

# **A taste of atmospheric chemistry in ORCHIDEE:**

## **Importance of the terrestrial biosphere for surface-atmosphere chemical interactions.**

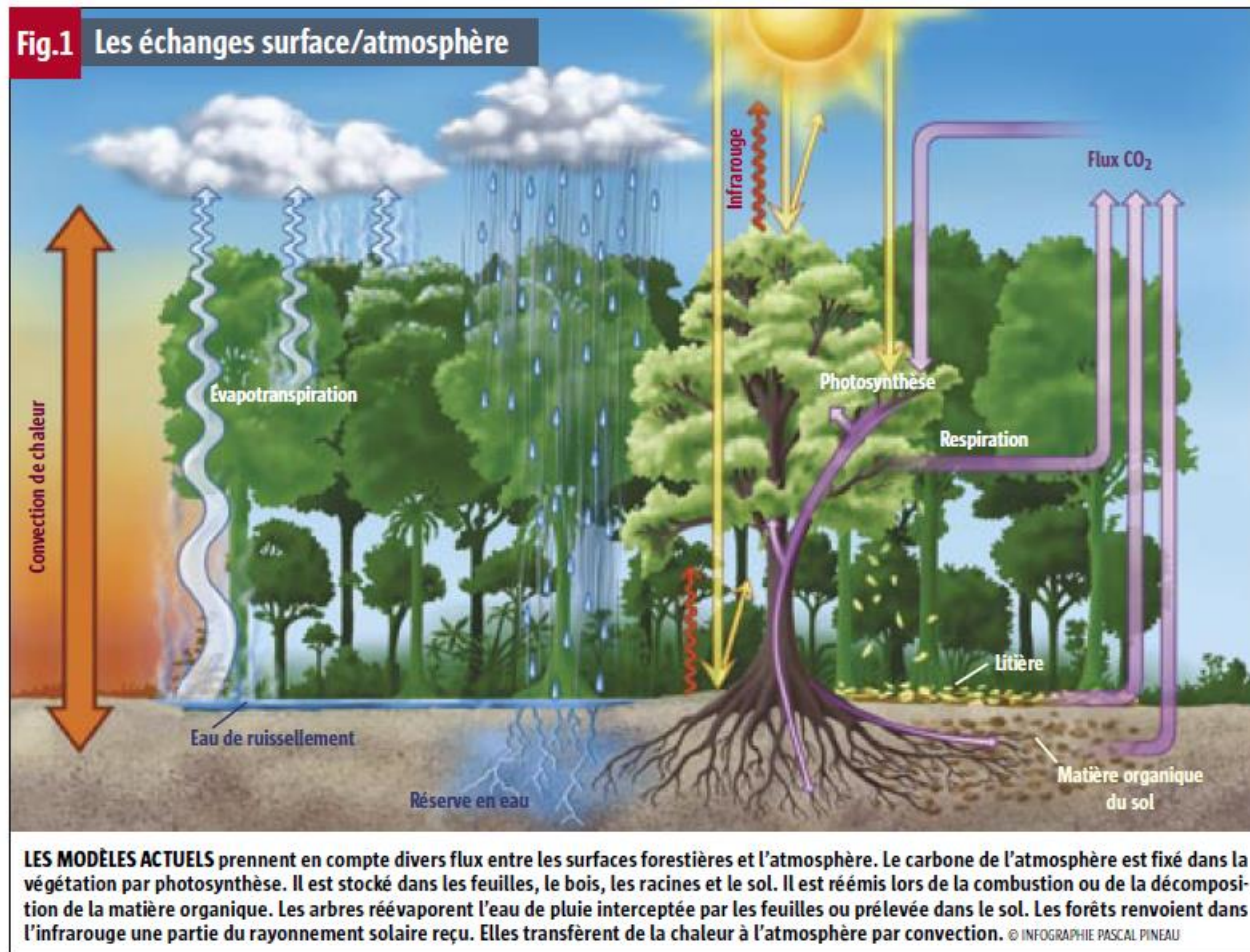
**Juliette Lathière and coworkers:**

Palmira Messina, Anne Cozic, Nicolas Vuichard, Sophie Szopa, Didier Hauglustaine, Nicolas Viovy, Josefina Ghattas, Yves Balkanski.

[juliette.lathiere@lsce.ipsl.fr](mailto:juliette.lathiere@lsce.ipsl.fr) - CNRS Researcher LSCE

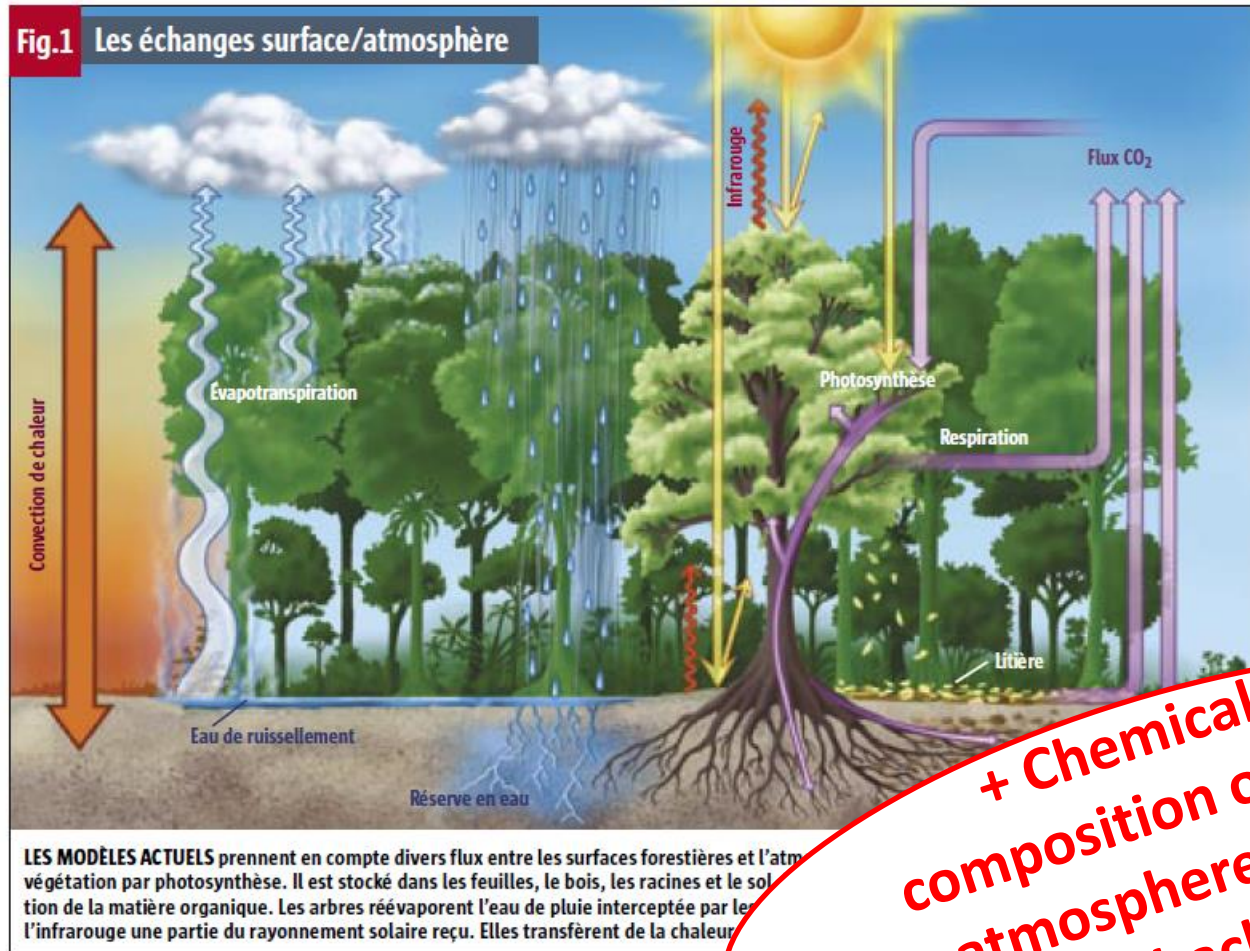


# Context



- Biophysical cycles (energy transfer, surface albedo)
  - Biogeochemical cycles (water, carbon, nitrogen...)
- Importance for the ESM and climate evolution

