Lecture, Summer term 2011, LMU München

An Introduction to Global Atmospheric Modelling

Lecture 4: Numerical Formulation in CCMs

<u>Content:</u>

- Numerical Formulation in Atmospheric Chemistry Models
- Methods to Solve Differential Equations
- Steps in Model Formulation

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Oberpfaffenhofen

Outline

- **Lecture 1 (27 April):** Introduction to Global Atmospheric Modelling
- **Lecture 2 (04 May):** Physical Climate Models & Fundamentals Atmospheric Radiation
- **Lecture 3 (11 May):** Fundamentals: Chemistry
- **Lecture 4 (18 May):** Numerical Formulation in CCMs & Steps in Model Formulation
- **Lecture 5 (25 May):** Introduction into NCAR Command Language (NCL)
- **Lecture 6 (1 June):** NCL practice (Dr Mattia Righi) **Doppelstunde**

Preliminary schedule:

- **Lecture 7 (8 June):** moved to 1 June
- **Lecture 8 (15 June):** Fundamentals: Dynamics
- **Lecture 9 (22 June):** Model Evaluation and uncertainties in climate projections
- **Lecture 10 (29 June):** International climate modelling activities: Part 1
- **Lecture 11 (6 July):** EXAM
- **Lecture 12 (13 July):** International climate modelling activities: Part 2
- **Lecture 13 (20 July):** Summary

Final Exam: 6 July 2012, 8:00-10:00

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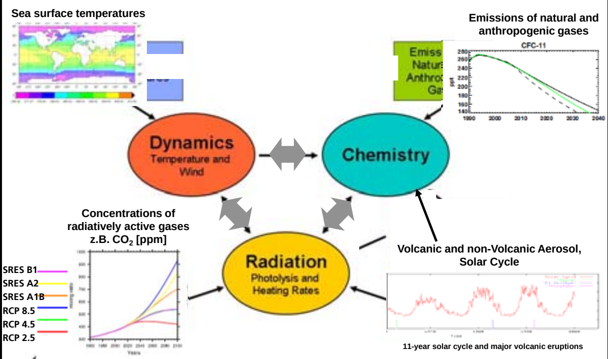
Gekoppelte Chemie-Klima Modelle (CCMs)



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Numerical Formulation

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Building a chemical model

$$\frac{d[y_i]}{dt} = P_i - L_i\,[y_i]$$

P: Chemical Production

L: Chemical Loss

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Equation for Chemical Box Models

Determination of C_i (Determination of chemical loss and production rates)

$$C_i = \frac{d[y_i]}{dt} = P_i - L_i\,[y_i]$$

$$P_i = \sum_{j\neq i, l\neq i} k_{jl}[j][l] + \sum_{m\neq i} j_m[m]$$

$$L_i = \sum_j k_{ij}[j] + k_i$$

k_{jl} : *reaction coefficients*

j_m : *photolysis rates*

Different chemical reactions

- bi-molecular
- tri-molecular
- thermal decay
- heterogeneous
- photolysis

Determination of C_i implies simultaneous solution of up to hundreds of coupled differential equations, containing many non-linear reactions.

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Reaction Rate Coefficients

How do we determine the reaction rate coefficients?

↓

Chemical Kinetics

The study of reaction rates (the change in reactant and product concentrations as a function of time).

Factors that Effect Reaction Rates

A. Concentration – As concentration increases, the reaction rate increases.

Reaction Rate ∝ Concentration

B. Physical State of Reactants – Reactants must mix and collide in order to react.

C. Temperature – As temperature increases, the reaction rate increases.

Reaction Rate ∝ Temperature

D. Catalyst – A substance that increases the rate of a reaction without being consumed in the process.

The Differential Rate Law

How does the rate of the reaction depend on concentration? E.g.

$$3A + 2B \rightarrow C + D$$

$$\text{rate} = k\,[A]^m[B]^n$$

m+n: Overall order of the reaction

(Specific reaction) rate constant

Order of reaction with respect to A

Order of reaction with respect to B

Each reaction is characterized by its own rate constant, depending on the nature of the reactants and the temperature

In general, the order with respect to each reagent must be found experimentally (not necessarily equal to soichiometric coefficienct)

Elementary Processes and Rate Laws

Reaction mechanism:

The collection of elementary processes by which an overall reaction occurs

The order of an elementary process is predictable

Unimolecular	$A^* \rightarrow B$	k [A]	First order
Bimolecular	$A + B \rightarrow C + D$	k [A] [B]	Second order
Termolecular	$A + B + C \rightarrow D + E$	k [A] [B] [C]	Third order

Chemical Kinetics

A reaction

A + B -> products

proceeds at a rate proportional to the concentrations raised to some power

$$\boxed{Rate = \frac{d[A]}{dt} = \frac{d[B]}{dt} = k[A]^{\alpha}[B]^{\beta}}$$

- k is the rate coefficient (rate constant). The powers a and b are the order of the reaction with respect to the reactants i.e.

  $\alpha A + \beta B \rightarrow$ products

- If for example a=b=1 then the reaction is called a second order reaction ($\alpha+\beta=2$) .

Chemical Kinetics: Bimolecular Reactions

A reaction

A + B -> C + D

proceeds at a rate proportional to the concentrations raised to some power

$$\boxed{\frac{d[A]}{dt} = -\frac{d[C]}{dt} = -k_b[A][B]}$$

- k is the rate coefficient (rate constant).
- k_b can be calculated by Arrhenius Law: **the rate of a chemical reaction increases exponentially with the absolute temperature.**

$$\boxed{k_b = Ae^{-\frac{E_a}{RT}}}$$

B. Arrhenius Equation

- Summarizes the tenets of collision theory into an equation that can be used to calculate the rate constant for a reaction.

$$k = \text{rate constant} = \underbrace{A}_{\text{Frequency factor}}\underbrace{e^{-E_a/RT}}_{\text{Fraction of molecules with sufficient energy}}$$

R = 8.315 x 10^{-3} kJ/K•mol
T = temperature (K)

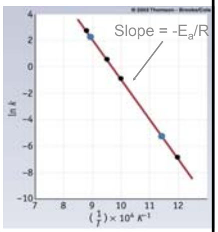
B. Arrhenius Equation

- $\mathbf{E_a}$ can be determined by finding ***k*** for a reaction experimentally at several temperatures.

$$k = Ae^{-E_a/RT}$$

Take *ln* and rearrange

$$\ln(k) = \ln\left(Ae^{-E_a/RT}\right) \Rightarrow \underbrace{\ln k}_{y} = \underbrace{-\frac{E_a}{R}\left(\frac{1}{T}\right)}_{mx} + \underbrace{\ln A}_{b}$$



A reaction

A + B + M -> C + M

proceeds at a rate proportional to the concentrations raised to some power

$$\boxed{\frac{d[A]}{dt} = -k_t[A][B]}$$

$$k_t(M,T) = \frac{k_0(T)[M]}{1+(k_0(T)[M]/k_\infty(T))} \cdot F(M, k_0(T), k_\infty(T)).$$

High pressure case

$$k_\infty = \lim_{[M]\to\infty} k_t(M,T).$$

Low pressure case

$$k_0 = \lim_{[M]\to 0} k_t(M,T).$$

Fit between low and high pressure case

$$\log_{10} F \cong \frac{\log_{10} F_c}{1+[\log_{10}(k_0(T)[M])/k_\infty(T)]^2},$$

Determination of k_0 and k_∞ in the lab at T=300K

$$k_{0(\infty)}(T) = k_{0(\infty)}^{300}(T/300)^{-n(m)}$$

JPL catalogue: k_0, n, k_∞, m

A reaction

$$\mathbf{A + B \xrightarrow{het} C + D}$$

$$\boxed{\frac{d[A]}{dt} = -k_{het}[A][B]}$$

Reactions that occur at the interface between condensed and gaseous phases, i.e. the surface

In liquids, the reactions tend to be inside the particle.

In solids, the diffusion from the surface is extremely small, and the reactions are confined to the surface.

On liquid surfaces

$$k_{het} = \frac{\omega A \gamma}{4}$$

$$\omega = \sqrt{8k_b T/\pi m}$$

A: surface

γ : uptake coefficient

On solid surfaces

$$k_{het,s} = \frac{\gamma \pi r^2 \omega [A] n}{1 + 3\gamma_s r/(4l_a)}$$

[A]: concentration
l_a : mean free path length
r: radius
γ : sticking coefficient (reaction probability)

First order reaction

$$\boxed{A + h\nu \to C + D}$$

Time Dependence for A (J is the photolysis frequency [s^{-1}]):

$$\frac{d[A]}{dt} = -J[A].$$

Example:

$$O_2 + h\nu\ (\lambda < 242\text{nm}) \longrightarrow 2\ O.$$

Species A undergoes photodissociation.

