_h v_a}{s(T_a)} \frac{E}{K_E v_a} - \frac{K_h v_a}{s(T_a)} \left[e_{sat}(T_a) - e_a \right]$$

$$E = \frac{K + L + \frac{K_h v_a}{s(T_a)} \left[e_{sat}(T_a) - e_a \right]}{\rho_w \lambda_v + K_H / K_E s(T_a)}$$

$$E = \frac{s(T_a)[K+L] + \gamma K_E \rho_w \lambda_v v_a e_{sat}(T_a)[1-RH]}{\rho_w \lambda_v [s(T_a) + \gamma]}$$

Penman Combination equation: mass transfer and energy balance approach combined such that no surface temperature data T_s , e_s are required!

Assumptions revisited:

- no ground heat flux
- no water advected energy
- no change in heat storage*

• uses approximation
$$s(T_a) \approx \frac{e_{sat}(T_s) - e_{sat}(T_a)}{T_s - T_a}$$

*If it is significant, ground heat conduction term can be included by replacing K+L by K+L-G.

Essence of Penman equation can be represented as

$F \propto$	$s(T_a) \times net \ radiation + \gamma \times "mass \ transfer"$	
$\Gamma \propto$	$s(T_a) + \gamma$	

Exercise: Evaporation from Lake Hefner, 12.7.1951

			Daily Averag	e		
Τ _a (°C)	<i>T</i> s (°C)	Wa	P (mb)	υ _a (cm s ⁻¹)	T _{span} (°C)	υ _{pan} (cm s ⁻¹)
27.2	26.9	0.69	973	581	27.5	279
			Daily Total		No lo e vij za	$a = 0.127 \mathrm{e}$
K _{in} (cal cm ⁻²	² day ⁻¹)	Albedo	L _{in} (cal cm ⁻² day ⁻¹)	Water-J Evapor) (cm)	Budget ation	Class-A Pan Evaporation (cm)
73	1	0.052	821	0.5	58	1.24

From U.S. Geological Survey (1954).

Case study Lake Hefner 12.7.1951: calculate a) net shortwave radiation, b) net longwave radiation, c) latent heat flux (neglecting all other types of heat fluxes). What is the corresponding evaporation rate in [mm/day]? Note: Latent heat of evaporation λ [kJ/kg] can be approximated by $\lambda = 2500 - 2.36 T_c$ (T_c: temperature in °C).

Physics of Transpiration

Transpiration is the evaporation of water from the vascular system of plants into the atmosphere. The entire process involves *absorption* of soil water by plant roots, *translocation* in liquid form through the vascular system of the roots, stem, and branches to the leaves; and through the vascular system of the leaf to the walls of tiny *stomatal cavities*, where evaporation takes place. The water vapour in these cavities then moves into the ambient air through openings in the leaf surface called *stomata*.



Figure: Diagram of the transpiration process and enlarged views of plant celluar structure where absorption, translocation and transpiration occur.

Plants live by absorbing CO_2 from the air to make carbohydrates, and that gas can enter the plant only when dissolved in water. The essential function of the stomatal cavities is to provide a place where CO_2 dissolution can occur and enter plant tissue; the evaporation of water is an unavoidable concomitant of that process.

Air in stomatal cavities is saturated at the temperature of the leaf, and water moves from the cavities into the air due to vapour-pressure difference, just as in open water evaporation. The major difference between transpiration and open-water evaporation is that plants can exert some physiological control over the size of the stomatal openings, and hence the ease of vapour movement, by the action of *guard cells*.



Figure: Photomicrograph of leaf surface showing one of the stomata and the crescent-shaped guard cells that regulate its opening.

Major factors affecting the opening and closing of guard cells are

- 1) light (most plants open stomata during the day and close them at night)
- 2) humidity (stomatal openings tend to decrease as humidity decreases below its saturation value)
- 3) water content of the leaf cells lif day-time water contents become too low, stomata tend to close)

Transpiration is a physical, not a metabolic process: water in the transpiration stream is pulled through the plant by potential energy gradients that originate with the movement of water vapour into the air through the stomata in response to a vapourpressure difference. When vapour exits through the stomata, water evaporates from the walls of the stomatal cavity to replace the loss; this loss of liquid water causes a potential-energy decrease that induces the movement of replacement water up through the vascular system: this movement ultimately produces a water-content gradient between the root and the soil; and this gradient induces movement of soil water into the root. Absorption at the root surface decreases soil water content in the adjacent soil, inducing some flow of water toward the root following Darcy's law.

The great cohesive strength of water due to its intermolecular hydrogen bonds maintains the integrity of the transpiration stream to heights of the tallest trees.

Modelling transpiration

Evaporation- revisited:

$$E = K_{at} \left[\frac{D_{WV} v_{a} k^{2}}{D_{M} \left[\ln \left[\frac{z_{m} - z_{d}}{z_{0}} \right] \right]^{2}} \right] \left[e_{s} - e_{a} \right]$$

with "atmospheric constant" $K_{at} = \frac{0.622\rho_a}{p\rho_w}$

E	=	K _{at}	×	C_{at}	×	[$e_s - e_a$]
evaporation		atmospheric	×	atmosph	eric	×	driving
rate		constant		conducta	ince		gradient

with
$$C_{at} = \frac{v_a k^2}{[\ln[\frac{z_m - z_d}{z_0}]]^2}$$
 [L T⁻¹]

Since evaporation from an open water surface is a "one-step" process in which water molecules pass directly from the liquid surface into the atmosphere, it can be conceptually represented by the electric-circuit analogy. In this analogy a current (water vapour) moves in response to a voltage (vapour-pressure difference) across a resistance (inverse of the atmospheric conductivity)



Figure: Relation between atmospheric conductance C_{at} and wind speed v_a for vegetations of various heights z_{veg} .

Leaf conductance

Is determined by the number of stomata per unit area and the size of the stomatal opening $(10,000-100,000 \ /cm^2)$



Figure: Conceptualization of (a) open water evaporation and (b) transpiration in terms of atmospheric resistance $(1/C_{at})$ and leaf resistance $(1/C_{leaf})$. Δe_v is the driving vapour-pressure difference between the evaporating surface and the atmosphere.

Plants control the size of their stomatal openings and hence leaf conductance by the response of the guard cells to

- 1) light intensity
- 2) ambient CO₂ concentration
- 3) leaf-air vapour-pressure difference
- 4) leaf temperature
- 5) leaf water content

 $C_{leaf} = C_{leaf, \max} \overline{G(K_{in}) G(\Delta \rho_{v}) G(T_{a}) G(\Delta \theta)}$

with

K_{in}: incident shortwave radiation

 $\Delta\rho_{\nu}$: humidity deficit (difference between saturated and actual absolute humidity of the air)

Ta: air temperature

 $\Delta \theta$: soil moisture deficit (difference between field capacity and actual water content of root zone)

Hardwoods		Conifers		
Species	C [*] _{leaf}	Species ^a	C [*] _{leaf}	
Grav birch	0.37	Douglas fir (c)	0.83	
Big-tooth aspen	0.33	Sitka spruce (c)	0.71	
White oak	0.33	Sitka spruce (1)	0.45	
Yellow birch	0.31	Sitka spruce (2)	0.30	
Black oak	0.30	Grand fir (c)	0.42	
American elm	0.29	Red pine (c)	0.32	
Ouaking aspen	0.29	Red pine (1)	0.23	
Black cherry	0.29	Red pine (2)	0.12	
Red maple	0.29	Red pine (3)	0.11	
American beech	0.25	Red pine (4)	0.091	
White ash	0.24	Western hemlock (c)	0.22	
Sugar maple	0.22	Ponderosa pine (c)	0.11	

^a Symbols in parentheses indicate leaf age: c is current year; 1–4 are previous years.

Maximum leaf conductances C^*_{leaf} (cm s-1) for forest tree leaves.

Factor Controlling Stomatal Opening	Quantity Representing Controlling Factor in Modet	Functional Relation
Light	Incident solar radiation, K_{in} (cal cm ⁻² s ⁻¹)	$G(K_{\rm in}) = \frac{46225K_{\rm in}}{41870K_{\rm in} + 104.4},$ $0 \le K_{\rm in} \le 0.0239 \text{ cal cm}^{-2} \text{ s}^{-1}.$
CO ₂ concentration	(not included)	(none)
Vapor-pressure deficit	Absolute-humidity deficit, $\Delta \rho_v$ (g m ⁻³)	$\begin{aligned} G(\Delta \rho_{\rm v}) &= 1 - 0.0666 \; \Delta \rho {\rm v}, \\ 0 &\leq \Delta \rho_{\rm v} \leq 11.52 \; {\rm g \; m^{-3}}; \\ G(\Delta \rho_{\rm v}) &= 0.233, \\ 11.52 \; {\rm g \; m^{-3}} &\leq \Delta \rho_{\rm v}. \end{aligned}$
Leaf temperature	Air temperature, T_a (°C).	$G(T_{\rm a}) = \frac{T_{\rm a}(40 - T_{\rm a})^{1.18}}{691},$ $0 \le T_{\rm a} \le 40 ^{\circ}\text{C}.$
Leaf water content	Soil-moisture deficit, $\Delta \theta$ (cm)	$G(\Delta \theta) = 1 - 0.00119 \exp(0.81 \ \Delta \theta),$ $0 \le \Delta \theta \le 8.4 \text{ cm}.$

Stewardt's (1988) model of leaf conductance as a function of environmental factors

Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere





Canopy conductance

 $C_{can} = LAI C_{leaf}$

with leaf area index LAI

$$LAI = \frac{total \ area \ of \ transpiring \ surface \ above \ ground \ area \ A}{A}$$

Transpirational Leaf-Area Indices, *L*_t, for Various Plant Communities.

Community	Leaf-Area Index
Desert	<1
Tundra	1
Grassland prairie	1
Savannah	1-3
Deciduous hardwood forest ^a	3-7
Tropical forests	>9
Temperate conifer forests	10-47

Information from Woodward (1987), Gholtz (1982), and other sources.

^a Maximum seasonal values for mature forests.

The Peman Monteith Model

Penman open water evaporation rewritten in terms of C_{at} and γ :

$$E = \frac{s(T_a)[K+L] + \rho_a c_a C_{at} e_{sat}(T_a)[1-RH]}{\rho_w \lambda_v [s(T_a) + \gamma]}$$

Monteith (1965) showed how the Penman equation can be modified to represent the evapotranspiration rate, ET, from a vegetated surface by incorporating canopy conductance:

$$ET = \frac{s(T_a)[K+L] + \rho_a c_a C_{at} e_{sat}(T_a)[1-RH]}{\rho_w \lambda_v [s(T_a) + \gamma [1 + C_{at} / C_{can}]]}$$

: Penman-Monteith equation

Note that for $C_{can} \rightarrow \infty$ Penman-Monteith reduces to Penman.

Potential evapotranspiration

Potential evapotranspiration (PET) is the rate at which evapotranspiration would occur from large area completely and uniformly covered with growing vegetation which has access to an unlimited supply of water and without advection or heat-storage effects.

Estimating actual evapotranspiration by soil moisture functions

The most widely used approach for estimating actual ET makes use of meteorological data to estimate PET and then computes actual ET as

$$ET = f(\theta) PET$$

where

 θ : water content of the root zone soil f(0): is based on relative water content 0.

 $f(\theta)$: is based on relative water content θ_{rel} as


General forms of relations between $f(\theta) = ET / PET$ and soil water content θ used to estimate ET. Different studies have used different functions to express the wetness of the soils. When the soil-water content variable is less than the critical value indicated by the vertical dashed line, ET is less than PET and plants are considered under water stress.

