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CALCULATION OF TNT AND RDX CONCENTRATION LIMITS FOR FEEDLOT WATER SUPPLIES

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INTRODUCTION

The occurrence of a contaminant in groundwater frequently reflects on the quality of a drinking water supply taken from that source for use by human beings; such a water supply may have to be replaced with another source, often at considerable expense. Should the groundwater be used for cattle in a feedlot, the demand is likely to be considerably higher than for a human population living in a similar area. Thus, it is prudent to ask whether the water, though unfit for direct human consumption, might not be satisfactory for cattle. Such a situation was brought to light in 1983-1984 at the Cornhusker Army Ammunition Plant near Grand Island, Nebraska, where the Army's investigations identified a groundwater plume containing significant levels of TNT and RDX. The problem was approached from two viewpoints: (1) Would the health of the cattle be seriously impaired? (2) Would their meat, after slaughter, contain excessive levels of the two munitions compounds?

CONTAMINANT LEVELS IN WATER BELOW WHICH TOXIC EFFECTS TO CATTLE ARE UNLIKELY

If a contaminant is not expected to be a carcinogen, toxicologists conduct chronic (lifespan) or sub-chronic (generally 90-day) exposure studies to define a no-observable-adverse-effects level (NOAEL) in a suitably sensitive species. They then apply a safety (or "uncertainty") factor to estimate an acceptable level for human exposure. Results of 90-day studies[1] in rats and in monkeys, to which a safety factor of 1,000 was applied, were used to provide the acceptable daily doses to humans, D_Ts, for TNT and RDX, respectively (Table 1). The safety factor adopted for humans is unduly high for application to cattle; concern for the latter is almost exclusively economic. Moreover, allowable chronic levels for humans are conceived in terms of a lifetime of exposure; feedlot cattle are typically slaughtered at 16-18 months,[2] as compared to their natural life span of approximately 20 years.[3-5] Only part of those short lives is spent in feedlots. For these reasons, application of a safety factor of 10, rather than 1,000, to the NOAEL should be appropriate, i.e., an acceptable exposure level for cattle would be 100 D_T. At such a degree of exposure, minimal toxic effects, such as diminished growth rate, might occur in an occasional steer—leading to virtually undetectable economic loss. Based on the values in Table 2, the value for C_w' (allowable contaminant concentration in drinking water for feedlot cattle) can be calculated:

$$C_w' = \frac{100 \times D_T \times BW_s}{W_w'} = 1100\ D_T$$

Values of C_w' are therefore 1.54 mg/L for TNT and 1.10 mg/L for RDX, almost 16 times higher than values of C_w, which are based on considerations of human health.

CONTAMINANT LEVELS IN DRINKING WATER FOR CATTLE BELOW WHICH EXCESSIVE ACCUMULATION IN THE MEAT IS UNLIKELY

Estimates Based on Published Bioconcentration Factor Equation - Bioconcentration factors, BF, for compounds that are not readily metabolized and that concentrate almost entirely in fatty tissue, have been expressed[9] in terms of the ratio of contaminant concentration in the fat of beef to the contaminant concentration in their feed (dry weight basis) at equilibrium, i.e., $BF = C_{fat}/C_{feed}$. The following equation, with input values listed in Table 2, involves internal conversion to a basis of the ratio of concentration in meat to that in the drinking water and introduction of a factor for meat consumption by humans:

$$C_w' = \frac{C_w \times R_w \times W_{feed}}{BF \times R_m \times W_w' \times f_f} = \frac{C_w \times 2.0 \times 16.5}{BF \times 0.29 \times 45.4 \times 0.3} = \frac{C_w \times 8.355}{BF}$$

Hence, C_w' = 141 mg/L for TNT and 308 mg/L for RDX. Both of these values are higher than the solubility limits shown in Table 1, so that there should be no concern for contamination of the meat of cattle whose only source of TNT is their drinking water supply.

Estimates Based on Approximate Experimental Biological Half-Lives of Contaminants - One-time dosage of animals with radiolabeled TNT[14] and of RDX[15] can provide estimates of the biological half-lives of these compounds.

It is obvious from the tissue analyses for the TNT radiolabel (summary in Table 3) that significant storage of the compound or its metabolites (not distinguished, one from the other, by the methods used) occurs in various organs, not only in fat.[14] Based on the fraction F of the label remaining in the internal organs, the value for k_1, 3.46 day^{-1}, leads to a half-life of about 0.200 day (4.8 hours); in these calculations, unrecovered material was ignored. A far more conservative calculation involves the assumption that any labeled material not in the excretum remained in the animal; the assumption, was for male dogs, and leads to a k_1 of 1.25 day^{-1}. With such a value, the allowable drinking water concentration for cattle, C_w', that would derive from it would be considered a worst-case approximation.

Residual carcass radioactivity of orally delivered RDX in rats after four days[15] was 9.5%, which translates into a value of $k_1 = \ln(1/0.095) \div 4 = 0.588\ day^{-1}$, or $t\,½ = 1.18$ days. The carcass residual concentration for the parent compound only (not a radiolabel) was only 0.6%, whence $k_1 = 1.279\ day^{-1}$ and $t\,½ = 0.54$ day.