Reaction *i*: A + hν → products

$$\underbrace{\left.\frac{d[A]}{dt}\right)_{reac\ i}}_{\text{A concentration rate of change due to photolysis reaction } i} = \underbrace{-[A]\cdot\int \underbrace{\underbrace{\sigma_X(\lambda)}_{\text{A absorption cross section}}\ \underbrace{\phi_i(\lambda,T,\ldots)}_{\text{Reaction } i \text{ quantum yield}}}_{\text{Action spectrum}}\ \underbrace{E(\lambda,\ldots)}_{\text{Spectral actinic flux}}\ d\underbrace{\lambda}_{\text{Wavelength}}}_{\text{Reaction rate coefficient j}}$$

$$J = \int_\lambda \sigma(\lambda)\varphi(\lambda)\int_\omega I(\lambda,\theta,\phi)\,d\omega\,d\lambda$$

Recommended Set of Equation for Stratospheric Modelling

	Photolysereaktion	Absorptionsquerschnitt	Quantenausbeute	Wellenlängen	
*	$O_2 + h\nu \longrightarrow 2O(^3P)$	*Minschwaner et al.* (1992)	QA = 1	175 – 240 nm	B1
		Yoshino et al. (1988)			
*	$O_3 + h\nu \longrightarrow O(^3P) + O_2$	*DeMore et al.* (1994),	*DeMore et al.* (1994)	175 – 850 nm	B2
		Paur und Bass (1985)			
*	$O_3 + h\nu \longrightarrow O(^1D) + O_2$	*DeMore et al.* (1994)	a) *DeMore et al.* (1994)	175 – 320 nm	B3
		Paur und Bass (1985)	b) *Ball et al.* (1994)	175 – 325 nm	
			c) *Michelsen et al.* (1994)	175 – 325 nm	
*	$H_2O + h\nu \rightarrow OH + H$	*DeMore et al.* (1994)	QA = 1 [1]	175 – 189 nm	
*	$H_2O_2 + h\nu \rightarrow 2\,OH$	*DeMore et al.* (1994)	QA = 1	190 – 350 nm	B4
*	$CH_2O + h\nu \longrightarrow HCO + H$	a) *DeMore et al.* (1994)	*DeMore et al.* (1994)	300 – 358 nm	B5
		b) *Meller* (1991)		225 – 376 nm	
*	$CH_2O + h\nu \longrightarrow CO + H_2$	a) *DeMore et al.* (1994)	*DeMore et al.* (1994)	300 – 358 nm	B5
		b) *Meller* (1991)		225 – 376 nm	
	$CH_3CHO + h\nu \rightarrow CH_4 + CO$	*Atkinson et al.* (1992)	*Atkinson et al.* (1992)	200 – 295 nm	B6
	$CH_3CHO + h\nu \longrightarrow CH_3 + HCO$	*Atkinson et al.* (1992)	*Atkinson et al.* (1992)	200 – 330 nm	B6
*	$CH_3O_2H + h\nu \longrightarrow CH_3O$ + Produkte	*DeMore et al.* (1994)	QA = 1 [1]	210 – 360 nm	
*	$CH_3O_2NO_2 + h\nu \rightarrow$ Produkte	*Atkinson et al.* (1992)	*Atkinson et al.* (1992)	200 – 325 nm	
*	$NO + h\nu \longrightarrow N + O(^3P)$	*Minschwaner und Siskind* (1993)	*Minschwaner und Siskind* (1993)	181 – 192 nm	B7
*	$NO_2 + h\nu \rightarrow NO + O(^3P)$	a) *DeMore et al.* (1994)	*DeMore et al.* (1994)	202 – 423 nm	B8
		b) *Schneider et al.* (1987)			
*	$NO_3 + h\nu \rightarrow NO + O_2$	*Wayne et al.* (1991)	*Wayne et al.* (1991)	584 – 641 nm	B9
*	$NO_3 + h\nu \longrightarrow NO_2 + O(^3P)$	*Wayne et al.* (1991)	*Wayne et al.* (1991)	400 – 641 nm	B9
*	$N_2O + h\nu \longrightarrow N_2 + O(^1D)$	*DeMore et al.* (1994)	QA = 1 [1]	175 – 240 nm	B10
*	$N_2O_5 + h\nu \rightarrow NO_3$ + Produkte	*Yao et al.* (1982) [1]	QA = 1 [1]	200 – 380 nm	B11
	$HONO + h\nu \longrightarrow OH + NO$	*Bongartz et al.* (1991) [1]	QA = 1	300 – 399 nm	
*	$HNO_3 + h\nu \rightarrow OH + NO_2$	*Burkholder et al.* (1993) [1]	QA = 1	186 – 350 nm	B12
*	$HNO_4 + h\nu \longrightarrow NO_2 + HO_2$	a) *DeMore et al.* (1994)	QA = 0.67 [1]	190 – 325 nm	B13
		b) *Singer et al.* (1989)		190 – 329 nm	
	$HNO_4 + h\nu \longrightarrow NO_3 + OH$	a) *DeMore et al.* (1994)	QA = 0.33 [1]	190 – 325 nm	B13

[1] empfohlen von [*DeMore et al.* (1994)]

Recommended Set of Equation for Stratospheric Modelling

p =3.11 mbar,
T = 252.3 K.
Photolysis
frequency for
SZA=60°,
h=39,63 km.

		b) *Singer et al.* (1989)		190 – 329 nm	
*	$Cl_2 + h\nu \rightarrow 2\,Cl$	*Maric et al.* (1993) [1]	QA = 1	250 – 500 nm	
	$ClO + h\nu \longrightarrow Cl + O(^3P)$	*Simon et al.* (1990)	QA = 1	237 – 312 nm	B14
*	$OClO + h\nu \longrightarrow ClO + O(^3P)$	*Wahner et al.* (1987) [1]	QA = 1 [1]	242 – 473 nm	B15
	$ClOO + h\nu \longrightarrow ClO + O(^3P)$	*DeMore et al.* (1994)	QA = 1	220 – 280 nm	
	$Cl_2O + h\nu \longrightarrow Cl + ClO$	*Simon* (1989)	QA = 0.75 [1]	237 – 500 nm	B16
		DeMore et al. (1994)			
	$Cl_2O + h\nu \longrightarrow Cl_2 + O(^3P)$	*Simon* (1989)	QA = 0.25 [1]	237 – 500 nm	B16
		DeMore et al. (1994)			
*	$ClOOCl + h\nu \longrightarrow Cl + ClOO$	*DeMore et al.* (1994)	QA = 1 [1]	190 – 450 nm	
*	$HOCl + h\nu \longrightarrow OH + Cl$	*DeMore et al.* (1994)	QA = 1	200 – 380 nm	B17
*	$HCl + h\nu \longrightarrow H + Cl$	*DeMore et al.* (1994)	QA = 1	175 – 220 nm	
	$ClONO + h\nu \longrightarrow Cl$ + Produkte	*DeMore et al.* (1994)	QA = 1 [1]	235 – 400 nm	
*	$ClNO_2 + h\nu \longrightarrow Cl$ + Produkte	*DeMore et al.* (1994)	QA = 1 [1]	190 – 370 nm	
*	$ClONO_2 + h\nu \longrightarrow Cl + NO_3$	a) *Burkholder et al.* (1994) [1]	QA = 0.9 [1]	196 – 432 nm	B18
		b) *DeMore et al.* (1992)			
	$ClONO_2 + h\nu \longrightarrow O(^3P) + ClONO$	a) *Burkholder et al.* (1994) [1]	QA = 0.1 [1]	196 – 432 nm	B18
		b) *DeMore et al.* (1992)			
	$CCl_4 + h\nu \longrightarrow Cl$ + Produkte	*DeMore et al.* (1994)	QA = 1 [1]	175 – 275 nm	
	$CCl_3F + h\nu \longrightarrow Cl$ + Produkte	*DeMore et al.* (1994)	QA = 1 [1]	175 – 260 nm	
*	$BrCl + h\nu \rightarrow Br + Cl$	*Maric et al.* (1994)	QA = 1	200 – 600 nm	B19
	$Br_2 + h\nu \longrightarrow 2\,Br$	*Maric et al.* (1994)	QA = 1	200 – 650 nm	B19
	$BrO + h\nu \longrightarrow Br + O(^3P)$	*Wahner et al.* (1988)	QA = 1	312 – 388 nm	B20
*	$BrONO_2 + h\nu \longrightarrow$ Produkte	a) *DeMore et al.* (1994)	QA = 1	186 – 390 nm	B21
		b) *Deters et al.* (1997)		209 – 509 nm	
		c) *Burkholder et al.* (1995)		200 – 500 nm	
	$Br_2O + h\nu \rightarrow$ Produkte	a) *Orlando und Burkholder* (1995)	QA = 1	196 – 432 nm	B22
		b) *Deters et al.* (1996)		208 – 444 nm	
	$HOBr + h\nu \rightarrow Br + OH$	a) *Orlando und Burkholder* (1995)	QA = 1	245 – 395 nm	B23
		b) *Deters et al.* (1996)		242 – 401 nm	
		c) *Rattigan et al.* (1996)		240 – 510 nm	
	$HOBr_{\lambda L} + h\nu \rightarrow$ Produkte	*Deters* (1996)	QA = 1	243 – 387 nm	
	$IO + h\nu \longrightarrow I + O(^3P)$	*Himmelmann* (1997)	QA = 1	373 – 480 nm	B24
		Harwood et al. (1997)		338 – 472 nm	
	$OIO + h\nu \longrightarrow$ Produkte	*Himmelmann* (1997)	QA = 1	480 – 667 nm	B24

