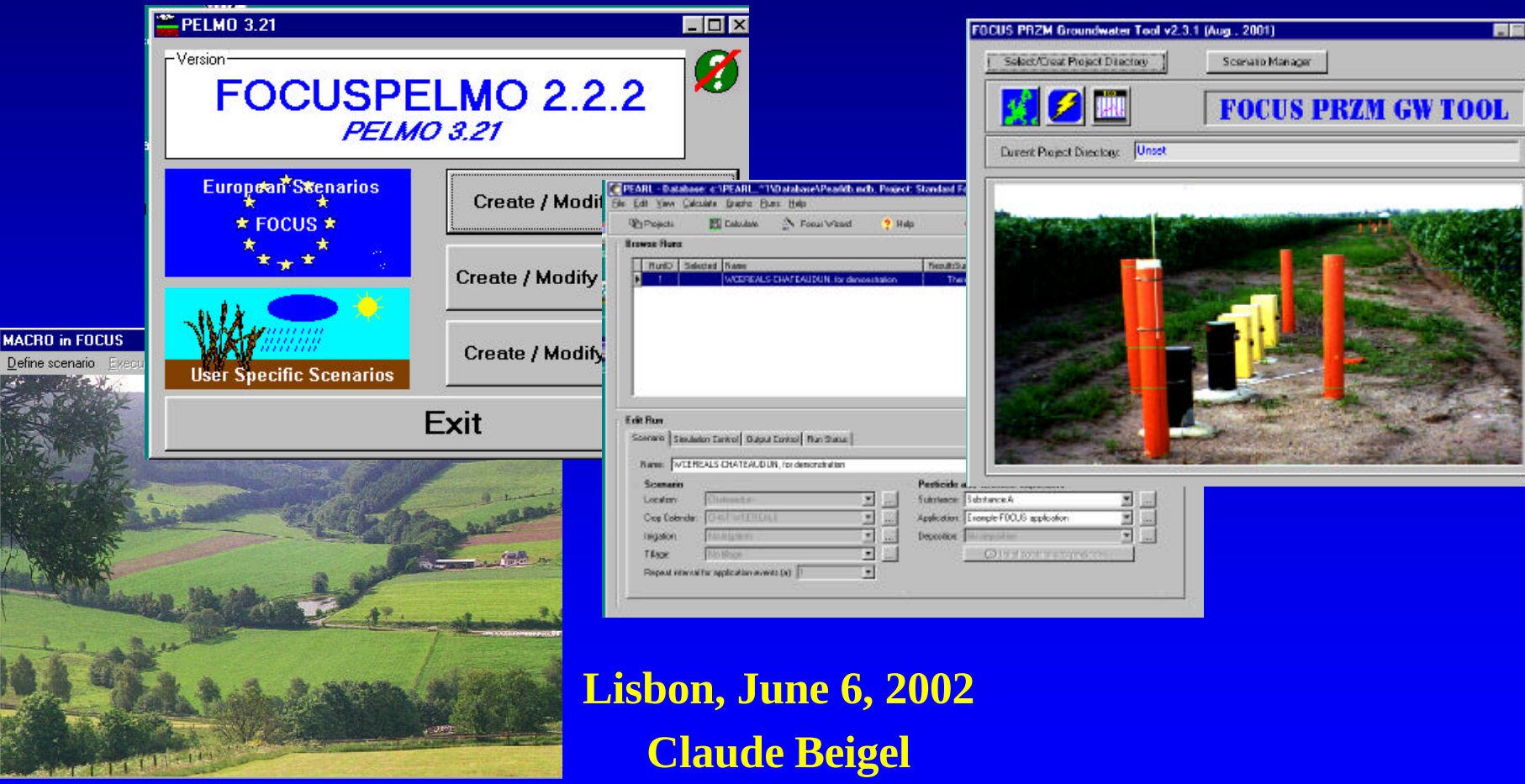
Experience in Industry with FOCUS Groundwater Scenarios and Shells



Lisbon, June 6, 2002

Claude Beigel

BASF Corporation, USA

BASF

FOCUS Groundwater Scenarios and Shells

- A major step towards harmonization and consensus at EU level
- Unresolved issues
- Interpretation of results
- What happens next at Member State level?

