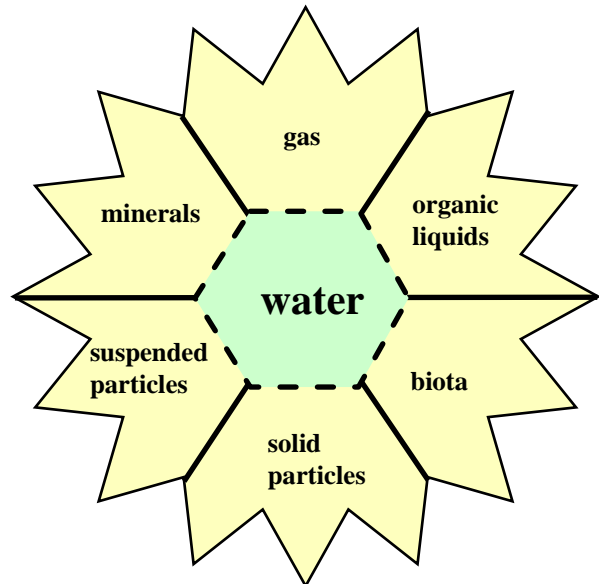


ECOSAT

Equilibrium Calculation of Speciation and Transport



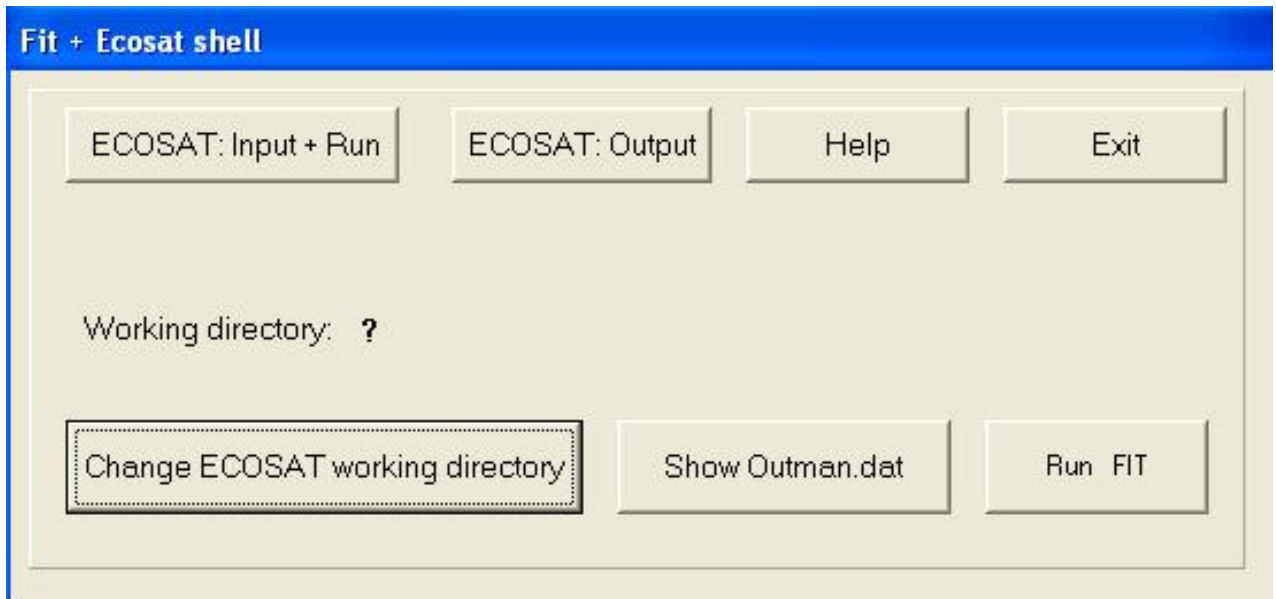
Distribution of Components over soil phases

ECOSAT is a computer program for the calculation of chemical speciation in soil-water systems.