# Context

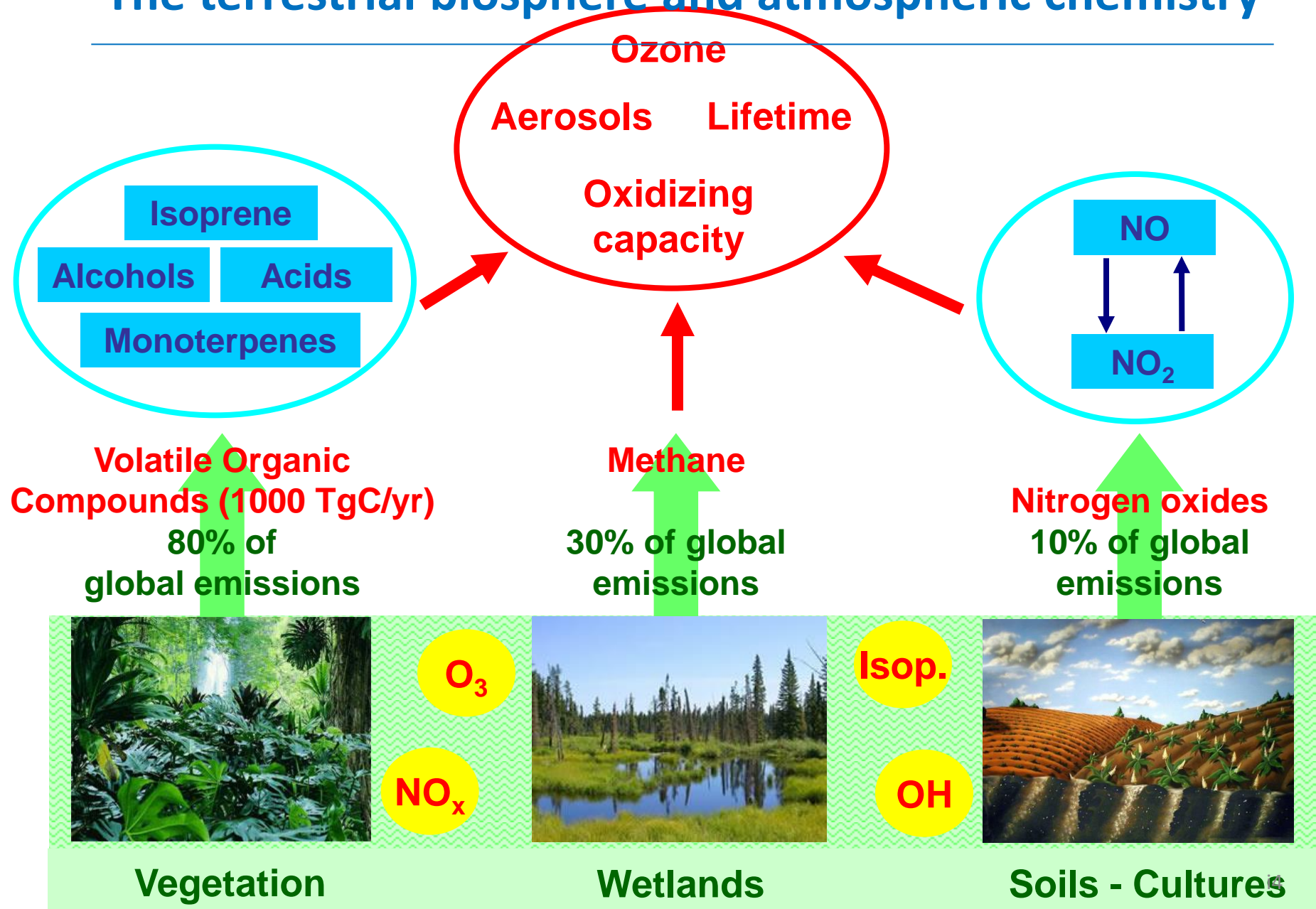


**+ Chemical composition of the atmosphere and feedbacks !**

- Biophysical cycles (energy transfer, surface fluxes...)
  - Biogeochemical cycles (water, carbon, nitrogen...)
- Importance for the ESM and climate evolution



# The terrestrial biosphere and atmospheric chemistry



# Chemistry-vegetation retroactions

Atmospheric chemical composition

CO<sub>2</sub>  
Pollution: O<sub>3</sub>, NO<sub>x</sub>, SO<sub>2</sub> and particles

Deposition



Deposition



Deposition



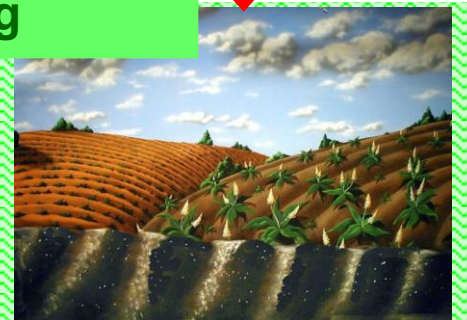
→ Growth, Distribution, Functioning



Vegetation



Wetlands



Soils - Cultures

## A few definitions...

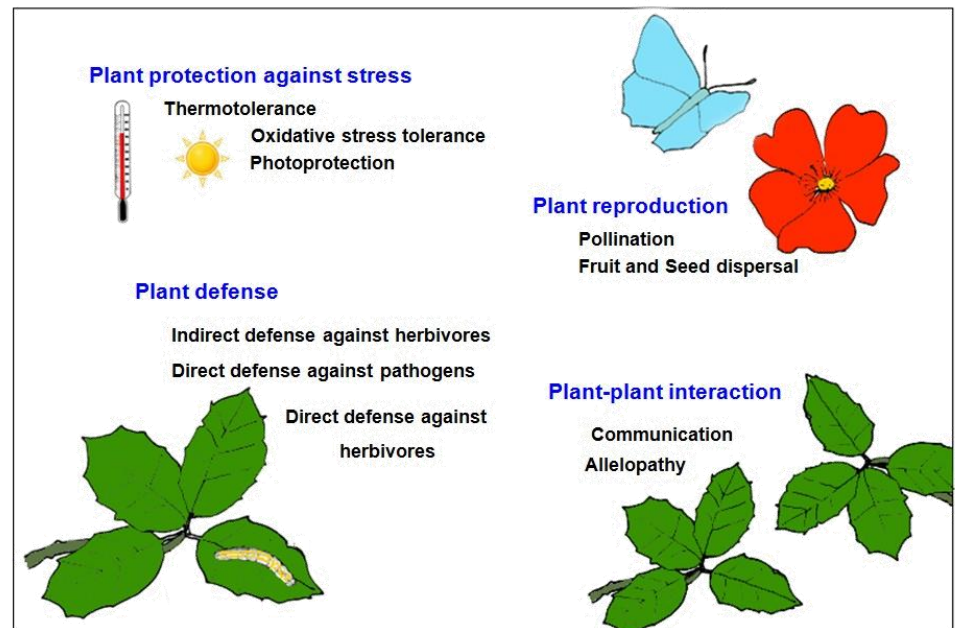
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➤ **Biogenic VOC (« biogénique » ou « biotique »)**: VOC emitted in the atmosphere from natural sources, marine or terrestrial. These emissions are related to soil microbial activity, volcanoes activity, natural gas leak, marine aerosols and marine and terrestrial biosphere.

# Biogenic VOCs : Importance for Ecology

- **Isoprene** : 0.5% to 2% of carbon assimilated and even more when stress occurs, up to 10% when accounting for every BVOCs
  - Antioxydant
  - Antibacterial protection
  - Blossom hormon
  - Keeping herbivorous away
  - Thermotolerance:  
Protecting against short high temperature episodes

## BVOCs functions in plants



# Biogenic VOCs : Importance for Ecology

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  - Thermotolerance: Protecting against short high temperature episodes
- **Monoterpenes and other VOCs (essential oils)**
  - Keeping herbivorous away
  - Antiseptic
  - Communication between plants
  - ...

