Use of nonlinear regression and nonlinear mathematical programming in the formulation of substrate mixtures for soil-less culture - a review -

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Abstract

With respect to four inorganic and organic substrates - tezontle (volcanic rock), perlite, peat and coir - we studied the relevant physical and chemical properties of mixtures of two of these substrates. A nonlinear regression model was used to analyse the physical properties of each possible mixture. Finally, a methodology is proposed for formulating mixtures of substrates as a deterministic nonlinear mathematical programming problem.

Keywords: Coir; Peat; Nonlinear regression, Nonlinear optimisation; Substrate mixtures; Tezontle.

1. Introduction

Soil serves as a support for plants and is the medium from which they obtain water, mineral substances and oxygen, which are essential for growth and vegetative development. An ideal soil has a porosity and particle disposition that enables root penetration while retaining appropriate amounts of water and air [Foth and Ellis (1988), Hablin *et al.* (1999), and Russell (2008)].

However, such soils may not be available, and then artificial soils may be used. This is the case of most flowerpot and containerised crops. Such plants have limited root growth, but they still need nutrients, air and water. For this reason, artificial substrates are sometimes required. These are often obtained by mixtures of various products, and the combination of the characteristics of each component provides the overall (and hopefully, optimal) characteristics of the substrate [Resh (2002a), Resh (2002b) and Russell (2008)].

The apparent density of a substrate should be low, so that the roots can penetrate it easily, and at the same time, to minimise the weight of the containerised crops. Organic matter has high porosity, ionic interchange and water retention capabilities, together with low density. All these properties are recommended for a substrate, which explains why most artificial substrates are essentially composed of organic matter; the remaining components are usually constituted of natural minerals or of artificial minerals such as tezontle, sand, perlite or vermiculite. These mineral products are very porous, with a high real density and a very low apparent density. In general, the grain size of an artificial substrate is higher than that of the soil, which facilitates air infiltration; at the same time, however, this property reduces water retention. This consideration explains why mixtures are usually composed of both organic and mineral substances, to achieve an equilibrium between air infiltration and water retention [Resh (2002a), Resh (2002b) and Russell (2008)].

The chemical properties of a substrate are important because they are the main factors responsible for the availability of nutrients. However, new crops are increasingly being constituted in such a way that the physical properties of a substrate prevail as its desired characteristics, with all the additional plant necessities being provided by nutritive substances, which are permanently available, being recycled to the plant by the irrigation system [Hablin *et al.* (1999), Resh (2002b) and Russell (2008)].

In many countries, substrates are still obtained by traditional trial and error methods; mixtures are formulated by arbitrarily establishing the proportions of the respective components, and the resulting mixture is then accepted if it improves the overall crop yield. The resulting mixture is not necessarily the optimal one, as the method does not explore all the possible combinations of the available components. The time employed in evaluating the mixtures, the cost of the materials used and the search for optimal resources are among the aspects contributing to the complexity of substrate formulation, given the number of variables involved in the problem (Zamora Morales *et al.* 2005).

Linear programming is a commonly-used empirical technique for formulating substrate mixtures used in a soli-less culture, and generally provides good approximations (Burés *et al.* (1988), Burés (1997) and Zamora Morales *et al.* (2005), among many others). However, most authors accept that the constraints imposed in the linear programming are not completely suitable, because they are established over design variables which do not present a linear behaviour.

This paper proposes a general methodology, based on nonlinear regression models and nonlinear mathematical programming, for obtaining substrate

mixtures for soil-less culture comprised of two inorganic or organic substrates, to be used for protected and containerised crops. For this purpose, we study the physical and chemical properties of four inorganic and organic substrates - tezontle (volcanic rock), perlite, peat and coir - together with those of the mixtures comprising different proportions of two of these four substrates, see Section 2.

Subsequently, the physical properties of the mixtures are modelled by nonlinear regression models, according to the respective substrate proportions in each mixture, see Section 3. These models are then used to replace the linear restrictions corresponding to the physical properties expressed in the linear mathematical programming problem; thus, we obtain a nonlinear mathematical programming solution. The corresponding linear and nonlinear problems are solved, compared and analysed using the commercial software LINGO.