E.g. Steward (1988):

$$f(\theta) = \frac{s(T_a) + \gamma \left\{ 1 + \frac{C_{at}}{C_{can}[G(\Delta \theta) = 1]]} \right\}}{s(T_a) + \gamma \left\{ 1 + \frac{C_{at}}{C_{can}[G(\Delta \theta)]]} \right\}}$$

Physics of Sensible and Latent Heat Fluxes Revisited: Physics of Turbulent Transfer

Diffusion

Diffusion is the process by which constituents of a fluid (such as momentum, heat content or dissolved constituent) are transferred from one position another within the fluid. Such transfers occur whenever there are differences in concentrations of the constituent in different parts of the fluid.

The rate of transfer of a constituent X in the direction z is directly proportional to the gradient of X in z-direction:

$$F_Z(X) = -D_x \frac{dC(X)}{dz}$$

 $F_Z(X)$: rate of transfer of X in direction z per unit area per unit time (flux of X)

C(X) concentration of X

D_x: diffusivity [Length²/Time]



Figure: Conceptual diagram of the general diffusion process. Concentration of dots indicates concentration of quantity X. More of the property X moves from z_1 to z_2 in a given time when the diffusivity D_x is higher.

Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere

Energy can be transferred between the ground surface and the air in the form of latent heat whenever there is a difference in vapor pressure.

A second mode of nonradiant heat transport occurs in the form of **sensible heat** that is heat energy that can be directly sensed via measurement of temperature.

Sensible heat transfer occurs whenever there is a temperature difference between surface and air.

$$H \propto (T_s - T_a)$$

H [Energy/Time/Length²]

Momentum transfer

Mechanisms of diffusion in the lowest layer of the atmosphere: when wind blows across a surface, the surface produces frictional drag and turbulence. The bulk vertical movement of air in turbulent eddies carries latent (in form of water vapor) and sensible heat vertically in the directions dictated by equations above.



Figure: Conceptual diagram of the process of momentum transfer by turbulent diffusion. Friction caused by surface roughness reduces average velocities (Straight arrows) near the surface and produces turbulent eddies (circular eddies), resulting in a net downward transfer of momentum. The vertical component of the eddies moves heat and water vapor upward or downward depending on the directions of temperature and vapor-pressure gradients.

Heat fluxes: quantitatively expressed by vertical transfer of momentum

$$\vec{p} = m \cdot \vec{v}$$

(Momentum p = mass times velocity, [kg m s^{-1}])

Concentration of momentum (momentum per unit volume) equals mass density times velocity ($\rho_a v_a$)

Thus, for momentum,

$$F_Z(M) = -D_M \frac{d(\rho_a v_a)}{dz} \approx -\rho_a D_M \frac{dv_a}{dz}$$

holds.

M: momentum

D_M: diffusivity of momentum

$$\frac{dv_a}{dz} > 0 \Longrightarrow F_Z(M) < 0$$

Momentum is being transferred downward from where velocities are higher to where they are lower. Turbulent eddies are the mechanism responsible for that.

F [Force /area]: Represents the horizontal **shear stress** due to differences of wind velocity at adjacent levels.

Because momentum is conserved, shear stress F_Z(M) is conserved

$$F_Z(M) = -\rho_a u_*^2$$

which leads to

$$-\rho_a D_M \frac{dv_a}{dz} = -\rho_a u_*^2$$
$$\Leftrightarrow \quad D_M = \frac{u_*^2}{dv_a / dz}$$

Assuming wind profile:

$$v_a = \frac{1}{k} u_* \ln\left(\frac{z - z_d}{z_0}\right), \ z > z_d + z_0$$

with

k = 0.4 von-Karman constant [.]

$$u_* = \frac{\kappa v_m}{\ln \left[\frac{z_m - z_d}{z_0}\right]}$$
: frictional velocity [ms⁻¹], v_m: wind velocity at height z_m.

[•] The friction velocity u* describes the intensity of turbulence. It is defined as $u^* \equiv \left(-\overline{v_a' \cdot w_a'}\right)^{1/2}$ with w_a' fluctuation of vertical wind speed ($w_a = \overline{w_a} + w_a'$). The minus sign is required because simultaneous values of w_a' and v_a' have opposite signs.

Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere





yields

$$\frac{dv_a}{dz} = \frac{u_*}{k(z - z_d)}$$

and therefore

$$D_M = k \ u_* \ (z - z_d)$$

Thus the diffusivity of momentum increases in proportion to distance above the zeroplane displacement height and in proportion to the velocity of the eddies which is characterized by u_* .

Latent Heat Transfer

Concentration of water vapor is given by absolute humidity (mass concentration of

water vapor)
$$\rho_v$$
. ($\rho_v = \frac{n_v RT}{V} = \frac{p_v}{R_v T}$)

Since molecular weight of water vapor is 0.622 molecular weight of dry air, the relation between p_v and ρ_v can be expressed as

 $\frac{p_v}{\rho_v} = \frac{p}{0.622\rho_a}$

Upward flux of water vapor [M/L²/T] equals evaporation rate ρE [M/L³][L/T] therefore

$$\rho_{w}E = -D_{vapor} \frac{d\rho_{v}}{dz}$$
$$= -D_{vapor} \frac{0.622\rho_{a}}{p} \frac{dp_{v}}{dz}$$

The upward latent heat transfer rate λE can be found directly as

$$\lambda E = -D_{vapor}\lambda_v \frac{0.622\rho_a}{p}\frac{dp_v}{dz}$$

Vapor and latent heat are transported vertically by the same turbulent eddies that are involved in momentum transfer.

Using

$$1 = \frac{{u_*}^2}{D_M dv_a / dz}$$

gives (multiplication by 1)

$$\begin{split} \lambda E &= -\frac{D_{vapor}}{D_M} \lambda_v \frac{0.622 \rho_a}{p} u_*^2 \frac{dp_v / d_z}{dv_a / d_z} = -\frac{D_{vapor}}{D_M} \lambda_v \frac{0.622 \rho_a}{p} \frac{k^2 v_m^2}{\left(\ln \frac{z_m - z_d}{z_0}\right)^2} \frac{dp_v}{dv_a} \\ &\approx -\frac{D_{vapor}}{D_M} \lambda_v \frac{0.622 \rho_a}{p} \frac{k^2 v_m^2}{\left(\ln \frac{z_m - z_d}{z_0}\right)^2} \frac{p_{v(z=m)} - p_{v,s}}{v_{(z=m)} - 0} = \\ &= \frac{D_{vapor}}{D_M} \lambda_v \frac{0.622 \rho_a}{p} \frac{k^2 v_m}{\left(\ln \frac{z_m - z_d}{z_0}\right)^2} (p_{v,s} - p_{v(z=m)}) = \\ &= K_{\lambda E} v_m (p_{v,s} - p_{v(z=m)}) \end{split}$$

Sensible Heat Transfer

Thermal capacity, cp:

$$c_p \equiv \frac{\Delta H}{m \, \Delta T}$$

relates a temperature change of a substance to a change in heat-energy content.

E.g. thermal capacity of water $c_p = 4216 J kg^{-1}K^{-1}$

The change of concentration of sensible heat h [Energy/Length³] can be expressed as

 $\Delta h = \rho_a c_a (T_a - T_b)$

c_a: heat capacity of air

T_a, T_b: air temperature

Diffusion equation of sensible heat:

$$F_Z(H) = -D_H \frac{d(\rho_a c_a T_a)}{dz}$$

 D_H : diffusivity of sensible heat

Similarly to latent heat:

$$H = \frac{D_H}{D_M} c_a \rho_a \frac{k^2 v_m}{\left(\ln \frac{z_m - z_d}{z_0}\right)^2} (T_s - T_{(z=m)}) =$$

= $K_H v_m (T_s - T_{(z=m)})$

where K_H is effectively constant for a given situation.

Soil Vegetation Atmosphere Transfer Modelling



Fig. 2. The Oregon State University one-dimensional coupled atmospheric-plant-soil model which simulates the atmospheric boundary layer, vegetated surface, and underlying soil physical processes. (note: four instead of two layers will be used with layer thicknesses 10cm, 30cm, 60cm and 100cm)

Objective:

- modeling heat fluxes (latent, sensible, ground heat flux)

- modeling water fluxes (soil moisture, surface runoff)

- driven only by meteorological variables

Case study:

- 7 days period in summer 1998, Illinois test site

- comparison to observed data

Energy Balance

$$R_n = H + E + G$$

Net radiation [Wm⁻²]

$$R_n = (1 - \alpha)SD + LD - \varepsilon \cdot \sigma \cdot t_{sfc}^{4}$$

SD: incoming shortwave radiation $[Wm^{-2}]$ LD: incoming songwave radiation $[Wm^{-2}]$ ε : emissivity [.] σ = 5.67 10⁻⁸ Stefan Boltzmann constant $[Wm^{-2} K^{-4}]$ Latent heat of evaporation [MJ kg-1]: (Energy absorbed (released) during evaporation (condensation))

 $\lambda = 2.5 - 0.002361 \left(t_a - 273.25 \right)$

t_a: air temperature [K]

Saturated water vapor pressure [kPa] (Clausius-Clapeyron equation):



Slope of e_{sat} [kPa K⁻¹]:



Vapor pressure [kPa]:

(Partial pressure exerted by water vapor)





Psychrometric constant (factor 0.1 converts pressure from mbar into kPa)

Dry air density at surface [kg/m³]:

$$\rho_{dry} = \frac{p_{sfc}}{t_a \cdot r_d} 100$$

with

 r_d =287 J/kg/K, gas constant for dry air



Moist air density at surface:

$$\rho_{moist} = \frac{p_{sfc}}{T_v \cdot r_d} 100$$

with T_v: virtual temperature [K]



Virtual temperature [K]

(Temperature of a sample of dry air at the same density and pressure as a sample of moist air at temperature t_a .)

$$T_v = t_a (1 + 0.608 \,\omega_v)$$

with

 ω_v : mass mixing ratio of water vapor



Virtual potential temperature [K]

(Is found by bringing a moist parcel to a pressure of 1000 mbar, then converting all moisture in the parcel to dry air and determining the parcel's temperature)



Mass mixing ratio of water vapor [.]

(kg of water vapor per kg of dry air)

$$\omega_v = \frac{0.622 \cdot e}{p_{sfc} \cdot 0.1 - e}$$



Saturated mass mixing ratio [.]:

$$\omega_{v \, sat} = \frac{0.622 \cdot e_{sat}}{p_{sfc} \cdot 0.1 - e_{sat}}$$

Slope of saturated mass mixing ratio:



Specific humidity at t_a[.]

(Mass of water vapor per unit mass of moist air (dry air plus water vapor))



Saturated specific humidity [.]:







Slope of saturated specific humidity [K⁻¹]:

Hydraulic conductivity [ms⁻¹]:

$$k = k_{sat} \left(\frac{\theta}{\theta_{sat}}\right)^{2b+3}$$

 θ_{sat} : Volumetric water content at saturation

k_{sat}: Saturated hydraulic conductivity

b: slope Parameter





with

 $\Psi_{\mbox{\tiny sat}}$: saturated matrix potential (suction head)



Soil water tension [m]:





Total volumetric heat capacity [Jm⁻³K⁻¹]:

 $C_{v} = \theta C_{v water} + (1 - \theta_{sat}) C_{v soil} + (\theta_{sat} - \theta) C_{v air}$

with

 $c_{v \text{ water}}$ = 4.2 10⁶ [Jm⁻³K⁻¹] water volumetric heat capacity $c_{v \text{ soil}}$ = 1.26 10⁶ [Jm⁻³K⁻¹] soil volumetric heat capacity $c_{v \text{ air}}$ = 1004 [Jm⁻³K⁻¹] air volumetric heat capacity

Thermal conductivity K_t [Wm⁻¹K⁻¹]:



FIG. 2. Thermal conductivity as function of volumetric soil moisture for four soil types: sand, silt, loam, and clay.

