

MATHEMATICAL MODELLING OF DOSE-RESPONSE RELATIONSHIP (HORMESIS) IN ALLELOPATHY AND ITS APPLICATION

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I. INTRODUCTION

Allelopathy arises from the release of chemicals by one plant species that affect other species in its vicinity, usually to their detriment. It has been demonstrated, in plant communities, to be a factor of ecological significance by influencing plant succession, dominance, climax formation, species diversity, structure of plant communities and productivity (Whittaker and Feeney, 1971; Rice, 1984; Chou, 1989). In agroecosystems, allelopathic effects between living weeds and crops, crops in mixtures, plant straw residue and succeeding crops during decomposition of residue are also well documented (Putnam, 1978; Rice, 1984).

This phenomenon has been observed for over 2000 years. Reports as early as 300 BC document that many crop plants (eg., chick pea, barley, bitter vetch) destroyed weeds and inhibited the growth of other crop plants. The soil sickness problem in agriculture was specifically related to exudates of crop plants (Rice, 1984). However, intensive scientific research on this phenomenon only started on 20th century. The term allelopathy was first introduced by a German scientist Molisch in 1937 to include both harmful and beneficial biochemical interactions between all types of plants including microorganisms. Rice (1984) reinforced this definition in the first monograph on allelopathy. Contemporary researchers have broadened the context of allelopathy to include interactions between plants and higher animals, and have suggested that allelopathy may be part of a whole network of chemical communication between plants, and between plants and other organisms, including bacteria, yeasts, insects and mammals, and that such communication may contribute to plant defence (Harborne, 1987; Lovett and Ryuntyu, 1992; Einhellig, 1995; Siemens *et al.*, 2002).

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Chemicals that impose allelopathic influences are called allelochemicals or allelochemicals (Putnam and Tang, 1986). They may be largely classified as secondary plant metabolites, which are generally considered to be those compounds (such as alkaloids, isoprenoids, phenolics, flavonoids, terpenoids, and glucosinolates etc.) which do not play a role in primary metabolic processes essential for a plant's survival, and are produced as offshoots of primary metabolic pathways. In contrast to primary metabolism, which comprises several hundreds of low molecular weight compounds, tens of thousands of secondary substances are known today, but only a limited number have been implicated as allelochemicals (Rice, 1984). Allelochemicals are present in virtually all plant tissues, including leaves, flowers, fruits, stems, roots, rhizomes, seeds and pollen. They may be released from plants into the environment by means of four ecological processes: volatilisation, leaching, root exudation, and decomposition of plant residues. Several chemicals can be released together and may exert toxicities in an additive or synergistic manner (Putnam and Tang, 1986).

During the last two decades, the science of allelopathy has attracted a great number of scientists from the diverse fields world wide and is now viewed from a multifaceted approach (Rice, 1984, 1985; Putnam and Tang, 1986; Rizvi and Rizvi, 1992; Inderjit, *et al.*, 1995, 1999; Narwal *et al.*, 1998; Macias *et al.* 1999; Chou *et al.*, 1999; Kohli *et al.*, 2001). This diverse interest has been greatly driven by the prospects that allelopathy holds for meeting increased demands for sustainability in agriculture and quality food production for humans, on reducing environmental damage and health hazards from chemical inputs, minimizing soil erosion, reducing reliance on synthetic herbicides, and for finding alternatives to replace them (Einhellig, 1995; Dakshini *et al.*, 1999; Singh *et al.*, 2001).

Of the disciplines involved in allelopathy research, mathematical modelling is making increasingly significant contributions. Such theoretical contributions range from separating allelopathy from competition (Weidenhamer *et al.*, 1989; Nakamaru and Iwasa, 2000), characterizing allelopathy and its ecological roles (Cheng, 1995; Dubey and Hussain, 2000; Goslee *et al.*, 2001; Sole *et al.*, 2005), elucidating fundamentals of allelopathy (An *et al.*, 1993; Liu *et al.*, 2003), simulating specific cases, eg. plant residue allelopathy (An *et al.*, 1996) and plankton allelopathy (Mukhopadhyay *et al.*, 1998, 2003), to the modelling of effects by external factors, such as density of target plants (Weidenhamer *et al.*, 1989; Sinkkonen, 2001).

This article, largely based on our previous modelling work, is to specifically discuss some fundamental issues associated with the dose-response phenomenon in allelopathic research, to review the latest developments in this area, and to further illustrate the above-mentioned contributions that mathematical modelling can make to this discipline.

II. A MODEL OF THE DOSE-RESPONSE RELATIONSHIP IN ALLELOPATHY AND ITS INTERPRETATION

Up to now, probably one of the most consistent features in studies of allelopathy has been the recognition of the characteristic responses of an organism to an allelochemical, i.e. stimulation or attraction at low concentrations of allelochemicals and inhibition or repulsion as the concentration increases (Carballeira *et al.*, 1988; Lovett 1979, 1989; Rice, 1984; Liu *et al.*, 2003). These phenomena have been widely observed in allelochemicals from living plants, in allelopathic effects from decaying plant residues, and from the gross morphological level to the biochemical level, and have also been widely recognized in other growth-regulating chemicals, including herbicides and even medicines (Devlin and Witham, 1983; Fedtke, 1982; Calabrese and Baldwin, 2003). However, we are still facing the challenge of interpreting such phenomena in allelopathy and their significance is yet to be fully explored.

