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A mathematical model of *Chenopodium album* L. dynamics under copper-induced stress

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ABSTRACT

Heavy metal contamination of the soil is a global problem that produces different harmful effects from an environmental and public health perspective. Although there have been numerous efforts to solve this problem, there is no precise methodology to decontaminate heavy-metal polluted soils. One of the strategies to develop such methods relies on mathematical modelling. Pursuing this goal, we propose a novel mathematical compartmental model consisting of a linear system of differential equations to address the suitability of the model plant (*Chenopodium album* L.) for the remediation of contaminated areas, such as sewage sludge lagoons. Our results show a tendency to maintain high concentrations of copper (Cu) in the roots with the possibility of continuing with good plants' dynamics. Moreover, the model theoretically proposes contaminant concentration in the plants' shoots and roots and predicts a more prolonged tendency to accumulate copper concentrations in the shoots and disrupt the shoots' dynamics. These results provide complementary support for the suitability of this model plant to be used in contaminated areas. In addition, we present asymptotic tendencies of the plants' biomass content and nitrogen-assimilatory (Nitrate reductase; NR) enzyme activity. In this way, we project the relationship between contaminant accumulation and plants' measurements. These projections are essential as they can potentially be used for optimization purposes and strategic harvesting planning. Finally, we present a parameter sensitivity analysis to complement the model examination.

1. Introduction

Heavy metal contamination produces harmful effects on plant development, and it is also an environmental threat of great magnitude for all living beings. Growth inhibition is the most common change observed in plants exposed to high heavy metal(s) concentrations (Prasad, 2004). In Gajewska and Sklodowska (2010), the authors stated that the primary plant part interacting with heavy metals is the root system. Therefore, the decrease in growth is observed more clearly in the roots than in the shoots. Heavy metals are taken into the cell through the roots' nutrient uptake pathways. Consequently, heavy metals may compete with essential elements' plant absorption. Therefore, the inability of the plant to absorb crucial nutrients may cause harmful effects on cellular structures, primary metabolism, and transport processes (Boojar and Goodarzi, 2007; Nedjimi and Daoud, 2009; Sharma and Dietz, 2009).

Nitrogen is one of the main structural components of the plant and constitutes 1.5%–2% of the dry weight of the plant (Frink et al., 1999). Therefore, it is crucial to infer nitrogen concentration in plants through different measurements. Plants usually take up nitrogen as nitrate (NO_3^-). In order to fulfil the essential metabolic functions, nitrate taken by the roots must first be reduced to nitrite and then to ammonia. Nitrate Reductase (NR) and Nitrite Reductase (NiR) enzymes actively reduce nitrate to ammonia. In particular, NR is one of the most important enzymes to infer the predominant form of nitrogen in plants (Marschner, 1995; Solanki and Dhankhar, 2011). NR is highly sensitive to the presence of nitrates. For this reason, it is suggested that NR activity reflects the nitrate content of the habitat where the plant is located (Lee and Stewart, 1978). Indeed, NR activity is accepted in ecological studies as an indicator of nitrate presence (Gebauer et al., 1988; Olsson and Falkengren-Grerup, 2003). NiR enzyme comes into play when NR enzyme converts nitrogen in nitrate form to nitrite. In particular, NiR is responsible for the reduction of nitrite to ammonia. With the assimilation of ammonia that occurs as a result of nitrogen

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fixation, the nitrogen source needed by the plants is converted to glutamine and glutamate by specific reactions, and amino acids and protein compounds are formed from these molecules (Zheng-Xun et al., 2007; Moschou et al., 2012).

Scientific evidence shows adverse effects of increased heavy metal concentration in the growing environment, plant development, and water (Malec et al., 2008, 2009). Due to this fact, various physiological, biochemical, and molecular markers have been established to determine the effects of heavy metal contamination (Malec et al., 2008, 2009; Maleva et al., 2009; Wan et al., 2011; Kumar et al., 2012). In this work, we are particularly interested in alterations from these markers under Cu contamination. Some of the adverse effects on plants due to Cu pollution have already been established. For example, the change in the plant's NR activity is a consequence of the decrease in the plant's nitrate uptake due to copper pollution (Llorens et al., 2000; Xiong et al., 2006). In addition, a reduction in NR enzyme activity may also occur due to the tendency of reactive Cu ions to bind to the sulfhydryl compounds (SH) contained in the NR enzyme. This state causes structural deterioration of the NR enzyme, resulting in irreversible consequences. Similarly, the NR enzyme may deteriorate structurally as a result of low molybdenum (Mo) intake from micronutrients due to high Cu concentrations. Specifically, Mo is a cofactor in the structure of NR, and its insufficient uptake reduces NR enzyme activity.

Phytoremediation, which is also called a "green solution", has a strategic potential to address the heavy metal pollution problem in the environment, and it has been implemented worldwide (Swaileh et al., 2004; Zeidler, 2005; González and González-Chávez, 2006; Ali et al., 2013). Phytoremediation aims to reduce the contaminant concentrations or toxic effects in the environment by using heavy metal-tolerant plants and related soil bacteria (Greipsoon, 2011; Rajkumar et al., 2013). Scientific studies have shown that some plants, such as *Chenopodium album* L., can survive in sewage sludge lagoons (Akpinar, 2021) or heavy metal contaminated areas (Mohan et al., 2019; Bhargava et al., 2007; Tozser et al., 2019; Alipour et al., 2015; Zulfiqar et al., 2012; Gupta and Sinha, 2007). Therefore, *Chenopodium album* L. is a candidate for monitoring heavy metal pollution in degraded areas (biomonitoring) and phytoremediation of heavy metals in contaminated sites.

Hand-in-hand studies of theoretical and experimental researchers play a significant role in unveiling the underlying working principles of biological mechanisms. Mathematical modelling is the primary tool used in theoretical studies. This approach provides a multidisciplinary framework for complementing, supporting, and producing new experimental settings of a system's dynamics. A mathematical model can potentially project a system's long-term behaviour under different physical constraints. On the one hand, a specialized model can include specific factors and relationships of the system at the cost of increasing the complexity of the model and hence limiting the incorporation of experimental data. On the other hand, a less complex mathematical model, so-called a "toy" model, can attenuate this complexity at the cost of missing specific features of the system. A toy model is primarily used for understanding the big picture more than the details. Therefore, a possible approach in mathematical modelling is to incorporate a minimum set of system features without losing the model tractability of the main variables. Additionally, one of the options when establishing a mathematical modelling strategy is to develop a compartmental model. The basis of compartmental models is to divide the system into multiple compartments to be analysed independently, which is supported by the so-called modular plant architecture approach. However, the meristematic nature of plants restricts the assertiveness of this approach (Cheeseman et al., 1996). This is because there is no exact distinction between a root and a shoot compartment in an actual plant. Nevertheless, this simplifying assumption can build up basic models to extract a set of the main dynamics that can be further refined later. In particular, a linear mathematical model provides a simple scenario to investigate the otherwise complex dynamics of a system.

Various mathematical models have been proposed to investigate and optimize phytoremediation techniques. We found a model for the phytoremediation of petroleum-contaminated soil (Thoma et al., 2003), an optimization model to comply with environmental criteria (Thomas and Vandemuelebroeke, 2005), a model for the accumulation of heavy metals in benthic algae (Seip, 1979), among many others (Cârdei et al., 2021; D'Acunto et al., 2019; Torres-Bejarano et al., 2019; Tantemsapya et al., 2011; Tawfiq and Wirojanagud, 2016). We also found a heuristic mathematical model to assess a contamination level or plan a harvesting strategy in these models. However, as far as the authors know, there is currently no mathematical model relating both the NR enzyme activity and the biomass content to the accumulation of contaminants in a plant. We propose that incorporating these feature dynamics into a mathematical model is crucial. Therefore, this approach relates contaminant accumulation to measurable experimental quantities intrinsic to the plant's dynamics. The model here developed aims to theoretically support the plausibility of the model plant to be used in a copper-contaminated environment by relating the model to experimental data. This work shows different scenarios of the main variables under copper-induced stress. Furthermore, our results provide model plants' consistent features with qualities observed in indicator species. In addition, our mathematical model assesses and predicts the NR enzyme activity, biomass content, and contaminant level in each of the plant's compartments as time evolves.

The work in this manuscript is developed as follows. In Section 2, we establish the experimental analysis of *Chenopodium album* L. under copper-induced stress. Section 3, sets the biological and mathematical fundaments that support our mathematical model. Section 4 establishes the mathematical model and analyzes different scenarios of the model plant under copper-induced stress. Our model parameters are calibrated and validated by the experimental data. Using these parameters we provide longer time projections of the variables. In addition to our forecasts, we provide asymptotic dynamics of the model's main variables, including information about the system's more extended time dynamics. In Section 4, we also provide parameter sensitivity analysis to address the model components and complement our mathematical analysis. Finally, in Section 5, we discuss some of the model's implications and limitations, and in Section 6, we establish our conclusions and future work to be developed.

2. Materials and methods

Chenopodium album L., which is seen to grow naturally in sewage sludge lagoons (Akpinar, 2021), was chosen as the model plant in this study. Uniform seedlings belonging to the *C. album* were collected from their natural environments in Turkey's Bursa Province. They were exposed to different concentrations of Cu (0 μM (control), 50 μM, and 500 μM). Plants were harvested on the 1st, 3rd, and 7th days after the Cu treatments. Then, they were washed thoroughly with de-ionized water, and the roots and shoots were separated (leaves+stems). The NR enzyme activity was immediately analysed in fresh plant material. NR in the fresh roots and shoots was determined according to the *in vivo* test described by Hageman and Hucklesby (1971), Jaworski (1971), and modified by Gebauer et al. (1984). This spectrophotometric method is based on measuring the absorbance of nitrite (NO_2^-) formed by the nitrate reduction in the incubation medium. NR (μM $NO_2^- g^{-1}$ DW h^{-1}) was calculated using the absorption value on a dry weight (DW) basis. Dry biomass was measured after oven-drying plant materials at 80 °C until constant weight. The biomass of roots and shoots was also measured on a DW basis. The same method indicated in Akpinar (2021) was used to determine Cu accumulation in plant parts.