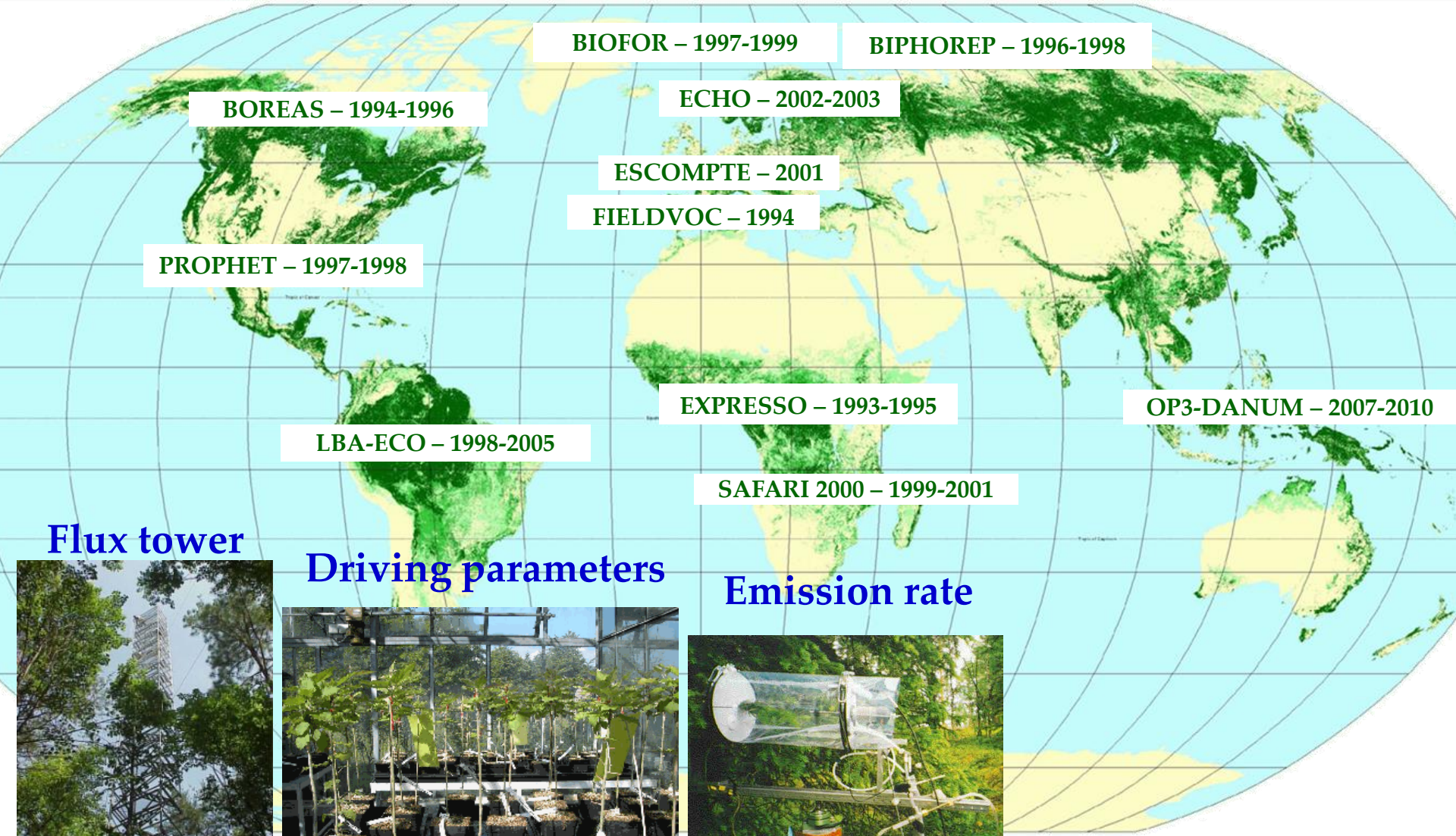


# Biogenic VOCs : Importance for Ecology

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    - Keeping herbivorous away
    - Antiseptic
    - Communication between plants
    - ...
- **Still many uncertainties: ecologic role, synthesis, ER, emission variation, compounds (difficulty to study and measure)...**

