A modular software architecture for a pesticide leaching model

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INTRODUCTION

The use of leaching models to predict the fate of pesticides starts since seventies, and EU directive 414/91 promotes their use in the registration process. These software produce result repeatable and comparables each others, nevertheless they are standalone, their source code is not easily available and this may create problems in inclusion in wider systems.
SEAMLESS, an integrated project of the 6th Framework aims the generation of an integrated framework with computer models and approaches for ex-ante assessment of alternative agricultural and environmental policy options for sustainable development in Europe. To analyse the externalities related to agrochemical application following agricultural activities, a pesticide model with the following characteristics was required:

- a modular software architecture,
- a programming language object oriented,
- a standardised way of communication among the other models,
- standardised interfaces to get and let information according project common rules.

At the beginning of 2006 the first prototype of the component has been uploaded in the SEAMLESS framework.

THE IT STRUCTURE

The structure is a container which describes a particular environmental context (for example the soil, the air or whatever else) and gives some tools and facilities to provide methods to estimate its properties.
This container provides three main structures, hierarchically linked and with their own properties:

- "Macro-component", representing the whole environmental compartment (i.e. the pesticide), whose main function is to regulate the communication with the external world (i.e. the "Modcom" framework);
- "Component", representing a particular environmental matter related to the "Macro-component" (i.e. the behaviour of pesticides in the soil), is an independent calculation unit that groups one or more Strategies;
- "Strategy", a particular way of modelling an environmental matter (i.e. the drift). Each strategy implements a calculation method (what is generally called "the model") in order to determine one or more output variables, provided some input variables and strategy parameters; parameters can assume a fixed value or they can be evaluated assigning an estimation method

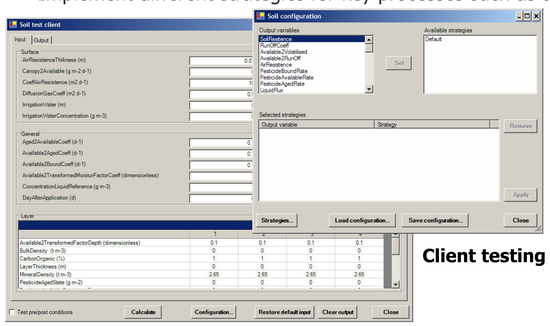
LINKS AMONG OTHER COMPONENTS

The modular approach of SEAMLESS made easy to focus only on pesticide aspects but this requires dependency from the other component supply. In particular the component requires information about field dimensions, soil layers and densities from soil structure component, water fluxes and contents from soil water component, rain from climate, crop development stage from crop component.