3. Theory

In this section, we provide the theory that supports the development of our mathematical model. To begin, we design a compartmental setting. The compartments are determined by the environment E, the roots R, and the shoots S, as is described in Fig. 1. We aim to incorporate the dynamics of a metal contaminant into each of these compartments in a simplified setting. Therefore, we assume that the independent compartments are only affected by the metal contaminant. We establish a linear system of 9 first-order differential equations with 13 free parameters that describe different plant dynamics. Although we greatly simplify the biological process by considering a simple linear model, we remain with the challenge of determining a plausible range for the model parameters to study the effect of copper pollution on the model plant. Therefore, we determine the parameters of our mathematical model by the experimental data described in Section 2. This provides a setting in which we theoretically explore the suitability of the model plant, *Chenopodium album* L., to be used in contaminated areas and assess the plant's contaminant concentration. Our main variables are determined by the biomass and the nitrogen-assimilatory enzyme (NR) activities. The latter measurement indirectly provides information about the plant's nitrogen (N). Indeed, as previously mentioned, NR has been established as one of the most important enzymes to determine the predominant form of nitrogen in plants. In addition, the dynamics of the nitrogen content and the NR enzyme activity had been successfully modelled as oscillatory in higher plants (Yang and Midmore, 2005), alluding to circadian oscillations. Therefore, we propose an initial model of NR enzyme activity described by a second-order constantly forced damped harmonic oscillator (Strogatz, 2015). To simplify the model simulations, we transform the second-order differential equation into two first-order differential equations. That is, we consider:

$$\begin{aligned} \frac{dNR}{dt} &= T \\ \frac{dT}{dt} &= d - bT - aNR, \end{aligned} \tag{1}$$

where $T = \frac{dNR}{dt}$ is the rate of change of NR enzyme activity, and a, b, c are constants such that $a > 0$, $b \geq 0$, and $d > 0$. We propose that the rate of change in nitrogen content (NC) is proportional to the rate of change in nitrate reductase enzyme activity:

$$\frac{dNC}{dt} = k_1 \frac{dNR}{dt}, \tag{2}$$

for some constant $k_1 > 0$. Furthermore, we propose that the biomass (B) content is determined by the dynamics of the nitrogen content, which is directly related to the amount of the NR enzyme in each compartment. Specifically, we propose that the biomass is determined by the difference between the amount of nitrogen and the decaying growth (Verkroost and Wassen, 2005), that is:

$$\frac{dB}{dt} = k_2 NC - k_3 B, \tag{3}$$

for some constants $k_2 > 0$ and $k_3 > 0$. Since we are primarily concerned with the NR enzyme activity, we combine Eqs. (2) and (3), and we propose the equation:

$$\frac{dB}{dt} = K_1 NR - K_2 B, \tag{4}$$

for some positive constants K_1 and K_2.

The contaminant dynamics of the model are motivated by the work of Thomas and Vandemuelebroeke (2005). A mathematical model is established in the abovementioned work to optimize harvesting strategies for metal phytoremediation. However, compared to Thomas and Vandemuelebroeke (2005), we directly relate the contaminant accumulation to the plant's intrinsic dynamics. Finally, we assume that the metal accumulation directly affects the nitrogen content as a negative linear forcing term. That is, we propose the following equation

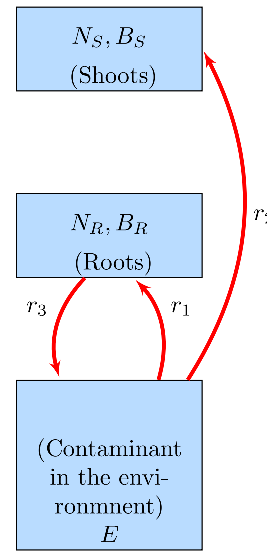

Fig. 1. Simplified compartmental flowchart of contaminant dynamics. N_S and N_R are the amount of NR enzyme activities in the shoots and the roots, respectively. B_S and B_R are the biomass content in the shoots and the roots, respectively. Under this scenario, the sum of the amount of contaminant in the compartments remains fixed. The contaminant uptake rate in the roots (r_1), the shoots (r_2), and the return rate to the environment (r_3) are almost equivalent according to the experimental data.

to describe the amount of the NR enzyme content under copper-induced stress:

$$\begin{aligned} \frac{dNR}{dt} &= T \\ \frac{dT}{dt} &= d - bT - aNR - eM, \end{aligned} \tag{5}$$

where M is the amount of metal absorbed by the plant and e is the uptake rate of the contaminant.

We limit our analysis to the previously described features in the present model. A future version of the model should include different elements, such as carbon dynamics, as carbon is one of the plants' essential structural components. An additional model description including specific information about water content, photosynthetic activity, temperature, humidity, pH, among others, should also be addressed in the future.

The main assumptions and variables of the model are summarized as follows:

- The model establishes two independent compartments of the plant determined by the plant roots and shoots that are independently affected by the contaminant. There is an additional compartment determined by the plant growing conditions which are simplified and described as the "environment".
- We exclude the intrinsic dynamics of the environment.
- We assume that a single contaminant dose is initially added to the environment.
- The main variables of the model are the NR enzyme activity, biomass content, and contaminant concentration in both the roots and the shoots. The experimental data constrains the NR enzyme activity and the biomass content variable. In addition, the contaminant concentration variable is constrained by the initial amount of contaminant added to the environment at the beginning of the experiment.
- The NR content is modelled as a damped harmonic oscillator. The forcing of this oscillator accounts for all external factors not considered in the modelling process. This is a central simplifying assumption aimed to minimize the number of variables in the system.

- The biomass content is related to the nitrogen content.
- The amount of metal in the environment affects the plant's roots and shoots linearly.
- The amount of contaminant in the system remains fixed at all times.
- An amount of metal is taken up directly by the roots, and another percentage goes immediately to the shoots.
- A portion of the contaminant not absorbed by the shoots is returned to the environment.
- All of the model parameters are assumed positive. These parameters are not directly measured from experimental data. Instead, they are determined by solving an optimization problem in which the NR enzyme activity, biomass content, and contaminant content variables fit the data.

4. Results

4.1. Mathematical model

Inspired by the experimental studies, we establish a model to capture the relationship between contaminant uptake, biomass content, and NR enzyme activity. The model is developed considering the simplifying assumptions previously established. To simplify notation, we denote the NR enzyme activity variable simply as $N_j(t)$. We also denote $B_j(t)$ as the biomass content, $T_j(t)$ as the rate of change of the N_j variable over time (i.e., $T_j(t) = \frac{dN_j(t)}{dt}$), and $M_j(t)$ as the amount of contaminant. All of the previous variables are evaluated at time t, and the subscripts $j = \{R, S, E\}$ denote the different compartments (R = Roots, S = Shoots, and E = Environment). The time is measured in days. All of the parameters are assumed positive, and their biological significance is described in Table 1. The proposed model is:

$$\begin{aligned}
\frac{dN_R}{dt} &= T_R \\
\frac{dT_R}{dt} &= d_R - b_R T_R - a_R N_R - e_R M_R \\
\frac{dB_R}{dt} &= \alpha_R N_R - \beta_R B_R \\
\frac{dN_S}{dt} &= T_S \\
\frac{dT_S}{dt} &= d_S - b_S T_S - a_S N_S - e_S M_S \\
\frac{dB_S}{dt} &= \alpha_S N_S - \beta_S B_S \\
\frac{dM_E}{dt} &= -(r_1 + r_2) M_E + r_3 M_R \\
\frac{dM_R}{dt} &= r_1 M_E - r_3 M_R \\
\frac{dM_S}{dt} &= r_2 M_E.
\end{aligned} \tag{6}$$

Additionally, the model's initial conditions are determined by the experimental initial conditions in each of the different scenarios herein presented. Considering the last three equations, we observe that:

$$\frac{dM_E}{dt}(t) + \frac{dM_R}{dt}(t) + \frac{dM_S}{dt}(t) = 0, \tag{7}$$

implying that the amount of contaminant in the three compartments remains fixed at all times. That is, $M_E(t) + M_R(t) + M_S(t) = N$, where N is the total amount of contaminant in the system.

We consider the proposed model under different parameter scenarios motivated by the experimental data. Under convenient parameter choices, a mathematical model can make either quantitative or qualitative predictions. We focus on quantitative predictions; however, we will show that the metal accumulation projections of our model might also be used to determine qualitative dynamics. The parameters of each of the scenarios studied here were obtained by solving an optimization problem defined by a higher-order interpolation of the experimental data. The optimization problem was solved using the MATLAB *fmincon* function (MATLAB, 2017). In all of the scenarios shown here (Subjects $A - F$ in Table 2), we calibrate the model parameters by considering the first five days (Subjects A, B, C, and D) or six days (Subjects E and F) of the experimental data. The remaining days of the experiment were used to validate the model's results. Since we aim to observe the effects of the contaminant in the system's dynamics, we use the model to project more extended time dynamics after the experiment. It is important to remark that since our model parameters are calibrated by data interpolation, future experimental settings that provide more satisfactory time resolution can give a more accurate description of the system's dynamics.

In Figs. 2–7, we consider the dynamics of different experiments under Cu contaminant levels. Each figure consists of a series of subfigures to describe the system's dynamics in the following way. In subfigures **(a)(b)(e)**, we observe the model calibration and validation periods. In subfigures **(c)(d)(f)**, we follow the projected long-term 14-days dynamics of the model variables. In all the subfigures, the experimental data are shown in red, and the model simulations are shown in blue.

