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Bigger, Stephen W, Ngeh, Lawrence and Orbell, John (2010) A mathematical model for the sequestering of chemical contaminants by magnetic particles. Journal of Environmental Engineering, 136 (11). pp. 1255-1259. ISSN 0733-9372

REVISED MANUSCRIPT

A Mathematical Model for the Sequestering of Chemical Contaminants by Magnetic Particles

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Synopsis

A mathematical model is developed and implemented to characterize the pick-up of various liquid chemical contaminants by polyethylene-coated magnetic particles. The model and its associated experimental and analytical protocols were applied to a wide range of liquid chemicals in order to gain insights into the physical basis for the pick-up phenomenon. The characteristics of the pick-up isotherms range between "ideal" and "non-ideal" behavior that are reflected in the mathematical model by a single parameter, α_0, where $\alpha_0 = 1$ corresponds to ideal behavior and $\alpha_0 > 1$ corresponds to a departure from idealized behavior that is directly quantified by the magnitude of α_0. The parameter α_0 is also related to the efficiency of pick-up and since the vast majority of isotherms observed in the study deviate from ideality, the high efficiency of pick-up observed in these systems has been attributed in part to this deviation. The proposed model and its associated experimental and analytical protocols demonstrate great potential for the systematic evaluation of the uptake of chemical contaminants using magnetic particle technology.

Key Words
iron powder; chemical contaminants; magnetic particles; oil

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Introduction

The application of magnetic particle technology to environmental remediation has attracted much interest in the literature over the years. Examples of this include the "Sirofloc" process for water clarification and decolourisation (Anderson *et al.* 1983; Priestly 1990; Booker *et al.* 1991) and functional magnetic particles that are used in the removal of pesticides from water (Lawruk *et al.* 1993). Magnetic particles have also been used in areas such as the magnetic separation of cancer cells (Wang *et al.*, 1993), in diagnosis (Nakamura and Matsunaga 1993), separation of radioactive materials (Nunez *et al.* 1996) and as catalyst supports (Wang *et al.* 2000).

It has also been found that polymer-coated magnetic particles can remove up to 90% of a standard grade of engine oil (Orbell *et al.* 1997) and that particles of uncoated iron powder are almost 100% effective in the magnetic harvesting of various contaminants (Orbell *et al.* 1999). Magnetite and maghemite particles have also been reported to exhibit high removal efficiency for dispersants and oils (Chun and Park 2001).

A sequence of detailed studies on iron powder as an efficient medium for the magnetic removal of oil contamination in environmental applications has appeared in the literature. These include: its use to remove contamination from oiled feathers (Orbell *et al.* 2004; Dao *et al.* 2006a), studies on the acute temperature dependence and thermodynamics of the pick-up process (Orbell *et al.* 2005; Dao *et al.* 2006b), the effect of pre-conditioners used in conjunction with iron powder for the removal of tarry and weathered oil (Dao *et al.* 2006c; Orbell *et al.* 2007) and its potential use to remove oil contamination from the surface of rock (Orbell et al. 2007).

In the investigations of oil pick-up and the pick-up of other chemical contaminants using either polymer-coated magnetic particles such as polyethylene-coated and poly(vinylchloride)-coated magnetic particles or iron powder, the percentage of chemical contaminant harvested by the particles, P, versus the particle-to-chemical ratio, R, is typically plotted for a given system (Orbell *et al.* 1997). Plots such as these characteristically increase from the origin and reach a plateau at the point (P_c,

R_c) whose respective coordinates correspond to the critical values of P and R at which the plateau is attained. Through observations made on many different systems it has been found that the approach to the plateau sometimes exhibits "ideal" behavior in that the pick-up isotherm is almost linear. An example is the pick-up of triethylamine with polyethylene-coated magnetic particles that demonstrates an almost linear relationship between the P and R parameters up to the plateau (Ngeh 2002). On the other hand, the isotherm for the pick-up of bromobenzene with the same type of particles demonstrates a significant departure from linearity and, as such, can be classified as an example of a "non-ideal" system (Ngeh 2002). Other variations in the behavior of the isotherm have been observed such as the high rate of approach to the plateau exhibited in the case of the pick-up of iodobenzene by polyethylene-coated magnetic particles (Ngeh 2002).