The present input-output argument involves equating the rate of ingestion of contaminant by cattle with the rate of loss when body concentration of the contaminant has reached equilibrium. (Note that no differentiation has been made between concentration in the whole animal and concentration in edible portions; that degree of fine-tuning is probably not justified in these calculations.)

$$C_w' \times W_w' = k_1 \times C_{meat} \times BW_s$$

Substituting $C_w \times R_w/R_m$ for C_{meat}, one obtains

$$C_w' = (k_1 \times C_w \times R_w \times BW_s) \div (W_w' \times R_m) = 76 \times k_1 \times C_w$$

For TNT, the more probable value of C_w' would be $C_w' = 76 \times 3.46 \times 0.049 = 12.8$ mg/L, while the worst case value would be $C_w' = 76 \times 1.25 \times 0.049 = 4.7$ mg/L.

For RDX, the more probable value of C_w' would be based on exclusion of metabolites, which were identified as "one-carbon intermediates," rather than potentially toxic RDX congeners, $C_w' = 76 \times 1.279 \times 0.035 = 3.4$ mg/L. The value derived on the basis of the radioactive label's fate is about half that.

Estimate for RDX Based on Subchronic Exposure in Rats[16] - Rats provided daily with drinking water saturated with RDX (50-70 mg/L) accumulated the compound more or less evenly in the various organs. At the end of 90 days, the concentration in the organs (brain, heart, liver, kidney, stomach, colon, and fat) ranged from 0.20 to 0.65 mg/kg. Thus, one may assume a value of C_w'/C_{meat} of 100. Since $C_{meat} = C_w \times R_w/R_m = 6.9C_w$, $C_w' = 690\ C_w = 24$ mg/L.

CONCLUSIONS

1. From the point of view of cattle safety, pollutant limits of 1.54 mg/L for TNT and 1.10 mg/L for RDX in drinking water are suggested. This statement does not imply dire consequences from exceeding these values to some degree; it only suggests the need for increased observation of the state of animal health.

2. On the basis of published bioconcentration equations, even drinking water saturated with TNT or RDX is predicted not to pose a problem of undue flesh contamination. These compounds do not concentrate heavily in body fat, but evidently do accumulate in experimental animals to a greater degree than the equations predict. Of the drinking water concentration levels estimated to be acceptable, with regard to flesh contamination, according to various assumptions, the most reasonable appear to be 13 mg/L for TNT and 24 mg/L for RDX. These permissible values are considerably higher than levels that have been found in off-post wells near Cornhusker Army Ammunition Plant.[17]

TABLE 1. PHYSICOCHEMICAL PROPERTIES AND ACCEPTABLE DAILY DOSE

Property	TNT	Reference	RDX	Reference
Log K_{ow}	1.84[a]	6,7	0.87	8
BF (calc'd)[b]	2.90×10^{-3}	9	9.51×10^{-4}	9
Solubility in Water (mg/L)	124 (20°C)	10	60 (23.5°C)	8
Acceptable Daily Dose, D_T (mg/kg)	1.40×10^{-3}	1	1.00×10^{-3}	1
Drinking Water Criterion,[c] C_w (mg/L)	0.049	1	0.035	1

a. Calculated from the value for trinitrobenzene,[6] with suitable adjustment for the methyl group.[7]
b. Through equation, $\log BF = -3.457 + 0.500 \log K_{ow}$.
c. $D_T \times 35$, expressed in mg/L.

TABLE 2. EQUATION INPUT DATA NOT SPECIFIC TO THE CONTAMINANTS

Definition of Symbol	Symbol	Value	Reference
Body weight of a steer	BW_s	500 kg	11
Fraction of fat in beef	f_f	0.3	12
Mass of fat in adult beef cattle	M_f	75 kg	13
Rate, per day, of human meat consumption	R_m	0.29 kg	12
Rate, per day, of human water consumption	R_w	2.0 L	13
Wt. of feed ingested daily by adult cattle	W_{feed}	16.5 kg	12
Daily wt. of water consumed by adult cattle	W_w'	45.4 kg	13

TABLE 3. LOSS OF TNT RADIOACTIVITY IN FOUR SPECIES 14 HOURS AFTER ORAL DOSING[14]

Distribution	Rat		Mouse		Rabbit		Dog	
	M	F	M	F	M	F	M	F
Internal[a] (% of dose)	1.09	1.89	2.68	1.18	2.08	3.54	6.02	6.91
Excretion[b] (% of dose)	90.53	100.54	77.38	59.25	75.57	85.40	71.33	81.34
Recovered (% of dose)	91.62	102.43	80.06	60.44	77.65	88.94	77.35	88.26
Internal ÷ Recovered = F	0.0119	0.0185	0.0335	0.0193	0.0268	0.0398	0.0778	0.0783
(100-Excretion) ÷ 100 = F_{max}	0.0947	-	0.2262	0.4075	0.2443	0.1460	0.2867	0.1866
$k_1(day^{-1})$[c] = ln (1/F)	4.43	3.99	3.40	3.94	3.62	3.22	2.55	2.55
$t\,½$[d] = $0.693/k_1$	0.156	0.174	0.204	0.176	0.191	0.215	0.272	0.272

[a] Blood, liver, kidneys, lungs, spleen, brain, muscle.

[b] GI tract plus contents, feces, and urine.

[c] The disappearance rate constant, k_1, is assumed to be first-order, i.e., the disappearance rate is proportional to the amount present at any given time.

[d] $t\,½$ is the half-life, assuming first-order disappearance kinetics.

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