

STUDY OF MATHEMATICAL METHODS AND MODELS USAGE IN THE PESTICIDE DEGRADATION AND RESIDUE PREDICTION

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Pesticide was widely used in agriculture industry to ensure the crops' yield and quality, followed that pesticide pollution had become one of the most serious issues for public health in the world. Therefore, it's necessary to develop mathematical models for the prediction of pesticide degradation and residue. In this paper, we introduced four kinds of mathematical models in pesticide prediction, and offered the basis theories and practical applications for each model. Then we compared their advantages and disadvantages systematically by analyzing the roles of each one. Finally, present challenges and future perspectives in pesticide residue prediction fields were discussed.

Key words: pesticide residues, pesticide degradation, mathematical model.

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Introduction. As with the rapid development of modern agriculture, massive pesticides are utilized to prevent crops from weeds, pests and diseases, and to guarantee the crops' yield and quality. Pesticide residues perform bad influences on human beings and environment [0–0], and it can be absorbed by our body through digestive and respiratory systems or via the skin, so as contacting pesticides by eating pesticide-contaminated food [0]. Therefore, pesticide pollution has become one of the most serious problems of public health in the world [0]. The world health organization and the United Nations food and agriculture organization define maximum residue limits (MRLs) to protect foods in the process of production [0–0]. Therefore, it is of great significance to study the pesticide degradation law and select appropriate mathematical model to simulate the dynamic process of pesticide residues. Among the quantitative methods of pesticide residues, many mathematical analysis methods and modeling methods are afforded to predict the determination of pesticide degradation and residues. In this paper, we firstly introduced four famous models and other forefront mathematical prediction methods for pesticide degradation and residue, including basis theory, application examples, then we summarized their advantages and shortcomings in applications respectively, and offered the basis theories and practical application examples for each model. Then by analyzing the role of each model, we compared their advantages and disadvantages systematically. Finally, we concluded the mathematical prediction models in pesticide residues, and made expectation about the development way in the future.

The classic mathematical models for pesticide residue prediction

(1) Exponential degradation model

According to the pesticides degradation regularity, the disappearance of pesticides in soil or on plants is like the decay of radioactive substances, which can be expressed by the first-order reaction kinetics formula [0], if other factors can be ignored. The degradation rate of pesticides is proportional to their concentration:

$$\frac{dc}{dt} = -kc (k > 0), c(0) = a \quad (1.1)$$

The expressions (1.1), $c = c(t)$ expressed as the concentration when time is t , t is time after pesticide applied, k is constant proportionality. a is the pesticide residue concentration when time $t = 0$ (initial concentration).

By solving differential equations (1.1), we get

$$c = ae^{-kt} \quad (1.2)$$

In the expressions (1.2) parameters a and k estimate from measured data, then we can gain the pesticide degradation exponential model. The half-life is $t_{\frac{1}{2}} = \ln 2 / k$.

Lourdes et al. [0] studied the degradation of phosphorus in soil by this exponential model, and calculated the half-life. The experiment results were rather closest to predict results, and this model was the simplest one. Song et al. [0] proposed an adaptive nonlinear exponential model for pesticide degradation through a variety of mechanisms such as exponential decay, linear and nonlinear effects, and constructed a nonlinearly effective function

of biotic and abiotic factors, $1 - a(c/c_0)^\theta$.

Exponential degradation model has the advantages including simple calculation, directly-viewed and easy understanding, which has important influence on the prediction of pesticide degradation. But the basic model is proposed in a relatively ideal situation, ignoring the nature environmental factors. Also, the predict results just describe the situation that the degradation rate is a monotonically decreasing function over time, which can't change following the special environments. It is limited in actual application due to its extremely idealization and simplification.

(2) Bivariate pesticide residue function model

Considering the influence of environmental factors,

pesticide residue model not only is related to time, but also is concerned to several variables' functions including beginning dosing, daily average temperatures, daily average illumination time objectively and daily average rainfall and so on.

$$\text{Let } y_{rs} = f(t_r, x_s) (r = 0, 1, \dots, u; s = 0, 1, \dots, v) \quad (2.1)$$

t is the time after pesticide; y is composite factor value, according to beginning dosing, daily average temperatures, daily average illumination time objectively and daily average rainfall, y is pesticide residues for variables t, x . Let the value of bivariate pesticide residue function $y_{rs} = f(t_r, x_s)$ shows as following Table 1.