In order to better understand the physical basis for the pick-up phenomenon a physical model together with the accompanying mathematical description was developed to fit the full range of experimental data obtained. The model is described in this paper and its applicability to a number of different systems of wide variability is demonstrated.

Theory

In an "ideal" system each particle picks up a fixed quantity of chemical, and so upon the addition of successive particles, a linear increase is expected in the total amount of chemical that is picked up. Under these conditions the value of P is expected to vary linearly with R up to the critical or "saturation" value P_c, whose corresponding value of R is denoted R_c. The saturated region where no more chemical can be adsorbed occurs at values of $R \geq R_c$.

For "non-ideal" systems, each particle usually picks up an amount of chemical that is disproportionately larger than that expected in the ideal case. The amount that is picked up also depends on the number of particles that are added to the system. Under these conditions the value of P varies non-linearly with R up to the critical value P_c. Hence a convex curvature of the isotherm compared with the ideal case is observed. Again, values of $R \geq R_c$ define the saturated region.

The adsorption of a chemical on magnetic particles such as iron particulates or polymer-coated magnetic particles can be mathematically modeled by considering the amount of chemical each particle can adsorb in the presence of other particles. Now, the particle-to-chemical ratio, R, is given by equation (1):

$$R = nm_1/m_2 \tag{1}$$

where n is the number of particles, m_1 is the average mass of one particle, and m_2 is the mass of chemical used in the experiment (Orbell et al. 1997). At the critical particle-to-chemical ratio, R_c, equation (2) applies:

$$R_c = n_c m_1/m_2 \tag{2}$$

where n_c is the critical number of particles that are responsible for the critical (maximum) percentage adsorption, P_c. The average mass of chemical, m_s, that is adsorbed by a single particle can be calculated from equation (3):

$$m_s = P_c m_2/(100n_c) \tag{3}$$

Substituting equation (2) in equation (3) yields an expression for m_s in terms of values P_c, m_1 and R_c that are convenient to determine experimentally:

$$m_s = P_c m_1/(100R_c) \tag{4}$$

Upon the step-wise addition of up to n_c particles in an "ideal" system, each particle adsorbs an amount of chemical equal to m_s and the percentage adsorption, $P(n)$, after the addition of n particles is given by equation (5) for n in the range $0 \leq n \leq n_c$:

$$P(n) = (nm_s/m_2) \times 100 \tag{5}$$

Under these conditions the value of $P(n)$ varies linearly with n up to the critical value P_c that corresponds to n_c. Using equations (1), (4) and (5), the simple function $P(R)$ can be confirmed for values of R in the range $0 \leq R \leq R_c$:

$$P(R) = RP_c/R_c \tag{6}$$

In many real systems, the viscous nature of the liquid chemical to be adsorbed as well as the complex surface interactions between the liquid and the particles means that disproportionately larger amounts of the liquid adhere to the particles at lower values of R compared with values of R close to R_c. Alternatively, it is possible that for organic compounds at low values of R, the particles can absorb the maximum amount of the compound, but at high values of R, some organic molecules can interact with two or more particles resulting in the observed deviation of the plot from the straight line. Clearly, the possible interaction with two or more particles is related to the chemical nature of the contaminant. If the contaminant is an organic compound it is anticipated that it would need to have two or more functional groups to interact simultaneously with several particles.

The capacity of the particles to adsorb an excess loading of chemical in the early stages of the adsorption isotherm can be modeled by introducing a parameter $\alpha(n)$ which is the fractional excess of chemical a particle can adsorb in the presence of n particles. The value of $\alpha(n)$ may be generated by an empirical function and depends on the number of particles present at any point in the adsorption process. In "non-ideal" cases, the percentage adsorption, $P(n)$, is thus given by equation (7):

$$P(n) = (M_n/m_2) \times 100 \tag{7}$$

where M_n is the mass of chemical adsorbed by n particles in a "non-ideal" system. The value of M_n may be related to $\alpha(n)$ as shown in equation (8) and can be calculated by an iterative process for values of n in the range $1 \leq n \leq n_c$:

$$M_n = M_{n-1} + M_s(n)\alpha(n) \tag{8}$$

where M_0 is zero, M_{n-1} is the mass of chemical adsorbed by $n - 1$ particles, and $M_s(n)$ is the average mass of chemical adsorbed by the nth particle in the presence of $n - 1$ particles which is iteratively adjusted to account for disproportionate adsorption. In particular:

$$M_s(n) = [(P_c m_2/100) - M_{n-1}]/(n_c - n) \qquad \text{where } M_0 = 0 \tag{9}$$