In Fig. 2, we consider the dynamics of the control experiment (Subject A). In this case, no contaminant is added to the plant growing condition. We observe a good resemblance between the experimental data and the model during the 7-day calibration and validation period. In Figs. 2**(a)(b)**, we observe a slightly oscillatory behaviour of the data, especially noticeable in the NR enzyme activity in the shoots. Further refinement in experimental settings may provide a more accurate description of oscillatory dynamics. In Figs. 2**(c)(d)**, we observe the projected 14-days dynamics of activities. In this control scenario, we observe a tendency of the shoots' biomass and NR enzyme activity to remain around "healthy" states. In the case of the roots variables, slight oscillations are observed around positive states that can also be considered healthy states of activity. In both the shoots and the roots variables, the preferred states in the long-time projection of the model are consistent with the observed activities during the experiment. In Fig. 2**(e)**, we observe a slight and almost insignificant increase in metal contaminant that might be naturally present in the environment and does not significantly affect the plant's dynamics. Fig. 2**(f)** shows a slight contaminant increase in the projected model dynamics. Overall, the increase of the projected contaminant in both the roots and the shoots is less than 1 DW unit. Additionally, in Table 2, we notice that the parameters for the control experiment differ in several orders of magnitude compared to the rest of the experiments in which Cu contaminant is added to the plant growing condition.

In Figs. 3–5, we consider the model dynamics under the addition of 50 μM of Cu to the plant growing conditions (Subject B, C, and D, respectively). There is a good resemblance between the experimental data and the model during the 7-day calibration and validation period in the three scenarios. In Figs. 3**(a)(b)**, we observe a slightly oscillatory behaviour in the roots' variables. There is a more pronounced oscillatory behaviour in the shoots' variables. In the projected model dynamics, we observe consistent oscillatory dynamics in the roots and a long-term toxic effect in the shoots, disrupting the shoots' variables after day 8 (NR enzyme activity) or day 13 (biomass content). The concentration of the contaminant is mainly in the roots during the experiment and the long-term projection. The model Cu concentration in the roots reaches around 140 DW units (150 DW units in the data) at the end of the experiment and about 220 DW units at the end of the projected time. The model Cu concentration in the shoots reaches around 90 DW units (80 DW units in the data) at the end of the experiment and around 140 DW units at the end of the projected time.

In Fig. 4, we observe different model projections compared to Fig. 3. There are oscillatory dynamics for both the roots' and the shoots' variables during the experiment. During the projected longer time dynamics of the system, the variables remain near slightly decreased positive activity states. In the shoots' variables, there is projected a

Table 1
Parameter description. The dry weight (DW) units are measured in mg/kg.

Parameter	Description	Units
a_R	NR harmonic proportionality constant in the roots	1/days^2
d_R	constant environmental forcing in the roots	DW/days^2
b_R	NR damping term in the roots	1/days
α_R	NR influence on the biomass rate in the roots	1/days
β_R	biomass influence rate in the roots	1/days
e_R	contaminant influence rate in the roots	DW/μM days^2
a_S	NR harmonic proportionality constant in the shoots	1/days^2
d_S	constant environmental forcing in the shoots	DW/days^2
b_S	NR damping term in the shoots	1/days
α_S	NR influence on the biomass rate in the shoots	1/days
β_S	biomass influence rate in the shoots	1/days
e_S	contaminant influence rate in the shoots	DW/μM days^2
r_1	contaminant uptake rate in the roots	1/days
r_2	contaminant uptake rate in the shoots	1/days
r_3	contaminant return rate to the environment	1/days

Table 2
Parameters fixed for different model simulations motivated by experimental data. Subject *A* is a control experiment. Subjects *B*, *C*, and *D* received 50 μM of Cu. Subjects *E* and *F* received 500 μM of Cu.

Parameter	A	B	C	D	E	F
a_R	$0.4153e^4$	2.5127	10.2825	4.1557	0.5793	1.7808
d_R	$0.4514e^4$	3.2323	14.7604	5.1497	0.0150	1.0686
b_R	$0.8017e^4$	3.6596	14.4398	0.1058	7.7625	3.6387
α_R	$0.1110e^4$	0.3062	7.9737	1.8582	0.0003	1.8735
β_R	$0.2923e^4$	1.0420	32.3239	6.4821	0.1261	4.2359
e_R	$0.0008e^4$	0.0058	0.0340	0.0051	0.0001	0.0021
a_S	$0.2743e^4$	0.0812	0.6782	0.5174	1.1344	0.3853
d_S	$0.5556e^4$	0.9005	1.4521	1.0683	0.1105	0.3705
b_S	$1.0410e^4$	0.0001	2.4012	0.5129	6.0540	0.0010
α_S	$0.0198e^4$	0.0236	0.4355	0.0716	0.0362	1.9000
β_S	$0.0533e^4$	0.0469	1.2148	0.2008	0.0420	3.6882
e_S	$0.1846e^4$	0.0150	0.0080	0.0002	0.0001	0.0008
r_1	$0.3993e^4$	0.0556	0.0648	0.0524	0.0198	0.0204
r_2	$0.0000e^4$	0.0349	0.0342	0.0314	0.0062	0.0062
r_3	$2.5915e^4$	0.0001	0.0001	0.0001	0.1755	0.1650

slight and slow decrease in both variables. The preferred states of each variable are consistent with the activity during the experiment. Thus, in this case, there is no disruption of the activity in the shoots but rather a slight decrease in its variables. Additionally, the contaminant is mainly absorbed in the roots. The Cu concentration in the roots reaches around 160 DW units (150 DW units in the data) at the end of the experiment and around 240 DW units at the end of the projected time. The Cu concentration in the shoots reaches around 85 DW units (85 DW units in the data) at the end of the experiment and around 130 DW units at the end of the projected time.

In Figs. 5**(a)–(d)**, we observe a medium oscillatory behaviour of the variables. The long-term projections show no significant change in the variables compared to the experiment. There is a long tendency to maintain positive "healthy" states. The concentration of the contaminant is mainly in the roots during the experiment and the projected activity. The Cu concentration in the roots reaches around 140 DW units at the end of the experiment, slightly different from the 160 DW units in the data, and approximately 220 DW units at the end of the projected time. The Cu concentration in the shoots reaches around 80 DW units at the end of the experiment and around 130 DW units at the end of the projected time.

In the overall analysis of Figs. 3–5, we found that the activity shown is consistent with the roots' ability to absorb contaminants facing the possibility (Fig. 3) of a longer-time toxic effect in the shoots. These three scenarios support the viability of the plant to be used in copper-contaminated areas. Moreover, there is a consistent metal accumulation in the proposed model in the three cases. At the end of the experiment, the model contaminant concentration in the roots ranges from 140 to 160 DW units and from 220 to 240 DW units for the long-time projected dynamics. On the other hand, the model contaminant concentration in the shoots ranges from 80 to 90 DW units at the end of the experiment and from 130 to 140 DW for the long-time projected dynamics.

Figs. 6–7 consider the model dynamics under 500 μM of Cu added to the plant growing condition (Subjects *E* and *F*, respectively). The resemblance between the experimental data and the model during the 7-day calibration/validation period is reasonable in the two cases. In Fig. 6, we observe a slightly oscillatory behaviour with a tendency to decrease over time during the experiment. The only exception is the shoots' biomass content that remains near a diminished activity state. The long-term model dynamics show a consistent toxic effect and an activity decrease as time evolves. Such reduction is oscillatory in the roots' variables. In addition, the NR enzyme activity in the shoots has the most significant activity decrease over time. The biomass content in the shoots is projected to stay near a stable state, similar to the experiment. The metal concentration in the roots reaches around 360 DW units at the end of the experiment, slightly different from the 330 DW units in the data and approximately 450 DW units at the end of the projected time. The metal concentration in the shoots reaches around 200 DW units (180 DW units in the data) at the end of the experiment and around 390 DW units at the end of the projected time.

In Fig. 7, we observe oscillatory dynamics of the data during the experiment with a tendency to decrease over time. The projected activities in the roots' variables show a significant decrease tending to disrupt the NR enzyme activity and the biomass content. On the other hand, the projected activities in the shoots' variables show oscillatory components tending to disrupt activity around day 14. The metal concentration in the roots reaches around 390 DW units (360 DW units in the data) at the end of the experiment and around 480 DW units at the end of the projected time. The metal concentration in the shoots reaches around 200 DW units (200 DW units in the data) at the end of