2. Physical and chemical properties of substrates and mixtures

Four substrates were used in the mixture formulation tests: perlite, tezontle, peat and coir. Following the methodology proposed by Pire and Pereira (2003), Gabriel *et al.* (1993) and North Carolina State University (2007), we determined, in triple analysis, the following physical and chemical properties: total porous space (TPS), air porosity (AP), humidity retention (HR), apparent density (AD), real density (RD), ashes(A), organic matter (OM), pH and electric conductivity (EC), which are shown in Table 1.

We also formulated six mixtures (denoted by M_1 - M_6 and defined in Tables 2 and 3) composed of two substrates with eleven different proportions. Using the above-mentioned procedure, their physical and chemical properties to be used in the formulation of mixtures of substrates were determined (Burés *et al.*, 1988); see Tables 2 and 3.

Table 1. Physical and chemical properties of each substrate

Substrate	TPS	AP	HR	AD	RD	A	OM	pH	EC
	%	%	%	gcc^{-1}	gcc^{-1}	%	%		dSm^{-1}
Perlite	62.40	5.43	56.97	0.19	0.51	100	0	7.6	1.3
Tezontle	50.70	7.81	42.89	1.17	2.36	100	0	8.0	1.3
Peat	72.65	8.38	64.27	0.07	0.28	10	90	6.4	1.2
Coir	81.83	4.48	77.35	0.09	0.49	10	90	7.2	3.7

Table 2. Physical and chemical properties of the mixtures

	M_1 = Perlite + Coir			M_2 = Perlite + peat			M_3 = Perlite + Tezontle		
	TPS	HR	OM	TPS	HR	OM	TPS	HR	OM
	%	%	%	%	%	%	%	%	%
0%+100%	81.83	77.35	90	72.65	64.27	90	50.70	42.89	0
10%+90%	84.77	81.06	70	77.23	66.66	90	51.77	47.20	0
20%+80%	85.34	79.34	50	85.17	75.46	70	54.17	50.46	0
30%+70%	82.86	77.71	40	84.80	74.51	50	51.91	50.20	0

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	M₁ = Perlite + Coir			M₂ = Perlite + peat			M₃ = Perlite + Tezontle		
	TPS	HR	OM	TPS	HR	OM	TPS	HR	OM
	%	%	%	%	%	%	%	%	%
40%+60%	76.06	71.49	30	82.77	75.63	60	50.31	48.60	0
50%+50%	73.29	69.86	30	79.60	75.60	40	51.80	49.80	0
60%+40%	72.69	69.83	20	79.00	73.86	40	55.54	53.26	0
70%+30%	67.20	63.20	20	71.20	68.06	20	58.43	53.29	0
80%+20%	64.83	63.40	10	67.51	64.66	20	57.89	54.74	0
90%+10%	66.11	64.11	0	63.49	60.63	10	59.89	57.03	0
100%+0%	62.40	56.97	0	62.40	56.97	0	62.40	56.97	0

Table 3. Physical and chemical properties

	M₄ = peat + Tezontle			M₅ = Coir + Tezontle			M₆ = peat + Coir		
	TPS	HR	OM	TPS	HR	OM	TPS	HR	OM
	%	%	%	%	%	%	%	%	%
0%+100%	50.7	42.89	0	50.7	42.89	0	81.83	77.35	90
10%+90%	51.23	49.8	0	48.43	46.71	10	83.74	76.89	90
20%+80%	53.45	51.74	0	51.89	50.17	10	82.46	76.17	90
30%+70%	52.91	50.91	0	54.77	53.34	10	65.23	57.51	90
40%+60%	58.99	56.71	10	59.29	57.86	10	65.31	59.03	90
50%+50%	61.39	59.39	10	62.29	60.86	10	75.89	68.46	90
60%+40%	65.45	62.88	0	64.2	62.2	20	60.43	51.86	90
70%+30%	66.57	62.85	20	69,17	67,17	20	63.54	56.4	90
80%+20%	67.17	62.88	20	72.8	70.23	20	77.94	63.09	90
90%+10%	73.62	67.62	30	76.8	73.66	30	74.11	51.54	90
100%+0%	72.65	64.27	90	81.83	77.35	90	72.65	64.27	90