Being inspired by Chinese Yin/Yang theory, an analogy is here employed in an attempt to interpret such allelopathic manifestations. It is hypothesized that the characteristic biological response to allelochemicals is a result of the character of the allelochemicals themselves. An allelochemical is assumed to have two complementary attributes: stimulation and inhibition, which are a complementary pair. These attributes act in a way that are antagonistic to each other as well as coexistent within the unity of an allelochemical. As a unity of opposites, stimulation and inhibition, although separate attributes, are really part of the same ultimate unity, i.e. stimulation implies inhibition, inhibition embodies stimulation, and each is, therefore, necessary to the other. As concentration changes for a given receptor organism, the relative dominance of stimulation and inhibition by the allelochemical alters. It is such alternation that determines the overall property of the allelochemical. This can only be shown through the biological responses when an allelochemical acts on an organism, and is referred to as the biological property of the allelochemical (as opposed to chemical or physical properties). Therefore the observed allelopathic phenomenon shall depend on the specific allelochemical, the given organism, the environmental conditions in which allelochemicals are produced and released, and in which the organism is grown, etc.

This hypothesis is mathematically expressed by the following model:

$$P = 100 + S - I$$

Where P represents the biological response to an allelochemical, S and I are biological responses to the stimulatory and inhibitory attributes of the allelochemical respectively, and are expressed in the model by enzyme kinetics (An *et al.*, 1993).

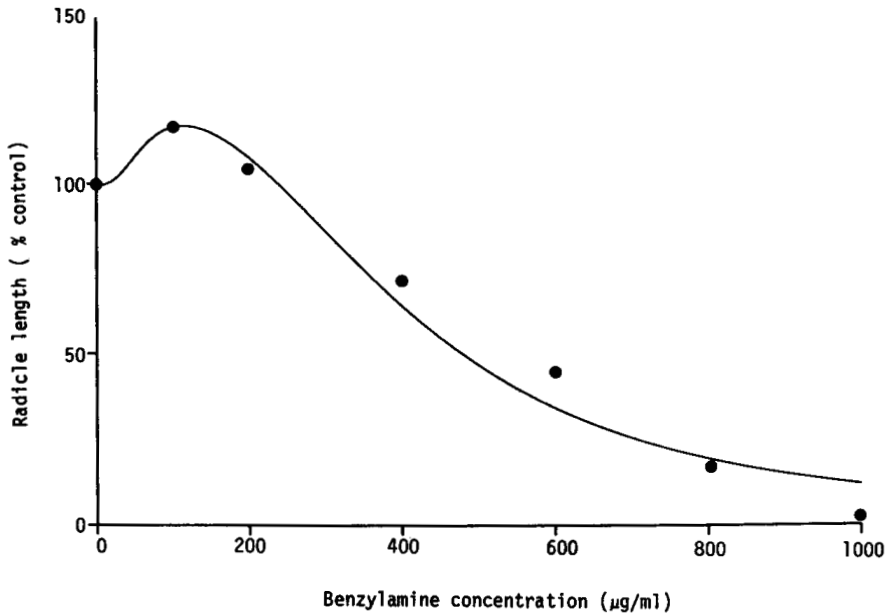


FIGURE 1 The response of linseed in radicle length to benzylamine (An *et al.*, 1993).

The illustration of the model is shown in Figures 1–5. It can be seen from the illustrations that the model simulates well the biological response to allelochemicals and is in a good agreement with a wide range of experimental data taken from the literature (An *et al.*, 1993). The model provides a useful platform for analysing experimental data, predicting allelopathic effects in practice, and for further theoretically exploring the fundamentals of allelopathy matters, which are discussed in the next sections.

III. INTERPRETATION OF THE FUNCTION OF ALLELOPATHY FROM A DOSE-RESPONSE MODELLING PERSPECTIVE

One important concept, derived from the operation of the above dose-response model, is that a plant always contains a certain amount of allelochemical whether under stress or not.

Under normal conditions, allelochemicals in a plant may be inactive and concentrations may be relatively stable. However, as environment conditions become stressful for plant growth, the allelochemical content dramatically increases. Stressful conditions include abnormal radiation (Koeppel *et al.*, 1970; Del Moral, 1972), mineral deficiencies (Loche and Chouteau, 1963; Lehman and Rice, 1972), water deficits (Del Moral, 1972; Gilmore, 1977), temperature extremes (Koeppel *et al.*, 1970), and attack by pathogens and predators (Gayed and Rosa, 1975; Woodhead, 1981) etc.

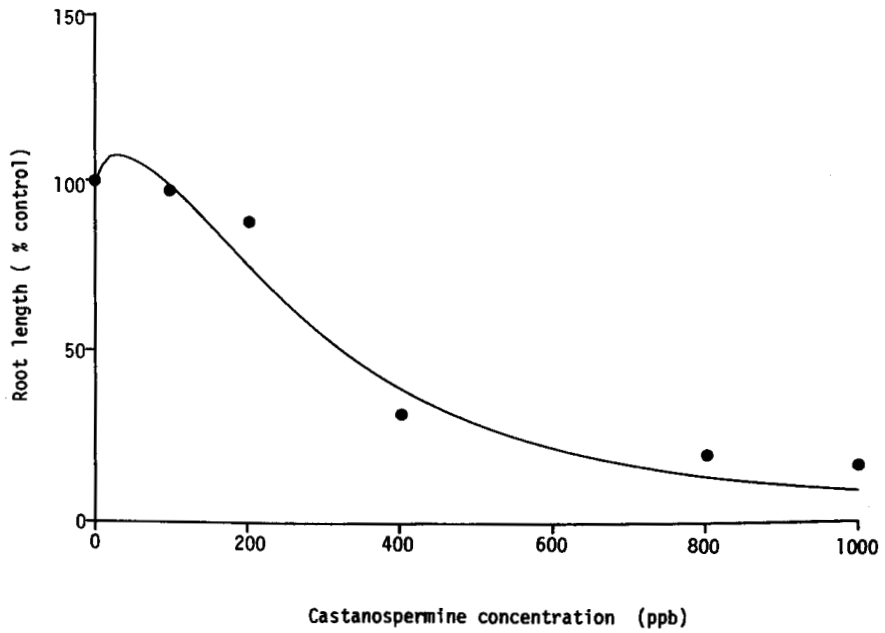


FIGURE 2 Effect of castanospermine on root growth of lettuce (An *et al.*, 1993).