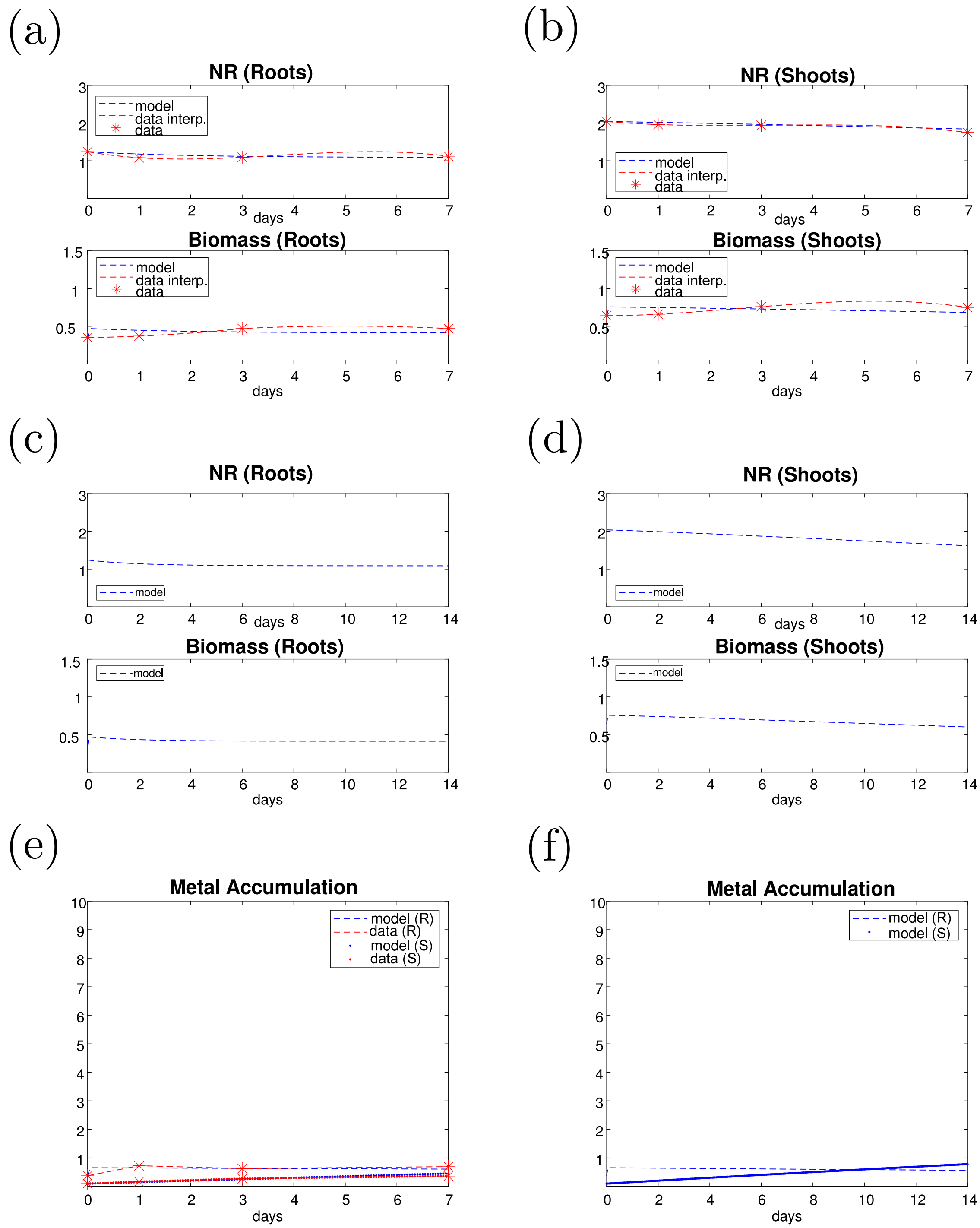

Fig. 2. NR enzyme activity, biomass content, and metal accumulation in the roots and the shoots of *C. album* in a control experiment (Subject *A*). **(a)(b)** NR enzyme activity and biomass content in the roots and the shoots of a 7-day experiment, respectively. **(c)(d)** Projection of the model in a 14-days scenario. **(e)(f)** Modelling of plausible contaminant dynamics in the 7-day experiment, and 14-days projection, respectively.

the experiment and around 390 DW units at the end of the projected time.

In the analysis of Figs. 6–7, our results show that the projected dynamics are consistent with the roots' ability to absorb contaminants, facing either a decrease in the shoots' variables or disruption of activities. These scenarios also support the viability of the model plant to be used in copper-contaminated areas. At the end of the experiment, the model contaminant concentration in the roots is around 360 DW units and ranges from 450 to 480 DW units for the projected dynamics. On the other hand, the model contaminant concentration in the shoots lies around 200 DW units at the end of the experiment and around 390 DW units for the long-time projected dynamics. In conclusion, there is a toxic effect in both of these scenarios due to the contaminant. However, the time scale in which this harmful effect is present is slow, which provides a solid indication and plausible theoretical and modelling justification of the model plant to serve as an indicator species.

As a final model analysis, we observe that the data and model dynamics are consistent during the first 7-days. The ranges of metal accumulation at the end of the experiment and the end of the long-time projections remain consistent for the different scenarios in each of

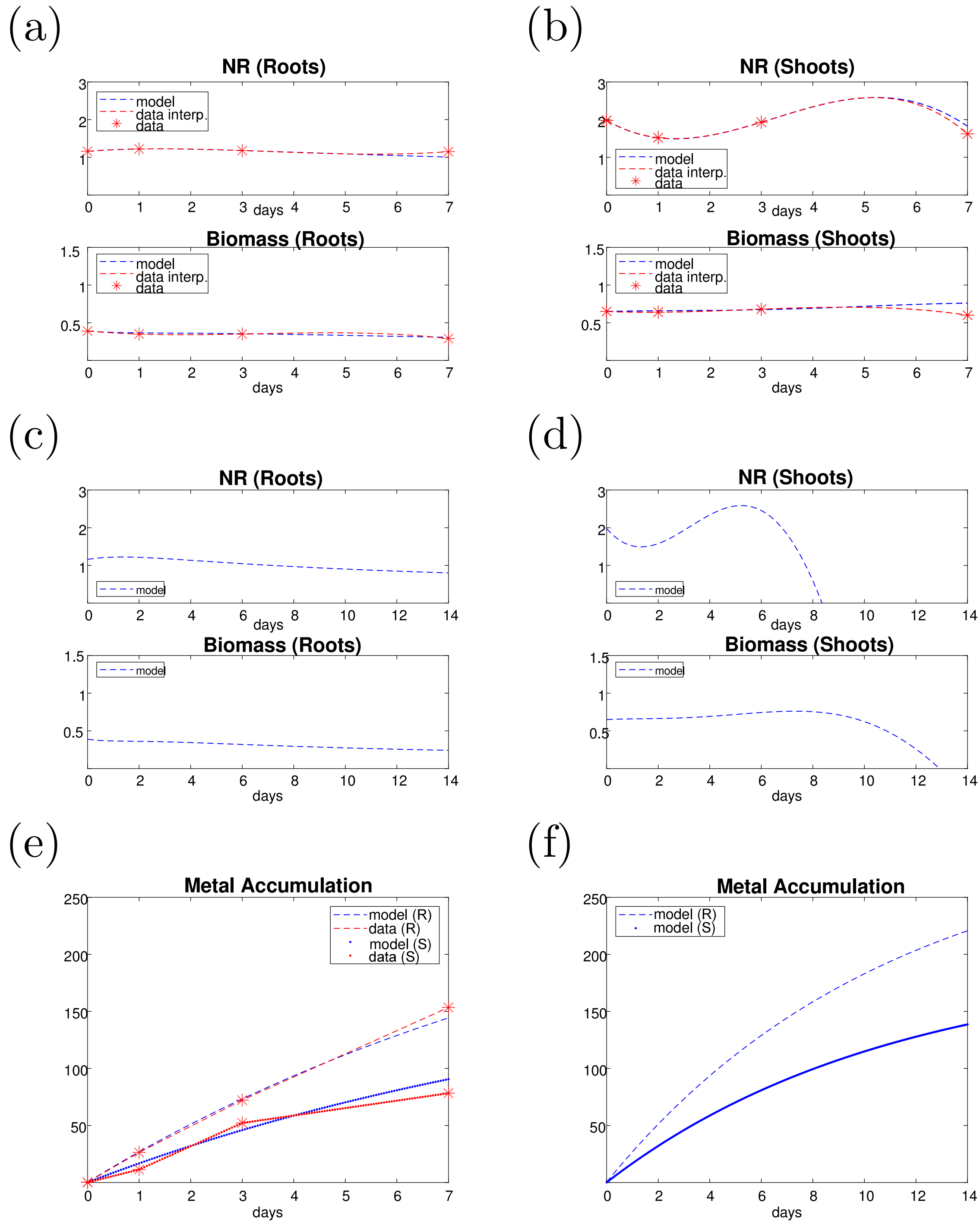

Fig. 3. NR enzyme activity and biomass content, in the roots and the shoots of *C. album* in an experiment with 50 μM of Cu added to the environment (Subject *B*) **(a)(b)** NR enzyme activity and biomass content in the roots and the shoots of *C. album* in a 7-day experiment, respectively. **(c)(d)** Projection of the model in a 14-days scenario. **(e)(f)** Modelling of plausible contaminant dynamics in the 7-day experiment, and 14-days projection, respectively.

the cases considered. Moreover, when analysing the parameter values in Table 2, we observe that the parameters related to the contaminant uptake (e.g., e_R, e_S, r_1, r_2, and r_3) lie in similar ranges. In particular, the contaminant uptake rate in the roots (r_1), the contaminant uptake rate in the shoots (r_2), and the contaminant return rate to the environment (r_3) are nearly identical in each of the cases considered (last three rows in Table 2).

The long-time tendency of the system's variables (i.e., the equilibrium solutions) is dependent on the different model parameters, as is detailed in the Appendix. Here, and motivated by our previous results, we analyse the contaminant's toxic effect in the shoots activities. Fig. 8 establishes a model scenario under an *in-silica* experimental setting. In our results, we obtain that the long-term tendency of the shoots' NR enzyme activity and biomass content is determined by three factors: the environmental factors, the amount of contaminant, and the absorption rates in the shoots. In particular, the longer time tendency of the system is established by the following relationships:

