FAP-2253/E-1

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November 5, 2004

Food & Drug Administration
Center for Veterinary Medicine
Director, Division of Animal Feeds (HFV-220)
7519 Standish Place
Rockville, MD 20855

Re: IFA # 10683 -- OPTIGEN® 1200 Controlled Release Nitrogen

Dear Sirs:

On September 28, 2004, Alltech Inc. submitted a Food Additive Petition for IFA # 10683, OPTIGEN® 1200 Controlled Release Nitrogen. On October 14, Dr. Mika Alewynse informed us that the submission could not be filed and that a re-submission of the report supporting the Environmental Assessment was in order.

Attached hereto, in triplicate, and consisting as part of the petition, is a replacement report for section H: Environmental Assessment.

We thank you for the opportunity to submit a revised report.

Sincerely,

ALLTECH, INC.

Karl A. Dawson

Karl A. Dawson, Ph.D.
Director of Worldwide Research

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Enclosures

2004F-0546

EA 1

POTENTIAL CONCENTRATIONS OF OPTIGEN RESIDUES IN THE ENVIRONMENT AND A COMPARISON TO SIMILAR RESIDUES FROM OTHER SOURCES

FOR THE ENVIRONMENTAL ASSESSMENT OF OPTIGEN CONTROLLED RELEASE UREA

Sponsor

Alltech, Inc.
3031 Catnip Hill Pike
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Nov. 5, 2004

Signature   Date

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October 29, 2004

CONTENTS

1. INTRODUCTION

This document presents the results of an analysis of the concentrations expected in the environment of polymer and other residues from use of the Alltech Optigen product in lactating dairy cattle, and a comparison of those residues with similar residues from other sources. These results are expected to be used for an environmental assessment (EA) of Optigen as part of a food additive petition to the U.S. Food and Drug Administration. This document contains the following sections: background; purpose and scope; predicted environmental concentration (PEC) values for Optigen residues in agricultural soils; PEC values for non-Optigen residues in agricultural soils; and comparisons and conclusions. An appendix lists the references used. Another appendix contains confidential information and thus may not be available in all copies of this document.

2. BACKGROUND

Optigen 1200 is a polymer-coated urea nitrogen supplement for lactating dairy cattle. Diffusion of the urea through micropores in the polymer coating delivers nitrogen to the rumen of the cattle at a slower rate than does uncoated urea. The polymer coating is created from a series of reactions including urea, hexamethylene diisocyanate trimer, alkyd resin, tung oil, and other catalysts and chemicals as described elsewhere (Appendix 2). The resultant cross-linked polyester polyurethane coating is resistant to degradation by the microbial fauna of the rumen, although during digestion, almost all of the nitrogen (93%) is removed from the Optigen 1200. Manure produced by dairy cattle generally is collected and stored for later use as a fertilizer in spring and summer on agricultural crops. The Optigen residue in the manure consists of the aliphatic polymer and polyurethane that is cross-linked to the alkyd resin as well as trace chemical constituents.

3. PURPOSE AND SCOPE

This document describes the calculations used to estimate a PEC of Optigen-derived polyurethane polymer and other residues in soils to which manure from Optigen-fed cattle is applied. This document also compares these PEC values with PEC values for polyester polyurethane and other residues derived from polymer-coated slow-release fertilizers and other sources. Although polymer-coated fertilizers comprise only a few percent of the current fertilizer industry, their use is growing. These fertilizers appear to be the only other significant source of polyurethane polymers and a significant source of the other studied residues in agricultural lands.

4. PEC VALUES FOR OPTIGEN RESIDUES IN AGRICULTURAL SOILS

4.1 Approach

We estimate two PEC values for the polymer and other residues: a possible "high-end" estimate and a likely typical-use estimate. For both estimates, we assume no metabolism of the polymer in the cow and complete excretion of the polymer in the feces. We further assume that the excreta are collected and stored and that the manure is applied to cropland to meet total growing season (i.e., annual) nitrogen and phosphorus requirements for the crop. The high-end estimate is intended to represent a near maximum (e.g., >99th percentile) environmental concentration. The typical-use estimate is intended to approximate a median value. The values used for input to the calculations are presented in Table 1.

4.2 High-end PEC Estimate for Optigen Polymer Residues

This section describes the calculations used to estimate a high-end PEC for Optigen-derived polymer residues, PEC_{HO}, in agricultural soils using the method of Spaepen et al. (1997).