# The terrestrial biosphere and VOCs



Flux tower



Driving parameters

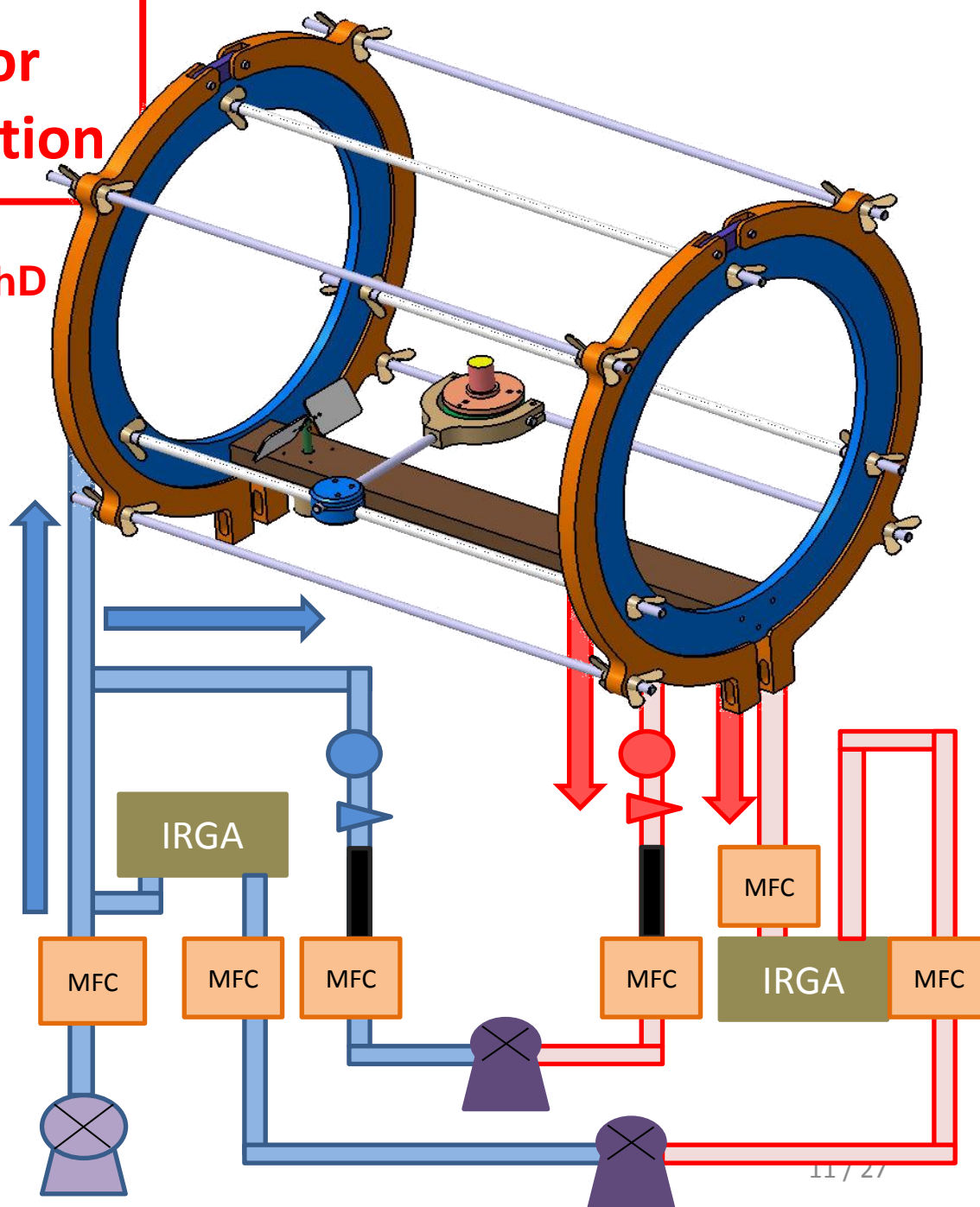


Emission rate



# Dynamic enclosure for Emission Rate investigation

Anne Cyrielle Genard-Zielinski PhD  
2014 IMBE-LSCE  
Christophe Boissard, LSCE



● Vanne d'arrêt

▲ Filtre O<sub>3</sub>

⊗ Pompe soufflante

⊗ Pompe aspirante

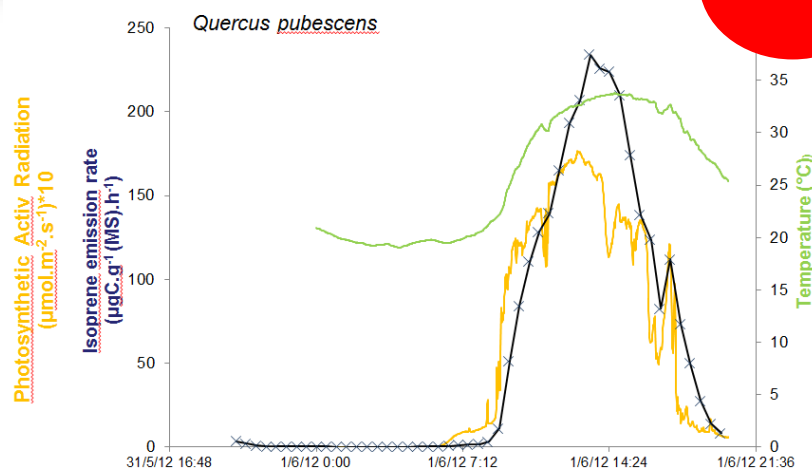
□ MFC Mass Flow Controller

■ IRGA Infra Red Gas Analyzer (H<sub>2</sub>O, CO<sub>2</sub>)