BASF

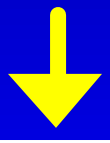
Situation Prior to FOCUS gw

- Which model?
  - National preferences, e.g. PELMO, PESTLA
  - Different model versions
- Which scenario(s)?
  - Existing national scenarios used as surrogates (e.g. Dutch, Hamburg, Denmark)
  - Specific scenarios developed by applicant
- Which parameters?
  - Little to no guidance available on model parameterization

BASF

Situation Prior to FOCUS gw

- Basic discussion at ECCO meetings
  - (e.g. concerning choice of model or use of laboratory vs. field DT_{50})
- Difficulty to attain consensus
- Questions on validity of the assessment



- Delay in decisions
- Unforeseeable decisions influenced by individual opinions

BASF

Main Achievements of FOCUS gw

Standard tool for harmonized assessment at EU level for Annex 1 listing

- Standard models and scenarios
- Guidance on assessment process including parameterization
- Ease of use (shells) and accessibility (website)
- Version control process in place for communicating issues and latest developments

BASF

Different Uses of the FOCUS gw Scenarios and Shells

- Primary use for assessment for Annex 1 listing of new compounds and re-registration of existing compounds (List 1 to 3)

- Screening tool for decision making for compounds in pre-development or for new use-patterns

BASF

Unresolved Issues

- Number and choice of models to run
- Parameterization
  - Averaging of data
  - Guidance for generation of degradation parameters
  - Moisture content correction
  - pH-dependent sorption
  - Application times and crop interception

BASF

Choice of Model

- FOCUS guidance
  - 1 chromatographic or capacity-based model (choice based on model-specific features)
  - MACRO for preferential flow
- In practice
  - Encouragement/request to run all 4 models
  - Choice based on RMS preferences

BASF

Parameterization

Averaging of Pesticide Input Parameter Values

- FOCUS guidance: use average values for pesticide input parameters
  - Degradation (DT_{50})
  - Sorption (K_{foc}, 1/n)
- Need for clear guidance
  - Averaging method (arithmetic, geometric, harmonic mean)

BASF

Parameterization

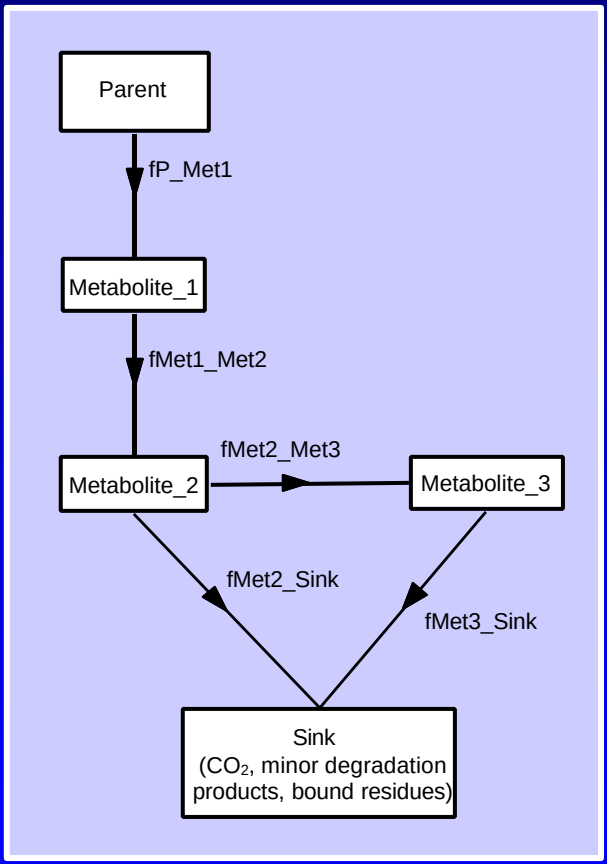
Generating Degradation Parameters

- Need for clear guidance
  - Accepted software and methods
  - Metabolites
    - Formation fraction and degradation rate
    - Derived from parent study or separate studies
    - Use of compartment models, e.g. ModelMaker
  - Use of field data