The **daily ingested dose, ID**, of polymer per cow is estimated as:

$$ID = Q_{Opt} \times C_{Poly} \times UC \qquad \text{Equation 0}$$

where:

ID = individual dose rate of polymer to cow (mg/cow-day);
Q_{Opt} = quantity of Optigen fed to cow (lbs/cow-day);
C_{Poly} = concentration of polymer in Optigen (percentage); and
UC = unit conversion factors (454 g/lb x 1000 mg/g).

For the high-end estimate of Optigen polymer residue levels in agricultural soils, we assume the maximum dose rate for Optigen of 0.8 lb per cow per day (see Table 1). The polymer comprises 4.0 % of the total Optigen formulation, however only 3.76 % of the constituents are incorporated into the polymer coating and thus inert in the gastrointestinal tract of the ruminant. Zinc stearate (0.19%) and yellow iron oxide (0.05%) are not incorporated into the polymer, but are added for anti-caking and coloration, respectively (Appendix 2). Thus,

$$\begin{aligned} ID &= 0.8\ \text{lb[Optigen]/cow-day} \times 0.0376\ \text{kg[polymer]/kg[Optigen]} \times \\ &\qquad\qquad 454\ \text{g/lb} \times 1000\ \text{mg/g}, \\ &= 13{,}656\ \text{mg[polymer]/cow-day}. \end{aligned}$$

The **quantity of polymer ingested per cow per year, Q_{Poly},** is:

$$Q_{Poly} = ID \times T \qquad \text{Equation 1}$$

where:

T = time (duration) of exposure (days) per year.

Optigen would be fed to cows 10 months per year (305 days) during lactation, and not fed to cows during the two-month "dry" period that precedes calving. However, some cows might not calve in a given year, and thus receive Optigen 365 days per year. Replacement heifers might be administered Optigen only 200 days per year. Assuming a mixed herd, therefore, we use the typical value of 305 days per year even for the high-end estimate for a herd:

Table 1. Input Parameter Values and Sources

Var.	Definition	Value	Reference
Q	Quantity Optigen (lbs) fed to cow daily	0.2 (low) 0.3 (typical) 0.8 (high)	J Downer, Pers. Comm. 2004
BW	Dairy cow body weight (kg)	500	European Union (EU) data; Spaepen et al. 1997
		600	Generic US dairy cow; NRC 1987
		606 (±58 SD)	US dairy cow after calving; Tuinstra et al. 1992
		635	high-producing US Holsteins; Van Horn et al. 1998
T	Time – duration of exposure (days/yr)	200 (minimum) 305 (typical) 365 (maximum)	10 months lactation per year is typical (J. Downer Pers. Comm. 2004); 200-365 days (Rhone Poulenc Animal Nutrition 1994)
P_E	Production of manure + urine by dairy cow (kg[excreta]/cow-yr)	20,391	EU data; Spaepen et al. 1997 (Table 1)
		22,883	50,450 lb/cow-yr, US; van Horn et al. 1998 (Table 1)
A_N	Amount of nitrogen applied to land (kg[N]/ha-yr)	100 (minimum) 200 (mid range) 600 (maximum)	Spaepen et al. 1997: maximum allowed amount that can be applied to land per year for various member countries of the EU
		139 (50^{th} percentile) 231 (85^{th} percentile) 464 (95^{th} percentile)	124 (50^{th} %), 206 (85^{th} %), 414 (95^{th} %) lbs[N]/acre-yr; application rates in the US; data from USEPA 1998 as reported in USEPA 1999
A_{P2O5}	Amount of phosphorous applied to land (kg[P_2O_5]/ha-yr)	10 (minimum) 120 (mid range) 700 (maximum)	Spaepen et al. 1997: maximum allowed amount that can be applied to land per year for various member countries of the EU
		94 (50^{th} percentile) 194 (85^{th} percentile) 283 (95^{th} percentile)	84 (50^{th} %), 173 (85^{th} %), 252 (95^{th} %) lbs[P_2O_5]/acre-yr; application rates in the US; data from USEPA 1998 as reported in USEPA 1999
P_N	Production of nitrogen in manure by dairy cow (kg [N]/cow-yr)	77.3	EU data; Spaepen et al. 1997 (Table 1)
		106 (low) 124 (high)	234-273 lbs[N]/cow-yr in US; NRC 1996 as cited in Van Horn et al. 1998
P_{P2O5}	Production of phosphorous in manure by dairy cow (kg[P_2O_5]/cow-yr)	39.08	EU data; Spaepen et al. 1997 (Table 1)
		42.6 (diet 0.40% P) 73.9 (diet 0.60% P)	40-71 lbs[P]/cow-yr = 94-163 lbs[P_2O_5]/cow-yr for diet from 0.40% to 0.60% P in US; NRC 1996 as cited in Van Horn et al. 1998
D	Depth of soil mixed with manure (m)	0.25	tilled soil: Spaepen et al. 1997
		0.05	untilled soil: Spaepen et al. 1997
ρ	Bulk density of soil (kg/m^3)	1500	loam soil with water content equal to 0.43[a]; USEPA 1999
		1500	EAEMP 1998 as cited in Spaepen et al. 1997

[a]Calculated by USEPA from data in Carsel and Parrish (1988), as referenced by USEPA (1999), based on dominant soil texture reported in CONUS soil database.