Table 1

The value of bivariate pesticide residue function $y_{rs} = f(t_r, x_s)$

t	x			
	x^0	x^1	...	x^v
t_0	y_{00}	y_{01}	...	y_{0v}
.....
t_u	y_{u0}	y_{u1}	...	y_{uv}

According to the value, we set the bivariate function as following:

$$Q_{m,n}(t, x) = \sum_{i=0}^m \sum_{j=0}^n a_{ij} p_i(t) q_j(x) \quad (2.2)$$

And make

$$I_{m,n} = \sum_{r=0}^u \sum_{s=0}^v [f(t_r, x_s - Q_{m,n})(t_r, x_s)] \quad (2.3)$$

to solve $\min(I_{m,n})$.

Wang et al. [0-0] studied the digestion process of BHD in rice paddy water, and designed a bivariate function model including environment factors according functional approximation theory. The half-life of pesticide residues was related to the initial dosage. The larger the initial dosage, the longer the half-life and vice versa. So, we could get the half-life by solving the function. The experiment results showed that this function is practical and useful in the prediction of pesticide residues.

Generally, the error case of pesticide residue function is related to the selection of m, n and the size of the interval between x and y . The smaller interval between x values, the smaller the relative error. The smaller interval between y values, the smaller the relative error, too. The value of m and n are larger, so that the error are smaller, but they should not be too large, because of rapidly increasing calculation, and increasing overall error. So it's difficult to choose the suitable value of x, y, m, n .

3) Rayleigh dynamic Model

Rayleigh dynamic Model is:

$$c = at^\alpha e^{bx^2} \quad (3.1)$$

The expressions (3.1), $c = c(t)$ expressed as the concentration when time is t , t is time after pesticide application, a, b is undetermined coefficients. After the logarithm based on (3.1), we will get

$$\ln c = \ln a + \alpha \ln x + bx^2 \quad (3.2)$$

Then, let $y = \ln c, x_1 = \ln x, x_2 = x^2$, the formula of (3.2) can be translated into a binary linear regression equation, as following:

$$y = a + a_1 x_1 + a_2 x_2 (a_0 = \ln a, a_1 = \alpha, a_2 = b) \quad (3.3)$$

Fang et al. [0] studied the degradation of methamidophos on rice leaves, mimicking the dynamic mathematics model. The regression of this model is remarkable and conform to the law of degradation, then they proposed three modified Rayleigh models to predict the pesticide residues, which showed better results. Zhu et al. [0] proposed a modified Rayleigh mathematics model for the degradation law of pesticide. In their study, parameter estimation method of modified Rayleigh model was introduced, which offered theoretical basis for the study on pesticide residue law.

Compared with exponential degradation model, Rayleigh dynamic model has more advantages like precision error, easy-to-use and high fitting accuracy, which avoid complicated calculations and range of independent variables in polynomials. Rayleigh dynamic model performs effective results and it's a utility model.

(3) Grey prediction GM (1.1) Model

Grey prediction is that the model using not the original data sequence but the generated data sequence. Based Grey Model, Grey prediction is a method that generates the approximate exponential law through accumulation (or other methods) of the original data and then carries out modeling.

Let pesticide residue sequence as

$$X^0 = (x^0(1), x^0(2), \dots, x^0(n)) \quad (4.1)$$

The original data sequence is accumulated once to obtain the new data sequence as

$$X^1 = (x^1(1), x^1(2), \dots, x^1(n)) \quad (4.2)$$

$$\text{in which } x^1(k) = \sum_{i=1}^k x^0(i), (k = 1, 2, \dots, n) \quad (4.3)$$

$z^{(1)}(k)$ is the adjacent to mean-generated sequence of $x^{(1)}(k)$, then

$$z^1(k) = \frac{1}{2}(x^{(1)}(k) + x^{(1)}(k-1)), (k = 2, 3, \dots, n) \quad (4.4)$$

Building the GM (1,1) model for pesticide residue sequence as

$$x^0(k) + az^1(k) = u \quad (4.5)$$

If $a = (a, u)^T$ is parameters sequence, then a is development coefficient and u is Grey action. Let the differential equation satisfying the data sequence generated by once accumulation as

$$\frac{dx^{(1)}}{dt} + ax^{(1)} = u \quad (4.6)$$

So parameter a and u can structure a matrix B, Y_n

$$B = \begin{bmatrix} -z^{(1)}(2), 1 \\ -z^{(1)}(3), 1 \\ \dots \\ -z^{(1)}(n), 1 \end{bmatrix} \quad Y_n = \begin{bmatrix} x^{(0)}(2) \\ x^{(0)}(3) \\ \dots \\ x^{(0)}(n) \end{bmatrix} \quad (4.7)$$