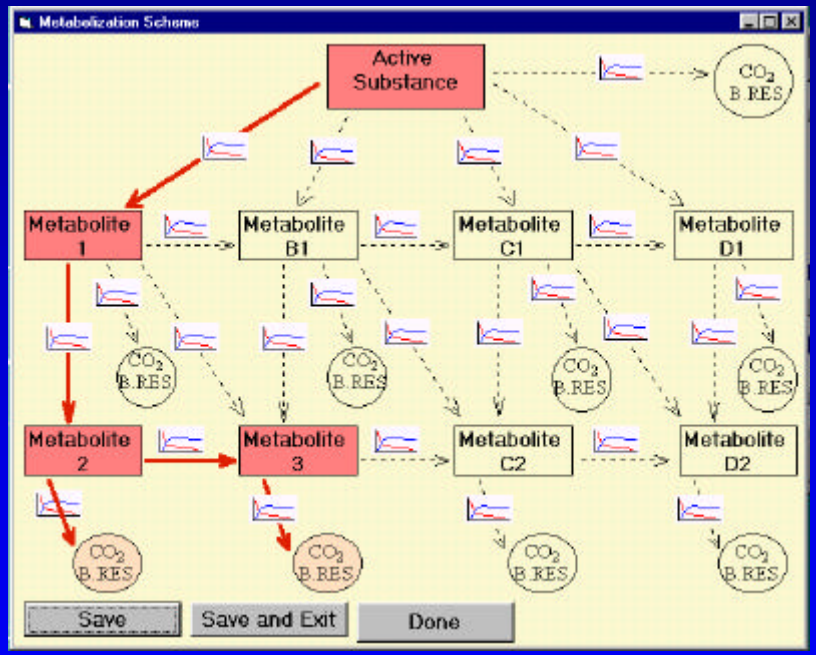
➔FOCUS kinetics workgroup

BASF

Example with Laboratory Degradation Including Metabolites



Multi-compartment model for description of the aerobic soil degradation of a substance including degradation products



Metabolization scheme in FOCUS-PELMO for evaluation of leaching of the substance and degradation products