Q_{Poly} = 13,656 mg[polymer]/cow-day x 305 days/yr,
= 4,165,080 mg[polymer]/cow-yr.

The **concentration of polymer in the excreta, C_E**, is the quantity of polymer ingested per year divided by the quantity of excreta produced per year per cow:

$$C_E = Q_{Poly} / P_E \qquad \text{Equation 2}$$

where:

C_E = concentration of polymer in excreta (mg[polymer]/kg[excreta]: and
P_E = yearly production of manure by dairy cow (kg[excreta]/cow-yr).

We identified two values for P_E from the literature (Table 1); we use the US value. Thus,

C_E = 4,165,080 mg[polymer]/yr / 22,883 kg[excreta]/cow-yr,
= 182.0 mg[polymer]/kg[excreta].

Note that the US P_E value of 22,883 kg/cow-yr is only about 10% higher than the P_E value of 20,391 kg/cow-yr recommended by Spaepen et al. (1997) based on data from member countries of the European Union (EU). Readily available data suggest that dairy cattle in the US typically are 20% heavier than dairy cattle in the EU (see Table 1). Thus, the value of 22,883 appears to be the best value to use for US dairy cattle, even though it might be a slight (~10%) underestimate of their yearly manure production.

The **application rate of manure, M, to farmland** is based on either its nitrogen (N) content or on its phosphorus (P_2O_5) content These can be calculated as:

$$M_N = (A_N/P_N) \times P_E \qquad \text{Equation 3}$$

and

$$M_{P2O3} = (A_{P2O5}/P_{P2O5}) \times P_E \qquad \text{Equation 4}$$

where:

M_N = manure application rate based on nitrogen content (kg[excreta]/ha-yr);
A_N = amount of nitrogen applied to land per year (kg[N]/ha-yr);
P_N = yearly production of nitrogen in manure by dairy cow (kg [N]/cow-yr);
M_{P2O5} = manure application rate based on phosphorus content (kg[excreta]/ha-yr);
A_{P2O5} = amount of phosphorus applied to land per year (kg[P_2O_5]/ha-yr); and
P_{P2O5} = yearly production of phosphorous in manure by dairy cow (kg[P_2O_5]/cow-yr).

Table 1 provides several values identified in the literature for A_N and A_{P2O5} The values from Table 2 of Spaepen et al. (1997) are maximum allowable application rates for the different EU member countries. The values reported by USEPA (1999) represent the distribution of actual application rates for different crops in different parts of the US. For the high-end estimate, we use the 95th percentile values to estimate a high-end manure application rate in the US.

Table 1 also provides several values for P_N and P_{P2O5}. Since these parameters are in the divisors of Equations 3 and 4, it is more conservative to use lower than higher values. In other words, lower values of those parameters will result in higher manure application rates, and hence higher application of the polymer residues to farmlands.

The 95 percentile manure application rates based on nitrogen and phosphorous can now be calculated as:

$$M_N = (464 \text{ kg[N]/ha-yr} / 106 \text{ kg[N]/cow-yr}) \times 22{,}883 \text{ kg[excreta]/cow-yr}, = 100{,}167 \text{ kg[excreta]/ha-yr};$$

$$M_{P2O5} = (283 \text{ kg}[P_2O_5]\text{/ha-yr} / 42.6 \text{ kg}[P_2O_5]\text{/cow-yr}) \times 22{,}883 \text{ kg[excreta]/cow-yr}, = 152{,}016 \text{ kg[excreta]/ha-yr}.$$

The **amount of polymer residue applied per unit surface area of land each year, C_{SA},** is calculated using the more restrictive manure application rate, M_N, for nitrogen. This is because application of manure at rates that could achieve the 95th percentile phosphorous levels would provide unacceptably high amounts of nitrogen, given the nitrogen and phosphorous composition of dairy cow manure. Therefore, the 95th percentile application rate for nitrogen, M_N, is used as the manure application rate, M, below:

$$C_{SA} = M \times C_E \qquad \text{Equation 5}$$

where:

C_{SA} = substance area application rate to land (mg[polymer]/ha-yr); and
M = manure application rate (kg[excreta]/ha-yr).