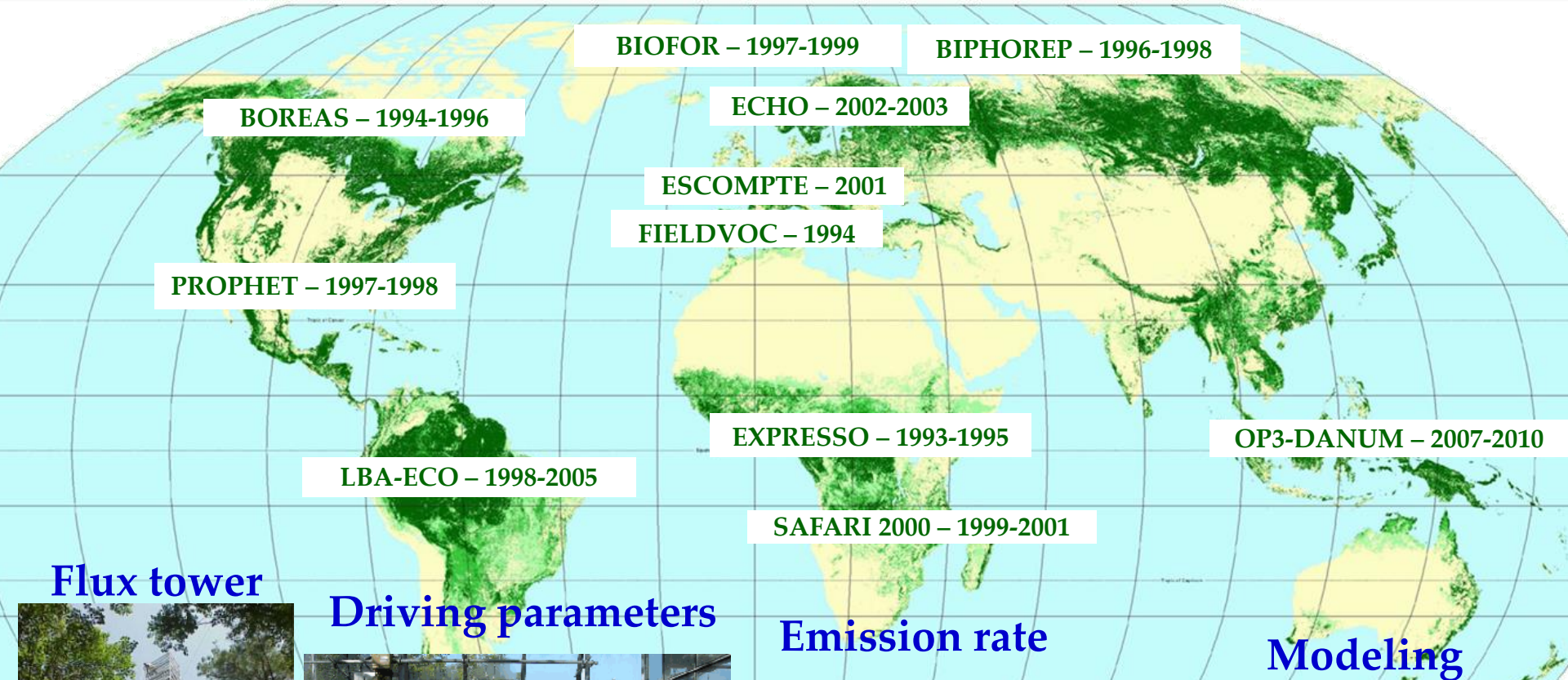


# Dynamic enclosure for Emission Rate investigation

Field campaign in Haute Provence – O3HP



# The terrestrial biosphere and VOCs



Flux tower



Driving parameters



Emission rate

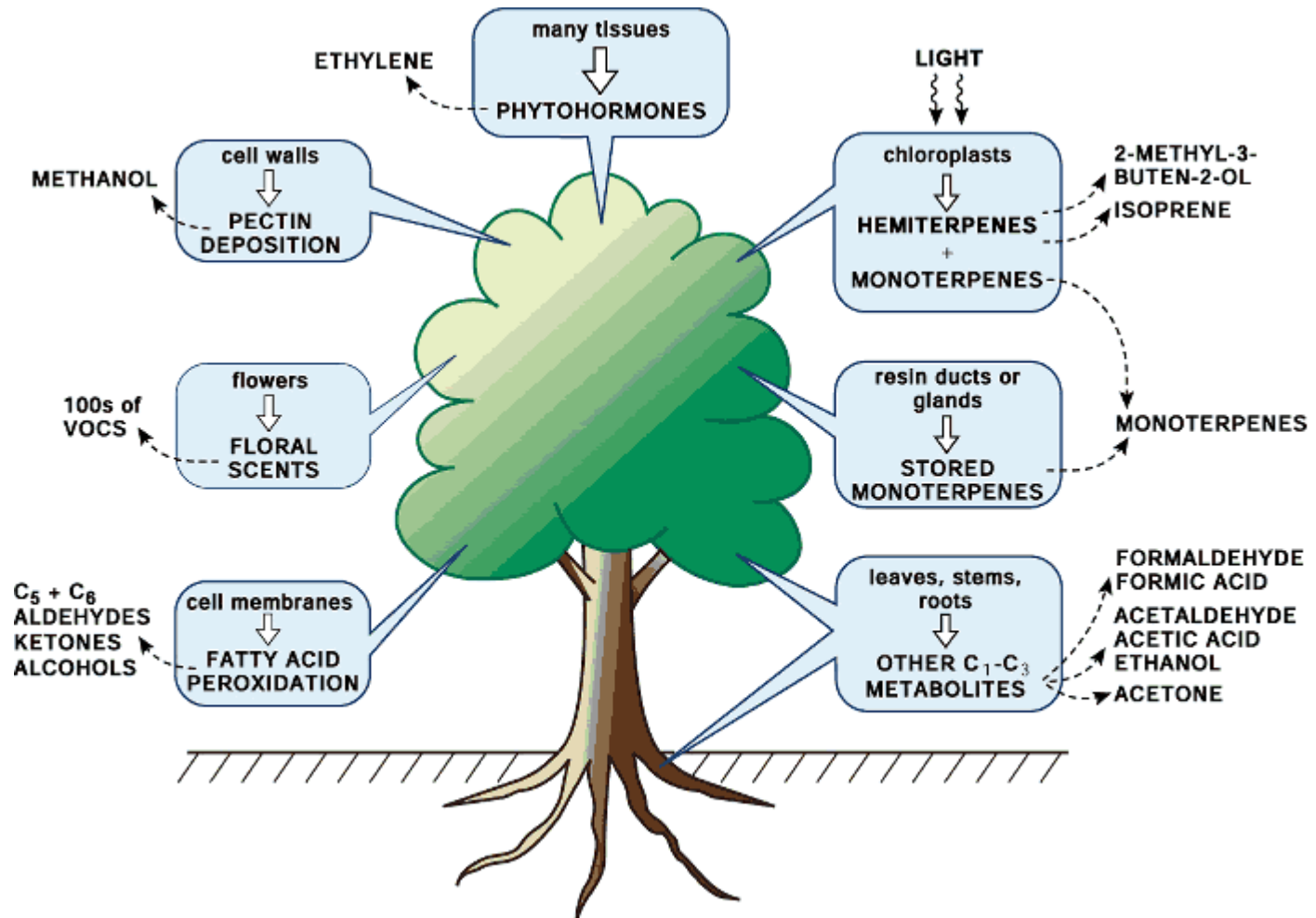


Modeling



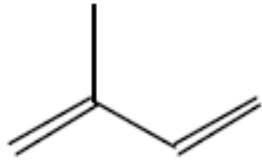


# BVOC : a great diversity of compounds



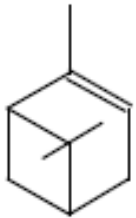
« BVOC tree »