Then the least squares estimation parameter column of \hat{a} satisfies $\hat{a} = (B^T B)^{-1} B^T Y_n$. Let \hat{a} into differential equation (10) to solve the time response function as

$$\hat{x}^{(1)}(t) = (x^{(1)}(1) - \frac{u}{a})e^{-at} + \frac{u}{a} \quad (4.8)$$

If $x^{(1)}(1) = x^{(0)}(1)$, then the time response sequence of GM (1,1) is

$$\hat{x}^{(1)}(t+1) = (x^{(0)}(1) - \frac{u}{a})e^{-at} + \frac{u}{a} \quad (4.9)$$

Then formula (4.9) is pesticide residue model in isometric time. t takes the natural numbers like 1, 2.

Wu et al. [0] set up three mathematical models including the gray GM (1,1) model on the basis of the observation of the amount of chlorpyrifos residues in peaches. The degradation process of chlorpyrifos could be regarded as some parts of information known, some parts of information unknown as uncertain gray system. Experiment results proved that the degradation process was simulated well by gray GM (1.1) degradation model. Yang et al. [0] established a IEA-GM (1.1) prediction model of the pesticide degradation according to immune evolutionary algorithm (IEA) and gray system theory.

And the degradation of residual quinalfthosion in cowpea, the degradation of residual mancozeb in *Lycopersicon esculentum* miller, the degradation dynamics of triadimefon in ear of wheat and the dynamic dispelling of pirimicarb residue in cucumber fruit were predicted based on the IEA- GM (1.1) prediction model.

GM (1.1) model has good accuracy in simulation and prediction, existing high practical application value. However, the solution of GM (1,1) model parameters involves matrix transpose, matrix multiplication and matrix inversion, which is too complex and not easy to apply, and has the characteristics of chaos.

4) Other Recent research models

In addition, many innovative research methods emerged for pesticide residues prediction. In 2016 Zuo et al. [0] studied the pesticide residue prediction based on fuzzy system. The mathematic Fuzzy System was established by using the MRL values (maximum residue limits of all kinds of pesticides in food) of Matlab Fuzzy. Taking chlorpyrifos as an example, the analysis results showed that the application of fuzzy system for pesticide residue prediction was feasible and reasonable, and it was conducive to solve the problem of the using amounts of pesticides in the process of agricultural. In 2018, Li et al. [0] proposed a multi-section model based on principal components analysis (PCA) and neural network. They solve the problem that the modeling data characteristics changes obviously and experimental results show that the multi-section models built by Back Propagation(BP)/Radial Basis Function (RBF) network can significantly reduce the prediction error compared with the single models, and reduce the output error to 0.8 % and 0.4 % for establishing multi-section models BP and RBF respectively.

Conclusions. Pesticides provide a strong guarantee for the large-scale incremental production of crops, but excessive and continuous usage of pesticides have aroused much fear in our life [0]. With the development of science and our environmental awareness being strengthened, the harmful impact of pesticide residues and their degradation behavior have attracted more and more attention. The pesticide degradation and residue are a highly complex physical and biochemical processes. Even though variety dynamic models with high fitting degree for the residual degradation process of different pesticide are established, they could not meet the requirement of universality [0]. Therefore, it is of great practical significance to study the pesticides degradation law, and select appropriate mathematical models to describe the dynamic process of pesticide residues, then to do the analyse and prediction works. This paper summarizes four kinds of classic mathematics models in pesticide residues prediction, and compare their strengths and weaknesses based on mathematics theory and experiments results for each other. It turns out that there still exist more works to do in the future. As the development of computer technology, digital simulation and molecular biotechnology technologies, the studies on pesticide degradation and residues will continue to be further developed [0–22].