A satisfactory fit of the experimental data can be obtained by assuming that the empirical function, $\alpha(n)$ varies linearly with n, and that the boundary conditions of (α, n) are $(\alpha_0, 1)$ and $(1, n_c)$. Under these conditions equation (10) can be readily derived:

$$\alpha(n) = \alpha_0 + (\alpha_0 - 1)(\mathrm{n} - 1)/(1 - n_c) \tag{10}$$

An optimum value of α_0 necessary to fit a given set of experimental data can be found by minimizing the sum of the squares of the residuals, $s(\alpha_0)$, in accordance with equation (11):

$$s(\alpha_0) = \sum_{\mathrm{i}=1}^{\mathrm{n}} [P(R_\mathrm{i}, \alpha_0) - P(R_\mathrm{i})]^2 \tag{11}$$

where $P(R_\mathrm{i}, \alpha_0)$ is the theoretical value of $P(R_\mathrm{i})$ calculated for a particular value of α_0 and $P(R_\mathrm{i})$ is the experimental value of the percentage adsorption determined at the particle-to-chemical ratio, R_i.

Materials and Methods

Polyethylene (PE) powder (grade 4612-05A) was obtained from Courtney Polymers Ltd., Dandenong, Australia. Steel "isoshot" pellets (grade S330, average particle size 1.0 mm) were kindly provided by Barton Abrasive Ltd., West Midlands, United Kingdom. All chemicals used in the experiments were AR grade reagents obtained from Aldrich Chemical Company Inc., Castle Hill, Australia.

The manufacture of PE-coated "isoshot" magnetic particles was conducted using a procedure involving the high-temperature heating of the pellets in a muffle furnace at 650°C and subsequent scattering of the particles in a fluidized bed of the polymer. The procedure is described elsewhere in detail (Orbell *et al.* 1997; Ngeh 2002) and it produces mechanically stable particles of average diameter *ca.* 1.2 ± 0.2 mm. Two hundred PE-coated particles were weighed and the average mass for a single particle was found to be 0.0820 g.

The chemical pick-up experiments were performed gravimetrically (Orbell *et al.* 1997; Ngeh 2002) at 20°C using a fixed mass (1.00 g) of chemical that was placed in a pre-weighed (w_1) Petri dish, which was then re-weighed (w_2). The PE-coated particles were applied to the chemical and the Petri dish was again re-weighed (w_3). The particle/chemical mixture was left in the Petri dish for 5 min after which the chemical-laden particles were harvested magnetically using a laboratory magnetic tester (Alpha Magnetics, Victoria, Australia). The Petri dish was then re-weighed (w_4). These measurements enable experimental values of R and P to be calculated from equations (12) and (13) respectively (Orbell *et al.* 1997; Ngeh 2002):

$$R = (w_3 - w_2)/(w_2 - w_1) \tag{12}$$

$$P = [(w_2 - w_4)/(w_2 - w_1)] \times 100 \tag{13}$$

The procedure was repeated in batches for increasing values of R until a maximum value of P was achieved (i.e. P_c), for a maximum value of R_c. The above procedure was carried out with five replicates in all subsequent experiments.

The experimental P and R data obtained for the affinity of a chemical compound for the magnetic particles were entered into an original computer program that was specifically written to analyze the data. The program determines the value of α_0 associated with the optimum fit to the experimental data.

Results and Discussion

Fitting Experimental Data to Theoretical Model

The derived mathematical model that is depicted by equation (1) together with equations (7) to (10) were used within an iterative computer program that generated the theoretical curves $P(R)$ for given values of the adjustable parameter, α_0. These plots appear in Fig. 1 and show that for an ideal system where $\alpha_0 = 1$, a linear relationship between $P(R)$ and R is established as expected. However, for non-ideal systems where $\alpha_0 > 1$, there is an increase in the curvature of the isotherm as the value of α_0 increases. Thus when $\alpha_0 = 1$, idealized adsorption occurs and values of α_0 that are successively greater than unity indicate successively greater departure from idealized adsorption behaviour.