These calculations include :

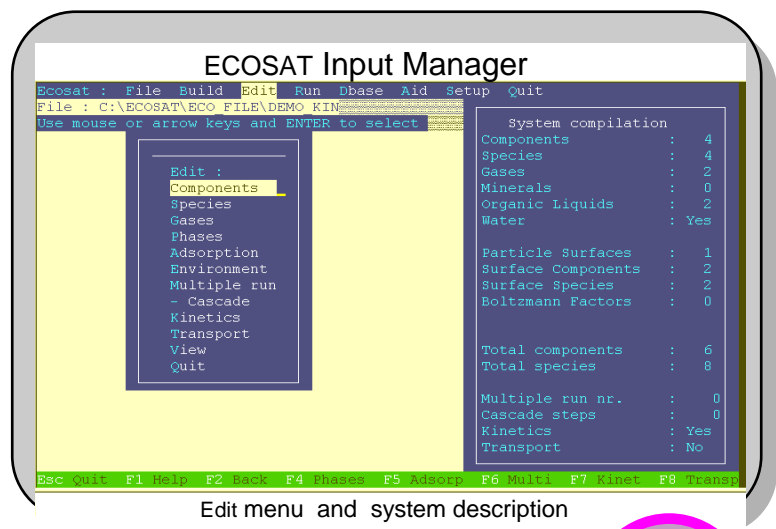
- **Speciation** : calculation of the distribution at equilibrium of compounds in different forms (species), present in different soil phases. Single run or **multiple run**.
- 1-dimensional or semi 2-dimensional transport in soil (columns) via the water or gas phase (**multicomponent transport**).
- **Reaction kinetics** : slow mass transfer (e.g. decay, slow desorption, slow dissolution)
- Parameter optimization in combination with the computer program FIT.

ECOSAT Windows shell



Input manager

- Drop down menus
- On line help
- Data input in various units
- (automatic) addition from database files



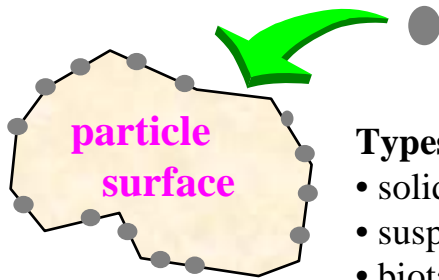
Name	Change	Constant	Total amount	Estimated	Moles/mole
Comp		Calc. Type	(mol/l)	log(Conc./Act.)	(g/mol)
benz	0	Total amount	1.0000000E+00	-4.000000	78.1000
Tol	0	Total amount	1.0000000E+00	-4.000000	92.1000
H	1	Activity	0.0000000E+00	-5.000000	1.0000
OH	-1	Total amount	0.0000000E+00	-9.000000	17.0000

Components edit table

Soil
Oxides
Organic matter
Clay
DOC
Biota

- Components
- Dissolved species
- Gases
- Minerals
- Organic liquids
- Particle surfaces
- Surface components (sites on surface)
- Surface species (adsorbed components)

Sorption



Types :

- solid
- suspended
- biota

Surface geometry :

- *Not relevant for nvc-models*
- *Plane (vc)*
- *Gel (vc-Donnan)*

Non Variable Charge models (nvc)

Freundlich
Langmuir one site (standard)
Langmuir two sites (advanced)
Ion-exchange (Gaines-Thomas)
Heterogeneous models

Variable Charge models (vc)

Diffuse Double Layer
Constant Capacitance
Basic Stern
Triple Layer
Donnan

Variable Charge + Heterogeneous models

NICA

Organic matter: NICA-Donnan

Oxides: CD-Music

Calculation Types

Multiple run

repeated speciation calculations

- titrations
- series calculations
- input data from file
- 5 series dimensions (nested loops)

Cascade

repeated soil solution extraction

Single run

default type

Kinetics

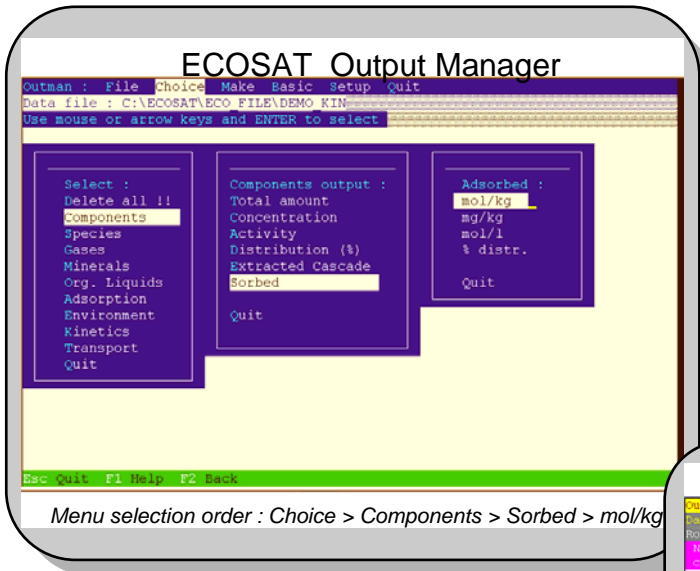
- slow mass transfer (decay, desorption, dissolution)
- combination with other types (e.g. 2-sites and 2-region model)