Recommended Set of Equation for Stratospheric Modelling

p =3.11 mbar,
T = 252.3 K.
Photolysis
frequency for
SZA=60°,
h=39,63 km.

			k
$O_2 + h\nu$	$\longrightarrow$	$2\,O$	2.44(-10)
$O_3 + h\nu(\lambda < 325nm)$	$\longrightarrow$	$O(^1D) + O_2$	9.46(-04)
$O_3 + h\nu$	$\longrightarrow$	$O(^3P) + O_2$	6.53(-04)
$O(^3P) + O_2 + M$	$\longrightarrow$	$O_3 + M$	7.98(-17)
$O(^3P) + O_3$	$\longrightarrow$	$2O_2$	2.28(-15)
$O(^1D) + O_2$	$\longrightarrow$	$O(^3P) + O_2$	4.22(-11)
$O(^1D) + N_2$	$\longrightarrow$	$O(^3P) + N_2$	2.78(-11)
$O(^1D) + H_2O$	$\longrightarrow$	$2\,OH$	2.2(-10)
$O(^1D) + H_2$	$\longrightarrow$	$OH + H$	1.0(-10)
$O(^1D) + CH_4$	$\longrightarrow$	$OH + CH_3(*)$	1.5(-10)
$H + O_2 + M$	$\longrightarrow$	$HO_2 + M$	6.52(-15)
$H + O_3$	$\longrightarrow$	$OH + O_2$	2.17(-11)
$H + HO_2$	$\longrightarrow$	$2\,OH$	7.3(-11)
$H + HO_2$	$\longrightarrow$	$H_2O + O(^3P)$	1.6(-12)
$H + HO_2$	$\longrightarrow$	$H_2 + O_2$	6.5(-12)
$OH + O_3$	$\longrightarrow$	$HO_2 + O_2$	3.86(-14)
$OH + HO_2$	$\longrightarrow$	$H_2O + O_2$	1.29(-10)
$OH + H_2$	$\longrightarrow$	$H_2O + H$	1.99(-15)
$OH + O(^3P)$	$\longrightarrow$	$O_2 + H$	3.54(-11)

Recommended Set of Equation for Stratospheric Modelling

p =3.11 mbar,
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Photolysis
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$OH + OH$	$\longrightarrow$	$H_2O + O(^3P)$	1.62(-12)
$HO_2 + O_3$	$\longrightarrow$	$OH + O_2$	1.52(-15)
$HO_2 + HO_2$	$\longrightarrow$	$H_2O_2 + O_2$	2.48(-12)
$HO_2 + O(^3P)$	$\longrightarrow$	$OH + O_2$	6.63(-11)
$H_2O_2 + h\nu$	$\longrightarrow$	$2\,OH$	3.24(-05)
$H_2O_2 + OH$	$\longrightarrow$	$H_2O + HO_2$	1.54(-12)
$H_2O_2 + O(^3P)$	$\longrightarrow$	$OH + HO_2$	5.05(-16)
$H_2O + h\nu$	$\longrightarrow$	$H + OH$	2.18(-10)
$OH + CO$	$\longrightarrow$	$CO_2 + H$	1.50(-13)
$OH + CH_4$	$\longrightarrow$	$H_2O + CH_3(*)$	2.11(-15)
$NO + h\nu$	$\longrightarrow$	$N + O(^3P)$	1.40(-07)
$N_2O + h\nu$	$\longrightarrow$	$N_2 + O(^1D)$	2.64(-07)
$N_2O + O(^1D)$	$\longrightarrow$	$2\,NO$	6.7(-11)
$N_2O + O(^1D)$	$\longrightarrow$	$N_2 + O_2$	4.9(-11)
$N + O_2$	$\longrightarrow$	$NO + O(^3P)$	9.53(-18)
$N + NO$	$\longrightarrow$	$N_2 + O(^3P)$	3.12(-11)
$N + NO_2$	$\longrightarrow$	$N_2O + O(^3P)$	1.39(-11)
$NO + O_3$	$\longrightarrow$	$NO_2 + O_2$	7.78(-15)
$NO + HO_2$	$\longrightarrow$	$NO_2 + OH$	9.97(-12)
$NO + NO_3$	$\longrightarrow$	$2\,NO_2$	2.94(-11)
$NO_2 + h\nu$	$\longrightarrow$	$NO + O(^3P)$	1.35(-02)
$NO_2 + O_3$	$\longrightarrow$	$NO_3 + O_2$	7.28(-18)
$NO_2 + O(^3P)$	$\longrightarrow$	$NO + O_2$	1.05(-11)
$NO_2 + OH + M$	$\longrightarrow$	$HNO_3 + M$	3.56(-13)
$NO_2 + NO_3 + M$	$\longrightarrow$	$N_2O_5 + M$	2.19(-13)
$N_2O_5 + M$	$\longrightarrow$	$NO_2 + NO_3 + M$	9.42(-06)
$NO_2 + HO_2 + M$	$\longrightarrow$	$HNO_4 + M$	2.57(-14)
$HNO_4 + M$	$\longrightarrow$	$NO_2 + HO_2 + M$	2.12(-06)

Recommended Set of Equation for Stratospheric Modelling

p =3.11 mbar,
T = 252.3 K.
Photolysis
frequency for
SZA=60°,
h=39,63 km.

$NO_3 + h\nu$	$\longrightarrow$	$NO_2 + O(^3P)$	2.56(-01)
$NO_3 + h\nu$	$\longrightarrow$	$NO + O_2$	3.17(-02)
$NO_3 + OH$	$\longrightarrow$	$HO_2 + NO_2$	2.2(-11)
$NO_3 + HO_2$	$\longrightarrow$	$OH + NO_2$	3.5(-12)
$N_2O_5 + h\nu$	$\longrightarrow$	$NO_2 + NO_3$	2.44(-04)
$HNO_3 + h\nu$	$\longrightarrow$	$NO_2 + OH$	4.84(-05)
$HNO_3 + OH$	$\longrightarrow$	$NO_3 + H_2O$	1.65(-13)
$HNO_4 + h\nu$	$\longrightarrow$	$NO_2 + HO_2$	8.13(-05)
$HNO_4 + OH$	$\longrightarrow$	$NO_2 + H_2O + O_2$	5.86(-12)
$Cl + O_3$	$\longrightarrow$	$ClO + O_2$	1.04(-11)
$Cl + H_2$	$\longrightarrow$	$HCl + H$	4.07(-15)
$Cl + HO_2$	$\longrightarrow$	$HCl + O_2$	3.53(-11)
$Cl + HO_2$	$\longrightarrow$	$ClO + OH$	6.89(-12)
$Cl + CH_4$	$\longrightarrow$	$HCl + CH_3(*)$	4.28(-14)
$Cl + OClO$	$\longrightarrow$	$2\,ClO$	6.41(-11)
$Cl + Cl_2O_2$	$\longrightarrow$	$Cl_2 + Cl + O_2$	1.0(-10)
$Cl + HOCl$	$\longrightarrow$	$Cl_2 + OH$	1.49(-12)
$Cl + ClONO_2$	$\longrightarrow$	$Cl_2 + NO_3$	1.28(-11)
$Cl_2 + h\nu$	$\longrightarrow$	$2\,Cl$	3.88(-03)
$Cl_2 + OH$	$\longrightarrow$	$HOCl + Cl$	3.95(-14)
$ClO + O(^3P)$	$\longrightarrow$	$Cl + O_2$	3.96(-11)

Recommended Set of Equation for Stratospheric Modelling

p =3.11 mbar,
T = 252.3 K.
Photolysis
frequency for
SZA=60°,
h=39,63 km.