$$\overline{N_S} \rightarrow \frac{d_S - e_S N}{a_S}, \tag{8}$$

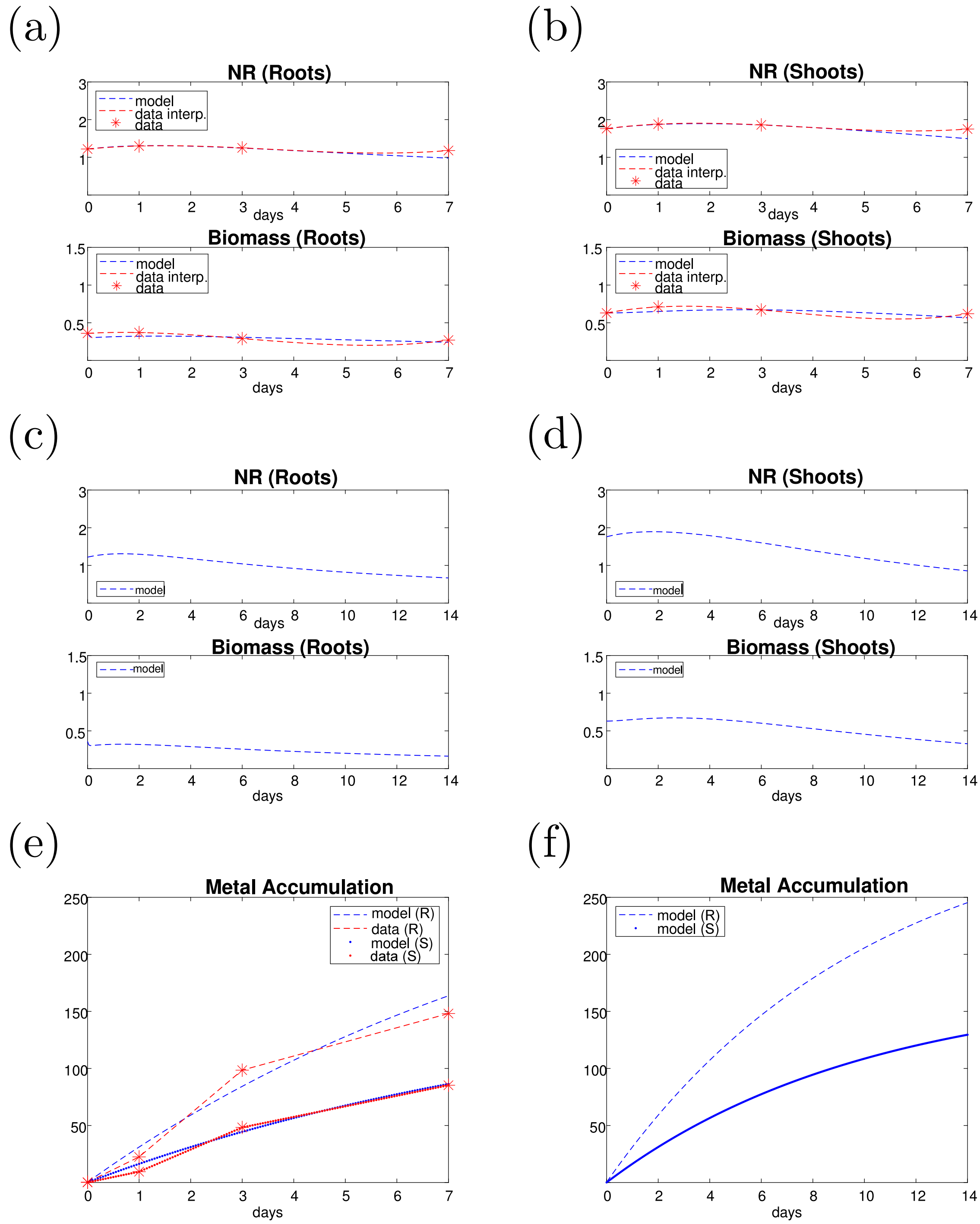

Fig. 4. NR enzyme activity and biomass content in the roots and the shoots of *C. album* in an experiment with 50 μM of Cu added to the environment (Subject *C*) **(a)(b)** NR enzyme activity and biomass content in the roots and the shoots of *C. album* in a 7-day experiment, respectively. **(c)(d)** Projection of the model in a 14-days scenario. **(e)(f)** Modelling of plausible contaminant dynamics in the 7-day experiment, and 14-days projection, respectively.

and

$$\overline{B_S} \to \frac{\alpha_S\left(d_S - e_S N\right)}{\beta_S a_S}, \tag{9}$$

where $\overline{N_S}$ is the projected NR enzyme activity in the shoots and $\overline{B_S}$ is the projected biomass content in the shoots. As shown in Fig. 8, strategic harvesting can be planned from the previous relationships, as the variables can provide a plausible scenario for the amount of contaminants in the environment and a theoretically proposed uptake rate. In particular, a minimum harvesting time can also be established, especially contemplating a framework in which the contaminant concentration in the environment is unknown.

4.2. Parameter sensitivity analysis

Sensitivity analysis serves to quantify how important each parameter is to each model variable. Sensitivity analysis is used to measure the effects of uncertainties on both the model's input and output. This mathematical tool can help create more accurate models by identifying

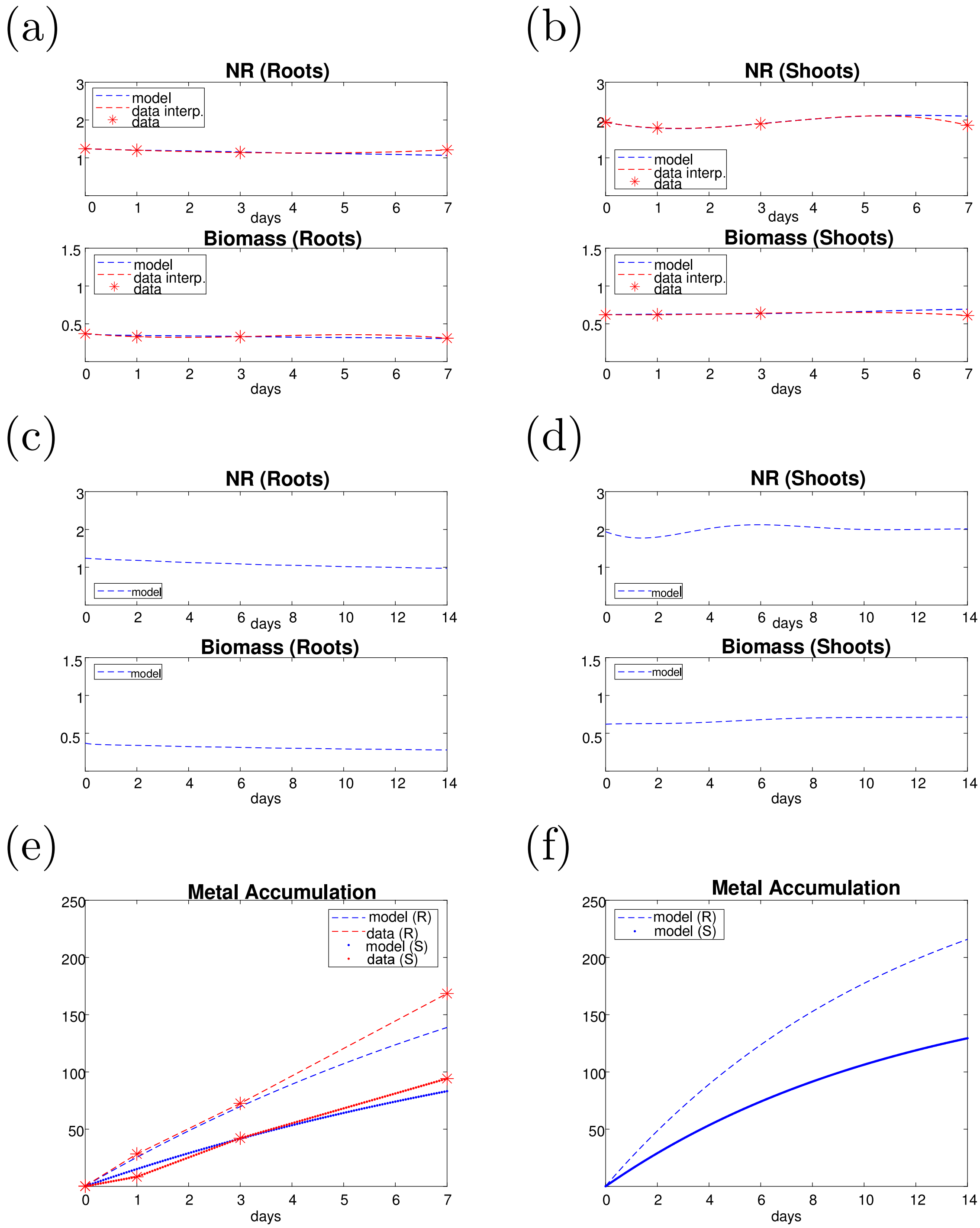

Fig. 5. NR enzyme activity and biomass content in the roots and the shoots of *C. album* in an experiment with 50 μM of Cu added to the environment (Subject *D*) **(a)(b)** NR enzyme activity and biomass content in the roots and the shoots of *C. album* in a 7-day experiment, respectively. **(c)(d)** Projection of the model in a 14-days scenario. **(e)(f)** Modelling of plausible contaminant dynamics in the 7-day experiment, and 14-days projection, respectively.

key parameters that predominantly affect the model dynamics. In this case, the *normalized forward sensitivity index* can measure the output variable's relative change regarding a change in a chosen input parameter. The normalized forward sensitivity index is defined in Arriola and Hyman (2009) as:

$$S_{u_p} := \lim_{\delta p \to 0} \left(\frac{\delta u}{u}\right)\left(\frac{\delta p}{p}\right)^{-1} = \left(\frac{p}{u}\right)\frac{\partial u}{\partial p}, \tag{10}$$

where u is a model variable, and p is a fixed model parameter. We are interested in quantifying which parameters influence the equilibrium solution most, as the stability of such an equilibrium solution is well understood. Therefore, we now measure the normalized sensitivity index of the biomass content and the NR enzyme activity in both the shoots and the roots to better understand the critical model dynamics. In Table 3, we show the non-trivial sensitivity indexes of our model. The most sensible parameters on the shoots' biomass variable are the constant environmental forcing term and the NR influence on the biomass change rate. In particular, increasing d_S or α_S by 10% implies modifying the shoots' biomass asymptotic tendency by more than 10% (as the sensitivity is greater than 1). In the same way, increasing d_S by 10% implies modifying the shoots' NR enzyme activity by more than 10%. Also, we observe that changing the shoots' contaminant influence