Transport

multicomponent

- 1-dimensional or semi 2-dimensional (axial symmetric) stationary water or gas flow
- variable feed composition
- soil column data sets with initial composition at different depths

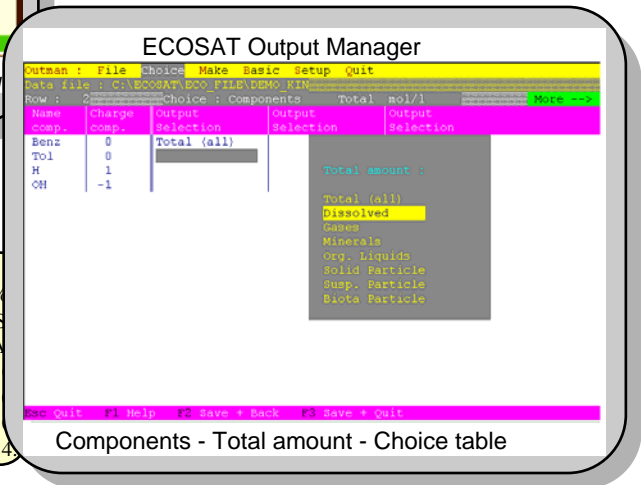
Output manager



Menu selection order : Choice > Components > Sorbed > mol/kg

User defined output selection

- Column ordered output (ready for import into spreadsheet)
- Concentrations, activities, total amounts, etc.
- Distributions (%) , different units (mol, mg)
- Time related output (kinetics and transport)
- Breakthrough 'curves' (only data)
- Soil column concentration profiles (only data)



Components - Total amount - Choice table

Example of output file (multiple run for pH)

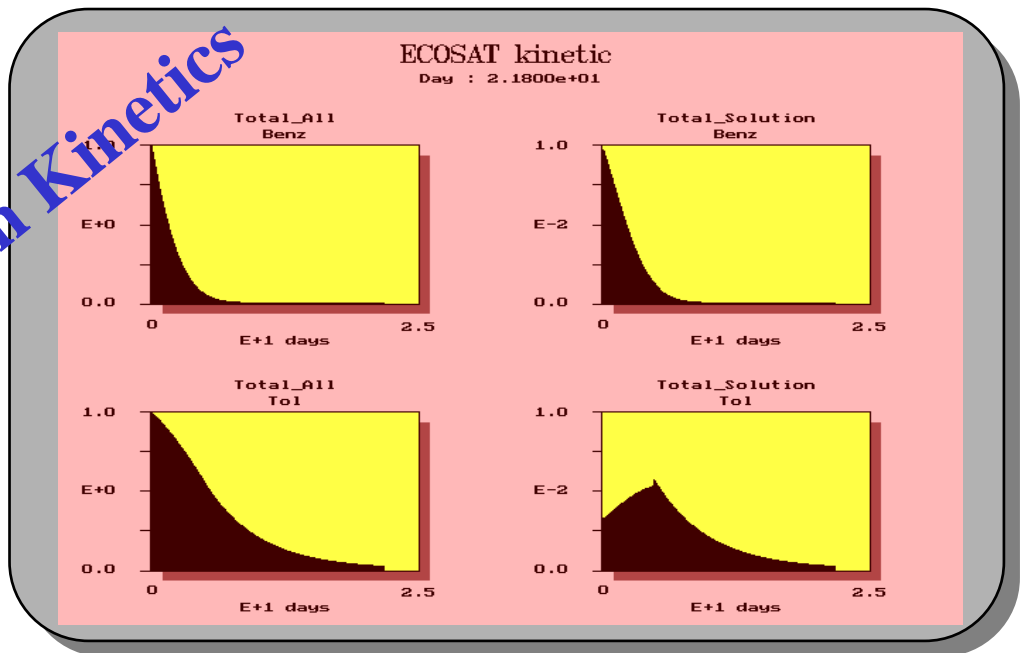
nr	Comp. Act. -log(mol/l)	Comp. Conc. mol/l	% of Al Solution	% of Al AIOH	% of Al Al(OH)2	% of Al Al(OH)3
1	4.0000	9.2669E-05	92.6692	5.2507	2.0146	0.0371
2	5.0000	2.4104E-05	24.1043	13.6577	52.4021	9.6384
3	6.0000	1.5976E-07	0.1598	0.9052	34.7301	63.8799
4	7.0000	2.2627E-10	0.0002	0.0128	4.9190	90.4765