3. Modelling the physical and chemical properties of the mixtures

As remarked above, in general the physical and chemical properties of substrates (and their mixtures) do not present a linear behaviour. In this section, we study the functional behaviour of the physical properties TPS, HR and OM in the mixtures M[1] – M₆[1].

The results were obtained by the implementation of a program in S-PLUS (Lam (2011)) to fit the different nonlinear regression models. The least squares method was applied to the following fitting models:

- Linear regression model

$$Y = p_1 x_1 + p_2 x_2 + \mathsf{x}$$

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[1]   The interest in this particular modelling is detailed in Section 4.

- Polynomial regression model

$$Y = p_1 x_1 + p_2 x_2 + p_3 x_1^2 + p_4 x_2^2 + \cdots$$
$$+ p_k x_1^k + p_{k+1} x_2^k + p_{k+2} x_1 x_2 + \xi$$

- Reciprocal regression model

$$Y = \frac{polynomial1}{Polynomial2} + \xi$$

- Logarithmic regression model

$$Y = p_1 \log x_1 + p_2 \log x_2 + \xi$$

- Exponential regression model

$$Y = p_1 \exp\{p_2 x_1 + p_3 x_2 + p_4 x_1^2 + p_5 x_1^3\} + \xi$$

The best model was selected by means of the minimum mean square error criterion (Graybill and Iyer (1994)).

In general, the models fitted take the form

$$Y = f(x_1, x_2) + \xi$$

where Y is the mixture variable to be modelled (TPS, HR or OM); $f(x_1, x_2)$ is the functional form of the model to be fitted; x_1, x_2 denote the proportions of two of the substrates(selected from perlite, tezontle, peat and coir) making up the mixture, where $0 \le x_k \le 1$, $k = 1,2$, and ξ is the error. Note also that x_1, x_2 satisfy $x_1 + x_2 = 1$ which means that x_1 and x_2 are linearly dependent, moreover, $x_1 = 1 - x_2$ or $x_2 = 1 - x_1$. A priori, all that is necessay is to fit a model in terms of x_1 (or x_2). However, in this study we wish to obtain a mathematical model for computing the physical property Y of the mixture, when the proportions and the individual physical

properties of the corresponding component of the substrate are known. This model is then used in the nonlinear optimisation program formulation. Strictly speaking, we do not estimate the model for any possible value of x_1 and x_2, but rather, in the subspace defined by the line $x_1 + x_2 = 1$. A possible drawback is the fact that few experimental points (eleven) are used for fitting the TPS, HR and OM characteristic models (see Tables 2-3). Fortunately, the experimental data present a smooth behaviour, and, most importantly, they provide information *over the whole domain* of x_1 and x_2 (specifically, the domain is the line $x_1 + x_2 = 1$ in the first octant of R^3). Moreover, it is important to take into account that models of the form $Y = p_0 + p_1 z_1 + p_2 z_2 + \xi$ (with $p_0 \neq 0$), or similar should not be considered, because when $x_1 = x_2 = 0$ we obtain $Y = p_0$, but the correct result is $Y = 0$. Finally, the most complicated aspect of this study is to propose the same *functional form* for each characteristic (TPS, HR and OM) and for all the possible mixtures obtained.

As shown in Tables 2-3, the variable OM presents a linear behaviour. Then, we just need to determine the behaviour of TPS and HR. In both cases, a well fitted model for TPS and HR for the six mixtures has the form

$$Y = p_1 z_1 + p_2 z_2 \exp\{p_3 z_1 + p_4 z_2 + p_5 z_1^2 + p_6 z_1^3\} + \xi$$
(1)

where $Z_k = dx_k$, $k = 1,2$, and d denotes the individual TPS or HR mixture component of the k-th substrate, respectively.