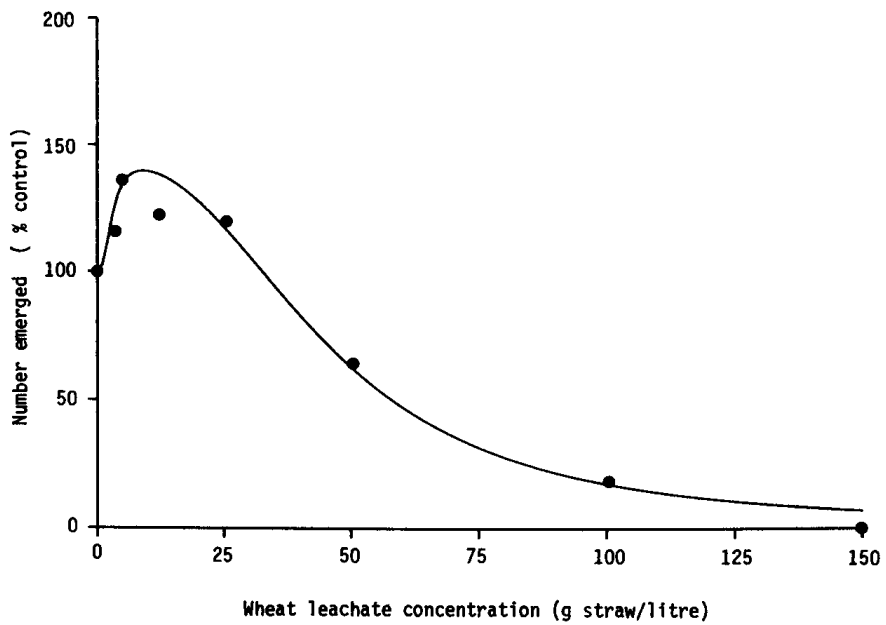


FIGURE 3 The response of wild oats (*A. ludoviciana*) in total number emerged to wheat straw leachate (An *et al.*, 1993).

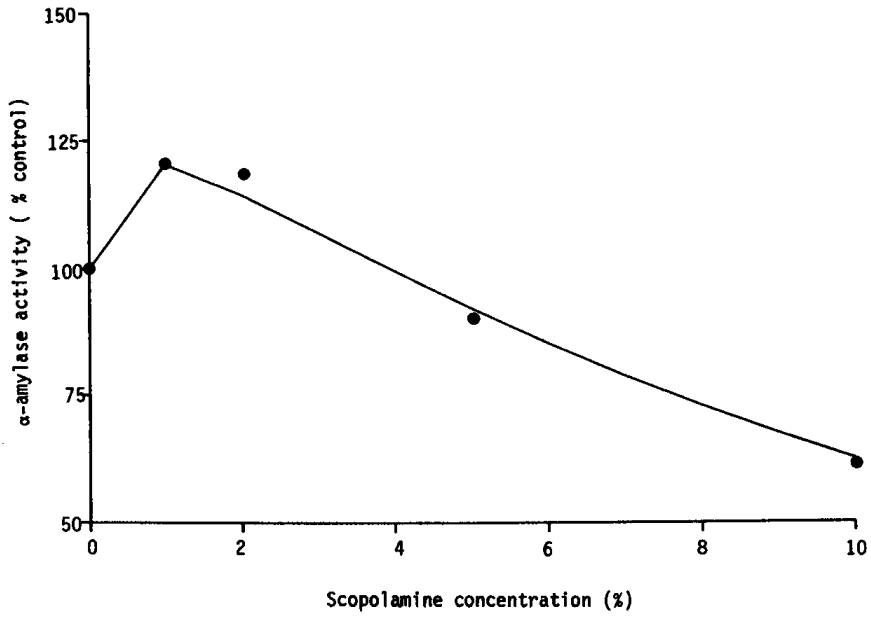


FIGURE 4 The response of α -amylase activity to scopolamine (An *et al.*, 1993).

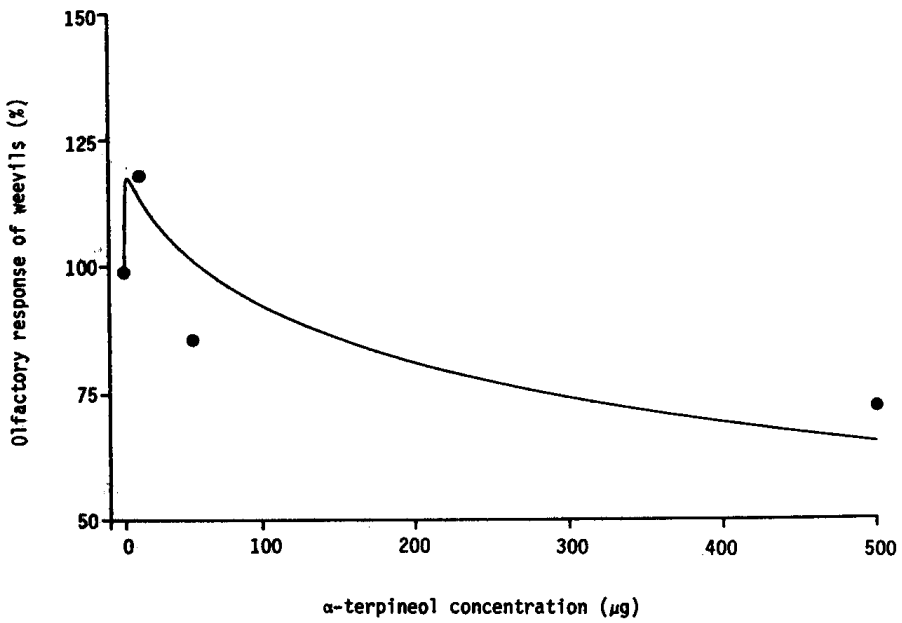


FIGURE 5 Olfactory response of weevil larvae to α -terpineol (An *et al.*, 1993).