# BVOCs : molecular structure

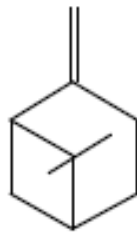


**Isoprene**

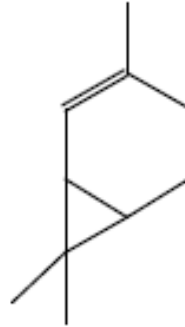
*Molécule d'isoprène*



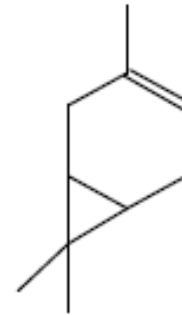
**α- Pinène**



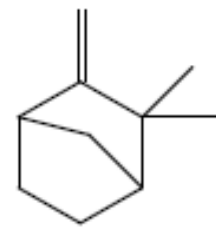
**β-Pinène**



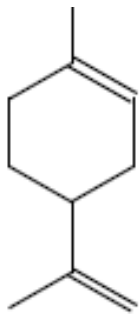
2-Carène



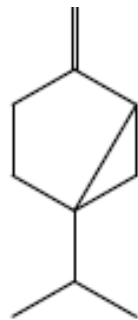
3-Carène



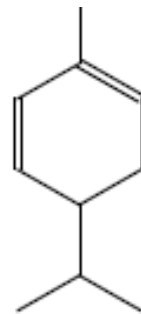
Camphène



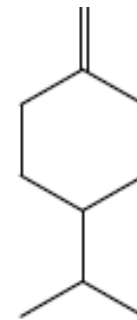
**Limonène**



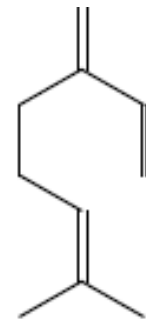
Sabinène



α-Phellandrène



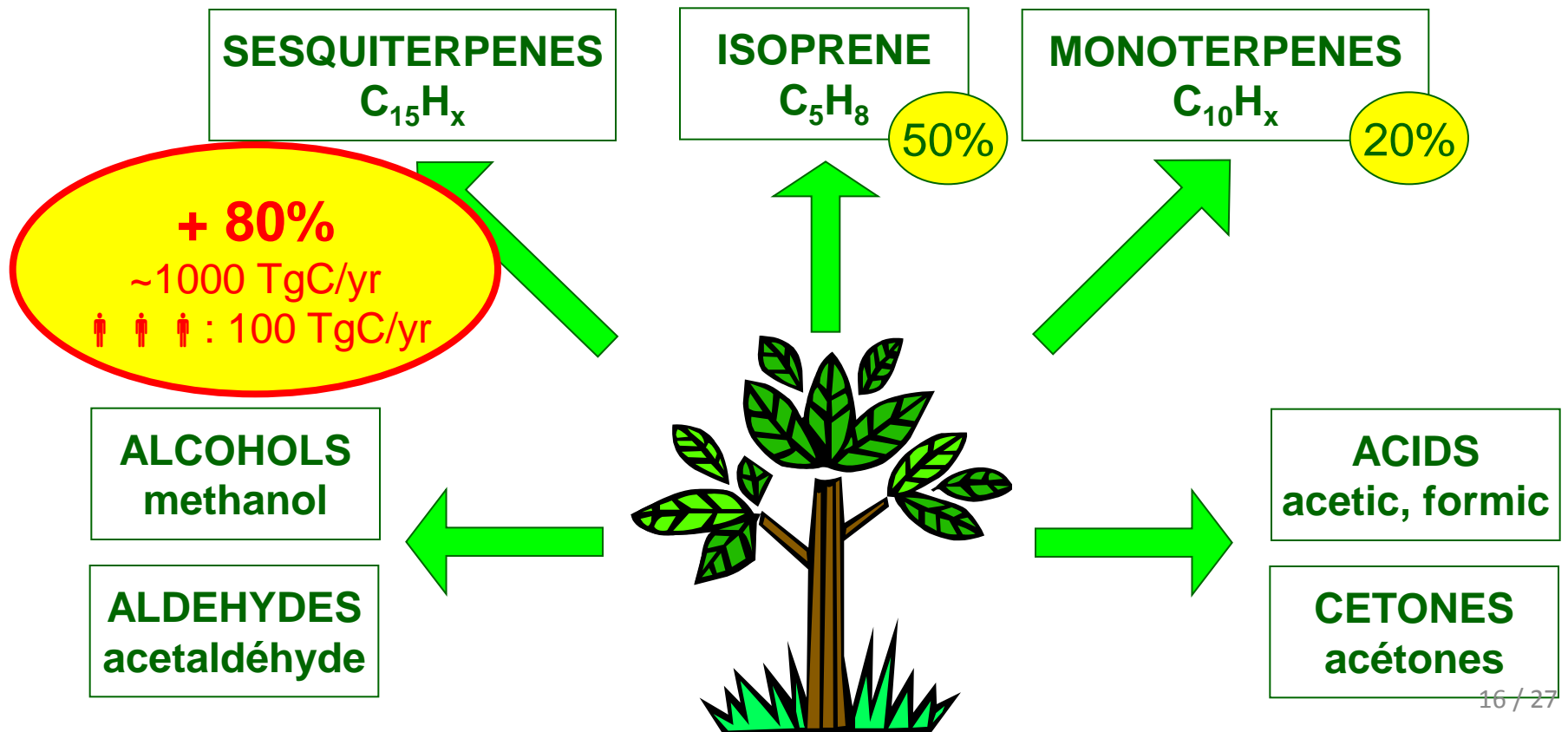
β-Phellandrène



Myrcène

**Main monoterpenes emitted by vegetation**

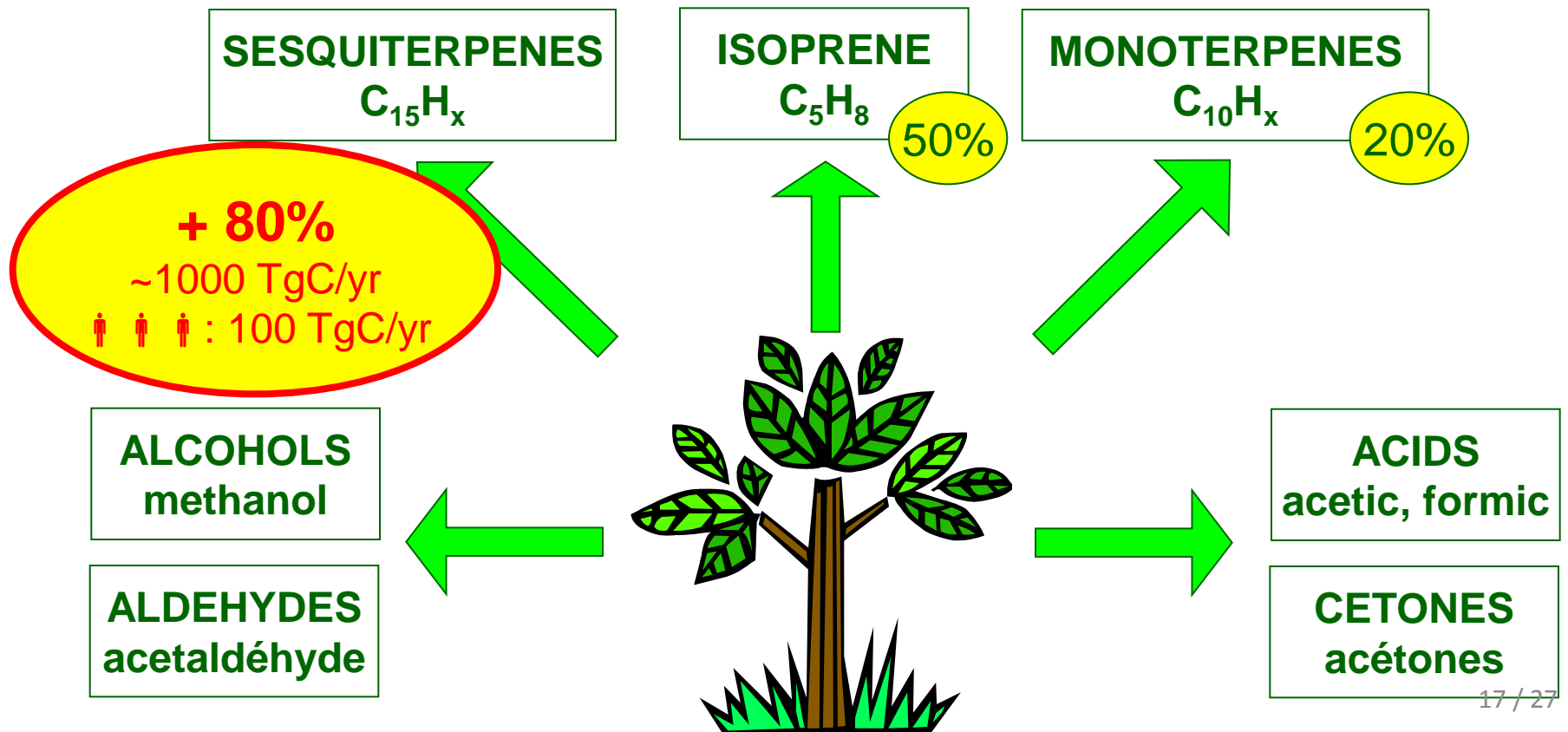
# BVOC : a great diversity of compounds



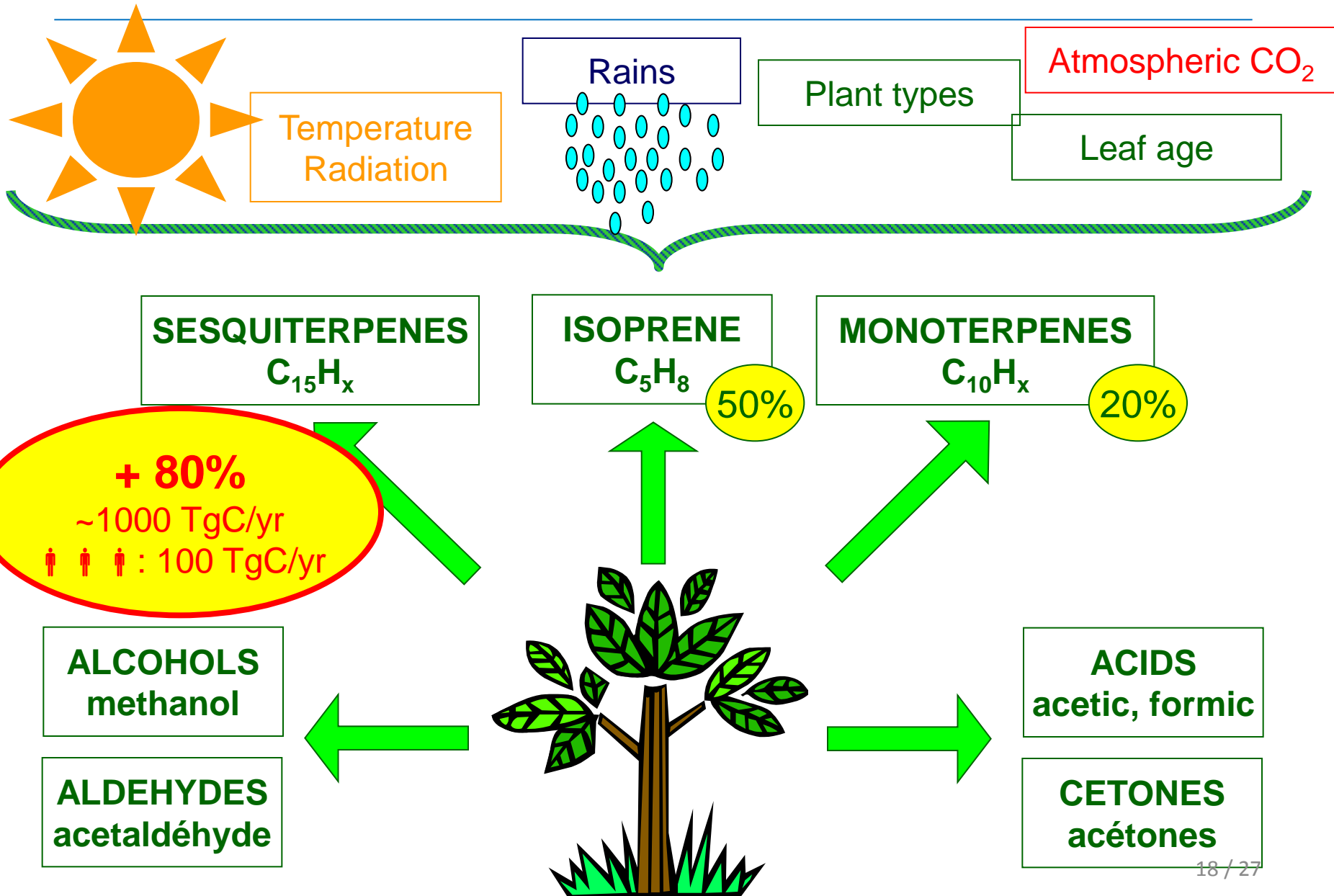
# BVOC : a great diversity of compounds

- **Other natural VOC sources:** Sharks (squalene), seaweed (cholesterol), living and human beings, oceanic biosphere, etc.