 $K_t = Min[1.9, K_{t,temp}]$



with

$$P_f = Log[10, \psi_{sat}(\frac{\theta_{sat}}{\theta})^b]$$



Maximum infiltration [mm d⁻¹]:

$$I_{\text{max}} = \frac{P_d Dx(1 - e^{-\frac{kdt \cdot dts}{86400}})}{\frac{P_d Dx dts}{86400 10^3} + Dx(1 - e^{-\frac{kdt \cdot dts}{86400}})}$$

with

$$k_{dt} = \frac{k_{dtref} \cdot k_{sat}}{k_{ref}}$$

 $k_{dt ref} = 3 [.]$ $k_{ref} = 2/10^{6} [.]$

$$Dx = dz_1 + dz_2 + dz_3 + dz_4$$

Ground heat flux G [Wm⁻²]:

$$G = \frac{K_t \cdot \left(t_{sfc} - t_{soil\,1}\right)}{0.5 \cdot dz_1}$$

Sensible heat flux H [Wm⁻²]:

$$H = \rho_{moist} \cdot c_p \cdot C_h \cdot (t_{sfc} - \theta_v)$$

Total evaporation [Wm⁻²; mm d⁻¹ : conversion factor ≈ 29]:

$$Etotal = Edir + Et + Ec$$

Potential Evaporation [mm d⁻¹] (*Penman Monteith*)

$$E_{pot} = \frac{\Lambda \cdot (R_n \cdot 0.0864)}{(\Lambda + \gamma)\lambda} + (\gamma (6.43 (1 + 0.536v_a)(e_{sat} - e)))/((\gamma + \Lambda)\lambda)$$



Direct soil evaporation E_{dir}: [mm d⁻¹]



 σ_f : vegetation fraction



Canopy transpiration [mm d⁻¹]:

$$E_{t} = \begin{cases} 0 & Wc = 0\\ \sigma_{f} \cdot E_{pot} \cdot B_{c} \left(1 - \left(\frac{Wc}{S}\right)^{n}\right) & else \end{cases}$$

 $W_c:$ canopy water content [mm] S=0.5 mm maximum allowed W_c

Wet canopy evaporation [mm d⁻¹]:

$$E_{c} = \begin{cases} 0 & Wc = 0\\ \sigma_{f} \cdot E_{pot} (\frac{Wc}{S})^{n} & else \end{cases}$$

Resistance term B_c:

$$Bc = \frac{1 + \frac{\Lambda\Lambda_{sat}}{R_r}}{1 + R_c \cdot C_h + \frac{\Lambda\Lambda_{sat}}{R_r}}$$



Factor R_r:



Canopy Resistance R_c: [sm⁻¹]

$$\mathbf{R}_{c} = \frac{r_{c\min}}{Lai \cdot f_1 \cdot f_2 \cdot f_3 \cdot f_4}$$

with

r_{cmin}: minimal stomatal resistance [sm⁻¹] Lai: Leaf area index [.]

Lai = (total area of transpiring surface above ground area A)/A



with





0.4 ∂ref

0.2

0 -0.5

0.1

0.2

⊖wilt

0.3

0.4

0.5

Exchange coefficient for heat [ms⁻¹]:



Neutral exchange coefficient [.]

kar² $C_n = \frac{n}{Log[\frac{h_a}{z0m}] * Log[\frac{h_a}{z0m}]}$ kar =0.4 Karman constant z0m: roughness length C'n neutral exchange coefficient 0.018 0.016 0.014 0.012 z0m 0.04 0.02 0.06 0.08 0.1 0.008

Functions modifying neutral exchange coefficient:

0.006

$$f_{h} = \begin{cases} e^{-Ri} , R_{i} > 0\\ 1 - (15Ri)/(1 + 75C_{n} \cdot (\frac{1}{z0m}(h_{a} * Abs[Ri]))^{0.5})], R_{i} <= 0 \end{cases}$$



Bulk Richardson number

(Quantifies the ratio of buoyancy to mechanical shear; Ratio: turbulence due to shear /turbulence due to buoyancy)

$$Ri = \frac{g \cdot h_a \cdot (\omega_v - t_{sfc})}{\omega_v \cdot v_a^2}$$

h_a: height of met-station measurement [m]

g: gravitational constant [ms⁻²]

 v_a : wind speed at h_a [ms⁻¹]



VEGETATION – RELATED PARAMETERS IN THE SVAT-MODEL

- roughness length (Z₀) in [m],
- minimal stomatal resistance (R_{cmin}) in [sm⁻¹]
- R_{gl} is the visible solar flux for which f_1 is about to double its minimum value,
- h_s is a parameter in f_2 .

Vegetation types	Albedo	$Z_0(m)$	$R_{c \min}$	R_{gl}	h_s
Broadleaf - evergreen trees	0.11	2.653	150	30	41.69
Broadleaf - deciduous trees	0.12	0.826	100	30	54.53
Broadleaf and needleleaf trees	0.12	0.8	125	30	51.93
Needleleaf - evergreen trees	0.1	1.089	150	30	47.35
Needleleaf - deciduous trees (larch)	0.11	0.854	100	30	47.3
Broadleaf trees with groundcover	0.19	0.856	70	65	54.53
Groundcover only	0.19	0.075	40	100	36.35
Broadleaf shrubs with groundcover	0.25	0.238	300	100	42
Broadleaf shrubs with bare soil	0.25	0.065	400	100	42
Dwarf trees/shrubs with groundcover	0.16	0.05	150	100	42
(tundra)					
Bare soil	0.12	0.011			
Cultivations	0.19	0.075	40	100	36.35
Wetland	0.12	0.04	150	100	60
Dry coastal complex	0.19	0.075	400	100	200
Water	0.19	0.01			
Glacial	0.8	0.011	999	999	999

Exercise: Case study Champaign, Illinois (88.37°W, 40.01°N)



Meteorological Input a) Wind

b) Temperature







d) Precipitation



13.7.92 0:00 14.7.92 0:00 15.7.92 0:00 16.7.92 0:00 17.7.92 0:00 18.7.92 0:00 19.7.92 0:00 20.7.92 0:00 21.7.92 0:00 22.7.92 0:00







f) Shortwave radiation

Date

g) Longwave radiation



Simulation Results a) Latent Heat Flux







b) Sensible Heat Flux

-50

Date

21,7.92 0:00

22.7.92

0:00

Part II: Meteorological Modelling and Applications to Hydrological Engineering

- Fundamentals of Atmospheric Science
- Water in the Atmosphere
- Continuity Equations
- Momentum Equations
- Global Circulation
- Nonlinear Dynamics and Chaos
- Numerical Solution of Partial Differential Equations using Finite Difference
 Schemes
EQUATIONS OF STATE

The equation of state describes the relationship among pressure, volume and absolute temperature of a real gas.

Equation of state for ideal gas

$$p = \frac{nR^*T}{V} = \frac{nA}{V} \left(\frac{R^*}{A}\right) T = Nk_B T$$
: Ideal gas law (simplified equation of state)

p: Pressure (mbar)

 R^{*} : Universal gas constant (R=0.083145 m³ mbar mole⁻¹ K⁻¹)

T: Temperature (Kelvin)

V: Volume (m³)

n: number of moles of a gas (mole)

 k_B : Boltzman's constant (=1.3807 10⁻²⁵ m³ mbar K⁻¹)

N: number concentration of gas molecules (molecules of gas per Volume) $\left(N = \frac{nA}{V}\right)$

A: Avogadro's number, A=6.02252 10²³ molecules

Example

Calculate the number concentration of air molecules in the atmosphere at standard sea-level pressure and temperature and at a pressure of 1 mb.

SOLUTION

At standard sea level, p = 1013 mb and T = 288 K.

N = $2.55 \ 10^{19}$ molecules cm⁻³.

p = 1 mb occurs at 48 km. At this altitude and pressure, T = 270 K,

 $N = 2.68 \ 10^{16} \text{ molecules cm}^{-3}$.



Figure: Temperature structure of the earth's lower atmosphere (Jacobson, 2005)

Troposphere: average rate of temperature decrease in free troposphere is about 6.5 K km^{-1} ; Thermal infrared radiation emitted by ground is absorbed by selective gases like CO₂ and water vapour. These gases are most concentrated near surface. Once they absorb the radiation, they reemit half of it upwards and the other half downward, but their emission is at lower temperature than is the emission of the radiation they absorbed. Because less radiation is available for absorption with increasing altitude, temperature decreases with increasing altitude in the troposphere.

Stratosphere: O_3 and O_2 absorb UV radiation and emit infrared radiation heating the region.

Thermosphere: molecular oxygen and nitrogen absorb very short wavelengths of radiation in this region.

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Equation of state for dry air

$$p_d = \frac{n_d R^* T}{V} = \frac{n_d m_d R'}{V} T = \rho_d R' T$$

 n_{d} : number of moles of dry air (mole) p_{d} : partial pressure exerted by dry air (mbar) ρ_{d} : mass density of dry air (kg m⁻³) R^{*} : gas constant for dry air (= 2.8704 m³ mbar kg⁻¹ K⁻¹) = R*/m_d m_{d} : molecular weight of dry air (=28.966 g mole⁻¹)

Equation of state for water vapor

$$p_v = \frac{n_v R * T}{V} = \rho_v R_v T$$

 p_{v} : partial water pressure exerted by water vapor (mbar)

 ρ_{v} : mass density of water vapor (kg m⁻³) (**absolute humidity**)

 R_{v} : gas constant for water vapor (= 4.6140 m³ mbar kg⁻¹ K⁻¹) $R_{v}=R^{*}/m_{v}$

 m_v : molecular weight of water vapour (=0.622 m_d [g mole⁻¹])

Mass mixing ratio of water vapour

 $\omega_{\nu} = \frac{\rho_{\nu}}{\rho_d} = \frac{m_{\nu}p_{\nu}}{m_d p_d} = \varepsilon \frac{p_{\nu}}{p_d} = \frac{p_{\nu}}{p_a - p_{\nu}}$

(kilograms of water vapour per kilogram of dry air)

Specific humidity (moist air mass mixing ratio)

$$q_{v} = \frac{\rho_{v}}{\rho_{a}} = \frac{\rho_{v}}{\rho_{d} + \rho_{v}} = \frac{\frac{p_{v}}{R_{v}T}}{\frac{p_{d}}{R'T} + \frac{p_{v}}{R_{v}T}} = \frac{\varepsilon p_{v}}{p_{d} + \varepsilon p_{v}}$$

= mass of water vapor per unit mass of moist air (.)

with
$$\varepsilon = \frac{R'}{R_v} = \frac{R^*}{m_d} \left(\frac{m_v}{R^*} \right) = \frac{m_v}{m_d} = 0.622$$

 ρ_{a} , ρ_{d} , ρ_{v} : density of most air, dry air and water vapor (kg m⁻³)

Example

If p_v =10 mbar and p_a =1010 mbar, p_a = p_d + p_v gives p_d =1000mbar; q_v =0.00618 kg/kg



Figure: Global distribution of surface specific humidity [g kg⁻¹]



Figure: Global vertical mean specific humidity [g kg⁻¹]

Equation of state for moist air

: Sum of the equations of state for dry air and water vapour

$$p_{a} = p_{d} + p_{v} = \rho_{d} R'T + \rho_{v} R_{v} T = \rho_{a} R'T \frac{\rho_{d} + \rho_{v} R_{v} / R'}{\rho_{a}}$$

with $\varepsilon = R'/R_v$, $\rho_a = \rho_d + \rho_v$, $\omega_v = \rho_v / \rho_d$ it follows

$$p_{a} = \rho_{a} R' T \frac{\rho_{d} + \rho_{v} / \varepsilon}{\rho_{d} + \rho_{v}} = \rho_{a} R' T \frac{1 + \frac{\rho_{v}}{\rho_{d} \varepsilon}}{1 + \frac{\rho_{v}}{\rho_{d}}} \text{ and therefore}$$

$$p_a = \rho_a R' T \frac{1 + \omega_v / \varepsilon}{1 + \omega_v} = \rho_a R_m T = \rho_a R' T_v$$

$$R_m = R' \frac{1 + \omega_v / \varepsilon}{1 + \omega_v} \approx R' (1 + 0.608\omega_v)$$
: gas constant for moist air

$$T_{\nu} = T \frac{1 + \omega_{\nu} / \varepsilon}{1 + \omega_{\nu}} = T \frac{R_m}{R'} \approx T(1 + 0.608\omega_{\nu})$$
: virtual temperature:

Temperature of a sample of dry air at the same density and pressure as a sample of moist air at temperature T.