According to Cruickshank and Perrin (1964), a similar conclusion was proposed by Muller and Borger in 1939, i.e. 'phytoalexin theory' of disease resistance, which proposed that phytoalexins are metabolites, which only form or become active when a parasite comes in contact with the host cells.

Plants have evolved means of adjusting the environment in their favour. It is well known that plants have developed physical means, such as the cuticle and trichomes, for their defense. Recently, it has been recognized that allelochemicals may also be employed in the defense systems of plants (Levin, 1971; Woodhead, 1981; Lovett, 1982; Lovett and Ryuntyu, 1992; Bais *et al.*, 2003). Plants may defend themselves by means of such chemicals in several ways. Phenolics, particularly flavonoids, are considered to protect plants from UV radiation (McClure, 1975). Under stressful conditions, such as drought or insufficient nutrients, allelochemicals may inhibit the growth of other plants and favour the producer (Kuo *et al.*, 1989). Allelochemicals, such as phenolics or their oxidation products, may affect the digestive enzymes of insects or fungal enzymes (Friend, 1979; Woodhead, 1981). Also, allelochemicals may cause the rapid death of a few cells in plants under disease attack, confine the pathogen to a restricted area and thus minimize the damage by the pathogen (Farkas and Kiraly, 1962). Recently by integrating ecological, physiological, biochemical, cellular, and genomic approaches Bais *et al.* (2003) demonstrated that *Centaurea maculosa* (spotted knapweed), an invasive species in the western United States, displaces native plant species by exuding the phototoxin (-)-catechin from its roots, which in susceptible species triggers a wave of reactive oxygen species (ROS) initiated at the root meristem that leads to a Ca^{2+} signalling cascade triggering genome-wide changes in gene expression and, ultimately, death of the root system.

It is conjectured that allelopathy may act as a defensive system in plants (Lovett and Ryuntyu, 1992). Visible allelopathic effects or increase of allelochemical contents in plants may be the results of operation of this system under stress. Its purpose is to mainly protect plants from stress and to keep an ideal or normal growth environment for plants. While under ideal conditions there are no allelopathic effects occurring, the allelochemicals are inactive and the plant content is stable. It is known that plants produce numerous allelochemicals, each of which (or a combination) may have different functions against different stress factors. Stress as referred to here, has a broad definition, which includes those external constraints, such as water deficits, mineral deficiencies, temperature extremes, abnormal radiation, herbivores feeding and disease *etc.*, that disturb normal plant growth and reduce the rate of dry matter production.

Allelopathy may have two functions in a plant: phytotoxic and autotoxic. Within the range of its capability to overcome stress, allelopathy is inhibitory to others except a producer. Under severe stress, which is beyond the adjusting capability of the plant, such as massive attack by pathogens or

severe mineral deficiencies, allelopathy may act autotoxically to decrease the population of the producer, which may be the best survival strategy for producer plants under unfavourable conditions (Chou, 1989). It has been observed that residues from plants grown under stressful conditions are more highly phytotoxic than under normal conditions (Mason-Sedun and Jessop, 1989). Chou (1983) also noted that the roots of rice seedlings under water-logged and oxygen-deficient conditions developed abnormally, and the plants tended to produce growth-inhibiting substances, resulting in decrease of yields. When the unfavourable conditions were removed by providing a good drainage system so that phytotoxins could be leached out of the soil, a significant yield increase of up to 40% occurred.

It is well documented that the concentration of secondary plant compounds in plant tissue is determined by the plant's genetic make-up in combination with its interaction with environmental conditions during growth (Bell and Charlwood, 1980; Mason-Sedun, 1986). Therefore, it is not surprising that allelopathic potentials, like other genetic characteristics, vary with and within species, and that this may reflect the extent of the plant's defense capability. For example, levels of phenolic acids in healthy plants of *Sorghum bicolor* differ considerably with cultivars. Cultivars with the highest normal phenolic levels are the most resistant to insects attack (Woodhead, 1981).

Putnam and Tang (1986) and Lovett (1982, 1987) indicated that allelopathic characteristics are more likely to occur in crop predecessors or 'wild types' that have evolved in the presence of allelopathic and competitive influences from other species. If allelopathy acts as a defense reaction to stress, then human interference, such as irrigation, the applying of fertilizers and pesticides etc., may help to overcome stress for plants, and hence currently used cultivars have diminished or reduced allelopathic capacity.

Allelochemical contents in plants are found to vary with experimental conditions. Woodhead (1981) reported that laboratory- and field-grown sorghum phenolics follow similar patterns, but that values for all field-grown plants are much higher than for the corresponding laboratory plants. This may be taken to imply that the ideal environment for plant growth is relative, and plants are always under some degree of stress. For example, Dicosmo and Towers (1984) pointed out that in plant cell cultures altered secondary metabolism implies some kind of stress even when conditions seem to be optimum. Even though under no apparent stress, plants may contain a certain amount of allelochemical. The equilibrium point, at which no allelopathic effects occur (i.e. when stimulation and inhibition are equal), is likely to vary with growth conditions. Therefore, it is not surprising that allelochemical concentrations at the equilibrium point of one condition may show allelopathic effect on the same test species under different conditions. This may help to explain the argument that allelopathic effects are observed under conditions of no stress.