>>> Insert Figure 1

Shown in Fig. 2 are experimental data for the pick-up of triethylamine and *m*-dichlorobenzene at 20°C using PE-coated magnetic particles. In each case the data were fitted using the iterative computer program and the solid lines represent the computer-generated optimum fits to the data. The triethylamine data ($\alpha_0 = 1.70$ in Table 1) display behaviour that is nearly ideal for which the value of α_0 is closer to unity relative to all of the other systems examined in the present study. In the initial stages of the triethylamine isotherm each particle picks up nearly the same amount of chemical resulting in an almost linear increase of the isotherm. On the other hand, the *m*-dichlorobenzene ($\alpha_0 = 3.57$ in Table 1) data show a marked departure from linearity and so this system can be classified as non-ideal. For *m*-dichlorobenzene in the initial stages of the isotherm, excess compound is picked up by particles resulting in a convex curvature of the isotherm. In the later stages, both the triethylamine and *m*-dichlorobenzene isotherms appear to plateau. This is due to the ultimate saturation of the particles by the compounds.

>>> Insert Figure 2

Other compounds show a varying degree of departure from ideality as reflected by their values of α_0. The computer fitting procedure was applied to the experimental data collected for a variety of compounds. Values of α_0 for these compounds are listed in Table 1.

>>> Insert Table 1

Efficiency of Chemical Pick-Up

The data analysis can be extended to determine the efficiency of a given system for the pick-up of a chemical contaminant. This can be achieved using either of two approaches. The first method involves using an efficiency parameter, E_1, which may be defined as the initial gradient of the pick-up isotherm, $(\mathrm{d}P/\mathrm{d}R)_0$, an approximation for which is given in equation (14):

$$E_1 = (\mathrm{d}P/\mathrm{d}R)_0 \approx (\Delta P/\Delta R) \approx P_1/R_1 \qquad (14)$$

where P_1 and R_1 are the respective initial values of P and R that lie on the pick-up isotherm. Clearly, this estimation of efficiency is an "average" estimated value for the initial part of the isotherm where $R << R_c$.

The second method involves mathematically deriving the initial gradient of the adsorption isotherm that represents the theoretical amount of chemical picked up by one infinitesimally small particle. Equation (15) can be derived from equations (8), (9) and (10):

$$\mathrm{d}M_\mathrm{n}/\mathrm{d}n = M_\mathrm{s}\alpha_0/(1 - n_\mathrm{c}) - \alpha P_\mathrm{c}M_2\ln(n_\mathrm{c} - n)/100 + \alpha M_\mathrm{n\text{-}1}\ln(n_\mathrm{c} - n) \qquad (15)$$

For $n = 1$, $M_0 = 0$, $M_\mathrm{s} = P_\mathrm{c}M_2/[100(n_\mathrm{c} - 1)]$, $\alpha = \alpha_0$ and so:

$$(\mathrm{d}M_\mathrm{n}/\mathrm{d}n)_{\mathrm{n=1}} = [\alpha_0 P_\mathrm{c}M_2/100)[1/(\mathrm{n_c} - 1) + \ln(n_\mathrm{c} - 1)] \qquad (16)$$

Since $\mathrm{n_c} >> 1$ then equation (17) applies:

$$(\mathrm{d}M_\mathrm{n}/\mathrm{d}n)_{\mathrm{n=1}} \approx \alpha_0 P_\mathrm{c}M_2\ln(\mathrm{n_c})/100 \qquad (17)$$

Thus equation (17) suggests that the initial gradient of the adsorption isotherm is proportional to α_0 and so α_0 is related to the adsorption efficiency.

Upon consideration of both the efficiency of pick-up and the extent to which a system behaves ideally, it is clear that a given system can be classified according to one of the following four types: (i) high efficiency and ideal, (ii) high efficiency and non-ideal, (iii) low efficiency and ideal, and (iv) low efficiency and non-ideal. From the range of chemical/polymer systems examined in the present study, the lowest value of R_c that was determined is *ca.* 3.0. Given that the maximum theoretical value of P_c is 100%, an average value of the efficiency parameter E_1 for all of these systems is thus estimated $E_1(\mathrm{av}) \approx P_\mathrm{c}/R_\mathrm{c} = 33.3$. On this basis a distinction can be made between "high efficiency and ideal" and "low efficiency and ideal" classifications at $E_1 \approx 33$. Similarly, the maximum observed value of α_0 is *ca.* 3 and so it is reasonable to propose that for many systems α_0 values typically lie in the following range: $1 \leq \alpha_0 \leq 3$. This enables a distinction to be made between "high efficiency and ideal" and "high efficiency and non-ideal" classifications at $\alpha_0 \approx 2$. The E_1 and α_0 data for the systems listed in Table 1 suggest that these systems belong mainly to the "high efficiency and ideal" or "high efficiency and non-ideal" classifications.

