MODELLING OF PESTICIDE UPTAKE IN PLANTS

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ABSTRACT

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The design of Pesticide formulation through a set of computer aided method and tools are discussed in this work relative to the physical properties of an array of pesticides. Computer-aided tools can be used for the selection of the formulation type, for processing and for formulation design. Also, the appropriate selection tools can enhance or simplify the process of ingredient optimization.

A suite of computer-aided tools based on the systematic methods for pesticide formulation design and analysis has been developed. These tools have been integrated into a framework that allows rapid and efficient access to the needed data, to the needed property and performance models and to the synthesis/design algorithms that generate and evaluate formulated product alternatives. The tools include property models for complex molecules and their solutions (including polymers and surfactants), multistage performance models (uptake, release models), algorithms for molecule and mixture design, database of knowledge (plants, pesticides, etc.), and guidelines for problem solution strategies.

The main aim of this project is to develop Pesticide uptake model with the database of plants, pesticide and surfactants, which can be integrated into the framework for efficient formulation design. The use of framework and its tools is highlighted through a practical case study where several feasible formulation alternatives were generated in an effective manner.

Therefore, through the use of framework and its tools, it will be possible to achieve the objective of fast evaluation of products, reduction of time to market and reduction of cost of the product. That is, convert molecules to money.

บทคัดย่อ

อาชาน มูเนอร์ : แบบจำลองการเกาะตัวของยาฆ่าแมลงบนใบไม้
(Modeling of Pesticide Uptake in Plants)
อ. ที่ปรึกษา: ผศ.ดร. กิติพัฒน์ สีมานนท์ ศ.ดร. มิกูเอล บากาเฮวิคซ์ xxx หน้า ISBN 974-9937-08-2

การออกแบบสูตรยาฆ่าแมลงด้วยวิธีการทางคอมพิวเตอร์คืองานวิจัยที่ต้องใช้คุณสมบัติทางกายภาพของลำดับชนิดยาฆ่าแมลงซึ่งจะช่วยในการคัดเลือกชนิดยาฆ่าแมลงที่เหมาะสม การออกแบบยาฆ่าแมลงได้ถูกพัฒนาขึ้นโดยรวมเข้ากับโครงสร้างของฐานข้อมูลที่จำเป็น คุณสมบัติ แบบจำลอง และขั้นตอนการผลิตและเลือกชนิดยาฆ่าแมลงได้อย่างแม่นยำและรวดเร็ว แบบจำลองนี้ประกอบด้วย แบบจำลองคุณสมบัติสำหรับโมเลกุลเชิงซ้อน พอลิเมอร์ กับ สารลดแรงตึงผิว แบบจำลองการเกาะตัวของยาฆ่าแมลงในหลายระดับ ขั้นตอนการออกแบบโมเลกุลกับของผสม ข้อมูลชนิดยาฆ่าแมลงกับพืช และ แนวทางในการแก้ไขปัญหา เป้าหมายหลักของงานวิจัยนี้ คือ การพัฒนาแบบจำลองการเกาะตัวของยาฆ่าแมลง ซึ่งได้ถูกทดสอบกับกรณีศึกษาจริง และ ให้ผลของสูตรยาฆ่าแมลงหลายแบบ ที่เหมาะสมกับชนิดพืชนั้นๆ โดยสรุป แบบจำลองนี้สามารถช่วยประเมินคุณภาพยาฆ่าแมลง และราคายาฆ่าแมลงถูกลง และ ออกสู่ตลาดได้เร็วขึ้น

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TABLE OF CONTENTS

CHAPTER **PAGE**

LIST OF TABLES

TABLE		PAGE

LIST OF FIGURES

FIGURE **PAGE**

NOTATIONS

xwax = wax thickness(m)

xcut = cuticle thickness (m)

hwax =Thickness of each layer in wax(m)

hcut =Thickness of each layer in cuticle(m)

t=time in hours

tu=uptake time in hours

tf=time factor

S=Surface area of droplet as a function of time (m^2)

S0=initial surface area of droplet

Sf=surface factor

v=Volume factor

Vd=Droplet Volume as a function of time (m^3)

V0=initial volume of droplet (m^3)

Vp= Volume of Plant

EO=Number of Ethoxy unit in surfactant

K4=Tortuosity Factor

SR=Surfactant rate (g/l)

Madjtotal=total moles of adjuvant in droplet (mol)

Madj=initial moles of solid adjuvant in droplet (mol)

Cdadj=initial concentration of adjuvant in droplet (mol/m^3)

Cadj0- Cadj30=concentration of adjuvant in 0 to 30 layer of wax and cuticle (mol/m^3)

Cpadj=concentration of adjuvant in plant (mol/m^3)

Kwdadj=partition coefficient of adjuvant between droplet and wax

Kwcadj= partition coefficient of adjuvant between wax and cuticle

Kcpadj= partition coefficient of adjuvant between cuticle and plant

MVadj=McGowan Volume of adjuvant (cm^3/mol)

MWadj=Molecular weight of adjuvant

Rhoadj=Density of adjuvant (g/cm^3)

Dadjwax0- Dadjwax15=Diffusivity of adjuvant in wax layers (m^2/s)

Dadjcut= Diffusivity of adjuvant in cuticle (m^2/s)

rhow= density of wax (kg/m^3)

MAItotal=total moles of active ingredient in droplet (mol)

MAI=initial moles of solid active ingredient in droplet (mol)

CdAI=initial concentration of active ingredient in droplet (mol/m^3)

C0 - C0=concentration of active ingredient in 0 to 30 layer of wax and cuticle (mol/m^3)

CpAI=concentration of active ingredient in plant (mol/m^3)

KwdAI=partition coefficient of active ingredient between droplet and wax

KwcAI=partition coefficient of active ingredient between wax and cuticle

KcpAI=partition coefficient of active ingredient between cuticle and plant

MVAI=McGowan Volume of active ingredient (cm^3/mol)

MWAI=Molecular weight of active ingredient

DAIwax0- DAIwax15=Diffusivity of active ingredient in wax layers (m^2/s)

DAIcut= Diffusivity of active ingredient in cuticle (m^2/s)

Sadj=solubility of active ingredient in adjuvant (g/l)

Swater= solubility of active ingredient in water (g/l)

RelUptAItot=Total relative uptake of active ingredient

RelUptadjtot= Total relative uptake of adjuvant