ECOSAT Reaction Kinetics

Different time curves in the diagrams :

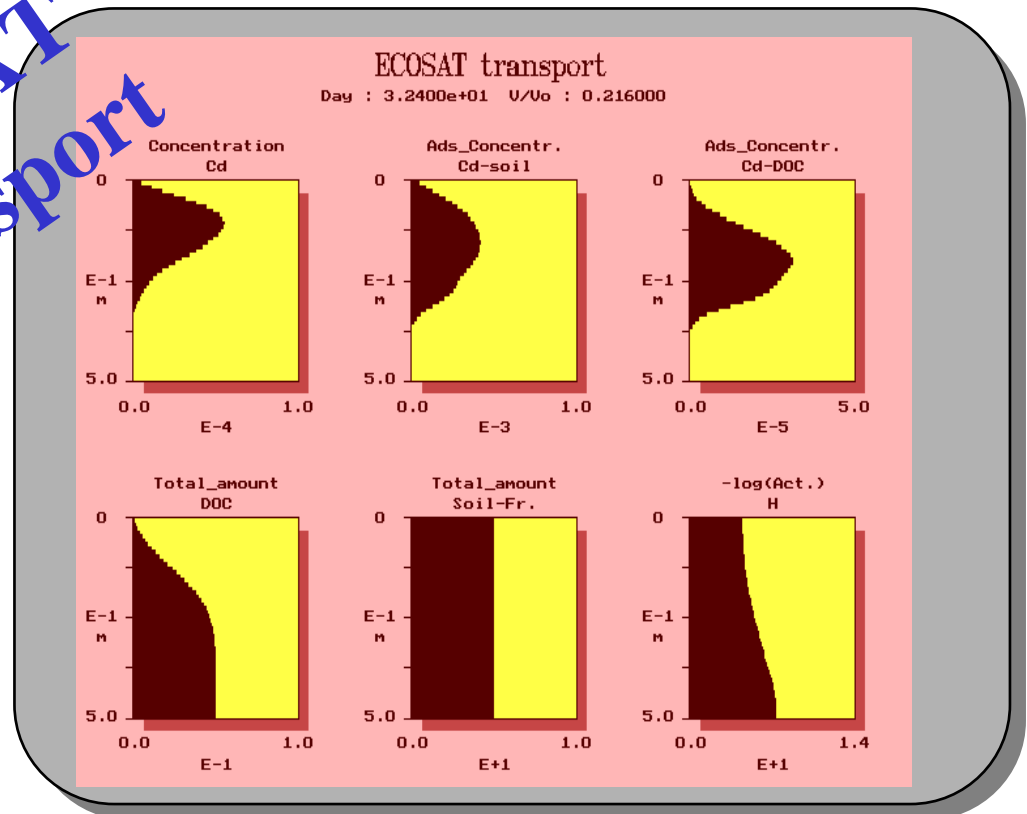
y-axis : variable value

x-axis : time (days)



Slow first order decay of benzene and toluene in the water phase
Equilibrium between water phase and mixture of the organic liquids benzene and toluene (Raoult's law)

ECOSAT Transport



Different soil column concentration profiles in the diagrams :

y_axis : soil depth
x-axis : variable value

*Leaching of Cadmium due to deposition of acid rain;
also leaching of DOC (dissolved organic carbon)*

ECOSAT

The ECOSAT package includes :

- *ecosat software*
- *user manual*

cost price euro 250,- ex sales tax

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