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ДОСЛІДЖЕННЯ МАТЕМАТИЧНИХ МЕТОДІВ І МОДЕЛЕЙ, ЩО ВИКОРИСТОВУЮТЬСЯ ДЛЯ ВИЗНАЧЕННЯ ДЕГРАДАЦІЇ ПЕСТИЦИДІВ ТА ПРОГНОЗУ ЇХ ЗАЛИШКІВ

Пестициди широко застосовуються в сільському господарстві для підвищення врожаю та якості сільськогосподарських культур. Внаслідок масового використання пестицидів, забруднення ними стало серйозною проблемою для екології та охорони здоров'я населення у світі. Тому необхідно застосовувати пестициди з урахуванням їх деградації у навколишньому середовищі. Незважаючи на те, що розраховані різноманітні динамічні моделі, що описують процес деградації залишків різних пестицидів, вони не відповідають вимозі універсальності. Тому важливим залишається практичне значення вивчення закономірності деградації пестицидів та вибору відповідної математичної моделі для опису динамічного процесу деградації залишків пестицидів.

У роботі розглянуто чотири види класичних математичних моделей для прогнозування залишків пестицидів.

1. Експоненціальна модель деградації. Згідно з нею швидкість деградації пестицидів пропорційна їх концентрації. Ця модель є найпростішою. Експоненціальна модель деградації має такі переваги: простий розрахунок, безпосередній перегляд та розуміння, що має суттєвий вплив на прогнозування деградації пестицидів. Але ця модель застосовується у відносно ідеальній ситуації, ігноруючи природні фактори навколишнього середовища. Також результати прогнозування описують ситуацію, згідно з якою швидкість деградації є лінійно зменшуваною функцією з часом, яка не може змінюватися внаслідок різних факторів. Вона обмежена у практичному використанні внаслідок ідеалізації та спрощення.

2. Біваріативна модель функціонування залишків пестицидів. Враховує вплив факторів навколишнього середовища,

пов'язана з часом, а також використовує декілька змінних функцій, а саме – початок обробки, середньодобові температури, тривалість світлового дня та середньоденну кількість опадів.

3. Динамічна модель Релея. Порівняно з експоненціальною деградаційною моделлю, динамічна модель Релея має більше переваг, таких як точність, простота у використанні та висока точність пристосування, що дозволяє уникнути складних обчислень та діапазону незалежних змінних у поліномах. Динамічна модель Релея дає ефективні результати.

4. Модель Грея. Модель GM має високу точність в моделюванні та прогнозуванні, а також практичну цінність застосування. Однак рішення параметрів моделі GM передбачає формування матриць, їх множення та інверсію, що є занадто складним і непротим у застосуванні, має характеристики хаосу.

5. Інші новітні моделі. У 2016 році Zuo та ін. вивчали прогнозування залишків пестицидів на основі нечіткої системи. Математична нечітка система була створена за допомогою значень MRL (максимальні межі залишків усіх видів пестицидів у їжі) MatlabFuzzy. У 2018 році Li та ін. запропонували модель муті-секцій на основі аналізу основних компонентів (PCA) та нейронної мережі. Вони вирішують проблему зміни даних моделювання. Експериментальні результати показують, що моделі мутісекцій, побудовані за допомогою мережі BackPropagation (BP)/RadialBasisFunction (RBF), можуть значно зменшити помилку прогнозування порівняно з окремими моделями. Похибка зменшується до 0,8 % і 0,4 % для встановлення мутісекційних моделей BP та RBF відповідно.

З розвитком комп'ютерних технологій, цифрового моделювання та молекулярних біотехнологічних технологій дослідження деградації залишків пестицидів будуть продовжуватись.

Ключові слова: залишки пестицидів, деградація пестицидів, математичні моделі.

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ИССЛЕДОВАНИЕ МАТЕМАТИЧЕСКИХ МЕТОДОВ И МОДЕЛЕЙ, КОТОРЫЕ ИСПОЛЬЗУЮТСЯ ДЛЯ ОПРЕДЕЛЕНИЯ ДЕГРАДАЦИИ ПЕСТИЦИДОВ И ПРОГНОЗИРОВАНИЯ ИХ ОСТАТКОВ

Пестициды широко используются в сельском хозяйстве для повышения урожайности и качества сельскохозяйственных культур. После массового их использования загрязнение ими стало одной из наиболее серьезных проблем всемирного здравоохранения. Поэтому необходимо разработать математические модели для прогнозирования деградации пестицидов и их остатков. В этой статье мы представили четыре вида математических моделей, которые позволяют прогнозировать деградацию пестицидов и изложили базовые теории и практическое применения для каждой модели. Мы критически сравнили их преимущества и недостатки, анализируя роль каждой из них. Были рассмотрены существующие проблемы и перспективы в области прогнозирования остатков пестицидов.

Ключевые слова: остатки пестицидов, деградация пестицидов, математические модели.

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