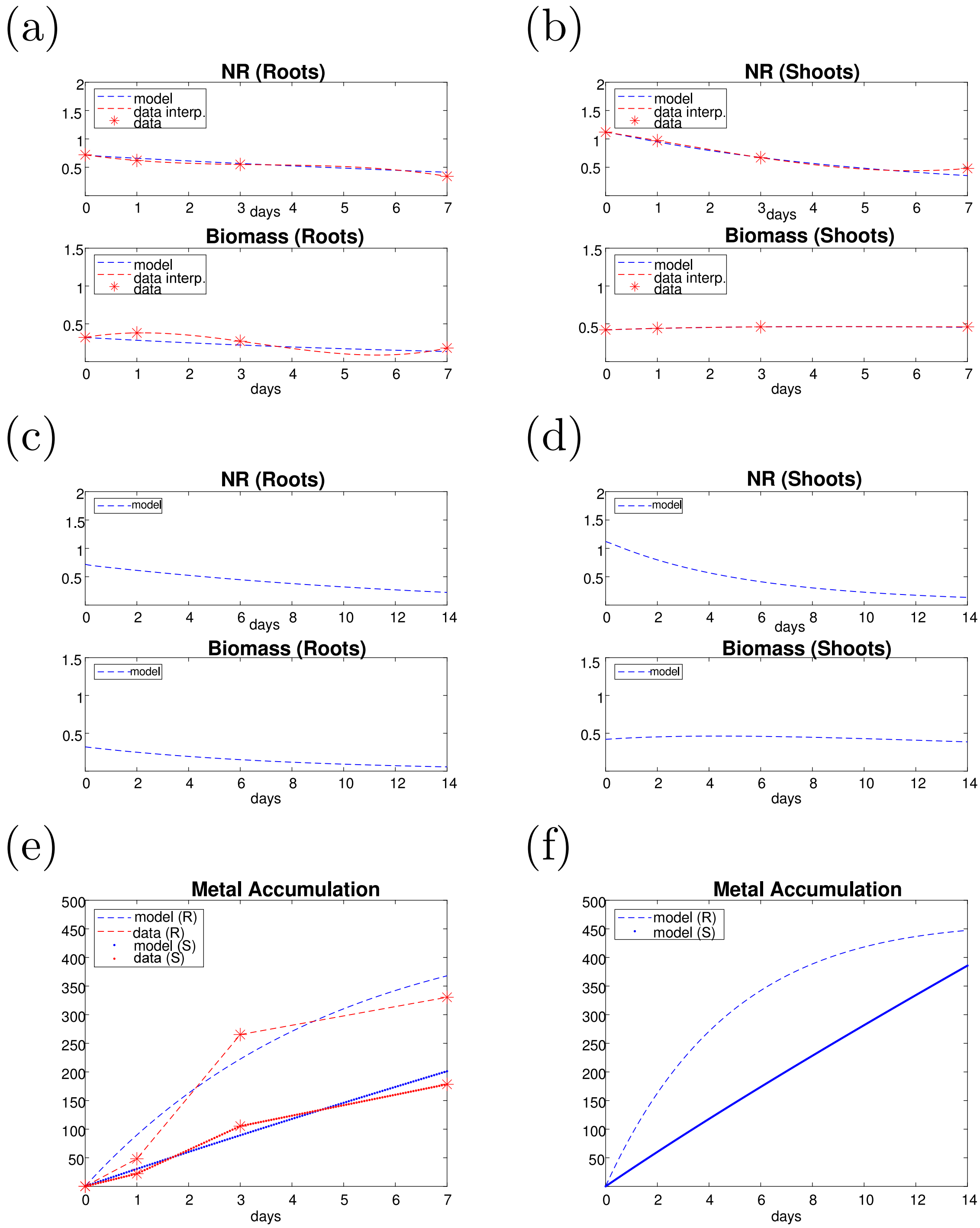

Fig. 6. NR enzyme activity and biomass content in the roots and the shoots of *C. album* in an experiment with 500 μM of Cu added to the environment (Subject *E*) **(a)(b)** NR enzyme activity and biomass content in the roots and the shoots of *C. album* in a 7-day experiment, respectively. **(c)(d)** Projection of the model in a 14-days scenario. **(e)(f)** Modelling of plausible contaminant dynamics in the 7-day experiment, and 14-days projection, respectively.

rate (e_S) by 10% implies modifying the shoots' NR enzyme activity by *less* than 10% (as the sensitivity index is smaller than 1).

5. Discussion

In the present study, we proposed a novel mathematical model providing a setting to relate the nitrogen-assimilatory enzyme activity and the biomass content to contaminant levels. The model parameters are calibrated and validated by experimental data to make the model biologically more plausible. Furthermore, different scenarios were considered to model contaminant-induced stress in the model plant. In this work, we have shown, the suitability of *C. album* to be considered in contaminated areas through mathematical modelling and numerical simulation. Our results show a tendency of the roots to maintain healthy levels of activity despite the presence of high levels of Cu. This roots' characteristic has provided the ability of the model plant to survive in sewage sludge lagoons. Indeed, in Akpinar (2021), *Chenopodium album* L. was observed naturally established in such an environment.

Different studies have analysed the plausibility of *C. album* for remediation of contaminated soil. Notably, in Mohan et al. (2019), the model

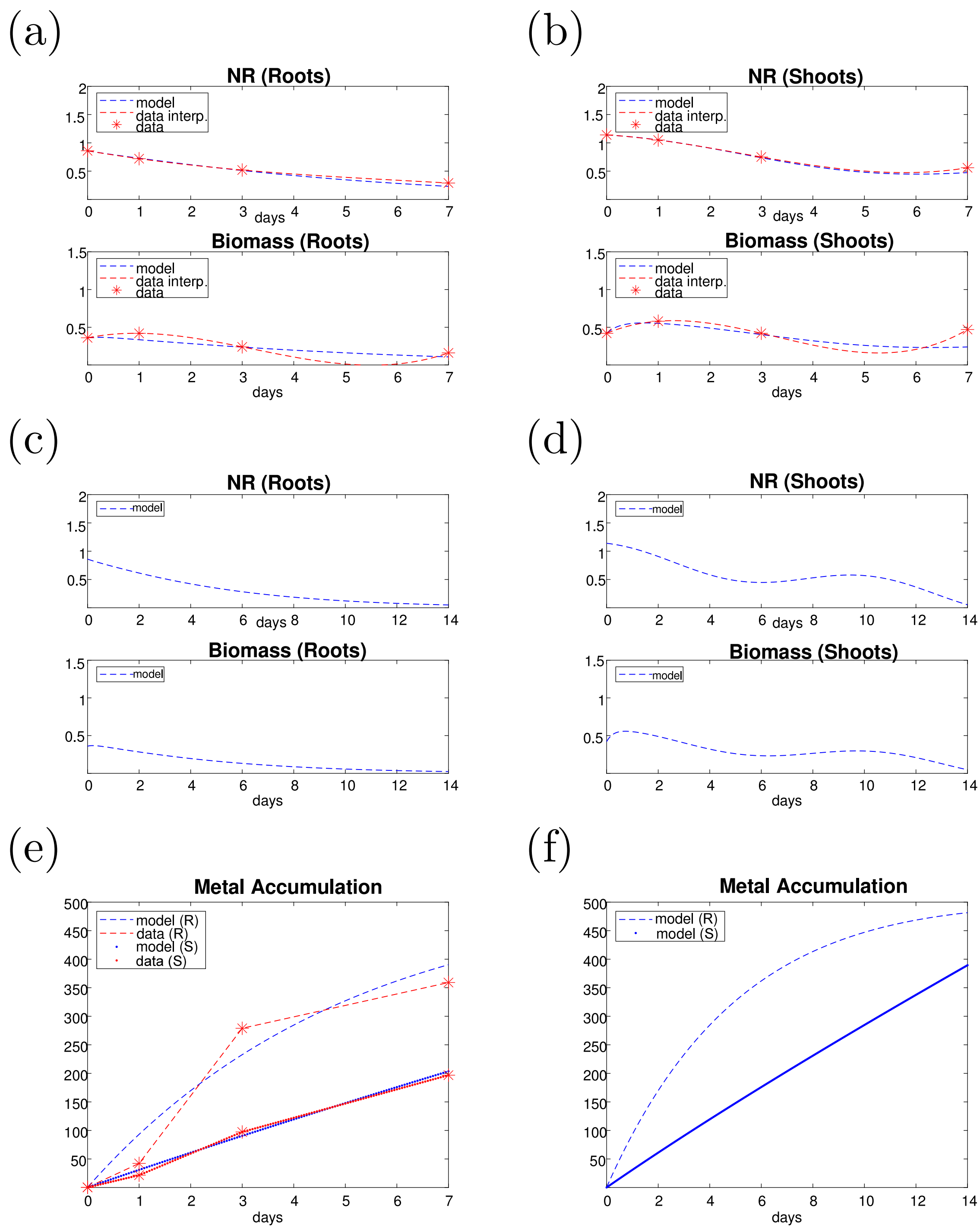

Fig. 7. NR enzyme activity and biomass content in the roots and the shoots of *C. album* in an experiment with 500 μM of Cu added to the environment (Subject *F*) **(a)(b)** NR enzyme activity and biomass content in the roots and the shoots of *C. album* in a 7-day experiment, respectively. **(c)(d)** Projection of the model in 7-day experiment, and 14-days projection, respectively.

plant removed heavy metals from the ground through a phytoremediation process. In Bhargava et al. (2007), there was an extensive study investigating the plausibility of *Chenopodium* spp. to endure six heavy metal contaminants. The abovementioned study established scientific evidence of *C. album* being a good copper accumulator. It was also suggested that the metal accumulation effectiveness of *Chenopodium* spp. made it a suitable choice for phytoextraction. In both of the previous studies, the assessment of metal uptake was made through different experimental settings. In comparison, our results of the experimental settings are supported through the evolution of the main model variables over time. This suggests that the ability of *C. album*, shown in the experimental data, to concentrate heavy metals in the roots and the shoots can also be maintained for longer times.

Tozser et al. (2019) analysed metal uptakes in *C. album*. In this study, it was suggested that to achieve efficiency in the remediation process, it is necessary to remove the plant organs lying above the ground once the contaminant is accumulated. Our model could potentially provide a theoretical strategy for such a removal process. Indeed, the removal process could be established as an optimization problem based on an estimated amount of contaminant in the soil.

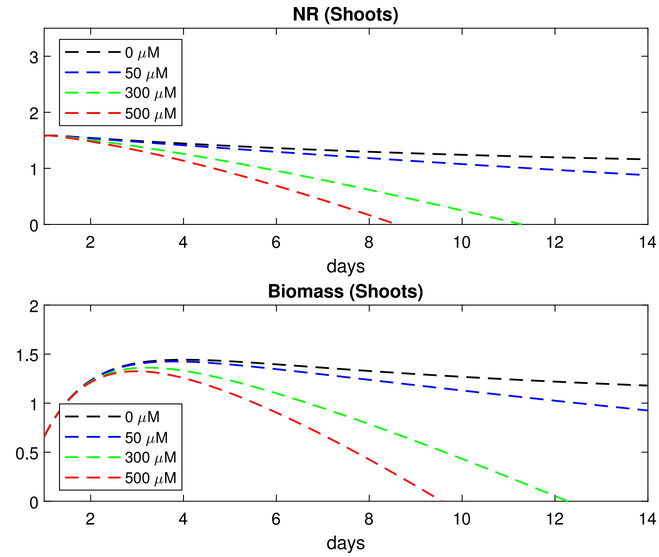

Fig. 8. Projection of the shoots' NR enzyme activity and the biomass content under different concentrations of Cu.