Shown in Fig. 3 is a plot of α_0 versus the efficiency parameter E_1 that pertains to the systems given in Table 1. The reasonable degree of linearity of this plot together with its vertical axis intercept close to unity confirms that the α_0 parameter is directly related to the efficiency of pick-up as indicated by equation (17). Moreover, the correspondence between the two variables is consistent with the notion that the high efficiency pick-up systems tend to be those that exhibit a more significant departure from ideality as reflected by their values of the α_0 parameter. As the outlying data in Fig. 3 tend to belong predominantly to non-ideal systems, a departure from linearity would therefore be expected for systems where $\alpha_0 >> 3$. Under these conditions E_1 would be expected to be a less reliable estimate of the overall efficiency of pick-up of the system.

>>> Insert Figure 3

It is expected that the pick-up characteristics of the systems will be primarily dependent on both the viscosity (η) and the surface tension (γ) of the liquid chemical as well as the extent of interaction between the chemical and substrate, and the particle size distribution and/or surface area. Although the dependency of α_0 on η and α_0 on γ (data given in Table 1) each shows an overall upward trend with a low level of correlation, no firm conclusions can be drawn. This suggests that these dependencies are complex ones that require further investigation. Nonetheless, this observation also supports the appropriateness of the mathematical modeling approach used in this study as a pragmatic and systematic way to characterize and assess the pick-up of chemical substances with magnetic particles.

Conclusions

A mathematical model has been successfully developed and implemented using a computer program in order to characterize the pick-up of various liquid chemical contaminants by polymer-coated magnetic particles. Using the model it has been demonstrated that the characteristics of the pick-up isotherms range between two extremes, represented by "ideal" and "non-ideal" behavior. A further dimension to each of these classifications is the efficiency with which a given chemical is picked-up with a given magnetic particle system. The efficiency can be defined as the initial gradient of the pick-up isotherm that, in turn, is shown to be proportional to the α_0 parameter. The use of a wide range of different chemicals has revealed that nearly all of the isotherms deviate from the ideal case and that PE-coated magnetic particles are highly efficient in the pick-up of these chemicals. The observed high efficiency of pick-up can be attributed in part to the departure from ideality that these systems exhibit.

Acknowledgement

The authors are grateful to Mrs. Elizabeth Bigger for her assistance with some of the computer calculations in this work.

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Table 1. Experimentally determined values of the parameters P_c, R_c, $E_1 = (dP/dR)_0$ and α_0 for the pick up of a range of chemicals with PE-coated magnetic particles together with corresponding values of the viscosity, η, and surface tension, γ, of the chemicals.

Chemical	P_c/%	R_c	E_1	α_0
benzene	98.3	3.4	64.5	3.13
bromobenzene	94.0	3.5	44.8	2.26
chlorobenzene	96.5	3.1	60.4	2.84
cyclohexane	94.9	3.7	42.7	2.45
ethylbenzene	93.7	4.1	42.6	2.44
iodobenzene	88.5	3.8	54.6	3.33
m-dichlorobenzene	96.8	3.5	64.0	3.57
m-xylene	90.5	3.8	35.9	1.92
pentan-2-one	95.2	5.0	36.4	2.41
triethylamine	97.0	5.6	30.2	1.70