→ High diversity and emission rate typical of the terrestrial biosphere

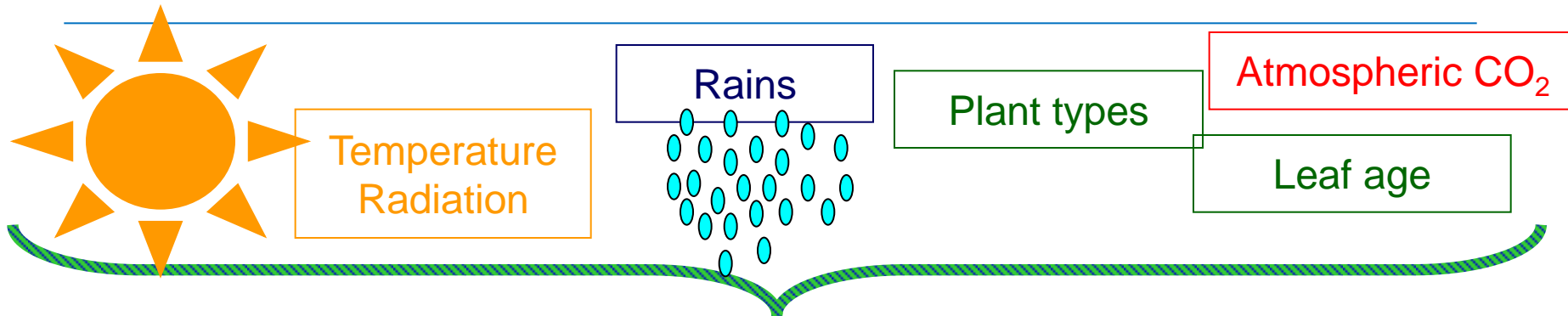


# BVOC : a great diversity of compounds

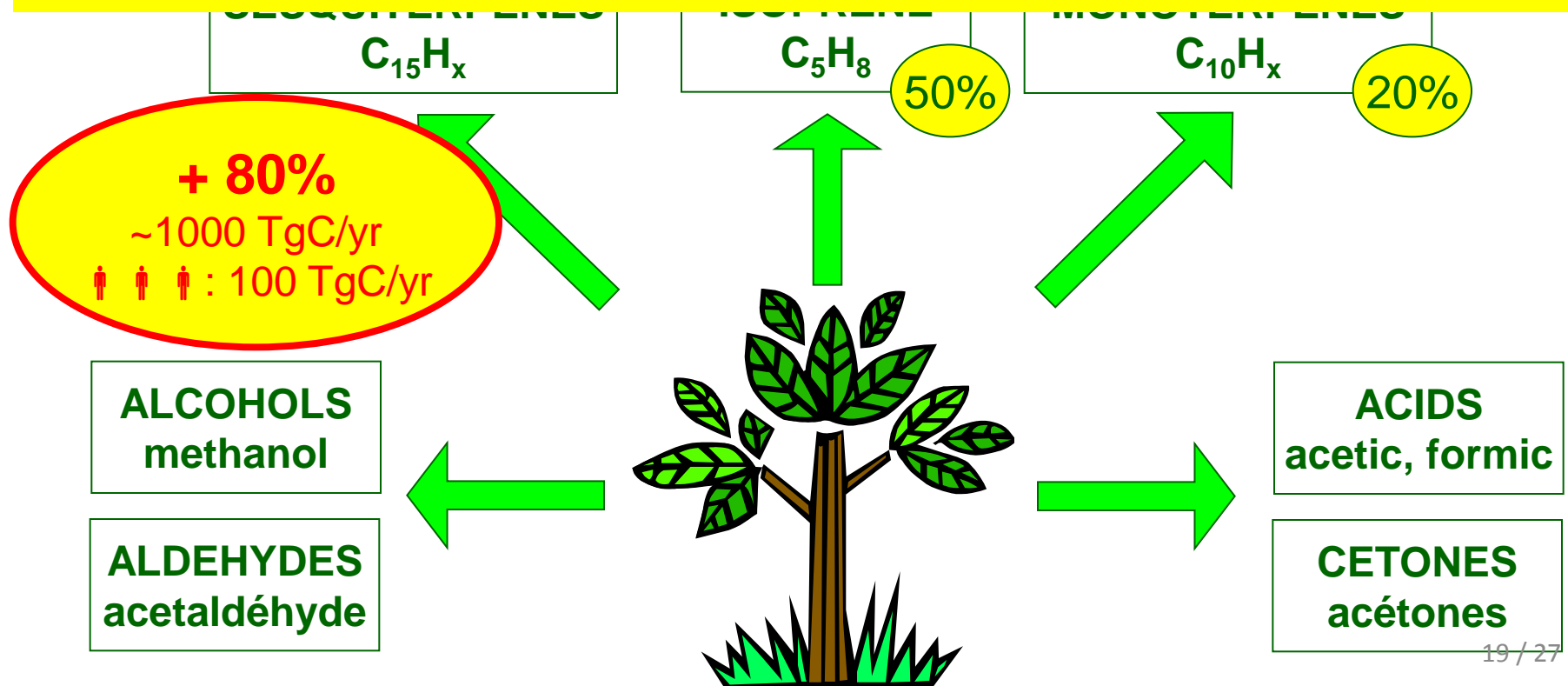




# BVOC : a great diversity of compounds



→ Implementation in models (regional, global; vegetation, chemistry)



# Biogenic VOCs in ORCHIDEE

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# Estimating VOC emissions from vegetation

Atmos. Chem. Phys., 16, 14169–14202, 2016  
www.atmos-chem-phys.net/16/14169/2016/  
doi:10.5194/acp-16-14169-2016  
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Atmospheric  
Chemistry  
and Physics  
Open Access  
EGU



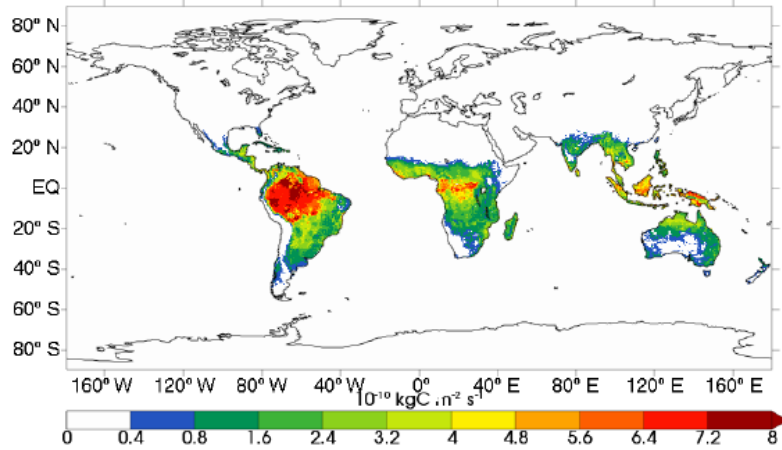
## Global biogenic volatile organic compound emissions in the ORCHIDEE and MEGAN models and sensitivity to key parameters

Palmira Messina<sup>1</sup>, Juliette Lathière<sup>1</sup>, Katerina Sindelarova<sup>2,3</sup>, Nicolas Vuichard<sup>1</sup>, Claire Granier<sup>2,4,5,6</sup>, Josefine Ghattas<sup>7</sup>, Anne Cozic<sup>1</sup>, and Didier A. Hauglustaine<sup>1</sup>

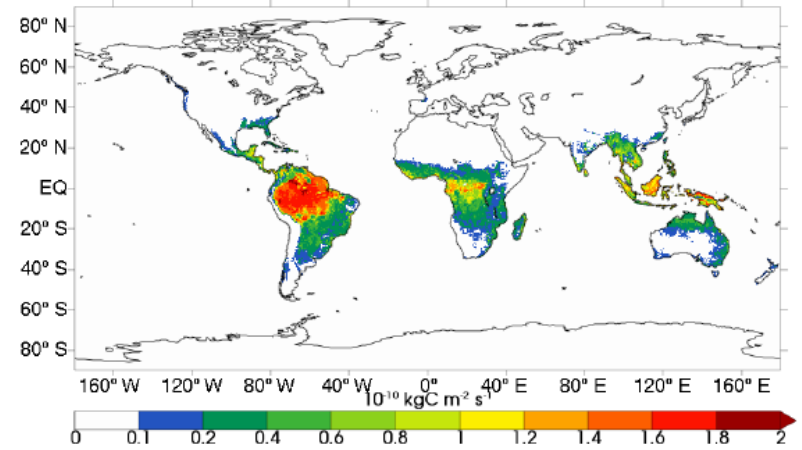
$$F_{c,i}(l) = \underbrace{\text{LAI}_i(l)}_{\text{ORCHIDEE}} \cdot \text{SLW}_i \cdot \underbrace{\text{EF}_{c,i}}_{\text{Prescribed}} \cdot \text{CTL}_c(l) \cdot L_c$$