Table 3
Non-trivial sensitivity index of the model. We assume $d_S - e_S N > 0$.

Parameter	Model equilibrium variable	Sensitivity index
d_S, α_S	$\overline{B_S}$	$1 + \frac{e_S N}{d_S - e_S N}$
d_S	$\overline{N_S}$	$1 + \frac{e_S N}{d_S - e_S N}$
d_R, α_R	$\overline{B_R}$	1
d_R	$\overline{N_R}$	1
e_S	$\overline{B_S}$	$1 - \frac{d_S}{d_S - e_S N}$
e_S	$\overline{N_S}$	$1 - \frac{d_S}{d_S - e_S N}$
a_S, β_S	$\overline{B_S}$	−1
a_S	$\overline{N_S}$	−1
a_R, β_R	$\overline{B_R}$	−1
a_R	$\overline{N_R}$	−1

Different studies have also assessed the ability of *C. album* to be suitable for phytoextraction of lead (Alipour et al., 2015), phytoextraction of different metals (Gupta and Sinha, 2007), and phytoremediation of cadmium from the soil (Zulfiqar et al., 2012), and they have obtained promising results. Additionally, we observe that the relevant contaminants previously mentioned have similar equivalence (Cu^{2+}, Cd^{2+}, among others). Therefore, mathematical modelling considering different contaminants with similar equivalence can provide information about the plausible long-term plant dynamics under various heavy metal contaminants. In this case, our model provided theoretical evidence of the capability of the model plant to maintain functional dynamics in the roots under Cu-induced stress.

Our results show that increasing contaminant concentrations mainly affect the shoot activities, and toxic effects can be observed. Another important observation of the model is that there is root capability to absorb the contaminant initially. However, as time increases, the shoots have a slower tendency to absorb contaminants. As is shown in Fig. 8, the slower trend of the shoots to assimilate contaminants is severely affected by the concentration in the system. In particular, as contaminant concentration increments, the activity in the shoots tends to be disrupted. Thus, being exposed to higher contaminant levels implies a higher absorption of contaminant and quicker disruption of healthy dynamics. Therefore, under the scenario shown in Fig. 8, our model can potentially establish a harvesting strategy dependent on the environmental dynamics.

A mathematical model is always improvable. Thus, future work can be directed to improve some of the model's limitations. A main future goal is to relate the shoots and the roots dynamics, here considered independent, by coupling the corresponding variables. However, this can potentially increase the model's complexity and ability to relate to experimental observations. Therefore, this modification needs to be carefully established to combine a more realistic model without losing the model's tractability and ability to relate to the experimental data. Also, further inclusion of plant features such as chlorophyll contents and total proteins content needs to be addressed in future modelling. Our sensitivity analysis also shows that the model is sensitive to modifying the parameters d_S, α_S, d_R, and α_R. Therefore, even though our model can correctly capture the contaminant dynamics and its accumulation in the shoots and roots, our simple model needs to be improved to consider more realistic complex internal processes in the plant's dynamics.

6. Conclusions

In this work, we established a mathematical model to support the suitability of the model plant (*Chenopodium album* L.) to be used in contaminated areas. Here, we provided a model for the nitrogen-assimilatory enzyme activity, the biomass content, and the contaminant concentration in the plant. As far as the authors know there is no similar existent model. Our numerical model simulation results provided qualitatively similar activities compared to the experimental data. Indeed, the main goal of the model was to give a qualitative description of the main variables and long-term projections of their dynamics. In these long-term projections, we observed a consistent tendency of maintaining normal or diminished activities of the main variables, depending on the contaminant-induced stress. We observed a plausible tendency to disrupt regular shoots' dynamics, whereas a consistent trend to maintain normal roots' dynamics. Moreover, we observed a consistent and longer-term tendency to absorb more significant amounts of contaminants in the roots. Even though our main goal was to provide a qualitative description of the main variables, our results can potentially be used to describe quantitative features of the main variables, e.g., the amount of metal accumulation in the plant, due to their ability to resemble the experimental data. Therefore, this model provides scientific progress related to quantifiable plant dynamics related to contaminant accumulation and provides the basis for further experimental observations.

Our theoretical results provided expressions for the long-term dynamics in the shoots variables. This complements the analysis developed in the manuscript, and it is a straightforward way to analyse the long-term dynamics of the system. Also, our sensitivity analysis provided information about some of the model's limitations and further directions for the mathematical improvement of the model.

Our mathematical model complemented experimental studies performed under copper-induced stress of *Chenopodium album* and provided the foundation of main variables to be analysed in future experimental settings. In this way, both experimental studies and mathematical modelling can provide complementary information that supports biological hypotheses. Future research opportunities can be directed towards incorporating more biological variables of the model, increasing model complexity, and comparing model performance under different heavy metal contaminants.

There is a need for continuing efforts to join both theoretical and experimental designs to establish further scientific advances to address the problem of heavy metal contamination in the environment. Multidisciplinary research teams need to continue working on this direction as it has successfully shown that better results can be achieved than solely theoretical or experimental approaches.

CRediT authorship contribution statement

Laura R. González-Ramírez: Conceptualization, Methodology, Investigation, Formal analysis, Writing - original draft and review, Software, Visualization. **Deniz Alaçam:** Supervision, Writing – original draft. **Aysegul Akpinar:** Methodology, Investigation, Data curation, Resources, Validation, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

This Appendix establishes the mathematical model used to set the parameter optimization problem. When considering the constant-coefficient matrix of the model (6), we obtain a unique equilibrium point determined by:

$$\left(\overline{N_R},\overline{T_R},\overline{B_R},\overline{N_S},\overline{T_S},\overline{B_S},\overline{M_E},\overline{M_R},\overline{M_S}\right) = \left(\frac{d_R}{a_R},0,\frac{\alpha_R d_R}{a_R\beta_R},\frac{d_S-e_S N}{a_S},0,\frac{\alpha_S(d_S-e_S N)}{\beta_S a_S},0,0,N\right). \tag{11}$$

The system's eigenvalues consist of a zero eigenvalue and 8 real eigenvalues with a negative real part. Finally, we note that the last three equations of the model (6) can be decoupled obtaining the system:

$$\begin{aligned} \frac{dM_E}{dt} &= -(r_1+r_2)M_E + r_3 M_R \\ \frac{dM_R}{dt} &= r_1 M_E - r_3 M_R \\ \frac{dM_S}{dt} &= r_2 M_E. \end{aligned} \tag{12}$$

The previous linear system can be explicitly solved by employing the eigenvalues and the eigenvectors of the corresponding constant coefficient matrix. Therefore, it is possible to obtain explicit expressions for the contaminant level. With the previous information, we can update the model to simplify the parameter inference to obtain:

$$\begin{aligned} \frac{dN_R}{dt} &= T_R \\ \frac{dT_R}{dt} &= d_R - b_R T_R - a_R N_R - e_R M_R \\ \frac{dB_R}{dt} &= \alpha_R N_R - \beta_R B_R \\ \frac{dN_S}{dt} &= T_S \\ \frac{dT_S}{dt} &= d_S - b_S T_S - a_S N_S - e_S M_S \\ \frac{dB_S}{dt} &= \alpha_S N_S - \beta_S B_S, \end{aligned} \tag{13}$$

where $M_E(t)$, $M_S(t)$, and $M_R(t)$ can be explicitly described. In this way, it is possible to reduce the number of differential equations and remain with 13 parameters to be determined.

By considering the fixed point of the new system and its stability, we provide the asymptotic tendency of the plants' shoots and roots activities:

$$\overline{N_R} \to \frac{d_R}{a_R}, \tag{14}$$

$$\overline{B_R} \to \frac{\alpha_R d_R}{\beta_R a_R}, \tag{15}$$

$$\overline{N_S} \to \frac{d_S - e_S N}{a_S}, \tag{16}$$

and

$$\overline{B_S} \to \frac{\alpha_S\left(d_S - e_S N\right)}{\beta_S a_S}. \tag{17}$$

As the contaminant increases, the shoots tend to decrease their variables. The rise in contaminants exerts a toxic effect, determined by the contaminants absorption rate. Nevertheless, we remark that this model's asymptotic limits are only helpful in the case of positive variable values. Therefore, detailed experimental data needs to motivate the choice of parameters for this analysis.

References

Akpinar, A., 2021. The role of chenopodium album L. on the on-site reclamation of sewage sludge lagoons. Fresenius Environ. Bull. 30, 11538–11547.

Ali, H., Khan, E., Sajad, M., 2013. Phytoremediation of heavy metals: Concepts and applications. Chemosphere 91, 869–881. http://dx.doi.org/10.1016/j.chemosphere.2013.01.075.

Alipour, N., Homaee, M., Asadi, K., Mazhari, M., 2015. Assessing chenopodium album L . to tolerate and phytoextract lead from heavy metal contaminated soils. Environ. Sci. 13, 105–112.

Arriola, L., Hyman, J.M., 2009. Sensitivity analysis for uncertainty quantification in mathematical models. In: Chowell, G., Hayman, J., Bettencourt, L., Castillo-Chavez, C. (Eds.), Mathematical and Statistical Estimation Approaches in Epidemiology. Springer, pp. 195–247. http://dx.doi.org/10.1007/978-90-481-2313-1_10.

Bhargava, A., Shukla, S., Srivastava, J., Singh, N., 2007. Chenopodium: A prospective plant for phytoextraction. Acta Physiol. Plant 30:1, 111–120. http://dx.doi.org/10.1007/s11738-007-0097-3.

Boojar, M., Goodarzi, F., 2007. The copper tolerance strategies and the role of antioxidative enzymes in three plant species grown on copper mine. Chemosphere 67 (11), 2138–2147. http://dx.doi.org/10.1016/j.chemosphere.2006.12.071.

Cârdei, P., Tudora, C., Vlădut, V., Pruteanu, M., Găgeanu, I., Cujbescu, D., Bordean, D., Ungureanu, N., Cristea, G.I.O., 2021. Mathematical model to simulate the transfer of heavy metals from soil to plants. Sustainability 13, http://dx.doi.org/10.3390/su13116157.