Thus,

$$C_{SA} = 100{,}167 \text{ kg[excreta]/ha-yr} \times 182 \text{ mg[polymer]/kg[excreta]}, = 18{,}230{,}394 \text{ mg[polymer]/ha-yr}.$$

The **volume, V, of soil** into which the polymer residue in the manure is mixed will determine the concentration of polymer residue in that top layer of soil. Tilling the soil after application of manure can mix the manure to a soil depth of 25 cm (see Table 1). Thus, the following equation can be used:

$$V = D \times A \qquad \text{Equation 6}$$

where:

V = volume of soil tilled per unit area (m^3/ha) each year,
D = depth to which soil is tilled (m), and
A = area of tilling (1 ha = 10,000 m^2).

However, some farmland applications of manure might not entail tilling. In cases of surface application without tilling, only the top 5 cm of soil might be expected to contain the polymer residue (see Table 1). The smaller the volume of soil associated with the polymer, the higher the concentration of polymer residue in the soil. Thus, for the high-end estimate, we assume a soil depth of 5 cm, and calculate the volume of soil as:

$$V = 0.05 \text{ m} \times 10{,}000 \text{ m}^2/\text{ha}$$
$$= 500 \text{ m}^3[\text{soil}]/\text{ha-yr}.$$

The **weight, W, of the volume of soil** in which the polymer residue is located is calculated as:

$$W = V \times \rho \qquad \text{Equation 7}$$

where:

W = weight of soil containing polymer residue per unit area (kg[soil]/ha-yr), and
ρ = bulk density of agricultural soil (kg[soil]/m^3[soil]).

Although the bulk density of soil depends on many soil characteristics, including moisture content, a value of 1500 kg/m^3 is used as a default value in assessments of contaminants in agricultural soils both in the US and in the EU (Table 1). Thus:

$$W = 500 \text{ m}^3[\text{soil}]/\text{ha-yr} \times 1500 \text{ kg}[\text{soil}]/\text{m}^3[\text{soil}],$$
$$= 750{,}000 \text{ kg}[\text{soil}]/\text{ha-yr}.$$

The **high-end predicted environmental concentration for Optigen polymer residues, PEC_{HO},** in the top 5 cm of the farmland to which the manure was applied now can be calculated:

$$PEC_{HO} = C_{SA} / (W + M) \qquad \text{Equation 8}$$

where:

PEC_{HO} = high-end Optigen polymer residue concentration in soil (mg[polymer]/kg[soil]).

This estimate assumes no polymer residues in the soil at the time of the manure application. If farmland soils already contain polymer residues, the calculated PEC represents the added concentration of polymer residue to be expected in one year.

$$PEC_{HO} = 18{,}230{,}394 \text{ mg}[\text{polymer}]/\text{ha-yr} \,/\, (750{,}000 \text{ kg}[\text{soil}]/\text{ha-yr} + 100{,}167 \text{ kg}[\text{excreta}]/\text{ha-yr}),$$
$$= 21.4 \text{ mg}[\text{polymer}]/\text{kg}[\text{soil+excreta}].$$

The applied manure can be considered as part of the soil, therefore:

PEC_{HO}= 21.4 mg[polymer]/kg[soil].

4.3 Typical PEC Estimate for Optigen Polymer Residues

A more typical PEC value for Optigen polymer residues in agricultural soils, PEC_{TO}, can be estimated using the more typical or central tendency values for the appropriate parameters. The values from Table 1 that we used for this estimate are listed below:

Q_{Opt} = 0.3 lb[Optigen]/cow-day, a "typical" value;
A_N = 139 kg[N]/ha-yr, the 50th percentile value;
A_{P2O5} = 94 kg[P_2O_5]/ha-yr, the 50th percentile value;
P_N = 115 kg[N]/cow-yr, mean of "high" and "low" values in Table 1;
P_{P2O5} = 58.3 kg[P_2O_5]/cow-yr, mean of high and low values in Table 1; and
D = 25 cm depth of soil tilled.

Substituting those values for those parameters, we estimate a typical-use scenario PEC value as described below.

ID = 0.3 lb[Optigen]/cow-day x 0.0376 kg[polymer]/kg[Optigen] x 454 g/lb x 1000 mg/g,
= 5,121 mg[polymer]/cow-day.

Q_{Poly} = 5,121 mg[polymer]/cow-day x 305 days/yr,
= 1,561,905 mg[polymer]/cow-yr.

C_E = 1,561,905 mg[polymer]/yr / 22,883 kg[excreta]/cow-yr,
= 68.26 mg[polymer]/kg[excreta].