Glossary of Symbols

$\alpha(n)$	fractional excess of chemical that a magnetic particle can adsorb in the presence of n particles
α_0	boundary value of the parameter $\alpha(n)$ corresponding to the theoretical case where $n = 0$; magnitude of α_0 quantifies extent to which a given system deviates from ideal case for which $\alpha_0 = 1$
E_1	arbitrarily defined efficiency of pick-up parameter
m_1	average mass (g) of one magnetic particle
m_2	mass (g) of chemical contaminant
M_n	mass (g) of chemical adsorbed by n particles in a "non-ideal" system
$M_\mathrm{n-1}$	mass of chemical contaminant adsorbed by $n - 1$ particles
m_s	average mass of chemical adsorbed by a single magnetic particle
$M_\mathrm{s}(n)$	average mass of chemical contaminant adsorbed by the nth particle in presence of $n - 1$ particles, iteratively adjusted to account for disproportionate adsorption
n	number of magnetic particles
n_c	critical number of particles responsible for critical (maximum) percentage adsorption, P_c
P	percentage (w/w%) of chemical harvested by magnetic particles
$P(n)$	percentage adsorption after addition of n particles where $0 \leq n \leq n_\mathrm{c}$
$P(R_\mathrm{i}, \alpha_0)$	theoretical value of $P(R_\mathrm{i})$ calculated for a particular value of α_0
$P(R_\mathrm{i})$	experimental value of the percentage adsorption determined at the particle-to-chemical ratio, R_i
P_1	initial value of P on the experimental pick-up isotherm
P_c	critical value of P at which a plateau commences on the P versus R plot
R	particle-to-chemical ratio; number of magnetic particles per gram of chemical

R_1	initial value of R on the experimental pick-up isotherm
R_c	critical value of R at which a plateau commences on the P versus R plot
$s(\alpha_0)$	sum of the squares of the residuals calculated in isotherm fitting algorithm

Figure Captions

Figure 1 Computer-generated theoretical isotherms for the sequestering of chemical contaminants by magnetic particles in accordance with the model depicted by equations (1) and (7) to (10) for P_c = 90.0%, R_c = 1.8, m_1 = 0.005 g and m_2 = 0.5 g. Values of α_0 are: (a) 1.00, (b) 2.0, (c) 3.0 and (d) 5.0.

Figure 2 Isothermal pick-up at 20.0°C of 1.00 g of: (i) triethylamine (open squares, P_c = 97.0%, R_c = 5.6, α_0 = 1.70) and (ii) *m*-dichlorobenzene (open circles, P_c = 96.8%, R_c = 3.5, α_0 = 3.57) using PE-coated magnetic particles with average particle mass of 0.0820 g. The solid curves are the computer-generated fit to the experimental data. The oblique straight lines represent the ideal isotherms in each case.

Figure 3 Plot of α_0 versus the efficiency parameter $E_1 = (\mathrm{d}P/\mathrm{d}R)_0$ derived from the data given in Table 1.

Figure 1

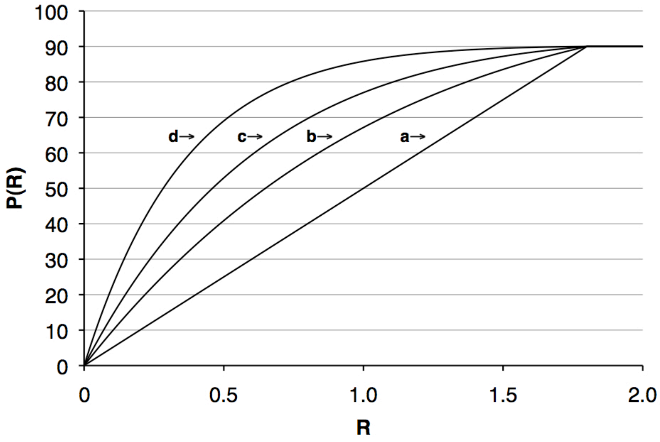

Figure 2

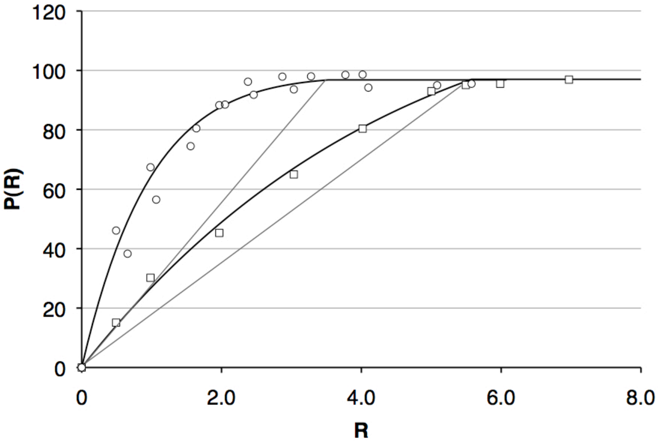

Figure 3