Cheeseman, J., Barreiro, R., Lexa, M., 1996. Plant growth modelling and the integration of shoot and root activities without communicating messengers: Opinion. Plant Soil 185, 51–64. http://dx.doi.org/10.1007/bf02257564.

D'Acunto, B., Frunzo, L., Luongo, V., Mattei, M., 2019. Modeling heavy metal sorption and interaction in multispecies biofilm. Mathematics 7 (9), 781. http://dx.doi.org/10.3390/math7090781.

Frink, C., Waggoner, P., Ausubel, J., 1999. Nitrogen fertilizer: retrospect and prospect. Proc. Natl. Acad. Sci. USA 96 (4), 1175–1180. http://dx.doi.org/10.1073/pnas.96.4.1175.

Gajewska, E., Sklodowska, M., 2010. Differential effect of equal copper, cadmium and nickel concentration on biochemical reactions in wheat seedlings. Ecotoxicol. Environ. Saf. http://dx.doi.org/10.1016/j.ecoenv.2010.02.013.

Gebauer, G., Melzer, A., Rehder, H., 1984. Nitrate content and nitrate reductase activity in Rumex obtusifolius L. I. Differences in organs and diurnal changes. Oecologia 63, 136–142. http://dx.doi.org/10.1007/BF00379795.

Gebauer, G., Rehder, H., Wollenweber, B., 1988. Nitrate, nitrate reduction and organic nitrogen in plants from different ecological and taxonomic groups of central europe. Oecologia 75, 371–385.

González, R., González-Chávez, M., 2006. Metal accumulation in wild plants surrounding mining wastes. Environ. Pollut. 144, 84–92. http://dx.doi.org/10.1016/j.envpol.2006.01.006.

Greipsoon, S., 2011. Phytoremediation. Nature Educ. Knowl. 3 (10).

Gupta, A., Sinha, S., 2007. Phytoextraction capacity of the chenopodium album L. grown on soil amended with tannery sludge. Bioresour. Technol. 98, http://dx.doi.org/10.1016/j.biortech.2006.01.015.

Hageman, R., Hucklesby, D., 1971. Nitrate reductase. Methods Enzymol 23, 497–503.

Jaworski, E., 1971. Nitrate reductase assay in intact plant tissues. Biochem. Biophys. Res. Commun. 43, 1274–1279. http://dx.doi.org/10.1016/s0006-291x(71)80010-4.

Kumar, A., Prasad, M., Sytar, O., 2012. Lead toxicity, defense strategies and associated indicative biomarkers in talinum triangulare grown hydroponically. Chemosphere 89, 1056–1165. http://dx.doi.org/10.1016/j.chemosphere.2012.05.070.

Lee, J., Stewart, G., 1978. Ecological aspects of nitrogen metabolism. Adv. Bot Res. 6, 1–43. http://dx.doi.org/10.1016/S0065-2296(08)60328-6.

Llorens, N., Arola, L., Blade, C., Mas, A., 2000. Effects of copper exposure upon nitrogen metabolism in tissue cultured vitis vinifera. Plant Sci. 160, 159–163. http://dx.doi.org/10.1016/s0168-9452(00)00379-4.

Malec, P., Maleva, M., Prasad, M., Strzalka, K., 2009. Identification and characterization of Cd-induced peptides in egeria densa (water weed): putative role in Cd detoxification. Aquat Toxicol. 95, 213–221. http://dx.doi.org/10.1016/j.aquatox.2009.09.007.

Malec, P., Waloszek, K., Prasad, M., Strzalka, K., 2008. Zinc reversal of cd-induced energy transfer changes in photosystem II of ceratophyllum demersum L. as observed by whole-leaf 77K fluorescence. Plant Stress 2, 121–126.

Maleva, M., Nekrasova, G., Malec, P., Prasad, M., Strzalka, F., 2009. Ecophysiological tolerance of elodea canadensis to nickel exposure. Chemosphere 77, 392–398. http://dx.doi.org/10.1016/j.chemosphere.

Marschner, H., 1995. Mineral Nutrition of Higher Plants, 2 Academic Press, London, http://dx.doi.org/10.1016/B978-0-12-473542-2.X5000-7.

MATLAB, 2017. R2017b. The Mathworks, Inc., Natick, Massachusetts.

Mohan, A., Kaur, R., Girdhar, M., 2019. Analysis of ability of chenopodium album for remediation of heavy metal degraded soil. Res. J. Pharm. Technol. 12 (10), http://dx.doi.org/10.5958/0974-360X.2019.00840.0.

Moschou, P., Wu, J., Cona, A., Tavladoraki, P., Angelini, R., Roubelakis-Angelakis, K., 2012. The polyamines and their catabolic products are significant players in the turnover of nitrogenous molecules in plants. J. Exp. Bot. 63 (14), 5003–5015. http://dx.doi.org/10.1093/jxb/ers202.

Nedjimi, B., Daoud, Y., 2009. Effects of calcium chloride on growth, membrane permeability and root hydraulic conductivity in two atriplex species grown at high (sodium chloride) salinity. J. Plant Nutr. 32:11, 1818–1830. http://dx.doi.org/10.1080/01904160903242342.

Olsson, M., Falkengren-Grerup, U., 2003. Partitioning of nitrate uptake between trees and understory in oak forests. Forest Ecol. Manag. 179, 311–320. http://dx.doi.org/10.1016/S0378-1127(02)00544-3.

Prasad, M., 2004. Heavy Metal Stress in Plants, From Biomolecules to Ecosystems. Springer-Verlag Berlin Heidelberg.

Rajkumar, M., Prasad, M., Swaminathan, S., Freitas, H., 2013. Climate change driven plant-metal-microbe interactions. Environ. Int. 53, 74–86. http://dx.doi.org/10.1016/j.envint.2012.12.009.

Seip, K., 1979. A mathematical model for the uptake of heavy metals in benthic algae. Ecol. Model. 6:3, 183–197. http://dx.doi.org/10.1016/0304-3800(79)90012-7.

Sharma, S., Dietz, K., 2009. The relationship between metal toxicity and cellular redox imbalance. Trends Plant Sci. 14, 43–50. http://dx.doi.org/10.1016/j.tplants.2008.10.007.

Solanki, R., Dhankhar, R., 2011. Biochemical changes and adaptive strategies of plants under heavy metal stress. Biologia 66 (2), 195–204. http://dx.doi.org/10.2478/s11756-011-0005-6.

Strogatz, S., 2015. Nonlinear Dynamics and Chaos: with Applications to Physics, Biology, Chemistry, and Engineering. Westview Press, http://dx.doi.org/10.1201/9780429492563.

Swaileh, K., Hussein, R., Abu-Elhaj, S., 2004. Assessment of heavy metal contamination in roadside surface soil and vegetation from the west bank. Arch. Environ. Contam. Toxicol. 47, 23–30. http://dx.doi.org/10.1007/s00244-003-3045-2.

Tantemsapya, N., Naksakul, Wirojanagud, W., 2011. Mathematical modeling of heavy metals contamination from MSW landfill site in Khon Kaen, Thailand. Water Sci. Technol. 64:9, 1835–1842. http://dx.doi.org/10.2166/wst.2011.751.

Tawfiq, L., Wirojanagud, W., 2016. Numerical model for estimation the concentration of heavy metals in soil and its application in Iraq. Glob. J. Eng. Sci. Res..

Thoma, G., Lam, T., Wolf, D., 2003. A mathematical model of phytoremediaton for petroleum-contaminated soil: model development. Int. J. Phytoremediation 5, 41–55. http://dx.doi.org/10.1080/16226510390856466.

Thomas, D., Vandemuelebroeke, L., 2005. A mathematical evolution model for phytoremediation of metals. Discrete Contin. Dyn. Syst.-B 5:2, 411–422. http://dx.doi.org/10.3934/dcdsb.2005.5.411.

Torres-Bejarano, F., Couder-Castañeda, C., Ramírez-León, H., Hernández-Gómez, J., Rodríguez-Cuevas, C., Herrera-Díaz, I., Barrios-Piña, H., 2019. Numerical modelling of heavy metal dynamics in a river-lagoon system. Math. Probl. Eng. http://dx.doi.org/10.1155/2019/8485031, Article ID 8485031.

Tozser, D., Tothmeresz, B., Harangi, S., Baranya, E., Lakatos, G., Fulop, Z., Simon, E., 2019. Remediation potential of early successional pioneer species chenopodium album and tripleurospermum inodorum. Nat. Conserv. 36, 47–69. http://dx.doi.org/10.3897/natureconservation.36.32503.

Verkroost, A., Wassen, M., 2005. A simple model for nitrogen-limited plant growth and nitrogen allocation. Ann. Bot. 96, 871–876. http://dx.doi.org/10.1093/aob/mci239.

Wan, G., Najeeb, U., Jilani, G., Naeem, M., Zhou, W., 2011. Calcium invigorates the cadmium-stressed brassica napus L. plants by strengthening their photosynthetic system. Environ. Sci. Pollut. Res. 18, 1478–1486. http://dx.doi.org/10.1007/s11356-011-0509-1.

Xiong, Z., Zhao, F., Li, M., 2006. Lead toxicity in brassica pekinensis rupr.:Effect on nitrate assimilation and growth. Environ. Toxicol. 21, 147–153. http://dx.doi.org/10.1002/tox.20167.

Yang, Z., Midmore, D., 2005. A model for the circadian oscillations in expression and activity of nitrate reductase in higher plants. Ann. Botany 96:6, 1019–1026. http://dx.doi.org/10.1093/aob/mci254.

Zeidler, M., 2005. Heavy metals in two herb species (river Morava, Czech Republic). Pol. J. Ecol. 53, 185–195.

Zheng-Xun, J., Chun-Rong, Q., Jing, Y., Hai-Ying, L., Zhong-Ze, P., 2007. Changes in activities of glutamine synthetase during grain filling and their relation to rice quality. Rice Sci. 14:3, 211–216.

Zulfiqar, S., Wahid, A., Farooq, M., Maqbool, N., Arfan, M., 2012. Phytoremediation of soil cadmium using chenopodium species. Pak. J. Agric. Sci. 49 (4).