# Estimating VOC emissions from vegetation

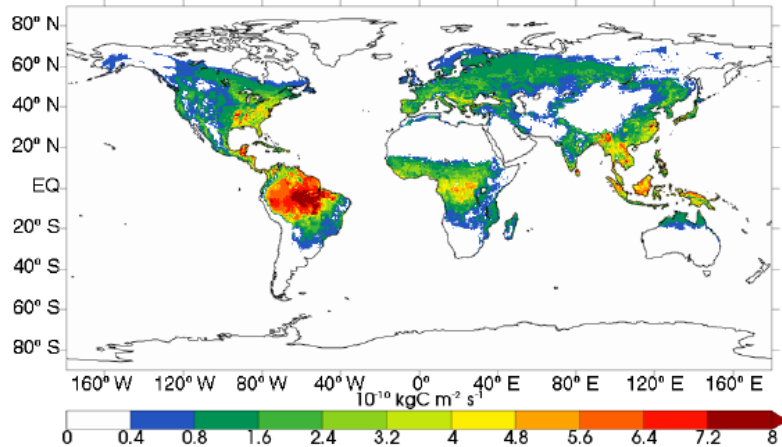
Isoprene in winter - ORCHIDEE



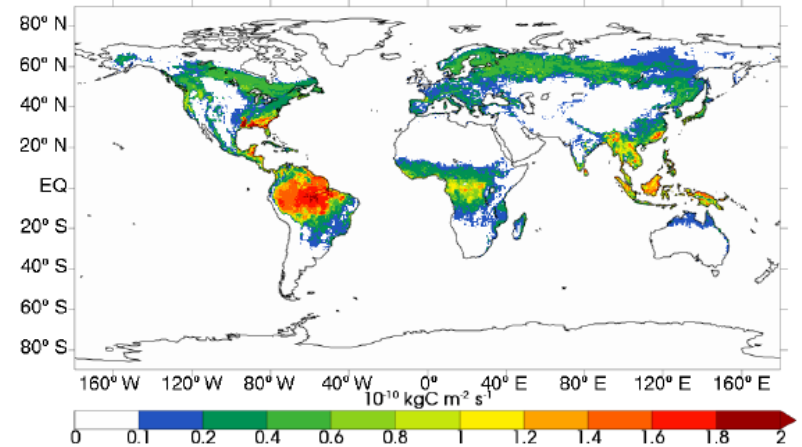
Monoterpenes in winter - ORCHIDEE



Isoprene in summer - ORCHIDEE



Monoterpenes in summer - ORCHIDEE



# In the ORCHIDEE code – Trunk version

```
p24lath@curie70:/ccc/work/cont003/dsm/p24lath/ORCHIDEE_CODE_VERSIONS/ORCHIDEE_TRUNK_22112016/modipsl/modeles/ORCHIDEE/src_sechiba> ls -l
total 2312
-rw-r--r--. 1 p24lath dsm 5625 Nov 22 15:29 AA_make
-rw-r--r--. 1 p24lath dsm 787 Nov 22 15:29 AA_make.ldef
-rw-r--r--. 1 p24lath dsm 5817 Nov 22 15:30 Makefile
-rw-r--r--. 1 p24lath dsm 101048 Nov 22 15:19 chemistry.f90
-rw-r--r--. 1 p24lath dsm 90496 Nov 22 15:29 condveg.f90
-rw-r--r--. 1 p24lath dsm 144305 Nov 22 15:29 diffuco.f90
-rw-r--r--. 1 p24lath dsm 96275 Nov 22 15:29 enerbil.f90
-rw-r--r--. 1 p24lath dsm 72364 Nov 22 15:29 explicitssnow.f90
-rw-r--r--. 1 p24lath dsm 341731 Nov 22 15:29 hydroL.f90
-rw-r--r--. 1 p24lath dsm 202155 Nov 22 15:29 hydroLc.f90
-rw-r--r--. 1 p24lath dsm 100717 Nov 22 15:29 intersurf.f90
-rw-r--r--. 1 p24lath dsm 192963 Nov 22 15:29 ioipslctrl.f90
-rw-r--r--. 1 p24lath dsm 41759 Nov 22 15:29 qsat_moisture.f90
-rw-r--r--. 1 p24lath dsm 381337 Nov 22 15:29 routing.f90
-rw-r--r--. 1 p24lath dsm 108424 Nov 22 15:29 sechiba.f90
-rw-r--r--. 1 p24lath dsm 17340 Nov 22 15:29 sechiba_io.f90
-rwxr-xr-x. 1 p24lath dsm 19636 Nov 22 15:29 sechiba_io_p.f90
-rw-r--r--. 1 p24lath dsm 183124 Nov 22 15:29 slowproc.f90
-rw-r--r--. 1 p24lath dsm 103633 Nov 22 15:29 thermosoil.f90
-rw-r--r--. 1 p24lath dsm 107013 Nov 22 15:29 thermosoilc.f90
```

**chemistry.f90**

✓ **SUBROUTINE chemistry\_bvoc**



# In the ORCHIDEE code – Trunk version

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- ❑ **Flags to add in run.def and activate for BVOC emissions (and NOx):**

```
CALL getin_p('CHEMISTRY_BVOC', ok_bvoc)
WRITE(numout,*) 'Biogenic emissions: ', ok_bvoc
```

```
IF ( ok_bvoc ) THEN
  ok_leafage      = .TRUE.
  ok_radcanopy    = .TRUE.
  ok_multilayer   = .TRUE.
  ok_pulse_NOx    = .TRUE.
  ok_bbgfertil_NOx = .TRUE.
  ok_cropsfertil_NOx = .TRUE.
```



All flags set to  
**FALSE** by default

- ❑ **Forcings used to add in sechiba.card in ListNonDel for NOx emissions:**

Located in /ccc/work/cont003/dsm/p86ips1/IGCM/SRF/chemistry/  
**orchidee\_bbg\_clim.nc**: Biomass burning  
**orchidee\_fertilizer\_1995.nc**: Fertilizer use

**CAUTION WITH NOx RESULTS !!!!**  
**IN DEVELOPMENT AND TESTS !**

# Other developments in progress in ORCHIDEE

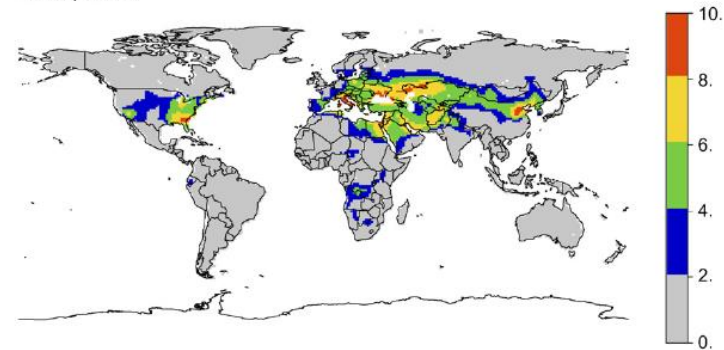
## Ozone impact on vegetation

Variable	O <sub>3</sub> Effect
Visible injury	↑
Photosynthesis	↓
Stomatal conductance	↓
Dark respiration	↑
Tree biomass	↓
Crop yield	↓
Root growth	↓
Decomposition	↓
Nitrogen uptake	↓

### ➤ Implementation in models

(a) JJA AOT40  
1980s, 1990s

Felzer et al., 2005, 2007



### ➤ Atmospheric ozone concentrations and impact on vegetation

Fig. 1. (a) Concentrations globales AOT40 d'ozone (ppmhr), issues des modèles MATCH et MIT IGSM pour les années 1980 et 1990.

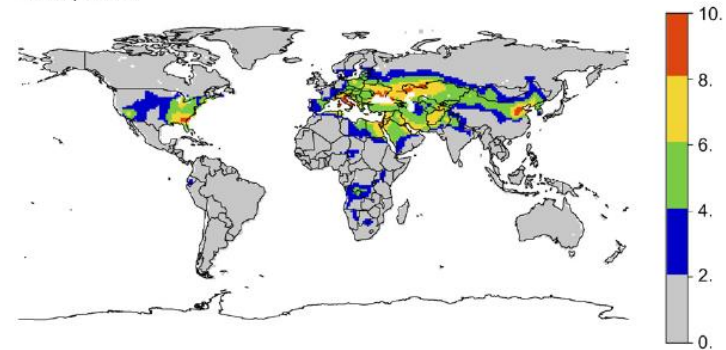
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(a) JJA AOT40 1980s, 1990s **Felzer et al., 2005, 2007**



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Fig. 1. (a) Concentrations globales AOT40 d'ozone (ppb-hr), issues des modèles MATCH et MIT IGSM pour les années 1980 et 1990.

### ➤ Thomas Verbeke PhD 2011-2015, LSCE, développements in ORCHIDEE, inclusion in trunk version to come

# Other developments in progress in ORCHIDEE

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- **Ozone Impact on vegetation:**
  - Thomas Verbeke PhD (D. Hauglustaine, N. Viovy, S. Szopa, J. Lathière), inclusion in the trunk version to come
- **Nitrogen Compounds in ORCHIDEE:**
  - Nicolas Vuichard (EURECA project)
- **Coupling with atmospheric chemistry:**
  - 2-way exchanges between ORCHIDEE and LMDzINCA (Anne Cozic, INCA group)