$ClO + OH$	$\longrightarrow$	$Cl + HO_2$	1.77(-11)
$ClO + HO_2$	$\longrightarrow$	$HOCl + O_2$	7.7(-12)
$ClO + NO$	$\longrightarrow$	$Cl + NO_2$	2.02(-11)
$ClO + NO_2 + M$	$\longrightarrow$	$ClONO_2 + M$	2.74(-14)
$ClO + ClO + M$	$\longrightarrow$	$Cl_2O_2 + M$	3.2(-15)
$Cl_2O_2 + M$	$\longrightarrow$	$ClO + ClO + M$	2.19(-03)
$Cl_2O_2 + h\nu$	$\longrightarrow$	$Cl + ClOO(*)$	3.44(-03)
$OClO + h\nu$	$\longrightarrow$	$ClO + O(^3P)$	1.30(-01)
$HOCl + h\nu$	$\longrightarrow$	$Cl + OH$	4.77(-04)
$HOCl + OH$	$\longrightarrow$	$ClO + H_2O$	4.14(-13)
$HOCl + O(^3P)$	$\longrightarrow$	$ClO + OH$	5.78(-14)
$ClNO_2 + h\nu$	$\longrightarrow$	$Cl + NO_2$	9.52(-04)
$ClONO_2 + h\nu$	$\longrightarrow$	$Cl + NO_3$	2.14(-04)
$HCl + h\nu$	$\longrightarrow$	$Cl + H$	2.22(-07)
$HCl + OH$	$\longrightarrow$	$Cl + H_2O$	6.49(-13)
$Br + O_3$	$\longrightarrow$	$BrO + O_2$	7.14(-13)
$Br + HO_2$	$\longrightarrow$	$HBr + O_2$	1.39(-12)
$BrO + O(^3P)$	$\longrightarrow$	$Br + O_2$	4.76(-11)
$BrO + HO_2$	$\longrightarrow$	$HOBr(*) + O_2$	4.5(-11)
$BrO + NO$	$\longrightarrow$	$Br + NO_2$	2.47(-11)
$BrO + NO_2 + M$	$\longrightarrow$	$BrONO_2 + M$	7.33(-14)
$BrO + ClO$	$\longrightarrow$	$Br + OClO$	8.8(-12)
$BrO + ClO$	$\longrightarrow$	$Br + Cl + O_2$	6.94(-12)
$BrO + ClO$	$\longrightarrow$	$BrCl + O_2$	1.14(-12)
$BrO + BrO$	$\longrightarrow$	$Br + Br + O_2$	1.88(-12)
$HBr + OH$	$\longrightarrow$	$Br + H_2O$	1.1(-11)
$BrCl + h\nu$	$\longrightarrow$	$Br + Cl$	1.57(-02)
$BrONO_2 + h\nu$	$\longrightarrow$	$BrO + NO_2$	2.42(-03)

Recommended Set of Equation for Stratospheric Modelling

p =3.11 mbar, T = 252.3 K. Photolysis frequency for SZA=60°, h=39,63 km.

$CH_2O + h\nu$	$\longrightarrow$	$CO + H_2$	8.17(-05)
$CH_2O + h\nu$	$\longrightarrow$	$HCO + H$	6.53(-05)
$CH_2O + OH$	$\longrightarrow$	$H_2O + HCO$	1.0(-11)
$CH_2O + Cl$	$\longrightarrow$	$HCl + HCO$	7.19(-11)
$CH_2O + Br$	$\longrightarrow$	$HBr + HCO$	7.14(-13)
$HCO + O_2$	$\longrightarrow$	$CO + HO_2$	6.1(-12)
$CH_3OH + OH$	$\longrightarrow$	$H_2O + CH_2O + H$	6.21(-13)
$CH_3OH + Cl$	$\longrightarrow$	$HCl + CH_2O + H$	5.4(-11)
$CH_3O_2 + HO_2$	$\longrightarrow$	$CH_3O_2H + O_2$	9.05(-12)
$CH_3O_2 + NO$	$\longrightarrow$	$CH_3O + NO_2$	8.57(-12)
$CH_3O + O_2$	$\longrightarrow$	$CH_2O + HO_2$	1.10(-15)
$CH_3O_2 + NO_2 + M$	$\longrightarrow$	$CH_3O_2NO_2 + M$	2.23(-13)
$CH_3O_2NO_2 + M$	$\longrightarrow$	$CH_3O_2 + NO_2 + M$	9.04(-05)
$CH_3O_2 + ClO$	$\longrightarrow$	$Cl + CH_2O + HO_2$	1.33(-12)
$CH_3O_2 + CH_3O_2$	$\longrightarrow$	$CH_2O + CH_3OH + O_2$	3.19(-13)
$CH_3O_2H + h\nu$	$\longrightarrow$	$CH_2O + OH + H$	2.09(-05)
$CH_3O_2H + OH$	$\longrightarrow$	$CH_3O_2 + H_2O$	5.88(-12)
$CH_3O_2H + OH$	$\longrightarrow$	$CH_2O + OH + H_2O$	2.52(-12)
$CH_3O_2H + Cl$	$\longrightarrow$	$HCl + CH_2O + OH$	6.41(-11)
$CH_3O_2NO_2 + h\nu$	$\longrightarrow$	$CH_3O_2 + NO_2$	1.05(-04)

Set of Ordinary Differential Equation for Chemical Models

Determination of C_i (Determination of chemical loss and production rates)

$$C_i = \frac{d[y_i]}{dt} = P_i - L_i[y_i]$$

$$P_i = \sum_{j \neq i, l \neq i} k_{jl}[j][l] + \sum_{m \neq i} j_m[m]$$

$$L_i = \sum_j k_{ij}[j] + k_i$$

k_{jl} : *reaction coefficients*

j_m : *photolysis rates*

Different chemical reactions

- bi-molecular
- tri-molecular
- thermal
- heterogeneous
- photolysis

Determination of C_i implies simultaneous solution of up to hundreds of coupled differential equations, containing many non-linear reactions.

Set of stiff differential equations => Numerical Solution difficult

ODEs and PDEs

Ordinary differential equation (ODE)
Equation with one independent variable

Partial differential equation (PDE)
Equation with more than one independent variable

Order
Highest derivative of an equation

Degree
Highest polynomial value of the highest derivative

Initial value problem
Conditions are known at one end of domain but not other

Boundary value problem
Conditions are known at both ends of domain

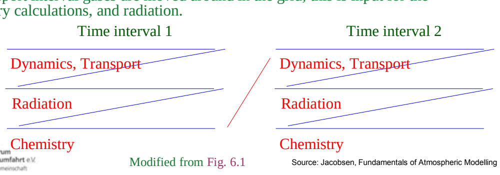
ODEs and PDEs

	Ordinary Differential Equations	Partial Differential Equations
First-order, first-degree	(a) $\frac{dN}{dt} = 16 - 4N^2$	(e) $\frac{\partial N}{\partial t} + \frac{\partial (uN)}{\partial x} = 0$
First-order, first-degree	(b) $\frac{dN}{dt} = 3AB - 4NC$	(f) $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = 0$
Second-order, first-degree	(c) $\frac{d^2 N}{dt^2} + \frac{dN}{dt} + 5t = 0$	(g) $\frac{\partial^2 N}{\partial t^2} + \frac{\partial^2 N}{\partial x^2} = 3t^2 + x$
Second-order, second-degree	(d) $\left(\frac{d^2 N}{dt^2}\right)^2 + \frac{dN}{dt} + 4 = 0$	(h) $\left(\frac{\partial^2 N}{\partial t^2}\right)^2 + \frac{\partial N}{\partial x} = t - x$

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Operator Splitting Scheme

Major processes in an atmospheric model are often solved separately from each other
Suppose a model has dynamics, transport, radiation and gas chemistry
Each of these processes may be solved sequentially during a common time interval
Time step
is an increment in time for a given process
Time interval
is the period during which several time steps of a process are solved
Example
time step dynamics 15 min, transport 15 min, radiation 45 min (every 3 time steps), chemistry variable, time interval common to all is 45 min => during the time interval 3 dynamics and transport time steps are taken, followed by 1 radiation time step, followed by a variable number of chemistry time steps; after the dynamics time interval, resulting wind speeds are taken as input for transport calculations; during the transport interval gases are moved around in the grid; this is input for the chemistry calculations, and radiation.