Tables 4 and 5 show the parameter estimator values of the model (1) and the corresponding mean square of the error (MSE) for the six samples M_1 - M_6 with the TPS and HR characteristics, respectively.

Table 4. Estimators of the model parameters and the mean square of the error for $Y = $ TPS

Mixture	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	$\hat{p}_4$	$\hat{p}_5$	$\hat{p}_6$	MSE
M_1	1.005	1.205	1.298e-2	-2.308e-3	-7.254e-4	8.008e-6	2.872
M_2	0.996	1.092	1.833e-2	-1.289e-3	-2.861e-4	-5.947e-7	3.253
M_3	0.992	0.718	1.037e-2	6.549e-3	-6.196e-4	9.648e-6	3.147
M_4	0.996	1.092	1.834e-2	-1.288e-3	-2.861e-4	-5.947e-7	3.253
M_5	1.004	0.493	-6.566e-3	1.378e-2	4.878e-4	-5.443e-6	0.899
M_6	0.998	1.214	-0.110	1.126e-2	2.968e-3	2.047e-5	52.71

Table 5. Estimators of the model parameters and the mean square of the error for $Y = $ HR

Mixture	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	$\hat{p}_4$	$\hat{p}_5$	$\hat{p}_6$	MSE
M_1	1.007	1.354	1.312e-2	-3.917e-3	-1.016e-3	1.530e-5	4.069
M_2	1.002	1.106	1.509e-2	-1.715e-3	-1.668e-5	-3.681e-6	3.051
M_3	0.998	0.7463	2.623e-2	6.815e-3	-1.239e-3	1.847e-5	1.364
M_4	1.005	5.744e-1	1.893e-2	1.338e-2	-2.936e-4	5.125e-6	5.087
M_5	1.001	4.061e-1	1.294e-2	2.099e-2	-1.521e-5	-3.200e-7	0.605
M_6	9.548e-1	1.184	-1.674e-3	-2.002e-3	-5.358e-4	5.536e-6	66.074

As shown in Tables 8 and 9, the mixture M6 has the poorest fit. However, note that the functional form of a particular physical characteristic modelled must be the same for all mixtures.

As an example, we include in Figure 1 the graphs of the estimated model and the experimental points for the TPS characteristic of mixture M$_1$
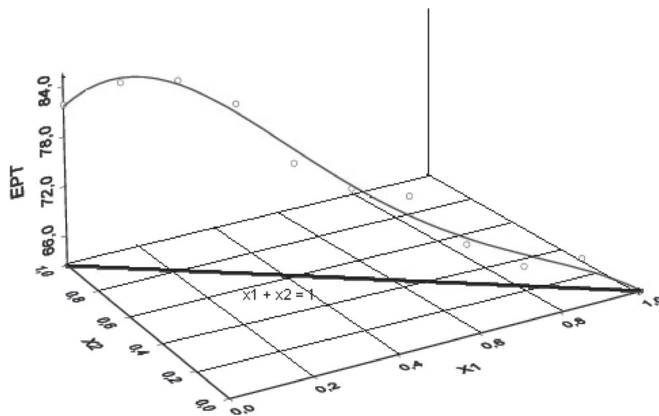

Figure 1. Graphs of the estimated model and the observed TPS data for the mixture M$_1$.

4. Formulation of mixtures by nonlinear mathematical programming

We consider the hypothesis proposed by Zamora Morales *et al.* (2005) as the basis for our formulation of the nonlinear mathematical programming problem. Since the mixture would essentially be used as a *support*, where the plant receives the nutrients via *nutritious solutions*, we only consider the physical properties as the design variables, except the variable OM, which is an important representative of the substrate's chemical properties and is therefore incorporated into the general model. In addition, we wish to achieve optimum control of the chemical properties of the nutritious solutions.