M_N = (139 kg[N]/ha-yr / 115 kg[N]/cow-yr) x 22,883 kg[excreta]/cow-yr,
= 27,659 kg[excreta]/ha-yr;

M_{P2O5} = (94 kg[P_2O_5]/ha-yr / 58.3 kg[P_2O_5]/cow-yr) x 22,883 kg[excreta]/cow-yr,
= 36,895 kg[excreta]/ha-yr.

Again, the amount of polymer residue applied per unit area of land each year, C_{SA}, is calculated using the more restrictive manure application rate, M_N, for nitrogen:

C_{SA} = 27,659 kg[excreta]/ha-yr x 68.26 mg[polymer]/kg[excreta],
= 1,888,003 mg[polymer]/ha-yr.

V = 0.25 m x 10,000 m^2/ha
= 2,500 m^3[soil]/ha-yr.

W = 2,500 m^3[soil]/ha-yr x 1,500 kg[soil]/m^3[soil],
= 3,750,000 kg[soil]/ha-yr.

PEC_{TO}= 1,888,003 mg[polymer]/ha-yr / (3,750,000 kg[soil]/ha-yr + 27,659 kg[excreta]/ha-yr)
= 0.500 mg[polymer]/kg[soil].

4.4 Summary PEC Estimates for Optigen-derived Polymer Residues in Soils

In summary, we estimated both typical and high-end values for soil concentrations of Optigen polymer residues in agricultural soils to which manure from Optigen-fed dairy cattle are applied based on the data presented in Table 1. Our **typical-use PEC estimate of 0.50 mg[polymer/kg[soil]** is based on a typical Optigen feeding rate of 0.3 lbs per cow per day, the median (50th percentile) value for manure application rates in US agricultural practices, and mixing the applied manure to a depth of 25 cm as it is tilled into the soil. Our **high-end PEC estimate of 21 mg[polymer]/kg[soil]** is approximately 2.5 orders of magnitude higher than the typical estimate. The high-end scenario assumes the maximum Optigen feeding rate of 0.8 lbs per cow per day, the upper 95th percentile manure application rates in the US, and little or no tilling of the manure into the soil. Because it is unlikely that all three of those assumptions would hold in any given location, the high-end-use scenario represents a maximum or overestimate of the maximum concentration of Optigen polymer residue that could be added to the soil in one year.

4.5 Other Potential Optigen-derived Residues in Agricultural Soils

We can now also estimate possible initial concentrations of the components of the Optigen polymer coating in soils assuming the polymer could degrade to those constituents without further reactions. HDI (hexamethylene diisocyanate) is the most abundant constituent of the polymer at 2.15 percent of total Optigen and 57.2 percent of the polymer coating. Using the typical-use and high-end estimates of 0.500 and 21.4 mg[polymer]/kg[soil], respectively, from Section 4.4, the typical-use and high-end HDI residues in soils would be 0.29 and 12 mg[HDI]/kg[soil], respectively.

Two constituents of Optigen contain zinc. Zinc oleate (0.12 percent of Optigen or 3.2 percent of the polymer coating after removal of urea) is incorporated into the polymer; however, zinc stearate (0.19 percent of Optigen) is not incorporated. Thus, we cannot estimate zinc residues on the basis of their proportion in the polymer residues in soil. Zinc comprises 10.3 percent of the molecular weight of zinc oleate, and 10.4 percent of the weight of zinc stearate. Assuming none of the zinc from these sources is absorbed and retained by the ruminant animal as Optigen passes through the gastrointestinal tract, the potential environmental contribution of zinc from Optigen can be calculated based on the total percentage of zinc in Optigen. The zinc from zinc oleate comprises 0.0124 percent of Optigen by weight (i.e., 0.12% x 10.3%) and the zinc from zinc stearate comprises 0.0198 percent of Optigen (i.e., 0.19% x 10.4%). Thus, zinc is 0.0322 percent of Optigen 1200 by weight.

The **daily ingested dose, ID**, of zinc per cow is estimated as:

$$ID_{Zn} = Q_{Opt} \times C_{Zn} \times UC \qquad \text{Equation 0}$$

where:

ID_{Zn} = individual dose rate of zinc to cow (mg/cow-day);
Q_{Opt} = quantity of Optigen fed to cow (lbs/cow-day);
C_{Zn} = concentration of zinc in Optigen (percentage); and
UC = unit conversion factors (454 g/lb x 1000 mg/g).

For the high-end scenario:

ID_{Zn} = 0.8 lb[Optigen]/cow-day x 0.000322 kg[Zn]/kg[Optigen] x 454 g/lb x 1000 mg/g,
= 117.0 mg[Zn]/cow-day.