Modified from Fig. 6.1

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Differences GCM and NWP models

- Major difference between **GCM** and **NWP model:** climate model is used to project the average behaviour of the atmosphere (its climate) as a result of **slow changes in some boundary conditions** (such as the solar constant) **or physical parameters** (such as the greenhouse gas concentration) and **not to make a deterministic prediction of the exact weather at a specific time**.
- A chaotic nature of the fluid dynamics equations is involved in weather forecasting. Extremely small errors in temperature, winds, or other initial inputs given to numerical models will amplify and double every five days, making it impossible for long-range forecasts—those made more than two weeks in advance—to predict the state of the atmosphere with any degree of forecast skill. Furthermore, existing observation networks have poor coverage in some regions (e.g., over Pacific Ocean), which introduces uncertainty into the true initial state.
- The unpredictable, chaotic nature of the atmosphere means that **deterministic predictions are not possible**. However, it is possible to **predict changes in climate due to changes in boundary conditions**, such as exchanges with the ocean or the land surface, or changes in external forcing factors, such as changes in solar radiation or GHGs.
- NWP models are used to predict the weather in the **short (1-3 days)** and **medium (4-10 days)** range future. GCM's are run much longer, for years on end, long enough to learn about the **climate in a statistical sense** (i.e. trends, means and variability).
- GCMs ignore fluctuating conditions when considering long-term changes, whereas NWP models take no notice of very slow processes.

A comparison between NWP models and GCMs

contrasts	NWP	GCM
goal	to predict weather	to predict climate
spatial coverage	regional or global	global
temporal range	days	years
spatial resolution	variable (20-100 km)	usually coarse
relevance of initial conditions	high	low
relevance of clouds, radiation	low	high
relevance of surface (land, ice, ocean...)	low	high
relevance of ocean dynamics	low	high
relevance of model stability	low	high
similarities		
physics	equations of motion (plus radiative transfer equations, water conservation equations ..)	
method	Finite difference expression of continuous equations, or spectral representation; run prognostically	

Methods to solve differential equations

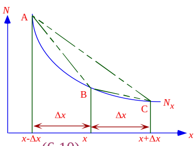
Finite Difference Approximation

First, replace continuous function u_x with a finite number of values in the x direction.
Second, define differences of du at point x_i

--> $\Delta u_i = u_{i+1} - u_{i-1}$ central difference

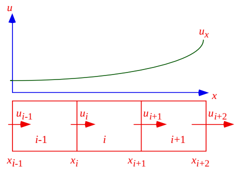
--> $\Delta u_i = u_{i+1} - u_i$ forward difference

--> $\Delta u_i = u_i - u_{i-1}$ backward difference



Central difference approximation to tangent slope at x_i (6.10)

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



Source: Jacobsen, Fundamentals of Atmospheric Modelling

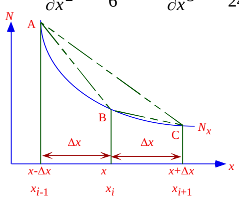
Taylor Series Expansion

Taylor series expansion of concentration N at point $x+\Delta x$ (6.11)

$$N_{x+\Delta x} = N_x + \Delta x \frac{\partial N_x}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 N_x}{\partial x^2} + \frac{1}{6}\Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} + ...$$

Taylor series expansion of concentration N at point $x-\Delta x$ (6.12)

$$N_{x-\Delta x} = N_x - \Delta x \frac{\partial N_x}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 N_x}{\partial x^2} - \frac{1}{6}\Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} - ...$$



Source: Jacobsen, Fundamentals of Atmospheric Modelling

Finite Difference Approximations

Sum the Taylor series expansions (6.13)

$$N_{x+\Delta x} + N_{x-\Delta x} = 2N_x + \Delta x^2 \frac{\partial^2 N_x}{\partial x^2} + \frac{1}{12}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} + ...$$

Rearrange (6.14)

$$\frac{\partial^2 N_x}{\partial x^2} = \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2} + O\left(\Delta x^2\right)$$

Truncation error (neglect 2nd-order terms and higher) (6.15)

$$O\left(\Delta x^2\right) = -\frac{1}{12}\Delta x^2 \frac{\partial^4 N_x}{\partial x^4} - ...$$

2nd-order central difference approx. of 2nd derivative (6.16)

$$\frac{\partial^2 N_x}{\partial x^2} \approx \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2}$$

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Finite Difference Approximations

Subtract the Taylor series expansions (6.17)

$$N_{x+\Delta x} - N_{x-\Delta x} = 2\Delta x \frac{\partial N_x}{\partial x} + \frac{1}{3}\Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + ...$$

Rearrange (6.18)

$$\frac{\partial N_x}{\partial x} = \frac{N_{x+\Delta x} - N_{x-\Delta x}}{2\Delta x} + O\left(\Delta x^2\right)$$

Truncation error (6.19)

$$O\left(\Delta x^2\right) = -\frac{1}{6}\Delta x^2 \frac{\partial^3 N_x}{\partial x^3} - ...$$

2nd-order central difference approx. of 1st derivative (6.20)

$$\frac{\partial N_x}{\partial x} \approx \frac{N_{x+\Delta x} - N_{x-\Delta x}}{2\Delta x} = \frac{N_{i+1} - N_{i-1}}{2\Delta x}$$

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Finite Difference Approximations

First two terms of Taylor series

1st-order forward difference approx. of 1st derivative (6.21)

$$\frac{\partial N_x}{\partial x} \approx \frac{N_{x+\Delta x} - N_x}{\Delta x} = \frac{N_{i+1} - N_i}{\Delta x}$$

1st-order backward difference approx. of 1st derivative (6.22)

$$\frac{\partial N_x}{\partial x} \approx \frac{N_x - N_{x-\Delta x}}{\Delta x} = \frac{N_i - N_{i-1}}{\Delta x}$$

Differencing Time Derivative

Central, forward, backward difference approximations (6.23)

$$\frac{\partial N_t}{\partial t} \approx \frac{N_{t+h} - N_{t-h}}{2h}$$

$$\frac{\partial N_t}{\partial t} \approx \frac{N_{t+h} - N_t}{h}$$

$$\frac{\partial N_t}{\partial t} \approx \frac{N_t - N_{t-h}}{h}$$

Consistency, Convergence

A numerical solution can replicate an exact solution to a PDE if several criteria are met:

Convergence of finite difference analog (6.6)

$$\frac{\partial N}{\partial x} = \lim_{\Delta x \to 0} \left\| \frac{\Delta N}{\Delta x} \right\|$$

Consistency of finite difference analog (6.7)

$$\lim_{\Delta x \to 0} \left\| \mathrm{T.E.}\left(\frac{\Delta N}{\Delta x}\right) \right\| = 0$$

Convergence of overall solution (N_e: exact solution; N_f: finite-difference solution (6.8)

$$\lim_{\Delta x, \Delta t \to 0} \left\| N_{e,x,t} - N_{f,x,t} \right\| = 0$$

Stability

Stablity occurs if the absolute-value difference between the numerical and the exact solution does not grow over time (often depends on the time step used).

Stability (6.9)

$$\lim_{t \to \infty} \left\| N_{e,x,t} - N_{f,x,t} \right\| \le C$$

Conditionally stable: Stable for limited time-step range
Unconditionally stable: Stable for all time steps
Unconditionally unstable: Unstable for all time steps

An unconditionally unstable scheme cannot be convergent overall, but individual finite-difference analogs in an unstable scheme may converge and may be consistent.

In other words, consistency and convergence of individual analogs do not guarantee stability.

Stability is guaranteed if a scheme is convergent overall and its finite-difference analogs are convergent and consistent.