Note:
$$\frac{1 + \frac{\omega_v}{\varepsilon}}{1 + \omega_v} \approx 1 + 0.608\omega_v$$
 (Taylor Expansion around $\omega_v = 0$)

$$f(\omega_{v}) \approx f(\omega_{v})\Big|_{\omega_{v}=0} + \frac{\partial f}{\partial \omega_{v}}\Big|_{\omega_{v}=0}(\omega_{v}-0)$$

with
$$\frac{\partial f}{\partial \omega_{v}} = \frac{\partial}{\partial \omega_{v}} \left(\frac{1 + \frac{\omega_{v}}{\varepsilon}}{1 + \omega_{v}} \right) = \frac{1}{\varepsilon (1 + \omega_{v})} - \frac{1 + \frac{\omega_{v}}{\varepsilon}}{(1 + \omega_{v})^{2}}; \Rightarrow \frac{\partial f}{\partial \omega_{v}} \Big|_{\omega_{v}=0} = \frac{1}{\varepsilon} - 1$$

 $\varepsilon = 0.622 \Rightarrow \frac{1 + \omega_{v}/\varepsilon}{1 + \omega_{v}/\varepsilon} \approx 1 + 0.608\omega_{v}$

$$\varepsilon = 0.622 \Rightarrow \frac{1}{1 + \omega_v} \approx 1 + 0.60$$

Example

If
$$p_d$$
=1013 mbar and p_v =10 mbar, T=298K, calculate $\omega_v, R_m, T_v, \rho_a$
 $\omega_v = 0.622 \cdot 10 mb / 1013 mb = 0.00614 \ kg \ kg^{-1}$
 $R_m = 2.8704 \cdot (1 + 0.608 \cdot 0.00614) = 2.8809 \ m^3 \ mb \ kg^{-1}K^{-1}$
 $T_v = 298 \cdot (1 + 0.6 \cdot 0.00614) = 299.1 \ K$
 $\rho_a = p_a / (R_m \cdot T) = 1023 / (2.8809 \cdot 298) = 1.19 \ kg \ m^{-3}$

CHANGE IN PRESSURE WITH ALTITUDE

Hydrostatic equation (Upward gradient in air pressure is balanced by downward force of gravity multiplied by air density)





$$dp_a = -\rho_a g dz$$

$$\frac{\partial p_a}{\partial z} = -\rho_a g$$

g: gravitational acceleration (9.81 ms⁻²)

- z: altitude (m)
 - Hydrostatic balance: air has no vertical acceleration
 - Reasonable assumption when averaged over large horizontal regions
 - Over small regions (<2-3 km) hydrostatic assumption is not accurate (e.g. cumulonimbus)

 $\frac{\partial p_a}{\partial z} \approx \frac{\overline{p_{a,1} - p_{a,0}}}{z_1 - z_0} = -\rho_{a,0} g$

 $p_{a,0}$ pressure at altitude z_0 , $p_{a,1}$ pressure at altitude z_1

Example

 $p_{a,0} = 1013 \text{mbar} \ \rho_{a,0} = 1.23 \text{ kg m}^{-3}, \ p_{a,100} = ?$ Solution: $p_{a,100} = 1013 mb - 1.23 kgm^{-3} \cdot 9.81 ms^{-2} \cdot 100 m = 1000.2 \ mbar$ $(1 \ bar = 10^3 \ mbar = 10^5 \ N / m^2 = 10^5 \ kg \ m / s^2 \ 1 / m^2 = 10^5 \ kg \ m^{-1} s^{-2})$ \Rightarrow Near the surface, pressure decreases approximately 1mbar for every 10m increase in altitude

$$dp_a = -\rho_a g dz = -p \frac{M \cdot g}{R^* \cdot T} dz$$

 $\left(\rho = \frac{M}{V} = \frac{M \cdot p}{R^* \cdot T}\right)$

T: absolute temperature [K], R*=0.083145 m³ mbar mole⁻¹ K⁻¹ universal gas constant, M: mean mol mass of air (M=28.97g/Mol)

Exponential decrease of pressure with height:

$$p = p_0 \cdot \exp\left(-\frac{M \cdot g}{R^* \cdot T}z\right)$$

p₀: surface pressure

Includes approximation: no temperature decrease with height

Scale height: $z_0 = \left(\frac{M \cdot g}{R^* \cdot T}\right)^{-1} \approx 8 \ km$ height in which pressure is reduced to 1/e.

(around 5.5 km for reduction to 1/2).

Standard atmosphere

$$p_{a,s} = 1013.25 \text{ mbar}$$
$$T_{a,s} = 288 \text{ K}$$
$$\Gamma_s = -\frac{\partial T}{\partial z} = +6.5 \text{ K km}^{-1}$$
$$\frac{\partial p_a}{\partial z} = -\frac{p_a}{R_m T} g$$

Substituting $T = T_{a,s} - \Gamma_s \cdot z$ (where *z*=0*km* corresponds to sea level), integrating from $p_{a,s}$ to p_a and 0 to *z* yields

$$\ln\left(\frac{p_a}{p_{a,s}}\right) = \frac{g}{\Gamma_s R_m} \ln\left(\frac{T_{a,s} - \Gamma_s \cdot z}{T_{a,s}}\right)$$

Rearranging again gives altitude as a function of pressure in a standard troposphere

$$z = \frac{T_{a,s}}{\Gamma_s} \left[1 - \left(\frac{p_a}{p_{a,s}}\right)^{\frac{\Gamma_s R_m}{g}} \right]$$



PHASE TRANSITIONS OF WATER

Figure: Global annual precipitation [dm/year]

Water appears in three states: gas, liquid, solid.

Sources and sinks of **water vapour** in the atmosphere are evaporation from soils, lakes, streams, rivers, and oceans, sublimation from glaciers, sea ice, and snow packs, and transpiration from plant leaves. Approximately 85 percent o water in the atmosphere originates from ocean surface evaporation. Sinks of water vapour are condensation to liquid phase, ice deposition to the solid phase, transfer to the ocean and other surfaces. Water vapour is not only a greenhouse gas (a gas that readily absorbs thermal-infrared radiation) but also a chemical reactant and carrier of latent heat.

Sources of **liquid water** include sea spray emission, volcanoes, combustion, condensation of water vapour, and melting of ice crystals. Sinks of liquid water include evaporation, freezing and sedimentation to the surface of aerosol particles, fog drops, drizzle, and raindrops.

Ice in the atmosphere forms from freezing of liquid water and solid deposition of water vapour. Losses of ice occur by sublimation to the gas phase, melting to the liquid phase, and sedimentation to the surface.

Types of energy

When water change state, it releases or absorbs energy.

Kinetic energy is the energy within a body due to its motion (E=0.5 M v^2). To change velocity and kinetic energy of a body, mechanical work must be done

Potential energy is the energy of matter that arises due to its position, rather than its motion

Internal energy is the kinetic and/or potential energy of molecules within an object.

Work is the energy added to a body by the application of a force that moves the body in the direction of force

Electromagnetic (radiant) energy is the energy transferred by electromagnetic waves that originate from bodies with temperatures above 0K

Latent heat

During condensation, freezing and deposition of a substance, energy is released. During evaporation, melting, and sublimation, energy is absorbed. The energy released or absorbed during such processes is **latent heat**. Latent heat absorbed (released) during evaporation (condensation) is latent heat of evaporation. It varies with temperature as

 $\frac{d\lambda_{e}}{dT} = c_{p,V} - c_{W}$

 $c_{p,V}$: Specific heat of water vapour at constant pressure [J kg⁻¹ K⁻¹]

 c_w : Specific heat of liquid water [J kg⁻¹ K⁻¹]



Figure: Phase changes of water. Freezing (melting) at 0°C releases (adsorbs) 333.5 Jg⁻¹, deposition (sublimation) at 0°C releases (absorbs) 2835 Jg⁻¹



Figure: Variation of specific heat of liquid water with temperature

Since changes in $c_{p,V}$ and c_W are small for temperatures above 0°C, these

parameters are often held constant

$$\lambda_e = \lambda_{e,0} - (c_w - c_{p,V})(T - T_0) \approx 2.501 \cdot 10^6 - 2370 \cdot T_c$$
 [J kg⁻¹]

Example

0°C: 2501 J is required to evaporate 1 g of liquid water. At 100°C, 2264 J is required.

Clausius-Clapeyron Equation

A parameter that affects liquid-water (and also ice-particle) formation is the saturation vapour pressure. The saturation vapour pressure is the partial pressure of gas at a specific temperature when the gas is in equilibrium with a liquid or solid surface. In a gross sense, it is the maximum amount of vapour the air can hold without the vapour condensing as a liquid or depositing as ice on a surface.

The temperature variation of the saturation vapour pressure of water over a liquid surface p_{vs} [mb] is approximated with the Clausius-Clapeyron equation

$$\frac{dp_{v,s}}{dT} = \frac{\rho_{v,s}}{T} \lambda_e = \frac{\lambda_e p_{v,s}}{R_v T^2}$$

 L_e : latent heat of evaporation [Jkg-1], $\rho_{v,s}$ [kg m⁻³]

$$\rightarrow \frac{dp_{v,s}}{p_{v,s}} = \frac{1}{R_v} \left(\frac{A_h}{T^2} - \frac{B_h}{T}\right) dT$$

 $T = T_0 = 273.15 \ p_{v,s,0} = 6.112 \ mb$

$$p_{\nu,s} = 6.112 \exp\left[6816\left(\frac{1}{273.15} - \frac{1}{T}\right) + 5.1309 \ln\left(\frac{273.15}{T}\right)\right]$$

with T[K], $p_{v,s}[mb]$.



Figure: Saturation vapor pressure $p_{v,s}$ [*mb*] over liquid water

Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere

Example T=253.15K (-20°C), p_{v,s} = 1.26mbar T=298.15K (25°C), p_{v,s} = 31.60mbar

Climate change:

T=288.15K (15°C), $p_{v,s}$ =17.03mbar T=289.15K (16°C), $p_{v,s}$ =18.16mbar Δ T=1°C -> Relative change of precipitable water by 5.5% -> impact on precipitation (e.g. intensity)



Figure: a) condensation occurs when the partial pressure of water vapour exceeds its saturation vapour pressure over liquid water, **b)** evaporation occurs when the saturation vapour pressure exceeds the partial pressure of water vapour (schematics not to scale).