Q_{Zn} = 117.0 mg[Zn]/cow-day x 305 days/yr,
= 35,685 mg[Zn]/cow-yr.

C_{E-Zn} = 35,685 mg[Zn]/yr / 22,883 kg[excreta]/cow-yr,
= 1.56 mg[Zn]/kg[excreta].

M_N = 100,167 kg[excreta]/ha-yr.

C_{SA-Zn} = 100,167 kg[excreta]/ha-yr x 1.56 mg[Zn]/kg[excreta],
= 156,261 mg[Zn]/ha-yr.

W = 500 m^3[soil]/ha-yr x 1500 kg[soil]/m^3[soil],
= 750,000 kg[soil]/ha-yr.

PEC (high-end estimate):

$\mathbf{PEC_{Zn}}$ = 156,261 mg[HDI]/ha-yr / (750,000 kg[soil]/ha-yr + 100,167 kg[excreta]/ha-yr)
= 0.18 mg[Zn]/kg[soil].

For the typical-use scenario:

ID_{Zn} = 0.3 lb[Optigen]/cow-day x 0.000322 kg[Zn]/kg[Optigen] x 454 g/lb x 1000 mg/g,
= 43.9 mg[Zn]/cow-day.

Q_{Zn} = 43.9 mg[Zn]/cow-day x 305 days/yr,
= 13,390 mg[Zn]/cow-yr.

C_{E-Zn} = 13,390 mg[Zn]/yr / 22,883 kg[excreta]/cow-yr,
= 0.585 mg[Zn]/kg[excreta].

M_N = 27,659 kg[excreta]/ha-yr.

C_{SA-Zn} = 27,659 kg[excreta]/ha-yr x 0.585 mg[Zn]/kg[excreta],
= 16,181 mg[Zn]/ha-yr.

W = 2,500 m^3[soil]/ha-yr x 1500 kg[soil]/m^3[soil],
= 3,750,000 kg[soil]/ha-yr.

PEC (typical-use estimate):

$$\mathbf{PEC_{Zn}} = 16.181 \text{ mg[Zn]/ha-yr} / (3{,}750{,}000 \text{ kg[soil]/ha-yr} + 27.659 \text{ kg[excreta]/ha-yr}) = \mathbf{0.0043 \text{ mg[HDI]/kg[soil]}}.$$

Table 2 summarizes the calculations for HDI and total zinc residues from Optigen 1200 fed to dairy cattle.

Table 2. Estimated Chemical Residues in Soils (mg[chemical]/kg[soil] =ppm)

Constituent	Typical-use Estimate	High-end Estimate
HDI	0.29	12
Total zinc	0.0043	0.18

5. PEC VALUES FROM OTHER SOURCES

5.1 Background

Polyurethane polymers are made by reacting diisocyanates and diols or diamines. They are used in a wide variety of products, including fibers, foams, and protective coatings in medical equipment, shoes, paints, wood preservers, and other medical, industrial, and residential products. In agricultural croplands, however, where Optigen might contribute to polyurethane in the environment, the only significant source of polyester polyurethane polymers is as a coating for slow-release fertilizers (M. Starsinic, pers. comm). Other types of polymers (e.g., polyacrylamide) are used to retain water and improve soil texture.

Almost all slow-release fertilizers deliver nitrogen, except for a few slow-release K sources. At the moment, slow release represents a small part of the total fertilizer industry in the US (3-4%), but their use is growing (Sartain and Kruse 2001). These products include ureaformaldehyde reaction products (e.g., Ntroform, Nutralene), Ureaform, methylene ureas (e.g., Nutralene), isobutylidene diurea (IBDU), sulfur-coated fertilizers, polymer-coated fertilizers, and sulfur/polymer-coated fertilizers. Thus, polymer-coated fertilizers comprise a small percentage of the total fertilizer industry in the United States.

5.2 Information Sources

Despite extensive searches on the Internet and published databases of the published literature (i.e., BIOSIS, Agricola, CAB, NTIS, Enviroline, General Science Abstracts, WasteInfo, Chemical Engineering and Biotec Abstracts), limited information on polymer-coated slow-release fertilizers was found. This reflects the relative recency of the technology, the current limited use of the more costly polymer-coated products for specialty crops, and the proprietary nature of the polymer coating formulations.