IV. APPLICATION OF THE DOSE-RESPONSE MODEL

A. The Dynamics of Allelochemicals from Living Plants in the Environment

Defence agents, allelochemicals or allelopathins, play an important role in allelopathic interactions or plant defence and act as important ecological mechanisms (Rice, 1984). The allelopathic characteristic of an allelochemical is defined as a biological property of the allelochemical, as opposed to its physical or chemical properties (An *et al.*, 1993). The content of allelochemicals in living plants, and the fate and dynamics of such compounds in the environment are important aspects in the study of allelopathy. Production of allelochemicals in living plants is affected by abiotic and biotic factors, which ultimately affect a plant's defence capability or allelopathic potential (Hedin, 1990; Lovett and Hoult, 1995; Einhellig, 1995). Various research efforts have been made in the identification of allelochemicals from living plants (Blua and Hanscom, 1986; Niemeyer, 1988; Wu *et al.*, 2001); in testing biological activities of identified allelochemicals (Waller *et al.*, 1995; An *et al.*, 2001); in observing their dynamics in plants and the environment (Woodhead and Bernays, 1978; Wolfson and Murdock, 1990); in characterising their modes of action (Wink and Bruning, 1995; Czarnota *et al.*, 2001); in determining the effect of abiotic and biotic factors (Koeppel *et al.*, 1970; Waterman *et al.*, 1984; Einhellig, 1989); and in identifying their genetic make-up (Niemeyer and Jerez, 1997; Quader *et al.*, 2001), etc.

An *et al.* (2003) developed a mechanistic model, by applying the concept of a diffusion process, which integrated earlier scattered research information with present knowledge. This model assembled a generalized picture of allelochemical production in living plants with the fate of allelochemicals and their dynamics in the environment, and also explored the possible ecological significance of plant allelopathy. Through their modelling work it is proposed that there are two kinds of allelochemical production in a plant, which are dictated by age and plant stress, and are reflected by the corresponding dynamics in the environment. Generally, allelochemical content in living plants declines with age after an early initial maximum, and there is a corresponding later fate in the environment, while periodic production may occasionally be a special case (An *et al.*, 2003). By combining this model with the above-mentioned dose-response model in section II, these authors demonstrated the possible existence of corresponding periodic dynamics in the environment; successfully simulated the response fluctuation of receiver plants to allelochemicals; theoretically interpret allelopathic results as reported in the literature; and attributed such results to the periodic production of allelochemicals. (Figures 6–7). The combined model has helped us to understand why the results from

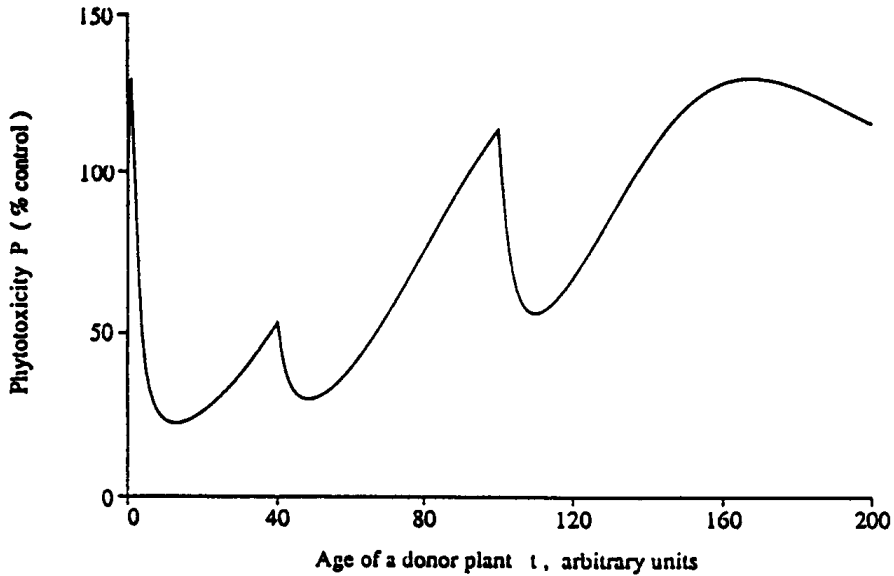


FIGURE 6 Simulated fluctuation of responses of receiver plants to periodic dynamics of allelochemicals in the environment, which is described by the combination of allelochemical—biological response model (An *et al.*, 1993) and the model (An *et al.*, 2003). P is response of test plants to allelochemicals, % control; t is time course of donor plant growth, arbitrary unit (An *et al.*, 2003).

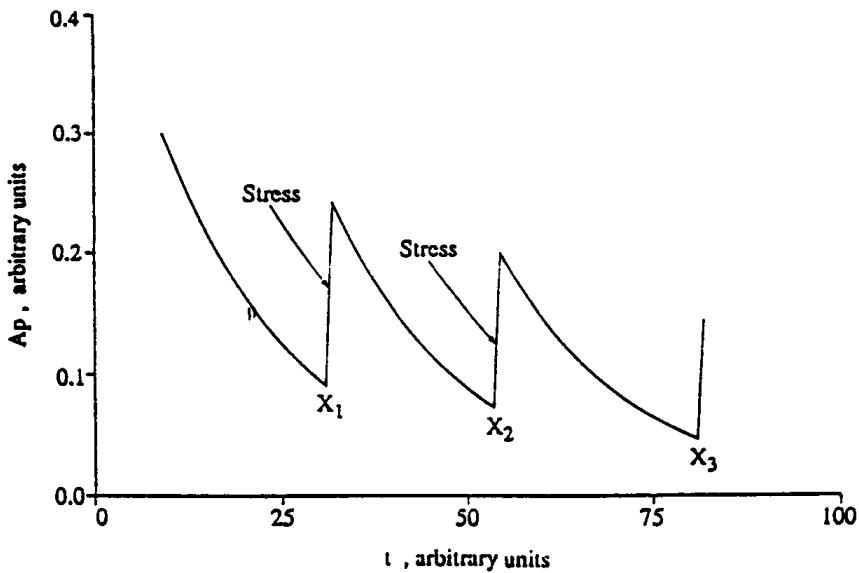


FIGURE 7 Simulated periodic production of an allelochemical under constant stress. A_p is allelochemical concentration in plant; t is time course of plant growth, both in arbitrary units. X_1 , X_2 , X_3 are concentrations at an equilibrium (An *et al.*, 2003).