Relative humidity





Figure: Global relative humidity in % at 850mbar

CONTINUITY EQUATIONS

Local and total differentiation

Total velocity in Cartesian coordinate system:

 $\vec{v} = \mathbf{i}u + \mathbf{j}v + \mathbf{k}w$

: i, j, k Cartesian-coordinate west-east, south-north, and vertical unit vectors

$$u = \frac{dx}{dt}, v = \frac{dy}{dt}, w = \frac{dw}{dt}$$
: scalar components of velocity [ms⁻¹]
$$|\vec{v}| = \sqrt{u^2 + v^2 + w^2}, |\vec{v}_h| = \sqrt{u^2 + v^2}$$



Figure: Zonally averaged west-east scalar velocities (m/s) for a) January and b) July (Jacobson, 2005)

The time rate of change of a variable such as concentration, momentum or temperature can be determined at a fixed location or in the frame of reference of the variable as it moves

 $\frac{dN}{dt}$: total derivative: time rate of change of N anywhere along the plume's trajectory

 $\frac{\partial N}{\partial t}$: partial derivative: time rate of change of N at fixed point

$$N = N(x(t), t) \Rightarrow \frac{dN}{dt} = \frac{\partial N}{\partial t} \frac{dt}{dt} + \frac{\partial N}{\partial x} \frac{dx}{dt} + \frac{\partial N}{\partial y} \frac{dy}{dt} + \frac{\partial N}{\partial z} \frac{dz}{dt} =$$
$$= \frac{\partial N}{\partial t} + u \frac{\partial N}{\partial x} + v \frac{\partial N}{\partial y} + w \frac{\partial N}{\partial z} =$$
$$= \frac{\partial N}{\partial t} + (\vec{v} \cdot \vec{\nabla})N$$

with $\vec{\nabla}$: Gradient Operator

Lagrangian frame of reference \Leftrightarrow Eulerian frame of reference

(Frame of reference that moves relative to a fixed coordinate system \Leftrightarrow frame of

reference fixed relative to a fixed coordinate system)

Example

Suppose the time rate of change of concentration of a gas along the path of a hot-air balloon travelling with the wind from east to west at u = -10 m s - 1 is $\frac{dN}{dt} = 10^8$ molecules cm⁻³s⁻¹. If the west-east gradient in concentration is $\frac{\partial N}{\partial x} = 10^{10}$ molecules cm⁻³km⁻¹ (concentration increases from west to east), determine the time rate of change of concentration at a fixed point A, which the balloon passes over.

SOLUTION:

 $u\frac{\partial N}{\partial x}$ = -10⁸ molecules cm⁻³s⁻¹ : rate of change of concentration in plume resulting from west-east velocity transporting the plume.

 $\left(\frac{\partial N}{\partial t}\right)_A \approx 2 \cdot 10^8 \text{ molecules cm}^{-3} \text{s}^{-1}$

Thus, transport from the east accounts for one-half of the production rate of N at point A, and transformations along the trajectory (dN/dt) account for the other half.

Derivation of continuity equations



Figure: Example of mass conservation (Jacobson, 2005)

[N]= Molecules cm⁻³ $[\Delta x], [\Delta y], [\Delta z] = cm$ [u]= ms⁻¹

$$\Delta N \Delta x \Delta y \Delta z = u_1 N_1 \Delta y \Delta z \Delta t - u_2 N_2 \Delta y \Delta z \Delta t$$

: Number of molecules leaving or entering control volume

$$\frac{\Delta N}{\Delta t} = -(\frac{u_2 N_2 - u_1 N_1}{\Delta x})$$

$$\frac{\partial N}{\partial t} = -\frac{\partial(uN)}{\partial x}$$

Continuity equation for a gas affected in one dimension

Generalization: Continuity equation for number concentration:

$$\frac{\partial N}{\partial t} = -\vec{\nabla} \cdot (\vec{v}N)$$

Similarly: Continuity equation for air density:

$$\frac{\partial \rho_a}{\partial t} = -\vec{\nabla} \cdot (\vec{v}\rho_a)$$



(Flux divergence form)

$$[\rho_a \vec{v}q] = \frac{kg}{m^2 s}$$
: flux of total mass of water in

air

¹ With $\vec{v}N = \vec{i}uN + \vec{j}vN + \vec{k}wN$

² $\vec{\nabla} \cdot (\vec{v}N) = N(\vec{\nabla} \cdot \vec{v}) + (\vec{v} \cdot \vec{\nabla})N$: identity

Considering sources and sinks:

$$\frac{\partial \rho_a q}{\partial t} + \vec{\nabla} \cdot (\rho_a \vec{v} q) = Q \rho_A$$

Q: source/sink term (g/kg/s)



TURBULENT HUMIDITY FLUXES

The spatial domain in a model is divided into grid cells of finite size. In most cases atmospheric motions occur over spatial scales much smaller than the resolution of the grid cell and over temporal scales smaller than the resolution of the time step. To account for subgrid scale disturbances, each variable in the model equations can be divided into an average and perturbation component.



Figure: Precise, mean and perturbation components of scalar velocity and gas concentration (*Jacobson, 2005*)

For instance, actual (precise) humidity and velocity can be decomposed as

$$q(t) = \overline{q} + q'(t);$$
$$v(t) = \overline{v} + v'(t)$$

 $\overline{q}, \overline{v}$ are constant in the averaging time interval

 $\overline{q}',\overline{v}'=0$

Therefore

$$\overline{qv} = \overline{q}\overline{v} + \overline{q'v'}$$
Additional turbulent

3

³ Combined temporal and spatial averaging:

yields

$$q = [q] + q^*; v = [v] + v^*$$

$$[qv] = [\overline{q}][\overline{v}] + [\overline{q'v'}] + [\overline{q}^*\overline{v}^*]$$

 $[\overline{q}][\overline{v}]$: "standing cell", $[\overline{q}^*\overline{v}^*]$: "standing eddies", $[\overline{q'v'}]$: "transient eddies"



Figure: Mechanism of turbulent humidity fluxes (Baumgartner & Liebscher, 1990)

Since density perturbation in the atmosphere are small, $\rho_a' \ll \overline{\rho_a}$, $\rho_a \approx \overline{\rho_a}$; thus

$$\frac{\partial \overline{\rho_a}(\overline{q}+q')}{\partial t} + \vec{\nabla} \cdot (\overline{\rho_a}(\overline{\vec{v}}+\vec{v}')(\overline{q}+q')) = \rho_a Q$$

Taking time and grid volume average of this equation, eliminating zero valued terms, removing unnecessary overbars results in

$$\overline{\rho_a} \left[\frac{\partial \overline{q}}{\partial t} + (\vec{v} \cdot \vec{\nabla}) \overline{q} \right] + \overline{q} \left[\frac{\partial \rho_a}{\partial t} + \vec{\nabla} \cdot (\overline{\vec{v} \rho_a}) \right] + \vec{\nabla} \cdot (\overline{\rho_a} \ \overline{\vec{v}' q'}) = \overline{\rho_a} \overline{Q}$$

which yields⁴

$$\frac{\partial \overline{q}}{\partial t} + (\vec{v} \cdot \vec{\nabla})\overline{q} + \frac{1}{\rho_a} \vec{\nabla} \cdot (\overline{\rho_a} \ \overline{\vec{v}'q'}) = \overline{Q}$$

 ${}^{_{4}}\frac{\partial\rho_{a}}{\partial t}+\vec{\nabla}\cdot(\vec{v}\,\overline{\rho_{a}})=0: \text{ continuity equation for air }$

Whereas models calculate spatially and temporally averaged values (e.g. $\overline{q}, \overline{\rho_a}, \overline{u}$), explicit equations for cinematic turbulent fluxes (e.g. $\overline{u'q'}, \overline{v'q'}, \overline{w'q'}$) have not been developed. Instead these quantities are estimated with parameterizations (e.g. Ktheory: gradient transport theory):

$$\overline{u'q'} = -K_{xx}\frac{\partial \overline{q}}{\partial x}, \overline{v'q'} = -K_{yy}\frac{\partial \overline{q}}{\partial y}, \overline{w'q'} = -K_{zz}\frac{\partial \overline{q}}{\partial z}$$

K: eddy diffusion coefficients (m²s⁻¹)

In general:

$$\frac{\partial q}{\partial t} + (\vec{v} \cdot \vec{\nabla})q + \frac{1}{\rho_a} \vec{\nabla} \cdot (\rho_a \mathbf{K} \vec{\nabla} q) = Q$$

where $K = \begin{bmatrix} K_{xx} & 0 & 0\\ 0 & K_{yy} & 0\\ 0 & 0 & K_{zz} \end{bmatrix}$: eddy diffusion tensor



Figure: Passing of cumulus-cloud, 1500 m vertical extension, 25m blow summit; horizontal extension: 1km. Correlation between q_w and w. *(Baumgartner & Liebscher, 1990)*

MOMENTUM EQUATIONS

... Solving for the velocities ...

Spherical coordinates

$$\vec{v} = \vec{i}_{\lambda}u + \vec{j}_{\phi}v + \vec{k}_{r}w, \quad \vec{v}_{h} = \vec{i}_{\lambda}u + \vec{j}_{\phi}v$$

 $dx = (R_e \cos \varphi) d\lambda_e$ $dy = R_e d\varphi$



Figure: Spherical coordinate symbols. R_e : Earth's radius (6371 km), φ : latitude, λ : longitude, \vec{i}_{λ} West-East, \vec{j}_{φ} South-Nord and \vec{k}_r vertical unit vectors

Forces cause objects such as air parcels to accelerate or decelerate, thereby creating or altering winds. The relationship between forces and winds is called **atmospheric dynamics**.

The momentum equation is derived from Newtons Second Law of motion

$$\vec{a}_{inertial} = \frac{1}{m} \sum \vec{F}$$

F [N or kg m s⁻²]: force, m [kg]: mass, a: acceleration [ms⁻²] Inertial acceleration is derived by considering that, to an observer in space, the absolute velocity of a body in motion near the surface is

$\vec{v}_{abs} = \vec{v} + \vec{\Omega} \times \vec{R}_e$

 \vec{v}_{abs} : absolute velocity [ms⁻¹] (as seen by observer from space)

 \vec{v} : local velocity of body as seen by observer at earth's surface

 $\vec{\Omega}$: angular velocity vector [rad s⁻¹]

 \vec{R}_e : radius vector for earth [m]

 $\vec{\Omega} \times \vec{R}_e$: rate of change in position of the body due to the earth's rotation [ms⁻¹]

$$\vec{\Omega} = \vec{j}_{\varphi} \Omega \cos \varphi + \vec{k}_r \Omega \sin \varphi , \ \vec{R}_e = \vec{k}_r R_e$$

where $\Omega = 2\pi \ rad \ / \ 86164s = 7.292 \cdot 10^{-5} \ rad \ s^{-1}$ magnitude of angular velocity, 86164: number of seconds for one revolution around axis (23h 56m 4s).