We called a company that produces polymer-coated fertilizers, Agrium, to obtain information on application rates for ESN, a urea-based controlled release fertilizer that consists of 1 to 2 percent polyurethane polymer coating (about half the amount found in some other polymer-coated fertilizers) and 44 percent nitrogen. ESN is a new product designed primarily for use as a corn fertilizer, with recommended application rates typically around 140 lbs/acre (157 kg/ha) depending on soil conditions and other factors, but as high as 220 lbs/acre (247 kg/ha) for some soil types and crops (A. Blaylock, Pers. Comm.). Most (80 percent) of the nitrogen is released within 40 to 60 days, depending on temperature. At temperatures under 43 to 44 degrees Fahrenheit, the fertilizer granules do not release any nitrogen, since nitrogen release is mediated in by microbial degradation of the polymer coating. (Note that release mechanism differs from Optigen, which releases urea via diffusion through micropores in the polymer coating). The stated typical and high-end application rates for ESN (above) would deliver 69 and 109 kg[N]/ha, respectively. As can be seen from Table 1, those nitrogen application rates are somewhat less than the median nitrogen application rate estimated for US agriculture as a whole. In general, less nitrogen is lost to runoff and leaching with slow-release nitrogen formulations; hence, less fertilizer needs to be applied.

5.3 Approach

We estimate both a typical-use and a high-end PEC value for the residues from polyurethane polymer-coated fertilizers, as was done for the residues from Optigen.

5.4 High-end PEC Estimate for Fertilizer Polymer Residues

The amount of polymer residue applied in slow-release fertilizer per year, C_{PFA}, is estimated as:

$$C_{FPA} = Q_{App} \times C_F \qquad \text{Equation 9}$$

where:

C_{FPA} = fertilizer polymer application rate to land (mg[polymer]/ha-yr);
Q_{App} = fertilizer application rate (kg[fertilizer]/ha-yr); and
C_F = concentration of polymer in fertilizer formulation (percentage).

We do not know what application rates might be considered typical or high-end for polymer-coated fertilizers other than ESN. Thus, to estimate polymer residues from polyurethane polymer-coated fertilizers, we assume a high-end application rate of 230 kg[N]/ha-yr to encompass the 85th percentile nitrogen application rate in the US (Table 1). We use the 85th instead of the 95th percentile nitrogen application rate because the 85th percentile rate is already more than twice the higher application rate stated for ESN (109 kg[N]/ha). The percentage of nitrogen in polymer-coated fertilizers appears to be typically in the range of 40 to 44 percent (Sartain and Kruse 2001). Thus, we calculate the fertilizer application rate, Q_{App}, for our high-end estimate as follows:

$$\begin{aligned} Q_{App} &= \text{nitrogen application rate/proportion nitrogen in fertilizer} \qquad \text{Equation 10} \\ &= 230 \text{ kg[N]/ha-yr} / 0.40 \text{ kg[N]/kg[fertilizer]}, \\ &= 575 \text{ kg[fertilizer]/ha-yr.} \end{aligned}$$

A review of available information suggests that polymer coatings of this type of fertilizer can range from 1-2 percent of the product to as high as 15 percent depending on the desired nitrogen release rate, with 4 percent being common (based on our review of data in Sartain and Kruse 2001). For our high-end estimate, we assume 12 percent of the product is polymer coating. Thus:

$$C_{FPA} = 575 \text{ kg[fertilizer]/ha-yr} \times 0.12 \text{ kg[polymer]/kg[fertilizer]}, = 69 \text{ kg[polymer]/ha-yr.} \quad \text{Equation 9}$$

For our high-end estimate, we assume that the fertilizer is mixed only with the top 5 cm of soil. Thus, the volume of soil containing polymer residue is calculated as:

$$V = 0.05 \text{ m} \times 10{,}000 \text{ m}^2\text{/ha} = 500 \text{ m}^3\text{[soil]/ha-yr.} \quad \text{Equation 6}$$

The weight, W, of the volume of soil in which the polymer residue is located is calculated as:

$$W = 500 \text{ m}^3\text{[soil]/ha-yr} \times 1500 \text{ kg[soil]/m}^3\text{[soil]}, = 750{,}000 \text{ kg[soil]/ha-yr.} \quad \text{Equation 7}$$

The predicted environmental concentration of the polymer from fertilizer, PEC_{HF}, in the top 5 cm of the farmland to which the fertilizer is applied is calculated as follows:

$$PEC_{HF} = C_{FPA} (\times 1{,}000{,}000 \text{ mg/kg}) / (W + Q_{App}) = 69{,}000{,}000 \text{ mg[polymer]/ha-yr} / (750{,}000 \text{ kg[soil]/ha-yr} + 575 \text{ kg[fertilizer]/ha-yr}), = 92 \text{ mg[polymer]/kg[soil+fertilizer]}; \quad \text{Equation 8}$$

PEC_{HF} = 92 mg[polymer from fertilizer]/kg[soil].