allelopathic research are disparate when conducted at different stages of plant growth and development, and why results fluctuate as experiments proceed. The model has also helped to reduce confusion on allelopathy and suggest directions for future research.

An *et al.* (2003) also further discussed the ecological significance of their modelling proposals in allelopathy. If it is considered that allelopathy acts as a defence system in a plant, then it is logical that the overall concentration of allelochemicals in plants declines with increasing plant age. Allelopathic potential, or allelochemical production, reflects the extent of the defence capability. It is well documented that the production of secondary plant compounds in plant tissue is determined by the plant's genetic make-up in combination with its interaction with environmental conditions during growth (Bell and Charlwood, 1980; Lovett, 1982; Mason-Sedun, 1986; Niemeyer and Jerez, 1997; Quader *et al.*, 2001). A defence system is an inherent character of the plant. Like other genetic characters, as the age of a plant increases, its defence capability inevitably manifests in weak, strong and then decreasing stages.

As environmental conditions become stressful for plant growth, the allelochemical contents in a plant dramatically increases. This phenomenon together with the periodic production of allelochemicals may be viewed as a wholistic response of plant chemical defence system to stress. Growth and development of a plant need a normal or ideal environment while stress is constant and indeterminate, in other words, a plant is always surrounded by stress. In order to optimise growth, a plant is constantly attempting to overcome stress. It may be that once stress occurs, a plant immediately responds by producing allelochemicals, which may result in the overcoming or inhibiting of stress. After that, allelochemical content declines, allowing the stress to affect the plant again. This means that stress may occur again, and the plant may respond by releasing allelochemicals again, thus showing a periodic pattern over time (Fig. 7). Allelochemical levels in plants generally appears to decrease with the maturing of plants, while throughout the whole time course of plant growth, allelochemical levels may fluctuate as a defence reaction to stress. The timing and extent of periodic production may depend on the frequency of stress occurring, its extent and the defence capability of a plant. Since stress is unpredictable and indeterminate in natural field conditions, the same pattern of periodic production is unlikely to be experimentally repeated.

B. Allelopathy Caused by Plant Residues During Their Decomposition

Plant residues undergoing decomposition may have allelopathic effects on the growth and yield of subsequent plants (Guenzi and McCalla, 1966; Kimber, 1967, 1973; An *et al.*, 1996a). Such effects have been attributed to the phytotoxic chemicals leached from the residues together with toxins

produced by micro-organisms during residue decomposition (McCalla and Duley, 1948; Cochran *et al.*, 1977; Harper and Lynch, 1982; Lovett and Jessop, 1982). The potential phytotoxicity is dependent on numerous factors that together govern the rate of residue decomposition, the net rate of active allelochemical production and the subsequent degrees of phytotoxicity (An *et al.*, 2002).

A mechanistic model was constructed to simulate such allelopathic phenomena (An *et al.*, 1996a), and later further developed by including intrinsic and extrinsic factors to examine this phenomenon under much wider conditions (An *et al.*, 2002). This model, combined with the dose-response model in section II, formed a new model, which provides an integrated view of the allelopathic pattern of plant residues during decomposition, in terms of both the response of a receiver plant and allelochemical dynamics in the environment (Figures 8–9). The new model showed that there are two aspects to phytotoxicity: stimulation and inhibition. The extent of each over the whole course of residue decomposition is not balanced. The most severe inhibition occurs at the early stages of residue decomposition. Phytotoxicity proceeds from stimulation to inhibition at this stage and reaches its maximum of inhibition soon after decomposition starts. Compared with the whole decomposition course, this stage is relatively short. At later stages of residue decomposition, the inhibition due to phytotoxicity is declining

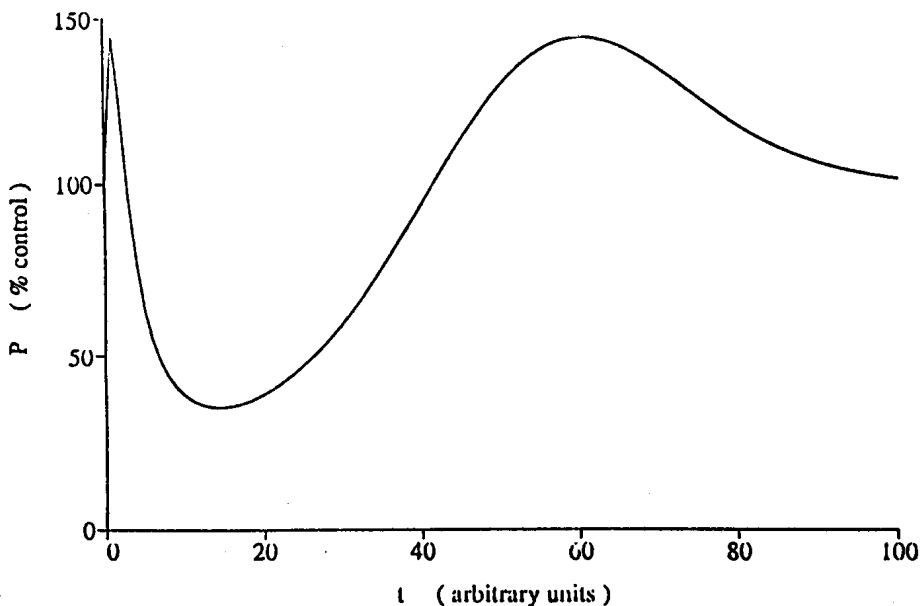


FIGURE 8 Simulating dynamics of residue phytotoxicity. P is phytotoxicity and t is decomposition time, both in arbitrary units (An *et al.*, 1996a).