Inertial acceleration is defined as

 $\vec{a}_{inertial} = \frac{d\vec{v}_a}{dt} + \vec{\Omega} \times \vec{v}_a$

$$\vec{a}_{inertial} = \frac{d}{dt}(\vec{v} + \vec{\Omega} \times \vec{R}_e) + \vec{\Omega} \times (\vec{v} + \vec{\Omega} \times \vec{R}_e) = \frac{d\vec{v}}{dt} + \vec{\Omega} \times \frac{d\vec{R}_e}{dt} + \vec{\Omega} \times \vec{v} + \vec{\Omega} \times (\vec{\Omega} \times \vec{R}_e)$$

With
$$\frac{d\vec{R}_e}{dt} = R_e \frac{d\vec{k}_r}{dt} \approx \vec{v}$$
, it follows:

$$\vec{a}_{inertial} = \frac{d\vec{v}}{dt} + 2\vec{\Omega} \times \vec{v} + \vec{\Omega} \times (\vec{\Omega} \times \vec{R}_e) = \vec{a}_{local} + \vec{a}_{Coriolis} + \vec{a}_{centripetal}$$

 $\vec{a}_{local} = \frac{d\vec{v}}{dt}$: Local acceleration: rate of change of velocity of a parcel of air in motion relative to a coordinate system fixed on earth $\vec{a}_{Coriolis} = 2\vec{\Omega} \times \vec{v}$: Coriolis acceleration: rate of change velocity of a parcel due to rotation of a spherical earth underneath the parcel $\vec{a}_{centripetal} = \vec{\Omega} \times (\vec{\Omega} \times \vec{R}_e)$: Earth's centripetal acceleration: inward-directed rate of change of velocity of a parcel due to its motion around the earth's axis.

$$\vec{a}_{local} + \vec{a}_{Coriolis} + \vec{a}_{centripetal} = \frac{1}{m} (\vec{F}_{gravitation} + \vec{F}_{pressure} + \vec{F}_{viscous})$$

$$\vec{F}_{gravitation} : \text{ true gravitational force}$$

$$\vec{F}_{pressure} : \text{ pressure gradient force}$$

$$\vec{F}_{viscous} : \text{ viscous force (drag)}$$

$$\vec{a}_{local} = \frac{1}{m} (\vec{F}_{gravitation} + \vec{F}_{pressure} + \vec{F}_{viscous} - \vec{F}_{Coriolis} - \vec{F}_{centripetal})$$

Whereas the centripetal and Coriolis effects are viewed as accelerations from an inertial frame of reference, they are viewed as **apparent forces** from a noninertial frame of reference. An apparent (or inertial) force is a fictitious force that appears to exist when an observation is made in a noninertial frame of reference.

 $\vec{F}_{gravitation}$, $\vec{F}_{pressure}$ $\vec{F}_{viscous}$ are **real** forces.

Moment equation from a reference frame fixed on earth's surface

Atmospheric models usually require expressions for local acceleration; thus momentum equation is written most conveniently for a reference frame fixed on the surface of the earth rather than fixed outside the earth-atmosphere system.

Local acceleration

$$\vec{a}_{local} = \frac{d\vec{v}}{dt} = \frac{\partial\vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v} =$$

$$\approx \vec{i}_{\lambda}\left(\frac{\partial u}{\partial t} + \frac{u}{R_{e}\cos\varphi}\frac{\partial u}{\partial\lambda_{e}} + \frac{v}{R_{e}}\frac{\partial u}{\partial\varphi} + w\frac{\partial u}{\partial z} - \frac{uv\tan\varphi}{R_{e}}\right) +$$

$$+ \vec{j}_{\varphi}\left(\frac{\partial v}{\partial t} + \frac{u}{R_{e}\cos\varphi}\frac{\partial v}{\partial\lambda_{e}} + \frac{v}{R_{e}}\frac{\partial v}{\partial\varphi} + w\frac{\partial v}{\partial z} - \frac{u^{2}\tan\varphi}{R_{e}}\right) +$$

$$+ \vec{k}_{r}\left(\frac{\partial w}{\partial t} + \frac{u}{R_{e}\cos\varphi}\frac{\partial w}{\partial\lambda_{e}} + \frac{v}{R_{e}}\frac{\partial w}{\partial\varphi} + w\frac{\partial w}{\partial z}\right)$$

(approximation: terms with uw/R_e , vw/R_e removed since small for large scale motions)

Coriolis acceleration

$$\vec{a}_{Coriolis} = 2 \cdot \vec{\Omega} \times \vec{v} =$$

$$= \vec{i}_{\lambda} 2\Omega(w\cos\varphi - v\sin\varphi) + \vec{j}_{\varphi} 2\Omega u\sin\varphi - \vec{k}_{r} 2\Omega u\cos\varphi \approx$$

$$\approx^{(1)} \vec{j}_{\varphi} 2\Omega u\sin\varphi - \vec{k}_{r} 2\Omega u\cos\varphi$$

$$\approx^{(2)} - \vec{i}_{\lambda} 2\Omega v\sin\varphi + \vec{j}_{\varphi} 2\Omega u\sin\varphi$$

Defining the Coriolis parameter as

$$f = 2\Omega \sin \varphi$$

gives another form of the Coriolis term as

$$\vec{a}_{Coriolis} \approx -\vec{i}_{\lambda} f v + \vec{j}_{\varphi} f u = f \vec{k}_r \times \vec{v}_h$$

with $|v_h|$ horizontal wind speed.

Note: Coriolis force is zero at equator $(\sin 0 = 0)$, and maximum at poles $(\sin \frac{\pi}{2} = 1)!$

(1) approximation if only zonal (i.e. west-east) winds are considered

(2) approximation if vertical component w and vertical components are neglected





Figure: Example of Coriolis deflections. The Coriolis force deflects moving bodies to the right in the northern Hemisphere and to the left in the Southern Hemisphere.



Figure: Coriolis acceleration components that results when the Coriolis force acts on a west-to-east wind travelling around the earth, parallel to the equator and into the page

Gravitational force

The true gravitational force vector acts towards the center of earth:

$$\vec{F}_{gravitation} = -m\vec{k}_r g$$

with $g = \frac{GM_e}{R^2_e} = 9.81 m s^{-2}$ $G = 6.6720 \cdot 10^{-11} m^3 k g^{-1} s^{-2}$: universal gravitational $M_e = 5.98 \cdot 10^{24} k g$: earth's mass

Pressure-gradient force

Pressure gradient force is a real force that causes air to move from regions of high pressure to regions of low pressure. The force results from pressure differences.

 $F_{p,l} = \left(p_c - \frac{\Delta p}{\Delta x}\frac{\Delta x}{2}\right)\Delta y \Delta z$ Force from air pressure left side of parcel: $F_{p,r} = -\left(p_c + \frac{\Delta p}{\Delta x}\frac{\Delta x}{2}\right)\Delta y \Delta z$ Force from air pressure right side of parcel: Force from total air in center of pressure box: $F_{p,x} = F_{p,l} + F_{p,r} = \left(p_c - \frac{\Delta p}{\Delta x}\frac{\Delta x}{2}\right)\Delta y \Delta z - \left(p_c + \frac{\Delta p}{\Delta x}\frac{\Delta x}{2}\right)\Delta y \Delta z$ $\Rightarrow \frac{F_{p,x}}{\Delta x \Delta y \Delta z} = -\frac{\Delta p}{\Delta x}$ $\Rightarrow \frac{F_{p,x}}{\rho_a \Delta x \Delta y \Delta z} = -\frac{\Delta p}{\rho_a \Delta x}$ $\Rightarrow \frac{F_{p,x}}{m} = -\frac{\Delta p}{\rho_a \Delta x}$ $\frac{\overline{F_{p,x}}}{m} = -\frac{\partial p}{\rho_a \partial x}$ $\Delta x, \Delta y, \Delta z \rightarrow 0$: Δy $p_{c} + \frac{\Delta p}{\Delta x} \frac{\Delta x}{2}$ $- F_{p,r}$ $p_{c} = \frac{\Delta p}{\Delta x} \frac{\Delta x}{2}$ $F_{p,l}$ p_{c} Δz

Figure: Example of pressure-gradient forces acting on both sides of a parcel of air

 Δx

Generalized:

$$\vec{F}_{p} = -\frac{m}{\rho_{a}} \vec{\nabla} p_{a} \overset{Cartesian \ Coordinates}{=} -\frac{m}{\rho_{a}} (\bar{i} \frac{\partial p_{a}}{\partial x} + \bar{j} \frac{\partial p_{a}}{\partial y} + \bar{k} \frac{\partial p_{a}}{\partial z}) = \\ \overset{Spherical \ Coordinates}{=} -\frac{m}{\rho_{a}} (\bar{i}_{\lambda} \frac{1}{R_{e} \cos \varphi} \frac{\partial p_{a}}{\partial \lambda_{e}} + \bar{j}_{\varphi} \frac{1}{R_{e}} \frac{\partial p_{a}}{\partial \varphi} + \bar{k}_{r} \frac{\partial p_{a}}{\partial z})$$



Figure: Pressure gradient force (heavy line) is perpendicular to isobars (medium lines) from high to low pressure. H and L indicate regions of high and low pressure



Viscous force

Viscosity is a measure of a fluid's ability to transmit forces laterally to the mean flow. When two layers of air slide over one another at different velocities, they exert a **viscous stress**, or force per unit area, on each other. The force acts parallel to the direction of motion and over the area of the plane between the two layers. The viscous force is an internal force : it is caused by molecular interactions within a parcel.

Viscous force can be described in terms of wind shear and shearing stress..

Wind shear ($\frac{\partial u}{\partial z} \neq 0$): change of velocity with height. Shearing stress ($\tau_{zx} = \eta_a \frac{\partial u}{\partial z}$ [Nm⁻²]): Force per unit area, parallel to the direction of motion due to wind shear.

with

$$\eta_a \approx 1.8325 \cdot 10^{-5} \left(\frac{416.16}{T+120}\right) \left(\frac{T}{296.16}\right)^{1.5}$$
: dynamic viscosity of air [kg m⁻¹ s⁻¹]



Figure: Example of shearing stress in x-direction on a volume of air.

$$F_{viscous,zx} = \frac{m}{\rho_a} \frac{\partial \tau_{zx}}{\partial z} =$$
$$= \frac{m}{\rho_a} \frac{\partial}{\partial z} \left(\eta_a \frac{\partial u}{\partial z} \right) \approx$$
$$\approx \frac{m}{\rho_a} \eta_a \frac{\partial^2 u}{\partial z^2}$$

Generalised

$$\vec{F}_{viscous} = m \cdot \frac{\eta_a}{\rho_a} \nabla^2 \vec{v} =$$

$$\overset{Cartesian Coordinates}{=} m \cdot \frac{\eta_a}{\rho_a} \cdot \left(\vec{i} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \vec{j} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + \vec{k} \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) \right)$$



Figure: A linear vertical wind shear results in a constant shearing stress at all heights and no net viscous force. A nonlinear wind shear results in a change of shearing stress with height and a net viscous force.

Example Near surface: $u_1=0 \text{ ms}^{-1} \text{ at } z_1=0\text{ m},$ $u_2=0.4 \text{ ms}^{-1} \text{ at } z_2=0.05\text{ m},$ $u_3=1 \text{ ms}^{-1} \text{ at } z_3=0.1\text{ m}$ $T=288\text{K}, \ \rho_a=1.225 \ kg \ m^{-3} \rightarrow \eta_a=1.792 \cdot 10^{-5} \ kg \ m^{-1} \ s^{-1}$ $\rightarrow \frac{F_{viscous,zx}}{m} \approx \frac{\eta_a}{\rho_a} \frac{1}{(z^3-z^1)/2} \left(\frac{u_3-u_2}{z_3-z_2} - \frac{u_2-u_1}{z_2-z_{21}}\right) = 1.17 \cdot 10^{-3} \ ms^{-2}$ Away from surface: $u_1=10 \ ms^{-1} \ at \ z_1=1000\text{ m},$ $u_2=14 \ ms^{-1} \ at \ z_2=1250 \ m,$ $u_3=20 \ ms^{-1} \ at \ z_3=1500 \ m$ $T=280\text{K}, \ \rho_a=1.085 \ kg \ m^{-3} \rightarrow \eta_a=1.753 \cdot 10^{-5} \ kg \ m^{-1} \ s^{-1}$ $\rightarrow \frac{F_{viscous,zx}}{m} \approx \frac{\eta_a}{\rho_a} \frac{1}{(z^3-z^1)/2} \left(\frac{u_3-u_2}{z_3-z_2} - \frac{u_2-u_1}{z_2-z_{21}}\right) = 5.17 \cdot 10^{-10} \ ms^{-2}$

Turbulent flux divergence

Obstacles at the surface, such as rocks, trees, structures, and mountains, deflect air. The deflected air gives rise to wind shear and eddies downwind of or adjacent to the obstacles. Wind shear and turbulence resulting from obstacles are **mechanical shear** and **mechanical turbulence**, respectively. In atmospheric models, the effects of mechanical shear and buoyancy on the acceleration of a parcel of air are modeled as subgrid scale effects and simulated with turbulent-flux divergence terms. These terms are derived from local acceleration, the continuity equation for air Reynolds decompositions and K-theory.