Stiff Problems

- Sets of chemical lifetimes of species vary by many orders of magnitude
- The analysis of stiff circuits requires the use of variable step sizes
- Not all the linear multistep methods can be efficiently used to integrate stiff equations

To be able to choose Δt based only on accuracy considerations, the region of absolute stability should allow a large Δt for large time constants, without being constrained by the small time constants

See further details for example in Sandu & Sander, 2006

Properties of ODE Solver

Stable
If the absolute-value difference between the numerical and the exact solution does not grow with time

Accurate
Check time-dependent solution from the solver with an exact solution

Mass-conserving
A scheme is mass-conserving if the mass of each element (e.g. N, O, H, etc.) summed over all species at the beginning of the simulation equals the mass of the element summed over all species at the end of the simulation

Positive definite
If a scheme always predicts non-negative concentrations

Fast
A good solver can take long time-steps and maintain accuracy

Methods for the chemical part

- **Analytical solution**
- **Classical numerical methods for stiff ODEs**
  - Taylor series solution
  - Forward-Euler Solution
  - Multi-step implicit Solution
  - Backward-Euler Solution
  - Gear's Method
  - Implicit and semi-implicit methods
  - Family Solution

Initial Value Problems

Values are known at an initial time and desired at a final time

Concentration of species *i* is known at time *t-h*=0 (12.2)

$$N_{i,t-h} = N_{i,0}$$

Vector of concentrations at time *t for a set of K species* (12.1)

$$\hat{N}_t = \left[N_{1,t}, N_{2,t}, ..., N_{i,t}, ..., N_{K,t}\right]$$

- During a time step, an ODE scheme solves for all $N_{i,t}$
- Once values at time t are found, t is replaced with t-h and a new time step is solved
- h: one time step

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Analytical Solution to ODEs (most accurate)

Nitrogen dioxide photolysis (12.4)

$$\dot{N}O_2 + h\nu \longrightarrow \dot{N}O + \dot{O}\cdot$$

Time rate of change of NO_2 concentration (12.5)

$$\frac{d[NO_2]}{dt} = -J[NO_2]$$

Analytical solution (12.6)

$$[NO_2]_t = [NO_2]_{t-h} e^{-Jh}$$

Example:

$[NO_2]_{t-h}$ = 10^{10} molec. cm^{-3}

J = 0.02 s^{-1}

---> $[NO_2]_t$ = 10^{10} e$^{-0.02t}$

- Analytical solutions to a set of ODEs are usually impractical to obtain
- => Numerical solutions are used in atmospheric models

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Taylor Series Solution to ODEs

Explicit Taylor series expansion for one species (12.7)

$$N_{i,t} = N_{i,t-h} + h\frac{dN_{i,t-h}}{dt} + \frac{h^2}{2}\frac{d^2N_{i,t-h}}{dt^2} + \frac{h^3}{6}\frac{d^3N_{i,t-h}}{dt^3} + ...$$

Taylor series expansion for NO (12.8)

$$[NO]_t = [NO]_{t-h} + h\frac{d[NO]_{t-h}}{dt} + \frac{h^2}{2}\frac{d^2[NO]_{t-h}}{dt^2} + \frac{h^3}{6}\frac{d^3[NO]_{t-h}}{dt^3} + ...$$

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Family Method

Organize short- and long-lived species into families, which are long-lived, solve for family concentration, then partition family concentrations into individual species concentrations

Odd oxygen family (12.92)

$$[O_T] = [O] + [O(^1D)] + [O_3] + [NO_2]$$

Odd hydrogen family (12.93)

$$[HO_T] = [OH] + [HO_2] + [H_2O_2]$$

Odd nitrogen family (12.94)

$$[NO_T] = [NO] + [NO_2] + [NO_3]$$

Odd chlorine family (12.95)

$$[Cl_T] = [Cl] + [ClO] + [ClO_2]$$

Source: Jacobsen, Fundamentals of Atmospheric Modelling

Grid and Time Resolution

- Computing power limits the amount of calculation that can occur
- Thus, calculations are performed on a "grid" of points
  - Typically 5° x 5° horizontal grid (~ 555 x 555 km at the Equator)
  - Also divide the atmosphere into vertical layers
- Since we are stepping forward in time, climate models have 4 dimensions

Model Stability

- As spatial resolution increases, the time resolution must also increase or climate models will not yield a stable solution (they will "blow up")
  - This is called the CFL criterion, named after Courant, Friedrichs, and Lewy, and is represented mathematically as:

Fastest signal propogating through the model domain (e.g. a gravity wave in the atmosphere with a speed of 300 m/s)

$$\frac{c\Delta t}{\Delta x} \leq 1$$

** Richardson used a 6 hour time step (Δx = 200 km) in his experiment. He would have had to used a time step of 8 minutes to find a stable solution

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Steps in Model Formulation

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Steps in Model Formulation

1. Define purpose of model (e.g., simulate tropospheric climate or stratospheric ozone)
2. Determine spatial and temporal scales of interest (e.g. global and centuries)
3. Determine dimension of model (e.g., 3D)
4. Select physical, chemical, dynamical processes treated (e.g., fully coupled)
5. Select variables (e.g. 10 meteorological variables and 150 chemical species)
6. Select computer architecture (e.g., parallel-processor machine)
7. Write code for model
8. Optimize memory and speed of model (e.g., minimizing global arrays)
9. Select time steps and time intervals (e.g., 300 s for a 5°x5° grid).
10. Set initial conditions (e.g., use observations or output from previous model run)
11. Set boundary conditions (e.g., set south-north velocities to 0 at poles)
12. Select input data (e.g., topography, chemical rate coefficients, absorption coefficients, emissions)
13. Select ambient observations for comparison (e.g., satellite data to judge performance)
14. Interpolate observations and model results for inputs and outputs
15. Select or write algorithms for statistics and graphics (e.g. by using NCL)
16. Run model simulations
17. Run sensitivity tests (e.g., to gauge the effect of model assumptions or processes)
18. Improve model based on results (e.g., through comparison with observations)

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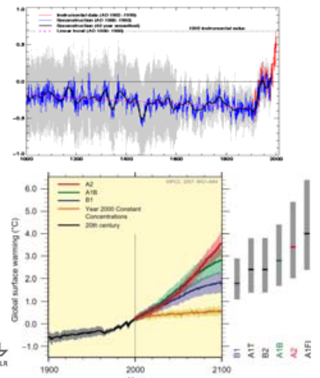
Steps in Model Formulation: 1. Define purpose



For example:
Understanding and Attributing Climate Change

Predicting the Future:
Climate Change; Source: IPCC 2007

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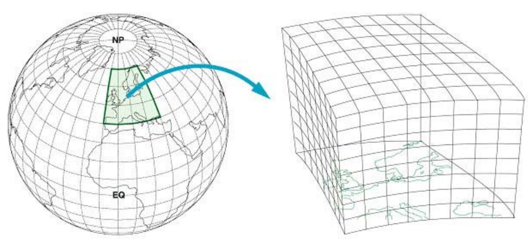
The Atmosphere over Europe in a discrete model



U.Cubasch

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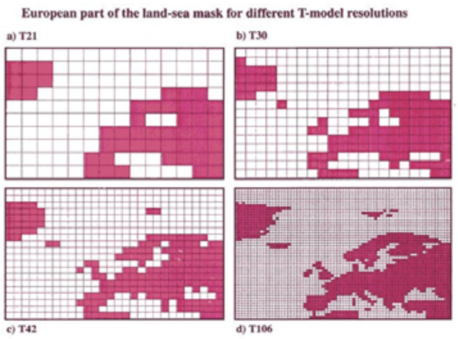
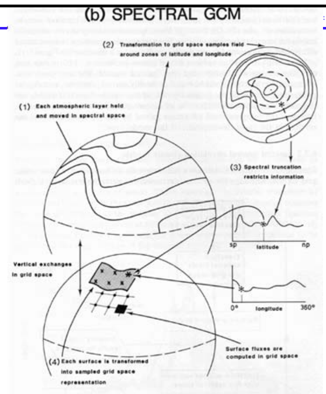
The Atmosphere over Europe in a discrete model



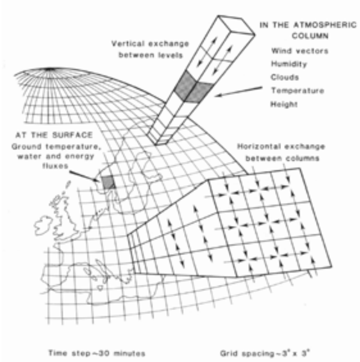
U. Cubasch

Spectral GCM



Source: *A Climate Modelling Primer*, Henderson-Sellers & McGuffie, *Figure 6.3(b)*

Grid GCM



Source: *A Climate Modelling Primer*, Henderson-Sellers & McGuffie, *Figure 6.3(a)*

Spaghetti Diagram for climate models

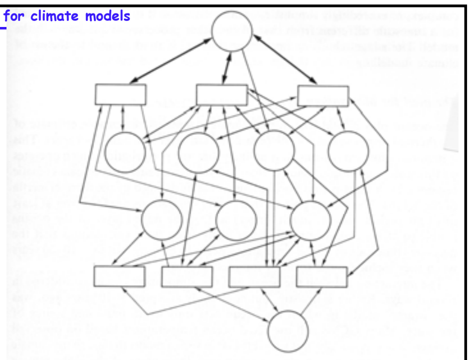


Figure 2.9 A generalized 'spaghetti' diagram for climate models. The arrows show the links between a set of unnamed processes and variables. The processes which could be entered in the boxes and the variables in the circles depend crucially on the timescale being modelled and the type of model employed.