5.5 Typical PEC Estimate for Fertilizer Polymer Residues

For the typical-use estimate of polymer residues from fertilizers in agricultural soils, PEC_{TF}, we calculate Q_{App} based on the typical application rate of 157 kg[fertilizer]/ha-yr stated for ESN. We also assume 4 percent of the product is polymer coating as a typical value. Finally, we assume tilling the fertilizer into the soil to a depth of 25 cm:

C_{FPA} = 157 kg[fertilizer]/ha-yr x 0.04 kg[polymer]/kg[fertilizer],
= 6.28 kg[polymer]/ha-yr.

V = 0.25 m x 10,000 m^2/ha
= 2500 m^3[soil]/ha-yr.

W = 2500 m^3[soil]/ha-yr x 1500 kg[soil]/m^3[soil],
= 3,750,000 kg[soil]/ha-yr.

PEC_{TF} = 6,280,000 mg[polymer]/ha-yr /
(3,750,000 kg[soil]/ha-yr + 575 kg[fertilizer]/ha-yr),
= 1.67 mg[polymer]/kg[soil+fertilizer].

PEC_{TF} = 1.7 mg[polymer from fertilizer]/kg[soil].

5.6 Summary PEC Estimates for Fertilizer-derived Polymer Residues in Soils

In summary, we estimated both typical and high-end values for soil concentrations of polymer residues in agricultural soils to which slow-release fertilizers coated with polyurethane polymers are applied. Our **typical-use PEC estimate of 1.7 mg[polymer/kg[soil]** is based on an application rate of 157 kg[fertilizer]/ha-yr of a product with 4 percent polymer coating tilled to a depth of 25 cm. Our **high-end PEC estimate of 92 mg[polymer]/kg[soil]** assumes an application rate of 230 kg[N]/ha-yr based on the 85th percentile nitrogen application rate in the US (see Table 1). That is equivalent to 575 kg[fertilizer]/ha-yr if nitrogen content is 40 percent. The high-end estimate also assumes a product with 10 percent polymer coating and tilling into only the top 5 cm of the soil surface.

5.7 Other Potential Residues in Agricultural Soils

According to USEPA (1998, as reported in USEPA, 1999), the average Zn application rate from fertilizer is 5 lbs/acre, or 5.6 kg[Zn]/ha-yr. Assuming tillage of soil to a depth of 25 cm for a typical use, that application rate means that 5.6 kg of Zn would be distributed in 3,750,000 kg soil (see value for W in Section 4.3), for a final typical-use estimate of 1.4 mg[Zn]/kg soil.

6. COMPARISONS AND CONCLUSIONS

Table 3 compares our estimates of Optigen polymer residues in agricultural soils to which manure from Optigen-fed dairy cattle are applied with estimates of polymer residues from polyurethane coated fertilizer formulations. The estimated typical-use and high-end polyurethane polymer residue levels in agricultural soils from manure from Optigen-fed dairy cattle are less than one third those from application of polyurethane-coated slow-release nitrogen fertilizers. For these estimates, we have assumed that either manure or slow-release fertilizer is supplying all of the needed nitrogen. Thus, it would be inappropriate to consider the fertilizer-derived polymer residues as a "background" to which the manure-derived residues might be added (or the reverse).

Table 3. Estimated Polymer Residues in Soils (mg[polymer]/kg[soil] = ppm)

Source	Typical-use Estimate	High-end Estimate
Optigen-derived	0.50	21
Fertilizer-derived	1.7	92

The largest uncertainties in our estimates derive from the potential variation in manure or fertilizer application rates depending on local conditions and the depth to which the soil might be tilled following those applications. Other uncertainties include the amount of Optigen polymer degradation that might occur during manure storage prior to spreading, which would tend to reduce the Optigen polymer residues in soils estimated above.

Of the constituents of Optigen that might appear in the residues, comparison of the PECs for the organic compounds with appropriate benchmarks for their evaluation has been conducted previously. Our primary concern was for accumulation of zinc in soils to which the manure is applied, given that zinc does not degrade. However, the amount of zinc in applications of manure from Optigen-fed cattle is negligible compared with the amount of zinc added as a micronutrient to soils in commercial fertilizers. That is, a typical-use estimate of the concentration of zinc from fertilizer is 1.4 mg[Zn]/kg[soil]. Thus, the typical concentration of Zn in agricultural soils resulting from direct application in fertilizers is approximately one order of magnitude higher than the high-end estimate of 0.18 mg[Zn]/kg[soil] potentially contributed by Optigen. Zinc is also an essential nutrient for dairy cattle and is generally added to diets at 50 mg[Zn]/kg[diet] (NRC, 1987).

APPENDIX 1

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