BASF

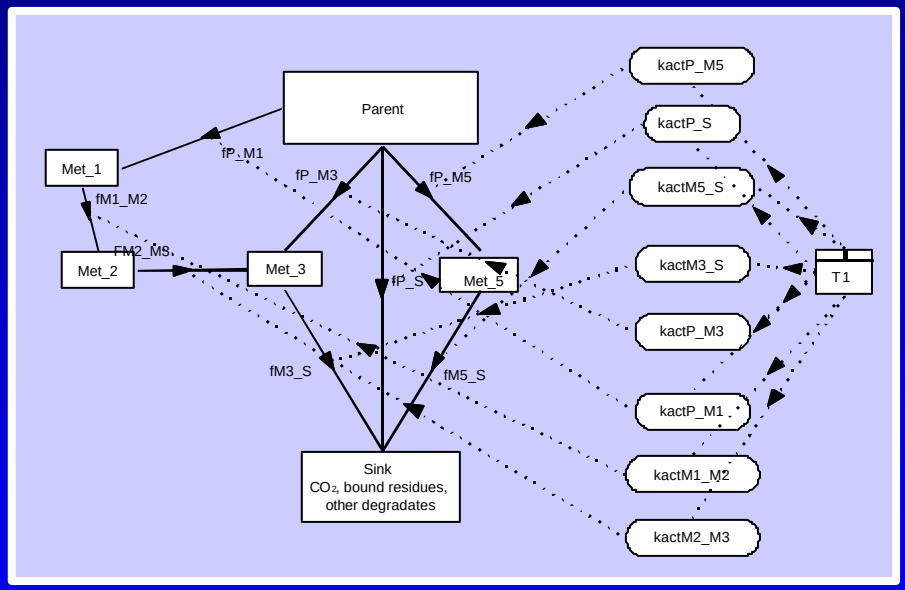
Parameterization

Standardization of Degradation Parameters

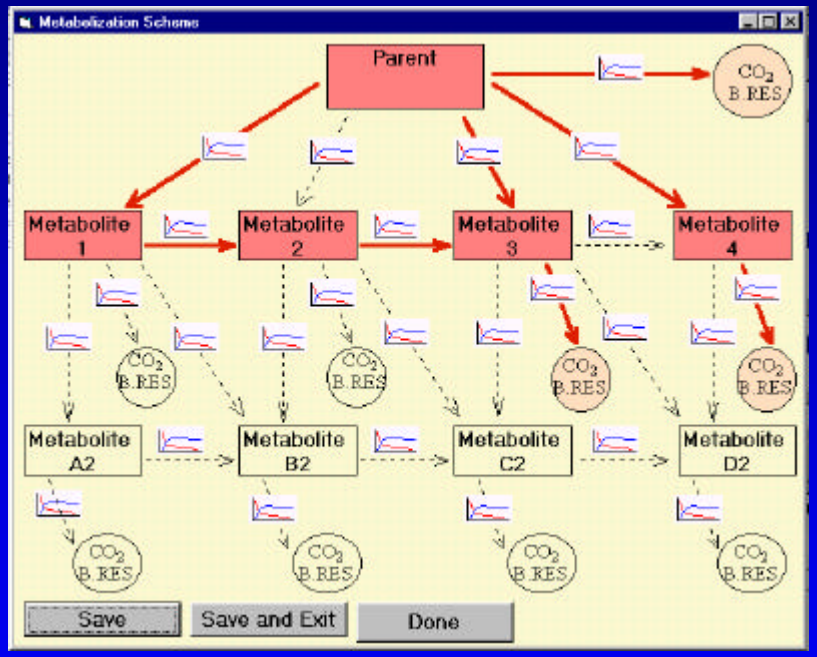
- Adjustment to reference moisture content
  - pF2 usually not available
  - FOCUS default values for soil types
- Biphasic degradation
- Standardization of field values
  - Temperature and moisture
  - Better description of observed data
  - Can be transferred between different regions
  - Difficult to generate

BASF

Example with Field Degradation Including Metabolites



Multi-compartment model for description of the field degradation of Parent and soil metabolites, with standardization to FOCUS reference soil temperature and moisture conditions



Metabolization scheme in FOCUS-PELMO for evaluation of leaching of the substance and its degradation products

BASF

Parameterization

pH-dependent sorption

- Cannot average K_{fOC} if pH-dependency
- pH-dependency option in PEARL
- Specific study needed
- Substances with several pKa values

BASF

Parameterization

Application Timing and Crop Interception

- Timing of applications
  - GAPs do not always agree with FOCUS planting and emergence dates
- Crop interception
  - Need for more detailed and agreed upon interception values function of BBCH growth stage

BASF

Interpretation of Results

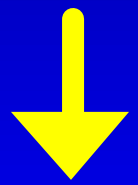
- Are the results realistic?
  - Assessment for groundwater based on predicted concentrations in shallow soil (at 1-m depth)
  - Results are fairly consistent with lysimeter results (worst-case conditions) for parent and metabolites

➔ **Conservative assessment representing worst-case conditions**

BASF

Interpretation of Results

- FOCUS guidance document:
  - 1 scenario < 0.1µg L^{-1} demonstrates 1 safe use

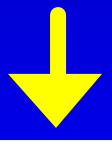


Sufficient for Annex 1 listing

BASF

FOCUS gw as a Basis for National Registrations

- Sound, harmonized approach
- Location scenarios designed to represent a variety of climate and soil conditions
- Wide range of crop scenarios
- Conservative assessment



Could be used as first step, starting point for national registration (already in some Member States)

BASF