Steps in Model Formulation

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14. Interpolate observations and model results for inputs and outputs
15. Select or write algorithms for statistics and graphics (e.g. by using NCL)
16. Run model simulations
17. Run sensitivity tests (e.g., to gauge the effect of model assumptions or processes)
18. Improve model based on results (e.g., through comparison with observations)

Physical Components in a climate model

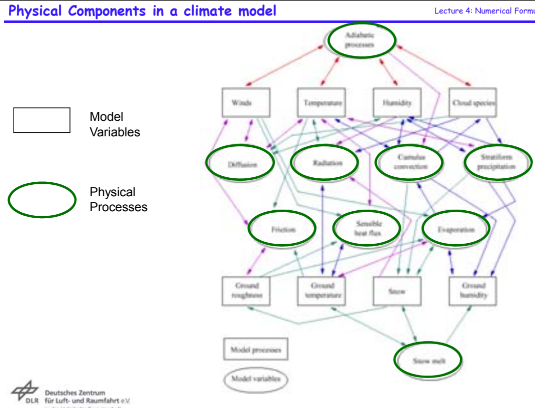
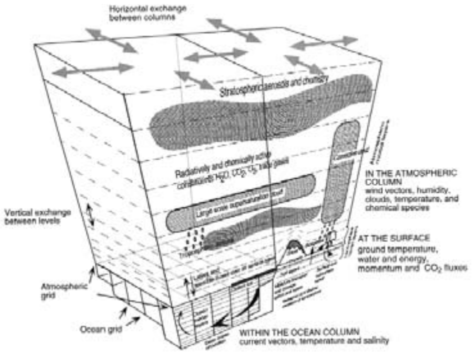


Illustration of the basic characteristics and processes within a GCM



Source: McGuffie and Henderson-Sellers, 2001

Parameterization

- Since by necessity our grid is large, many things occur at scales smaller than the grid size
  - Clouds
- Model cannot "see" these things
- Parameterizations are employed to simulate the large-scale feedback that small scale features produce
  - Calculate an "average" cloudiness over a grid box

Typical Climate Model Parameterizations

- Convection and Clouds
  - Mass, momentum, heat, moisture fluxes
  - Fluxes are usually much larger at scales smaller than a climate model grid size
  - Radiation interactions
- Turbulence
- Radiation
- Boundary Layer
  - Fluxes of heat, moisture, momentum

Components of a global climate model

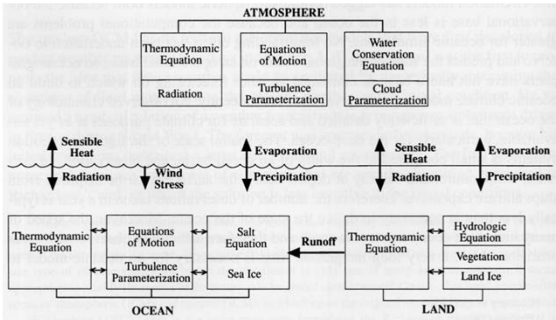


Fig. 10.1 Schematic diagram showing the components of a global climate model.

Source: *Global Physical Climatology*, D.L. Hartmann, *Figure 10.1*

Steps in Model Formulation

1. Define purpose of model (e.g., simulate tropospheric climate or stratospheric ozone)
2. Determine spatial and temporal scales of interest (e.g. global and centuries)
3. Determine dimension of model (e.g., 3D)
4. Select physical, chemical, dynamical processes treated (e.g., fully coupled)
5. Select variables (e.g. 10 meteorological variables and 150 chemical species)
6. Select computer architecture (e.g., parallel-processor machine)
7. Write code for model
8. Optimize memory and speed of model (e.g., minimizing global arrays)
9. Select time steps and time intervals (e.g., 300 s for a 5°x5° grid).
10. Set initial conditions (e.g., use observations or output from previous model run)
11. Set boundary conditions (e.g., set south-north velocities to 0 at poles)
12. Select input data (e.g., topography)
13. Select ambient observations for comparison (e.g., satellite data to judge performance)
14. Interpolate observations and model results for inputs and outputs
15. Select or write algorithms for statistics and graphics (e.g. by using NCL)
16. Run model simulations
17. Run sensitivity tests (e.g., to gauge the effect of model assumptions or processes)
18. Improve model based on results (e.g., through comparison with observations)

What do we need to start a GCM simulation?

1. Initial Conditions

- **Possible existence of multiple attractors make the choice of initial conditions far from trivial**
- **Possibilities for initial conditions:**
  - start from stable solution (e.g. an atmosphere without horizontal gradients)
  - start close to an observed state (weather predictions, decadal simulations in CMIP5).
- Spinup: time until the simulations is independent from the initial conditions
  - depends on the application
  - short in the atmosphere due to the lack of inertia (few months)
  - processes at the land surface (in particular cumulative processes that depend on the storage of water below the ground) have a large inertia and need several years spinup
  - even longer spinup is needed if the GCM runs with a coupled ocean

What do we need to start a GCM simulation?

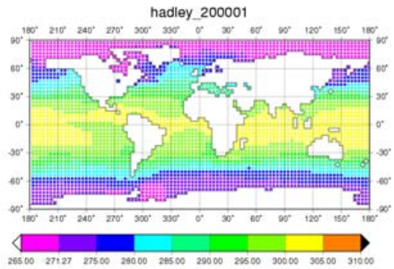
2. Surface boundary conditions

a) Sea Surface Temperatures (SSTs) and sea-ice (or a coupled ocean)
b) Land-sea mask
c) Orography
d) Roughness length *(Sea, Sea-ice, Land)*
e) Vegetation
f) Albedo for different surface types
g) Emissions (GHGs, CFCs, ozone precursors etc.)
h) Prescribed 3D concentration for aerosols and ozone (if not interactively modeled)
i) Solar forcing data
j) volcanic aerosol dataset

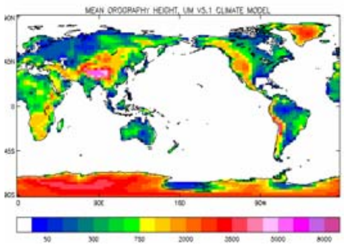
a,b) Sea Surface Temperatures and Sea Ice; Land-sea mask

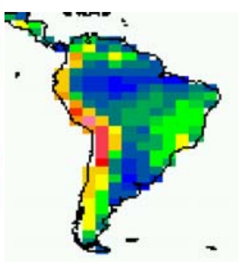
Pink grid points:

Sea ice



c) Orography





Andes only poorly resolved
Alps not really visible

Source: A. Brown

d) Roughness Length

The **roughness length** is used in numerical models to **express the roughness of the surface**. It affects the intensity of **mechanical turbulence** and the **fluxes** of varies quantities above the surface.

The 'roughness length' depends on the **frontal area of the average element** (facing the wind) **divided by the ground width it occupies. Vertical sub-gridscale heat exchange (by turbulent eddies)** can be expressed as the **vertical gradient of potential temperature times the roughness length**.