Local acceleration: (I)
$$\vec{a}_{local} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \vec{\nabla})\vec{v} |\cdot \rho_a$$

Continuity equation (II)
$$\frac{\partial \rho_a}{\partial t} = -\rho_a (\vec{\nabla} \cdot \vec{v}) - (\vec{v} \cdot \vec{\nabla}) \rho_a) | \vec{v}$$

$$|\mathbf{H}|: \qquad \qquad \rho_a \cdot \vec{a}_{local} = \rho_a \left[\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \vec{\nabla}) \vec{v} \right] + \vec{v} \left[\frac{\partial \rho_a}{\partial t} + \vec{\nabla} \cdot (\vec{v} \rho_a) \right]$$

Variables in this equation are decomposed as

$$\vec{v} = \vec{v} + \vec{v}', \rho_a = \overline{\rho}_a + \rho'_a$$

Because density perturbations are generally small ($\rho'_a \ll \overline{\rho}_a$), the density simplifies to $\rho_a \approx \overline{\rho}_a$. Substituting the decomposed values into above formula gives

$$\overline{\rho}_{a} \cdot \vec{a}_{local} = \overline{\rho}_{a} \left\{ \frac{\partial(\vec{v} + \vec{v}')}{\partial t} + [\vec{v} + \vec{v}') \cdot \vec{\nabla}](\vec{v} + \vec{v}') \right\} + (\vec{v} + \vec{v}') \left\{ \frac{\partial \overline{\rho}_{a}}{\partial t} + \vec{\nabla} \cdot [(\vec{v} + \vec{v}')\rho_{a}] \right\}$$

Takling time and grid volume average of this equation, eliminating zero terms and removinbg unnecessary overbars gives

$$\overline{\rho}_{a} \cdot \vec{a}_{local} = \overline{\rho}_{a} \left\{ \frac{\partial \overline{\vec{v}}}{\partial t} + (\overline{\vec{v}} \cdot \overline{\vec{v}}) \overline{\vec{v}} \right\} + \overline{\vec{v}} \left\{ \frac{\partial \overline{\rho}_{a}}{\partial t} + \overline{\vec{v}} \cdot (\overline{\vec{v}} \rho_{a}) \right\} + \overline{\rho}_{a} (\vec{v}' \cdot \overline{\vec{v}}) \overline{\vec{v}}' + \overline{\vec{v}}' \overline{\vec{\nabla}} \cdot (\vec{v}' \overline{\rho}_{a})$$
Remember: $\frac{\partial \overline{\rho}}{\partial t} + \overline{\vec{v}} \cdot (\overline{\vec{v}} \overline{\rho}_{a}) = 0$
Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere

This yields $\overline{\vec{a}_{local}} = \overline{\vec{a}_{local}} + \vec{a}'_{local}$ with

$$\overline{\vec{a}}_{local} = \frac{\partial \overline{\vec{v}}}{\partial t} + (\overline{\vec{v}} \cdot \vec{\nabla}) \overline{\vec{v}}$$

$\vec{a}'_{local} =$	$\vec{F}_{turbulent} = 1$		$\frac{1}{\overline{\rho}_{\mu}(\vec{v}'\cdot\vec{\nabla})\vec{v}'+\vec{v}'\vec{\nabla}\cdot(\vec{v}'\overline{\rho}_{\mu})}$
	m_a	$\overline{\rho}_{a}$	

 $\vec{F}_{turbulent}$ accounts for mechanical shear, buoancy and other eddy effects.

Expanding the turbulent flux divergence term in Cartesian altitude coordinates gives

$$\begin{split} \frac{\vec{F}_{turbulent}}{m_a} &= \frac{1}{\vec{\rho}_a} \left[\overline{\rho_a(\vec{v}' \cdot \vec{\nabla}) \vec{v}' + \vec{v}' \vec{\nabla} \cdot (\vec{v}' \, \vec{\rho}_a)} \right] = \\ &= \vec{i} \frac{1}{\rho_a} \left[\frac{\partial(\rho_a \overline{u' u'})}{\partial x} + \frac{\partial(\rho_a \overline{v' u'})}{\partial y} + \frac{\partial(\rho_a \overline{w' u'})}{\partial z} \right] + \\ &+ \vec{j} \frac{1}{\rho_a} \left[\frac{\partial(\rho_a \overline{u' v'})}{\partial x} + \frac{\partial(\rho_a \overline{v' v'})}{\partial y} + \frac{\partial(\rho_a \overline{w' v'})}{\partial z} \right] + \\ &+ \vec{k} \frac{1}{\rho_a} \left[\frac{\partial(\rho_a \overline{u' w'})}{\partial x} + \frac{\partial(\rho_a \overline{v' w'})}{\partial y} + \frac{\partial(\rho_a \overline{w' w'})}{\partial z} \right] \end{split}$$

Averages such as $\overline{u'u'}$, $\overline{w'v'}$ are kinematic turbulent fluxes. Each such average must be parameterized. With K-theory, vertical kinematic turbulent fluxes are approximated with e.g.

$$\overline{w'u'} = -K_{m,zx} \frac{\partial \overline{u}}{\partial z}, \ \overline{w'v'} = -K_{m,zy} \frac{\partial \overline{v}}{\partial z}$$

where Km's are eddy diffusion coefficients for momentum.

$$\frac{\vec{F}_{turbulent}}{m_a} = -\vec{i} \frac{1}{\rho_a} \left[\frac{\partial}{\partial x} \left(\rho_a K_{m,xx} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\rho_a K_{m,yx} \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\rho_a K_{m,zx} \frac{\partial u}{\partial z} \right) \right] - - \vec{j} \frac{1}{\rho_a} \left[\frac{\partial}{\partial x} \left(\rho_a K_{m,xy} \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\rho_a K_{m,yy} \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\rho_a K_{m,zy} \frac{\partial v}{\partial z} \right) \right] - - \vec{k} \frac{1}{\rho_a} \left[\frac{\partial}{\partial x} \left(\rho_a K_{m,xz} \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left(\rho_a K_{m,yz} \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial z} \left(\rho_a K_{m,zz} \frac{\partial w}{\partial z} \right) \right]$$

Each term in this equation is an acceleration in one direction due to transport of momentum normal to that direction. The *zx* term is an acceleration in the *x*-direction due to a gradient in wind shear and transport of momentum in the *z*-direction Kinematic turbulent fluxes are analogous to shearing stresses in that both result when momentum is transported down a gradient of velocity. In case of viscosity, momentum is transported by molecular diffusion. In the case of turbulence, momentum is transported by eddy diffusion.

In tensor (matrix) form

$$K_{m} = \begin{bmatrix} K_{m,xx} & K_{m,yx} & K_{m,zx} \\ K_{m,xy} & K_{m,yy} & K_{m,zy} \\ K_{m,xz} & K_{m,yz} & K_{m,zz} \end{bmatrix}$$

In vector and tensor notation

$$\frac{\vec{F}_{turbulence}}{m_a} = -\frac{1}{\rho_a} \left(\vec{\nabla} \cdot \rho_a K_m \vec{\nabla} \right) \vec{v}$$

Example

300 m

Vertical eddy diffusion coefficient in middle of boundary layer : $K_m = 50m^2s^{-1}$ $u_1 = 10 ms^{-1}$ at $z_1 = 300m$, $u_2 = 12ms^{-1}$ at $z_2 = 350m$, $u_3 = 15ms^{-1}$ at $z_3 = 400m$ $\frac{F_{turbulence, zx}}{m} = \frac{1}{\rho_a} \frac{\partial}{\partial z} \left(\rho_a K_{m,zx} \frac{\partial u}{\partial z} \right) \approx \frac{K_{m,zx}}{(z_3 - z_1)/2} \left(\frac{u_3 - u_2}{z_3 - z_2} - \frac{u_2 - u_1}{z_2 - z_1} \right) = 0.02ms^{-2}$: west east acceleration of wind due to transfer of westerly momentum from 400 to

SUMMARY MOMENTUM EQUATIONS

Complete momentum equation

$$\frac{d\vec{v}}{dt} = -f\vec{k} \times \vec{v} + \frac{F_g}{m_a} - \frac{1}{\rho_a}\vec{\nabla}p_a + \frac{\eta_a}{\rho_a}\nabla^2\vec{v} + \frac{1}{\rho_a}(\vec{\nabla}\cdot\rho_aK_m\vec{\nabla})\vec{v}$$

Term	Acceleration or Force/Mass Expression	Horizontal Accel. (m s ⁻²)	Vertical Accel. (m s ⁻²)
Local acceleration	$\bar{\mathbf{a}}_l = rac{\mathrm{d} \bar{\mathbf{v}}}{\mathrm{d} t} = rac{\partial \bar{\mathbf{v}}}{\partial t} + (\bar{\mathbf{v}} ullet abla) \bar{\mathbf{v}}$	10^{-4}	^a 10 ⁻⁷ -1
Coriolis force per unit mass	$\frac{\mathbf{F}_{c}}{M_{a}} = f \mathbf{k} \times \mathbf{v}$	10^{-3}	0
Effective gravitational force per unit mass	$rac{\mathrm{F}_g}{M_a} = rac{\mathrm{F}_g^*}{M_a} + rac{\mathrm{F}_r}{M_a} = - abla \Phi$	0	10
Pressure-gradient force per unit mass	$\frac{\mathbf{F}_p}{M_a} = -\frac{1}{\rho_a} \nabla p_a$	10^{-3}	10
Viscous force per unit mass	$\frac{\mathbf{F}_v}{M_a} = \frac{\mathbf{\eta}_a}{\rho_a} \nabla^2 \mathbf{v}$	$^{b}10^{-12} - 10^{-3}$	$b10^{-15} - 10^{-5}$
Turbulent flux divergence of momentum	$\frac{\mathbf{F}_t}{M_a} = -\frac{1}{\rho_a} (\nabla \cdot \rho_a \mathbf{K}_m \nabla) \mathbf{v}$	^c 0–1	^c 0–1

^aLow value for large-scale motions; high value for small-scale motions (<3 km).

^bLow value for free atmosphere, high value for air adjacent to the surface.

^cLow value for no wind shear, high value for large wind shear.

Table: Terms in the momentum equations and their horizontal and vertical magnitudes

GLOBAL CIRCULATION





FIGURE 3.1.3

A plan view of the life cycle of a Northern Hemisphere frontal cyclone: (a) surface front between cold and warm air; (b) wave beginning to form; (c) cyclonic circulation and wave have developed; (d) fastermoving cold front is overtaking retreating warm front and reducing warm sector; (e) warm sector has been eliminated and (f) cyclone is dissipating.