Taking these considerations into account, we study the following design variables: the balance of volumes, OM, TPS and HR. The minimising objective function is the cost of the mixture, which is studied via linear functions of the substrate proportions in the mixtures and their individual costs. A basic problem type takes

the form (2), where C_k is the cost in dollars per litre of the k-th substrate (perlite: 0.073, tezontle: 0.218, peat: 0.21 and coir: 0.106); x_k denotes the proportion in litres of the k-th substrate; m_k is the OM percentage per litre of the k-th substrate; e_k is the TPS percentage per litre of the k-th substrate and C_k is the HR percentage per litre of the k-th substrate. Now, OM_s and OM_i are limits or levels of the upper and lower restrictions for OM, respectively. In this study, we consider the limits (0-45) and (46-90); similarly, we define the upper and lower limits for TPS and HR, establishing the following two levels: (55-70) and (71-86) for TPS, and (45-60) and (61-76) for HR. These intervals or levels of restriction, for each of the variables OM, TPS and HR, were established following the recommendations of Abad *et al.* (1988), for substrates used in a soil-less culture and considering labeling specifications for commercial sustrates. Finally, the respective $\hat{p}_j^k$ were obtained from Table 5.

$$\min_{x_1,x_2} c_1 x_1 + c_2 x_2$$

Subject to

$$x_1 + x_2 = 1$$

$$m_1 x_1 + m_2 x_2 \le OM_s$$

$$m_1 x_1 + m_2 x_2 \ge OM_i$$

$$\hat{p}_1^1 e_1 x_1 + \hat{p}_2^1 e_2 x_2 \exp\{\hat{p}_3^1 e_1 x_1 + \hat{p}_4^1 e_2 x_2 + \hat{p}_5^1 e_1 x_1^2 + \hat{p}_6^1 e_1 x_1^3\} \le TPS_s$$

$$\hat{p}_1^1 e_1 x_1 + \hat{p}_2^1 e_2 x_2 \exp\{\hat{p}_3^1 e_1 x_1 + \hat{p}_4^1 e_2 x_2 + \hat{p}_5^1 e_1 x_1^2 + \hat{p}_6^1 e_1 x_1^3\} \ge TPS_i$$

$$\hat{p}_1^2 c_1 x_1 + \hat{p}_2^2 c_2 x_2 \exp\{\hat{p}_3^2 c_1 x_1 + \hat{p}_4^2 c_2 x_2 + \hat{p}_5^2 c_1 x_1^2 + \hat{p}_6^2 c_1 x_1^3\} \le HR_s$$

$$\hat{p}_1^1 e_1 x_1 + \hat{p}_2^1 e_2 x_2 \exp\{\hat{p}_3^1 e_1 x_1 + \hat{p}_4^1 e_2 x_2 + \hat{p}_5^1 e_1 x_1^2 + \hat{p}_6^1 e_1 x_1^3\} \ge HR_i$$

$$0 \le x_1 \le 1, \ 0 \le x_2 \le 1,$$

Potentially, if we combined the four substrates in the two-substrate mixtures $_4C_2$ with all the possible combinations of the two upper and lower levels for OM, TPS and HR (2^3) we would have 48=6×8 possible mixtures. However, Table 6 shows only the mixtures selected by linear or nonlinear mathematical programming. In other words, mixtures for which neither a linear nor a nonlinear optimisation program present a feasible region (i.e. the corresponding optimisation program has no solution) have been removed from Table 10, leaving only the substrate mixtures for soil-less culture with a feasible solution, as either a linear or a nonlinear optimisation program. In cases where the mixture of substrates has no feasible solution in the linear or nonlinear optimisation program, this is noted as NF (there

is no feasible solution to the optimisation problem). In addition, the restrictions to the coded variables OM, TPS and HR are coded by assigning "1" to the range with the smaller values and "2" to the higher range.

