# ROLE OF COMPUTER SIMULATION MODELING IN PESTICIDE ENVIRONMENTAL RISK ASSESSMENT<sup>1</sup>

R. Don Wauchope
U.S. Department of Agriculture – Agricultural Research Service
Southeast Watershed Research Laboratory
P.O. Box 946,Tifton, Georgia 31794 USA
don@tifton.usda.gov

Jan B. H. J. Linders
National Institute for Public Health and the Environment
Expert Centre for Substances
PO Box 1, NL-3720 BA, Bilthoven, Netherlands
Jan.Linders@RIVM.NL

#### **ABSTRACT**

It has been estimated that the equivalent of approximately \$US 50 billion has been spent on research on the behavior and fate of pesticides in the environment since Rachel Carson published "Silent Spring" in 1962. Much of the resulting knowledge has been summarized explicitly in computer algorithms in a variety of empirical, deterministic, and probabilistic simulation models. These models describe and predict the transport, degradation and resultant concentrations of pesticides in various compartments of the environment during and after application.

In many cases the known errors of model predictions are large. For this reason they are typically designed to be "conservative", i.e., err on the side of over-prediction of concentrations in order to err on the side of safety. These predictions are then compared with toxicity data, from tests of the pesticide on a series of standard representative biota, including terrestrial and aquatic indicator species and higher animals (e.g., wildlife and humans). The models' predictions are good enough in some cases to provide screening of those compounds which are very unlikely to do harm, and to indicate those compounds which must be investigated further. If further investigation is indicated a more detailed (and therefore more complicated) model may be employed to give a better estimate, or field experiments may be required. A model may be used to explore "what if" questions leading to possible alternative pesticide usage patterns which give lower potential environmental concentrations and allowable exposures.

We are currently at a maturing stage in this research where the knowledge base of pesticide behavior in the environmental is growing more slowly than in the past. However, innovative uses are being made of the explosion in available computer technology to use models to take ever more advantage of the knowledge we have. In this presentation, current developments in the state of the art as practiced in North

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America and Europe will be presented. Specifically, we will look at the efforts of the 'Focus' consortium in the European Union, and the 'EMWG' consortium in North America. These groups have been innovative in developing a process and mechanisms for discussion amongst academic, agriculture, industry and regulatory scientists, for consensus adoption of research advances into risk management methodology.

## OUTLINE

## I. INTRODUCTION

A. Risk Paradigm

Often environmental Chemists and toxicologists each assume the other can do more than they can...

- B. Need for models
  - 1. Complex parameter space & extrapolation
  - 2. Risk is probabilistic (Crystal Ball)

# II. HISTORY (mainly US)

- A. Surface water NPS (clean water act -- runoff: CREAMS
- B. Groundwater NPS (Drinking water act -- groundwater) PRZM and Europe
- C. FQPA: cumulative and aggregate exposure; risk cup
  - 1. dietary modeling
  - 2. regression models

## III. CURRENT STATE OF THE ART (tour of the Web)

- A. US/Canada: EMWG (URL)
- B. EU: FOCUS (URL)
- C. Agricultural Environmental Modeling: the future
- D. Scale Effects

## IV. CONCLUSION

Desperation replaces suspicion (we have to use them)

## **RELEVANT URL's:**

USDA-ARS: http://www.ars.usda.gov/

SWAT model site: <a href="http://www.brc.tamus.edu/swat/index.html">http://www.brc.tamus.edu/swat/index.html</a>

Southeast Watershed Research Laboratory : http://sacs.cpes.peachnet.edu/sewrl/

REMM model: http://sacs.cpes.peachnet.edu/remmwww/

Object Modeling System <a href="http://oms.ars.usda.gov/">http://oms.ars.usda.gov/</a> RZWQM model: <a href="http://arsagsoftware.ars.usda.gov/">http://arsagsoftware.ars.usda.gov/</a>

Chemical Properties Databases http://chemfinder.com

EPA

National Environmental Research Laboratory: http://www.epa.gov/athens

BASINS site: http://www.epa.gov/ost/basins/

CEAM home page: http://www.epa.gov/ceampubl/ceamhome.htm

CARAT web page: www.epa.gov/pesticides/carat/

EFED Models site: <a href="http://www.epa.gov/oppefed1/models/water/index.htm">http://www.epa.gov/oppefed1/models/water/index.htm</a>
Field dissipation Workshop, July/01 <a href="http://esc.syrres.com/fdw/default.htm">http://esc.syrres.com/fdw/default.htm</a>
Pesticide fact sheets—new Al's: <a href="http://www.epa.gov/opprd001/factsheets/">http://www.epa.gov/opprd001/factsheets/</a>

Registration Eligibility Documents (RED;s):

http://www.epa.gov/pesticides/reregistration/status.htm

EMWG web site: https://lists.epa.gov/cgi-bin/lyris.pl?enter=emwglist

FOCUS web site for GW modeling (PRZM, PEARL, PELMO, MACRO)

http://viso.ei.jrc.it/focus/

FIFRA Environmental Modeling Work Group (FEMWG) site http://www.femvtf.com/Welcome.html

WIN-PST pesticide screening tool:

HTTP://www.wcc.nrcs.usda.gov/pestmgt/winpst.html

PEARL web site: http://www.alterra.dlo.nl/english/

PEST model parameter optimization software:

http://www.rockware.com/catalog/pages/freepest.html

Pest Management Science: <a href="http://www.wiley.co.uk/wileychi/sci/ps.html">http://www.wiley.co.uk/wileychi/sci/ps.html</a>
Pesticide Fate Models Web Site: <a href="http://www.pfmodels.org/index.html">http://www.pfmodels.org/index.html</a>

PRZM (by FOCUS) site: http://arno.ei.jrc.it:8181/focus