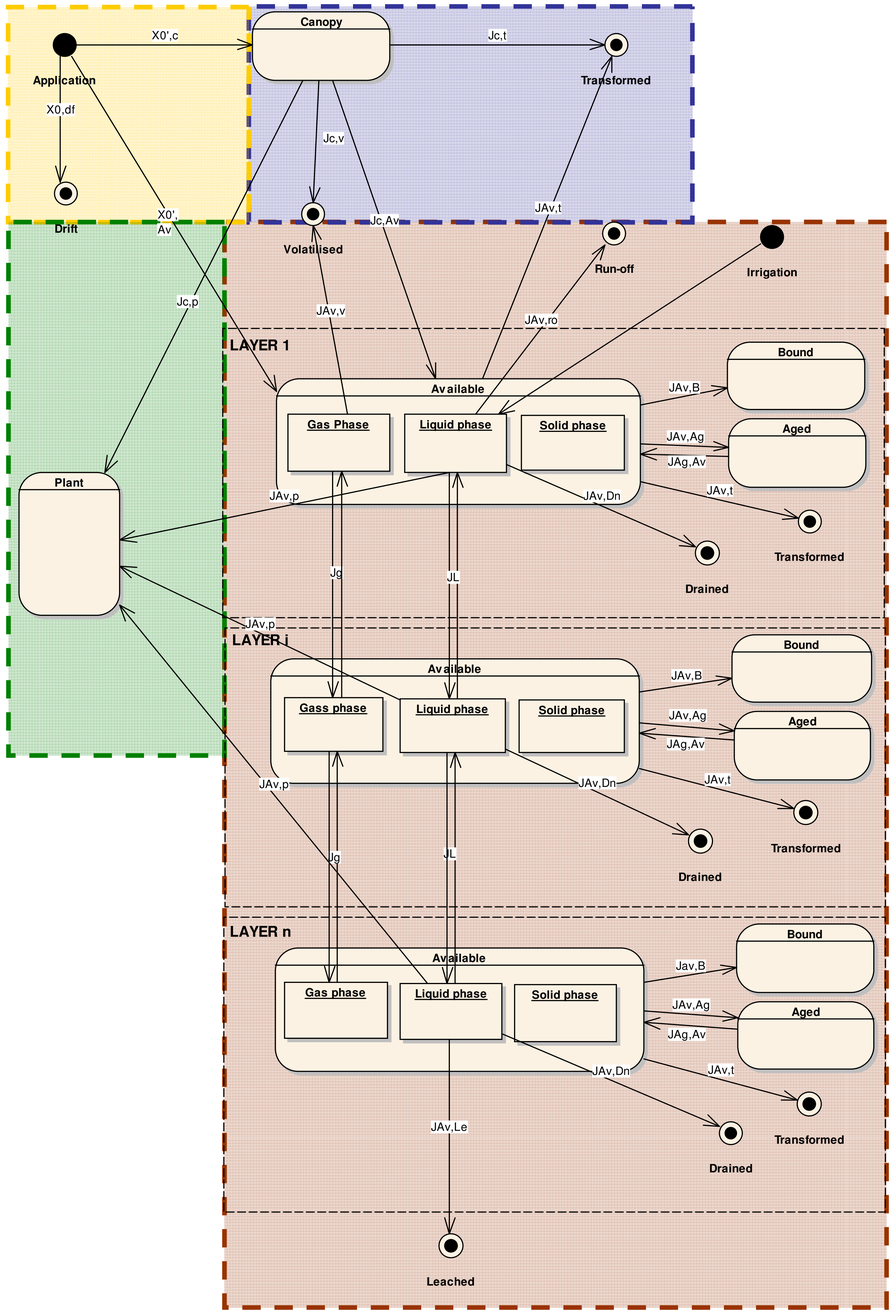
TOWARDS PROTOYPE 2

The next version of component is going to:

- Simulate crop association
- Simulate metabolites
- Simulate pesticide behaviour in micro and macropores
- Implement different strategies for key processes such as degradation.



Client testing form: soil component



Application — Flow in: where the pesticide enters the system

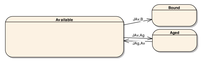
Bound — Compartment: where pesticide is stored

Transformed — Flow out: where the pesticide leave the system

The logical view of Macro-component Pesticide

Air component
Canopy component
Crop component
Soil component

SOIL

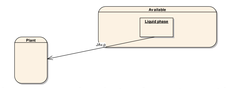


The pesticide equilibrium in the soil has been modelled according the model developed by Fragoulis et al. (2004) which considers 3 different pool:
1.The available pool is the pesticide quantity which can move and can be transformed by biotic processes. It is partitioned in 3 phases: solid, liquid and gaseous.
2.The bound pool is the pesticide quantity which cannot extracted from the soil without altering it physical-chemical structure. This supposes that the molecule is not in its original form but has been bound irreversibly to the soil particles. The first prototype implement the Fragoulis approach ($X_{B,max}$ - maximum bound concentration, k_B - binding coefficient, t_i - days after the last application):

$$J_{Av,B} = k_B X_{B,max} e^{-k_B t_i}$$

3.The aging pool is the pesticide quantity which becomes less available with time to ecological receptors as the results of entrapment within soil micropores and organic matter. In the prototype 1 this is modelled by 2 first order constants: one fast that describes the flow from Available to Bound and the second slower that describes the reverse process.

ROOT UPTAKE



Pesticide root uptake is calculated using the transpiration stream concentration factor which is calculated by the Burken e Schnoor (1998) relationship :

$$J_{Av,P} = 0.756\, C_L\, q_p\, e^{\frac{-(\log k_{OW} - 2.50)^2}{2.58}}$$

DRIFT

Drift is the amount of pesticide that leave the field during the application because of the nebulisation of the solution or the dusting. Drift is calculated using the integral of the equations of EU drift calculator which is used in the European pesticide registration procedure
The drift loss ($X_{0,df}$) has been calculated (X_0 - applied amount, L_{df} - drift loss, P -field perimeter, S -field area):

$$X_{0,df} = \frac{X_o\, L_{df}\, P}{2\, S}$$

Crop	L_{df} [m]
Annual crop	0.162084658
Orchard (early)	3.08205739
Orchard (late)	1.5255739
hops	1.8935553
vineyard (early)	0.2506977
vineyard (late)	0.758173
Aerial application	11.47617

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http://www.seamless-ip.org

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