The results were computed using the commercial software Hyper LINGO/PC, release 6.0 (Winston, 1995). The default optimisation method used by LINGO to solve the nonlinear mathematical programming is that of Generalised Reduced Gradient (GRG) (Bazaraa *et al.* 2006). As can be seen, the linear programming reduces the total of mixtures by 66.66%, while the nonlinear mathematical programming reduces them by 68.75%; thus, both methods reduce the number of mixtures by very similar amounts. However, note the following two aspects:

Table 6. Mixtures of substrates via nonlinear mathematical programming

Restriction level			Solution with Linear programming		Solution with Nonlinear programming	
OM	TPS	HR	x_1	x_2	x_1	x_2
			%	%	%	%
Perlite-coir						
1	1	1	100	0	100	0
1	1	2	80.2	19.8	94.0	6.0
1	2	2	55.7	44.3	57.8	42.2
2	2	2	48.8	51.2	48.8	51.2
Coir-tezontle						
1	1	1	49.6	50.4	48.9	51.1
2	1	2	62.0	38.0	73.5	26.5
2	2	2	96.1	3.9	96.3	3.7
Perlite-peat						
1	1	1	100	0	100	0
1	1	2	NF		88.2	11.8
1	2	2	NF		71.9	28.1
2	1	2	44.8	55.2	NF	
2	2	2	15.7	84.3	48.9	51.1

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Restriction level			Solution with Linear programming		Solution with Nonlinear programming	
OM	TPS	HR	x_1	x_2	x_1	x_2
			%	%	%	%
Perlite-tezontle						
1	1	1	100	0	NF	
2	1	1	100	0	NF	
Peat-coir						
2	2	2	10.3	89.7	0	100
Peat-tezontle						
1	1	1	50	50	47.9	52.1
1	1	2	NF		50	50
2	1	1	80	20	NF	
2	1	2	87.9	12.1	69.7	30.3
2	2	2	100	0	NF	

a) The mixture substrate proportions assigned by the two techniques can vary significantly, as can be seen, for example, in peat-tezontle with restriction levels 2 1 2.

b) Linear mathematical programming is a useful and widely used tool in mixture problems, however, in general the nonlinear programming model achieves a better mixture formulation. But, if a user insists in using a linear solution, he/she could face two situations: One, is that the optimal linear solution might not be feasible under the nonlinear model, and second, that the optimal linear solution might be suboptimal with the respect to the nonlinear solution. Thus, from a practical point of view, the interpretation of these results would be that on occasions non-feasible substrate mixtures used in a soil-less culture are tested or produced, which results in a waste of research time and/or money. Worse still, when linear programming leads us to reject a mixture that would have been accepted by the nonlinear method, we might be rejecting the best possible mixture.

5. Conclusions

The aim of this study is to propose a general methodology which can be applied to various situations, with only simple modifications. For example, a mixture formulation in the absence of nutritive substances, or one comprised of substrates that are rich in nutrients and artificial nutrition, could be studied by modifying nonlinear mathematical programming, through restrictions on chemical properties and/or via alternative objective functions.

Alternatively, the presence in the mixture of certain undesirable (desirable) ions or cations could be minimised (maximised). This methodology could be extended to the simultaneous optimisation of several objective functions; for example, to minimise the cost and to maximise the amount of nitrogen in a mixture, which implies the use of nonlinear multiobjective optimisation methods (Steuer, 1986).

Note that the procedure described in Section 3 can be used for modelling various kinds of physical and chemical properties of the mixtures. In addition, the

nonlinear mathematical programming approach can be adapted by adding new restrictions and/or objective functions for a particular characteristic.

Finally, note that there are few experimental points and a large number of parameters. Nevertheless, on the one hand, we have a sample of equally–spaced experimental points *throughout the domain* of the variables x_1 and x_2 (i.e. the line $x_1 + x_2 = 1$), and the mathematical behaviour considered is a smoother of these variables. Furthermore, our aim is to obtain the best mathematical approximation possible to these points and thus obtain the best results.

A potential user of this methodology (e.g. the commercial producer of a protected crop) could consider using a greater number of experimental points, taking into account the higher initial investment that would be required.

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