A **lower** roughness length implies **less exchange between the surface and the atmosphere**, but also stronger wind near the ground (e.g. at the standard height of 10 m).
A terrain classification based on roughness length is given in the following table:

class		roughness	landscape features
no.	name	length m	
1	sea	0.0002	open water, tidal flat, snow with fetch above 3 km
2	smooth	0.005	featureless land, ice
3	open	0.03	flat terrain with grass or very low vegetation, airport runway
4	roughly open	0.10	cultivated area, low crops, obstacles of height H separated by at least 20 H
5	rough	0.25	open landscape, scattered shelter belts, obstacles separated by 15 H or so
6	very rough	0.5	landscape with bushes, young dense forest etc separated by 10 H or so
7	closed	1.0	open spaces comparable with H, eg mature forest, low-rise built-up area
8	chaotic	over 2.0	irregular distribution of large elements, eg city centre, large forest with clearings

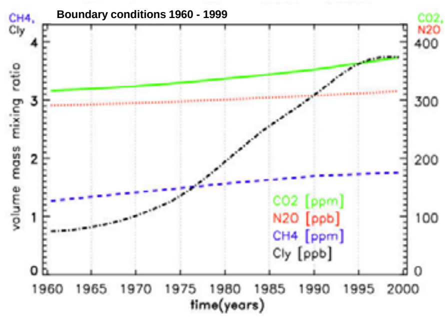
f) Typical Surface Albedos

Surface type	Albedo (α)
Soil, dark and wet	0.05
Soil, light and dry	0.40
Desert	0.20-0.45
Savanna grassland, wet season	0.18
Savanna grassland, dry season	0.23
Grass, long	0.16
Grass, short	0.26
Cropland	0.18-0.25
Orchards	0.15-0.20
Forest	0.05-0.20
Water, small zenith angle	0.03-0.10
Water, large zenith angle	0.10-1.00
Snow	0.40-0.95

[note that 0.25 represents 25% of radiation reflected]

http://www.gpa.uq.edu.au/courses/GEOS2101/lectures/lecture2.pdf

g) Emissions



Simulation design, preparation, integration, interpretation

Simulation design:

- Choice of model configuration, including model vertical and horizontal resolution and complexity
- choice among the different subgrid scale parameterisations & parameters for it
- precise definition of the intial and boundary conditions that will be used for the experiment
- incorporate the material and personal constraints that can limit the scope of the simulation and try to find a reasonable balance between the scientific interest of the simulation and the overall costs and human and computer time.

Preparation:

- prepare and check initial conditions and boundary conditions

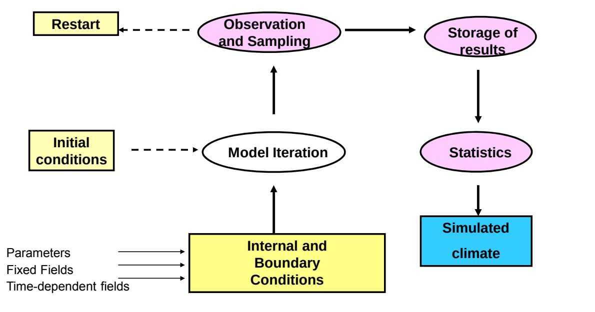
Integration:

- start test runs (few months)
- Start run and check regularly
- Postprocess the output in order to bring out interesting results

Interpretation:

- interpretation of the results

The different steps in a GCM simulation



Short Description of the GCM ECHAM5 (1 of 8)

1.1 Short Desciption

The ECHAM model has been developed from the ECMWF model (cycle 31, November 1988). It contains several changes, mostly in the parameterization, in order to adjust the model for climate simulations.
The reference resolution is T42, but the model is set up to use resolutions in the range T21 to T106. Long term integrations have so far only been done for T21, T30, T42 and T63. The layout is as follows (indicates changes from the original ECMWF model):

1.2 Numerical solution

- **Prognostic variables:** e.g., vorticity, divergence, temperature, log surface pressure, water vapour, cloud species
- **Horizontal representation:** spectral transform, triangular truncation (T42/T63/T106); in all practical applications the series expansion of spherical harmonic functions must be truncated at some finite point.
- **Vertical representation:** hybrid coordinate system, second order finite differences, 19, 39, and 69 layers
- **Time integration:** semi-implicit | leap frog with time filter, t = 40 min (T21), t = 30min (T30), t = 24 min (T42), t = 15 min (T63), and t = 12 min (T106)

Short Description of the GCM ECHAM5 (2 of 8)

1.3 Surface boundary conditions

- **SST and sea-ice:** e.g. Hadley data set
- **Orography:** mean terrain heights computed from high resolution USGS GTOPO30 data set
- **Land-sea mask:** from USGS GTOPO30 data set
- **Roughness length:**
  - *Sea:* Charnock formula, modified after Miller et al. (1992)
  - *Sea-ice:* constant (0.01 m)
  - *Land:* function of vegetation and orography (variance)
- **Vegetation:** fraction of grid area covered by vegetation based on Wilson and Henderson - Sellers (1985) data
- **Albedo:**
  - *Sea:* function of solar zenith angle bare
  - *Land:* satellite data (Geleyn and Preuss (1983))
  - *Sea ice:* function of temperature (Robock,1980)
  - *Land ice:* function of temperature (Robock, 1980; Kukla and Robinson, 1980)
  - *Snow:* function of temperature and fractional forest area (Robock, 1980; Matthews, 1983)

Short Description of the GCM ECHAM5 (3 of 8)

1.4 Physical parameterization

Radiation: (Hense et al.,1982; Rockel et al, 1991; Eickerling, 1989)

- *two-stream approximation*
- *six spectral intervals in the terrestrial part*
- *four spectral intervals in the solar part*
- *gaseous absorbers:* H_2O, CO_2 and O_3 (CO_2 and O_3 prescribed)
- *aerosols:* prescribed
- *clouds:* computed cloud optical depth and cloud cover
- *emissivity:* function of cloud water path (Stephens, 1978)
- *continuum absorption:* included
- *cloud overlap:* maximum for contiguous clouds layer and random otherwise
- *diurnal cycle:* included
- *radiation time step:* 2 hours

Short Description of the GCM ECHAM5 (4 of 8)

1.4 Physical parameterization

Clouds: (Sundquist, 1978; Roeckner and Schlese, 1985; Roeckner et al, 1991)

Cloud water transport equation

Subgrid-scale condensation and cloud formation with different thresholds for convective and stratiform clouds (Xu and Krueger, 1991)

Temperature dependent partitioning of liquid/ice phase (Matveev, 1984)

Rain formation by auto-conversion of cloud droplets (Sundquist, 1978)

Sedimentation of ice crystals (Heymsfeld, 1977)

Evaporation of cloud water
Evaporation of precipitation

See video on CLOUDS (EU-EUCLIPSE project) at http://www.youtube.com/watch?v=5UCb38WzkII

Short Description of the GCM ECHAM5 (5 of 8)

1.4 Physical parameterization

Connvection: (Tiedtke, 1989)

Mass flux scheme for deep, shallow and mid-level convection

Clouds are represented by a bulk model and include updraft and downdraft mass fluxes

Convective momentum transport
is parameterized according to Schneider and Lindzen (1976)

Evaporation of rain is parameterized according to Kessler (1969)

Stratocumulus convection
is parameterized as a vertical diffusion process with enhanced eddy diffusion coefficients (Tiedtke et al., 1988)

Short Description of the GCM ECHAM5 (6 of 8)

1.4 Physical parameterization

Land-surface processes: (Sellers et al., 1986; Blondin, 1989; Du"menil and Todini, 1992)

- *Heat transfer:* diffusion equation solved in a 5-layer model with zero heat flux at the bottom (10 m)
- *Water budget equation for three reservoirs:* soil moisture, interception reservoir (vegetation), snow
- *Vegetation effects:* stomatal control on evapotranspiration and interception of rain and snow
- *Run-off scheme:* based on catchment considerations including sub-grid scale variations of field capacity over inhomogeneous terrain
- *Sea-ice temperature* calculated from surface energy budget

Short Description of the GCM ECHAM5 (7 of 8)

1.4 Physical parameterization

Planetary boundary layer: (Louis, 1979)

- *Surface fluxes of momentum, heat, moisture and cloud water* are calculated from Monin-Obukhov similarity theory with transfer coefficients depending on roughness length and Richardson number
- *Above the surface layer:* eddy diffusivity approach with coefficients depending on wind shear, thermal stability and mixing length
- *Above the PBL:* vertical diffusion only for unstable stratification
- *Cloud species*
- *Moist Richardson number* (Brinkop, 1991; 1992)

Short Description of the GCM ECHAM5 (8 of 8)

1.4 Physical parameterization

Horizontal diffusion: (Laursen and Eliasen, 1989)

- *Scale selective operator* applied beyond a threshold wave number

Gravity wave drag (Palmer et al, 1986; Miller et al, 1989)

- *Surface stress due to gravity waves*, which are exited by stably stratified flow over irregular terrain is calculated from linear theory and dimensional considerations
- *Orographic forcing* prescribed as a directionally dependent sub-grid scale orographic variance computed from the high resolution USGS GTOPO30 data set
- *Vertical structure of momentum flux* induced by gravity waves calculated from a local wave Richardson number, which describes the onset of turbulence due to convective instability and the turbulent breakdown approaching a critical level
- *The GWD scheme* is not used at T21 resolution

End of Lecture 4