

CHAPTER VI

CONCLUSION AND RECOMENDATIONS

A general framework for efficient computer-aided pesticide formulation design has been presented in this work. A database containing a group of compounds, and their properties, has been combined with the needed mathematical models so that the behavior of the pesticide product can be studied. The uptake model is improved and further developed to take into account the solubilisation of the pesticide into the water droplet by the surfactants; a new set of diffusivity correlations is also added in the model for the movement of pesticide and surfactants into the leaf. Droplet vaporization was also included to make the model able to predict how this phenomenon influences the uptake behavior. The mathematical models have been converted to their predictive forms through the development of predictive models for their parameters. The final model has been validated against the experimental data and it was found that it is able to produce acceptable results. The knowledge of exactly how the pesticides diffuse into the plant and what role surfactant plays in this process is very limited. Uptake model developed in this work can help to prove some of theories, which are proposed.

Hopefully, the framework plus its resident tools (uptake model) will simplify and optimize the experimental work required in the complicated and time-consuming pesticide product design process by generating and testing a great number of feasible alternatives in an effective manner. Much work is needed to increase the application range of the property/performance models as well as increasing the population of the databases.