NONLINEAR DYNAMICS AND CHAOS

Numerical Weather Prediction (NWP) is an **initial value problem**, where these initial values are based on observed weather conditions. Unfortunately these observations include instrumentation and sampling errors. How do these errors affect the long range predictability?

Equations of motion are nonlinear (because they contain products of variables like *uv*,*uw*,*etc*) are very **sensitive to initial conditions**. Such sensitivities means that substantially different weather forecasts can result from slightly different initial conditions.

One **famous illustration** of sensitive dependence to initial conditions was suggested by **Ed Lorenz**: 2-D convection within a tank of water, where the bottom of the tank is heated. The vertical temperature gradient from bottom to top drives a circulation of water, with warm fluid trying to rise. The circulation can modify the temperature distribution within the tank.

A very specialised, highly simplified set of equations that approximates this flow is

$$\frac{\partial C}{\partial t} = \sigma \cdot (L - C)$$
$$\frac{\partial L}{\partial t} = r \cdot C - L - C \cdot M$$
$$\frac{\partial M}{\partial t} = C \cdot L - b \cdot M$$

with

C: circulation (positive for clockwise, greater magnitude for a more vigorous circulation)

L: left-right distribution of temperature (positive for warm water on the left)

M: amount of vertical mixing (0 for linear temperature gradient, positive when temperature is more uniformly mixed within the middle of the tank)



Figure: Tank of fluid (shaded), showing circulation C. The vertical M and horizontal L distributions of temperature are also shown



Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere



Figure: "Butterfly" showing evolution of the solution to the Lorenz equations in phase space.

Modelling Water and Energy Fluxes at the Land Surface and in the Atmosphere



Figure: Time evolution of circulation C and mixing M; M(0)=45



Lorentz Attractor

Figure: Time evolution of circulation C and mixing M; M(0)=44

SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS USING FINITE DIFFERENCE SCHEMES

An ordinary differential equation (ODE) is an equation with one independent variable, such as time; a Partial Differential Equation (PDE) is an equation with more than one independent variable, such as time and space.

Order of a PDE,ODE: highest derivative rank of the equation

Degree of a PDE,ODE: highest polynomial exponent of the highest derivative

Finite Difference Approximations to Advection–Diffusion Equations

$$\frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} - \frac{1}{\rho_a} \frac{\partial}{\partial x} (\rho_a K_{xx} \frac{\partial q}{\partial x}) = Q$$

A finite difference approximation involves the replacement of each continuous differential operator with a discrete analog.









$$\frac{\partial u}{\partial x} \approx \frac{\Delta u_i}{\Delta x_i} = \frac{u_{i+1} - u_{i-1}}{x_{i+1} - x_{i-1}}$$

Order	т	q	Approximation
(a) 1st order backward	1	2	$\frac{\partial N}{\partial x} \approx \frac{N_i - N_{i-1}}{\Delta x}$
(b) 1st order forward	1	2	$\frac{\partial N}{\partial x} \approx \frac{N_{i+1} - N_i}{\Delta x}$
(c) 2nd order central	1	3	$\frac{\partial N}{\partial x} \approx \frac{N_{i+1} - N_{i-1}}{2\Delta x}$
(d) 2nd order backward	1	3	$\frac{\partial N}{\partial x} \approx \frac{N_{i-2} - 4N_{i-1} + 3N_i}{2\Delta x}$
(e) 2nd order forward	1	3	$\frac{\partial N}{\partial x} pprox \frac{-3N_i + 4N_{i+1} - N_{i+2}}{2\Delta x}$
(f) 3rd order backward	1	4	$\frac{\partial N}{\partial x} \approx \frac{N_{i-2} - 6N_{i-1} + 3N_i + 2N_{i+1}}{6\Delta x}$
(g) 3rd order forward	1	4	$\frac{\partial N}{\partial x} \approx \frac{-2N_{i-1}-3N_i+6N_{i+1}-N_{i+2}}{6\Delta x}$
(h) 4th order central	1	5	$\frac{\partial N}{\partial x} \approx \frac{N_{i-2} - 8N_{i-1} + 8N_{i+1} - N_{i+2}}{12\Delta x}$
(i) 4th order backward (I)	1	5	$\frac{\partial N}{\partial x} \approx \frac{-N_{i-3} + 6N_{i-2} - 18N_{i-1} + 10N_i + 3N_{i+1}}{12\Delta x}$
(j) 4th order forward (I)	1	5	$\frac{\partial N}{\partial x} \approx \frac{-3N_{i-1}-10N_i+18N_{i+1}-6N_{i+2}+N_{i+3}}{12\Delta x}$
(k) 4th order backward (II)	1	5	$\frac{\partial N}{\partial x} \approx \frac{-3N_{i-4} + 16N_{i-3} - 36N_{i-2} + 48N_{i-1} - 25N_i}{12\Delta x}$
(l) 4th order forward (II)	1	5	$\frac{\partial N}{\partial x} \approx \frac{25N_i - 48N_{i+1} + 36N_{i+2} - 16N_{i+3} + 3N_{i+4}}{12\Delta x}$
(m) 2nd order central	2	3	$rac{\partial^2 N}{\partial x^2} pprox rac{N_{i+1} - 2N_i + N_{i-1}}{\Delta x^2}$
(n) 4th order central	2	5	$\frac{\partial^2 N}{\partial x^2} \approx \frac{-N_{i-2} + 16N_{i-1} - 30N_i + 16N_{i+1} - N_{i+2}}{12\Delta x^2}$

Table: Finite difference approximations of
$$\frac{\partial N}{\partial x}$$
, $\frac{\partial^2 N}{\partial x^2}$ (Jacobson, 2005)

Stability criteria for the Advection-Diffusion Equation

If the eddy diffusion term is removed and no sinks/sources are present, the humidity equation reduces to the west-east advection equation

$$\frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} = 0$$

For certain explicit finite difference scheme approximations, stability is maintained when

$$\Delta t < \frac{\Delta x_{\min}}{\left| u_{\max} \right|}$$

(Courant-Friedrich-Levy-Criterium)

with

u_{max}: maximum west-east scalar velocity

 Δx_{min} : minimum west-east grid cell-length in the domain

 Δt : time step

A parcel of air is not allowed to travel across a grid cell during a single time step

Example 5:

 $u_{max}=20 \text{ ms}^{-1}$, $\Delta x_{min}=5 \text{ km gives } \Delta t_{max}=250 \text{ s}$

If advection is ignored, the humidity equation reduces to the west east diffusion equation

$$\frac{\partial q}{\partial t} - \frac{1}{\rho_a} \frac{\partial}{\partial x} (\rho_a K_{xx} \frac{\partial q}{\partial x}) = 0$$

Stability criterion:

$$\Delta t < \frac{\Delta x^2_{\min}}{K_{\max}}$$

K_{max}: largest eddy diffusion coefficient in the domain

Example 6:

 Δx_{min} =5 km, $K_{max,vertical}$ = 50 m²s⁻¹ gives Δt_{max} =200 s

 Δx_{min} =5 km, $K_{max,horizontal}$ = 2,500 m²s⁻¹ gives Δt_{max} =10,000 s

Explicit solutions to the diffusion equation are more likely to become unstable in the vertical than in the horizontal direction in an atmospheric model.

Forward Euler scheme (explicit)

$$\frac{q_{i,t} - q_{i,t-\Delta t}}{\Delta t} + u \frac{q_{i+1,t-\Delta t} - q_{i-1,t-\Delta t}}{2\Delta x} - K_{xx} \frac{q_{i+1,t-\Delta t} - 2q_{i,t-\Delta t} + q_{i-1,t-\Delta t}}{\Delta x^2} = 0$$



Implicit Scheme

$$\frac{q_{i,t} - q_{i,t-\Delta t}}{\Delta t} + u \frac{q_{i+1,t} - q_{i-1,t}}{2\Delta x} - K_{xx} \frac{q_{i+1,t} - 2q_{i,t} + q_{i-1,t}}{\Delta x^2} = 0$$

Solution along i = 1, ..., *I* is obtained by rearranging the equation as

$$A_{i}q_{i-1,t} + B_{i}q_{i,t} + D_{i}q_{i+1,t} = q_{i,t-h}$$

with

$$A_{i} = -\Delta t \left(\frac{u}{2\Delta x} + \frac{K}{\Delta x^{2}} \right)_{i-1}$$
$$B_{i} = 1 + \Delta t \left(\frac{2K}{\Delta x^{2}} \right)_{i}$$
$$D_{i} = \Delta t \left(\frac{u}{2\Delta x} - \frac{K}{\Delta x^{2}} \right)_{i+1}$$

leading to a matrix equation

$$\begin{bmatrix} B_{1} & D_{1} & 0 & 0 & & & & \\ A_{2} & B_{2} & D_{2} & 0 & & & & \\ 0 & A_{3} & B_{3} & D_{3} & & & & \\ 0 & 0 & A_{4} & B_{4} & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & &$$

of form

 $\mathbf{M} \cdot \vec{x} = \vec{s}$

which can be solved e.g. via

 $\vec{x} = \mathbf{M}^{-1} \cdot \vec{s}$

Finite Differencing in Two Directions

$$\frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} + v \frac{\partial q}{\partial x} - \frac{1}{\rho_a} \frac{\partial}{\partial x} (\rho_a K_{xx} \frac{\partial q}{\partial x}) - \frac{1}{\rho_a} \frac{\partial}{\partial y} (\rho_a K_{yy} \frac{\partial q}{\partial y}) = Q$$

$$\left|\frac{q_{i,t} - q_{i,t-\Delta t}}{\Delta t} + \left(u\frac{q_{i+1,j} - q_{i-1,j}}{2\Delta x} + v\frac{q_{i,j+1} - q_{i,j-1}}{2\Delta y}\right)_{t} - \left(K_{xx}\frac{q_{i+1,j} - 2q_{i,j} + q_{i-1,j}}{\Delta x^{2}} - K_{yy}\frac{q_{i,j+1} - 2q_{i,j} + q_{i,j-1}}{\Delta y^{2}}\right)_{t} = 0\right|$$

(*j*: index in north-south direction)

The equation is linear for all *i*,*j* and can be solved implicitly in matrix form.

Disadvantage: 100x100 horizontal grid required matrix is 10,000x10,000. Advantage: solution is unconditionally stable for all values u, v, K_{xx}, K_{yy}

OVERVIEW VECTORS ANALYSIS

Cartesian coordinates

 $\vec{a} = (a_x, a_y, a_z) = \vec{i} a_x + \vec{j} a_y + \vec{k} a_z$

 $\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y + a_z b_z = \left| \vec{a} \right| \left| \vec{b} \right| \cos \theta$: scalar or dot product



Figure: Illustration dot product

 $\vec{c} = \vec{a} \times \vec{b} = (a_y b_z - a_z b_y, a_z b_x - a_x b_z, a_x b_y - a_y b_x) : \text{ cross product}$ $|\vec{c}| = |\vec{a}| |\vec{b}| \sin \theta$



Figure: Illustration vector product

Nabla operator notation

 $\vec{\nabla} = \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}$: Nabla operator

$$\vec{\nabla}N = (\mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z})N = \mathbf{i}\frac{\partial}{\partial x}N + \mathbf{j}\frac{\partial}{\partial y}N + \mathbf{k}\frac{\partial}{\partial z}N$$

$$\vec{\nabla} \cdot \vec{v} = (\mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}) \cdot (\mathbf{i}u + \mathbf{j}v + \mathbf{k}w) = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

$$(\vec{v} \cdot \vec{\nabla})N = (u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z})N = u \frac{\partial N}{\partial x} + v \frac{\partial N}{\partial y} + w \frac{\partial N}{\partial z}$$