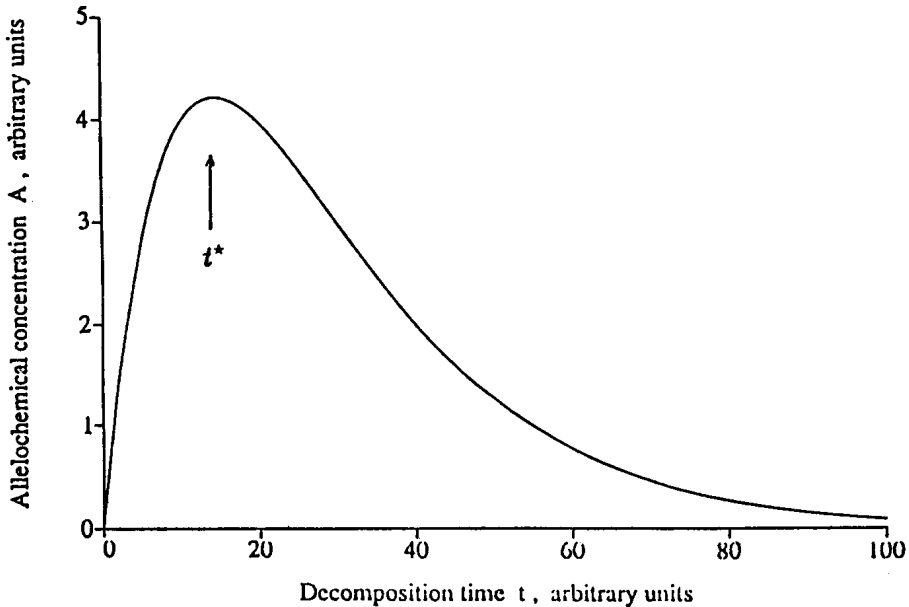


FIGURE 9 Dynamics of allelochemical production from decomposing plant residues. A is amount of allelochemical produced and t is decomposition time, both in arbitrary units (An *et al.*, 1996a).

while stimulation gradually emerges. Generally speaking, over the whole course of residue decomposition in terms of agronomic practice, inhibition dominates residue phytotoxicity, which is declining with increasing decomposition time.

The most interesting aspects that this modelling work revealed are at the initial and later stages of dynamic residue allelopathy. At the initial stage of residue decomposition, plant responses are stimulated, although only for a short time, while at later stages plants gradually recover from high inhibition and move towards stimulation, eventually returning to 'control' levels of response. However, such important phenomena have often been overlooked in the literature due to, perhaps, a lack of effective experimental means, incomplete short-range experimental results, widely variant experimental conditions, limited data accumulation and interpretation.

Such modelling analysis has great application potential in the managing of plant residues for weed control and in overcoming the negative effects of plant residues to meet the increased demand for conservation and no-tillage farming systems by means of managing the inhibition and stimulation periods. For example, with a knowledge of residue decay dynamics, and by analysing risk situations with respect to residue retention, a crop manager may avoid the inhibitory period of decaying residues, thus minimising their negative effects and await the stimulatory effect to crop plants, thereby enhancing the benefits of residue retention on the soil. By ex-

tending the inhibitory period of decaying residues and enhancing its effects, weeds may be controlled (An *et al.*, 1998). A successful example in applying this principle in practice was presented by An *et al.* (1996b) in controlling vulpia. *Vulpia* (*Vulpia* spp.) is a notorious annual weed in pastures and cereal crops in southern Australia. Pasture establishment often failed due to the presence of vulpia residues which possess strong allelopathic potential. The use of cultivation and then delaying sowing for about three weeks enabled the allelochemicals to dissipate, avoided the peak inhibitory period from vulpia residues, and allowed successful pasture establishment to follow (An *et al.*, 1996b).

C. Density-Dependent Chemical Interference

Sinkkonen (2001) further developed the above dose-response model (Section II) by combining it with the density-dependent graphic model of Weidenhamer *et al.* (1989) to form a new model to describe plant response to change in phytochemical concentration in those cases of density-dependent phytotoxicity. According to this extension model, direct chemical interference is density-dependent; with increasing target plant density, the effects of phytochemicals are diluted. As a result, inhibition is the most probable outcome in density-dependent phytochemical interactions at low target plant densities, but phytotoxic effects often become stimulatory as target plant density increases (Sinkkonen, 2001). The author also claimed that his extension of the dose-response model by An *et al.* (1993) is useful when estimating whether the response of plants to direct chemical interference can be distinguished from pure competition (Sinkkonen, 2001), an important but often-argued issue in allelopathy research. The same author concluded that, based on the examples presented in his paper, the dose-response model by An *et al.* (1993) is suited for modelling plant responses to density-dependent chemical interference. He also made suggestions to further modify the model equations in some cases. These include the cases where an environmental factor, such as adsorption of phytochemicals by soil particles or degradation of phytochemicals by soil microorganisms, alters the model in predictable way; and to add a density-dependent stress factor to the model, which would change the power of stimulat and inhibitory attributes at different plant densities, etc.. However, Sinkkonen also cautioned that every modification must be based on empirical data showing a distinctive pattern that can be modelled (Sinkkonen, 2001).

Later by combining the model by An *et al.* (1996), Sinkkonen (2003) extended the density-dependent model (Sinkkonen, 2001) to describe residue allelopathy at different densities of growing plants. While the original residue allelopathy model predicts inhibitory effects in most cases, the new density-dependent extension of the residue allelopathy model predicts

that the density of target plants determines whether or not inhibition occurs. According to the new model, the intensity of inhibition decreases and the final stimulatory period begins earlier if target plant density increases (Sinkkonen, 2003). The author claimed that combining the effects of density-dependency with the residue allelopathy model enhances our understanding of chemical interference. In addition, the new model may partially explain why several field studies have not observed chemically driven inhibitory effects similar to those observed in laboratory experiments (Sinkkonen, 2003). Recently, Sinkkonen (2005) further developed the density-dependent model to simulate the effects of phytochemicals on seed germination and seedling emergence by considering seed densities and germination probability. The details of this model are shown in the Sinkkonen article of this special issue.

V. OTHER APPROACHES IN MODELLING ALLELOPATHY DOSE-RESPONSE (HORMESIS)

A. Model for Curve-Fitting Allelochemical Dose Responses (Hormesis)

Liu *et al.* (2003) acknowledged that when bioassay techniques are used to study the effects of allelochemicals on plant processes it is generally observed that the processes are stimulated at low allelochemical concentrations and inhibited as the concentrations increase. They developed a highly flexible but simple empirical model to describe the general pattern for this type of response (hormesis) and used the model to analyze some experimental data from allelochemical effects. The stimulation-inhibition properties are described by the parameters in the model. The index, $p\%$ reduction, is calculated to assess the allelochemical effect. The features of this model are that the biologically significant indices, such as maximum value for stimulation and specific doses for giving no effect and 50% reduction of untreated control, are derived, and the estimations of the parameters of the model and of the indices are computationally easy due to the model being based on a quadratic equation. The model is compared with experimental data for the response of lettuce seedling growth to Centaurepsin, the olfactory response of weevil larvae to α -terpineol, and the response of annual ryegrass (*Lolium multiflorum* Lam.), creeping red fescue (*Festuca rubra* L., cv. Ensylva), Kentucky bluegrass (*Poa pratensis* L., cv. Kenblue), perennial ryegrass (*L. perenne* L., cv. Manhattan), and Rebel tall fescue (*F. arundinacea* Schreb) seedling growth to leachates of Rebel and Kentucky 31 tall fescue. The results show that the model gives a good description of the observations and can be used to fit a wide range of dose responses. Assessment of the effects of leachate from Rebel and Kentucky 31 tall fescue clearly differentiate the properties of the allelopathic sources and the relative sensitivities of indicators such as the length of root and leaf (Liu *et al.*, 2003). The authors concluded that the model is considerably

flexible and can be useful in fitting a wide range of stimulation response at low dose and inhibition at increasing dose.

B. Application of Nonlinear Regression Models in Allelopathy

Backed by an ancient statement that ‘the poison is in the dose’ by physician Paracelsus some 500 years ago, Belz and Hurlle (2001, 2002), and Belz *et al.* (2002, 2004) experimentally reinforced the recognition of dose-response relationships in allelopathy. Their efforts were not just limited to the confirmation of such phenomena, but also to the exploring of allelopathy’s fundamentals and practical utilization, aided by the mathematical modelling of hormesis.

They transferred the methodology of dose-response experiments in weed science and data analysis using log-logistic model and other nonlinear regression methods on curve parallelism, ED50, and curve slopes etc. into the allelopathy field. They screened over one hundred wheat cultivars against a test species for their allelopathic potential, compared the responses by synthetic allelochemicals, and verified the dose-responses by density-dependent phytotoxicity of allelochemicals produced and released by living plants. They concluded that dose-response studies as used in bioassays in other biological sciences, are an appropriate method for analysing allelopathic interactions between living plants. The four-parameter log-logistic model (or its peaked expansion) adequately described most of the observed dose-response patterns and provided a valuable tool for various approaches and comparative studies in allelopathy. The potential application of their research is that it can be used to identify the primary cause of observed allelopathic interactions, to point to the mode of action of allelochemicals, and to preselect cultivars with allelopathic traits based upon allelochemicals with a different mode of action. For details, see Belz *et al.* in this special issue.

VI. CONCLUDING REMARKS

Practically, scientists are often asked questions such as “what period of time must elapse between the first and second crops in a given region so that inhibition of the second crop does not occur?” and “what rate of the residue from a certain crop should be left on the soil in order to avoid residue phytotoxicity and bring benefits to the soil?”

To answer such questions, scientists have to conduct individual experiments under a set of controlled conditions. However, if the conditions on which experiments are based are asked to change, the whole procedure has to start again. It is obvious that such an approach is time-consuming, high cost and low accuracy.

The question naturally emerges, “is there any other approach which can overcome these limitations?” Mathematical modelling offers a positive

answer. By means of such an approach, scientists can synthesize present information as it is obtained, and provide quantitative predictions for different conditions.

However, the role of mathematical modelling is not limited to that of a prediction tool. From the discussion of the previous sections, it is clear that mathematical modelling works, and, combined with other disciplines, has contributed to increasing our understanding of allelopathy, has helped establish the fundamentals of allelochemical function, has highlighted directions for future research by integrating scattered information, generalising the phenomenon observed in fields and laboratories, and has provided a theoretical framework and insights into the mechanisms of allelopathy phenomena. It can be stated that the current mathematical modelling works in allelopathy have just scratched the surface of this developing area, and that more in-depth conceptual treatments are yet to come.

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