UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

March 25, 1998

MEMORANDUM

SUBJECT: Tier II Modeling of Surface Water EECs for Propazine Use on Grain Sorghum and Comparison of Model Output with Monitoring Data
(PC Code: 080808; DP Barcode: D242425; not EPA registered)

TO: Steven Schaible, PM Team Reviewer
Robert Forrest, Product Manager
Minor Use, Inerts and Emergency Response Branch
Registration Division

FROM: Rudy A. Pisigan, Jr., Chemist RPisigan Jr 4/6/98
Sid Abel, Environmental Scientist Sid Abel 4/6/98
Environmental Risk Branch IV
Environmental Fate and Effects Division

THROUGH: Mah T. Shamim, Ph.D., Chief [signature] for Mah Shamim 4/6/98
Environmental Risk Branch IV
Environmental Fate and Effects Division

SUMMARY

This report presents the Tier II estimated environmental concentrations (EECs) of propazine (MILO-PRO 4L) in surface water as predicted from PRZM3.1/EXAMS II modeling for a grain sorghum field scenario in Texas with an application rate of 1.2 lbs a.i./acre. The predicted maximum (acute) pesticide residue level is 85 ug/L and the upper 90% confidence bound on mean (chronic) is 57 ug/L, both of which are within the concentration range of 0.1 to 105 ug/L of propazine in the surface water monitoring data. The estimated maximum and mean residue levels generated from the model, instead of the monitoring data, are recommended for use in human health risk assessment for propazine as part of the registration process. The data qualtiy and reliability of the surface monitoring data considered in the report could not be evaluated due to limitations related to historical pesticide application, sampling site characterization, sampling

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techniques, and analytical methods. Although the model results are recommended to be used, the monitoring data tend to support the contamination of surface water by propazine. The groundwater concentration of 3.5 ug/L previoustly predicted from SCI-GROW model in Tier I assessment is retained for screening risk assessment purposes. The current Tier II results for propazine are not recommended for Section 3 assesssment.

1.0 INTRODUCTION

The Tier II assessment was conducted to provide refined estimates of surface water concentrations of propazine for drinking water assessment. A refined estimate of groundwater concentration of propazine will not be determined in this report. Instead, the groundwater screening concentration (3.5 ug/L) previously predicted by SCIGROW in the Tier I assessment will be retained for risk assessment purposes. EFED currently does not have an existing model to provide more refined estimates of ground water exposure concentrations of pesticide.

2.0 ENVIRONMENTAL CHEMISTRY

MILO-PRO 4L (Propazine) is a liquid flowable selective herbicide. It is applied for the control of many annual broadleaf weeds. It can be applied by aerial spray and broadcast (ground) application. For the preplant application, the product is applied in the spring after plowing. In the preemergence application, the product is used at planting or immediately after planting before weeds and sorghum emerge.

Propazine is a weakly basic triazine chemical (pKb=12.15) that typically exists as a neutral species in most natural environments. The major routes of dissipation are aerobic and anaerobic microbial degradation and leaching to the aquifer. It is relatively persistent and expected to be mobile in the environment.

Hydrolysis: Propazine is hydrolytically stable at pH 5, 7, and 9. Thus, hydrolysis would not be expected to be an important chemical degradation pathway for propazine.

Photolysis: Propazine is relatively resistant to photolytic degradation. It has been observed to be photolytically stable in pond water.

Soil and Aquatic Metabolism: Under soil aerobic conditions, propazine slowly undergoes microbial degradation in loam sand with a half-life of 15 weeks or 105 days. The major metabolite is 2-hydroxypropazine. Other metabolites present in trace quantities (<5% of applied dosage) are deethylatrazine and atrazine-desethyl-2-hydroxy. Anaerobic metabolism proceeds relatively faster in loam sand with a half-life of 8 weeks or 56 days. In studies involving field soil dissipation that include metabolism and other fate processes, metabolites that were detected are 2-hydroxypropazine, deethylatrazine, and diaminoatrazine. No data are available to indicate the rate and extent of both aerobic and anaerobic metabolism in aquatic environments.

Soil-Water Partition Coefficient: Values of the organic carbon adsorption coefficients (Koc) from adsorption/desorption studies using several soils indicated that Propazine is fairly mobile. The organic content appear to be an important factor influencing the mobility of propazine in soils. Mobility of the pesticide is expected to decrease with increase of organic carbon content of the soils or sediments.

3.0 SURFACE WATER MODELING

The EECs of propazine in surface water were calculated using two models: PRZM3.1, dated December 16, 1997 to simulate the transport of the pesticide off the field, and EXAMS II, Version 2.97.5, to simulate the fate of the chemical in the water body.

3.1 Scenario

The scenario chosen represents a high-end exposure site for propazine used on sorghum in Texas. The site is assumed to be a 10-hectare field draining into a 1-hectare pond, 2 meters deep with no outlet. The site is selected so that it generates exposures larger than for most sites (about 90%) used for growing the selected crop in Texas. It is further assumed that 75% of the applied pesticide stayed on the target site, 5% drifted into the pond, and the remaining 20% either deposited offsite (pond drainage basin) or remained airborne.

The sorghum site is in the Southern High Plains of Western Texas near panhandle. The fields are located in Lubbock, Hockley, Crosby, and Cochran Counties. The area represents approximately 14 percent of Texas acreage. A Pullman clay loam soil was selected to represent a reasonable "at risk" soil for the region. An "at risk" soil is one that has a high potential for runoff, erosion, and a shallow depth to groundwater. Pullman clay loam taxonomically belongs to fine, mixed thermic Torretic Paleustolls. The scenario is also characterized by conventional tillage with residues left in place and with no crop rotation. Therefore, the selection of the site is based primarily on several factors that include runoff characteristics and hydrology.

3.2 Procedure and Input Parameters

The PRZM 3.1 simulation was run for a period of 36 years on sorghum on January 1, 1948 and ending December 31, 1983. The 10 yr return EECs (or 10% yearly exceedance EECs) listed in Table 1 were calculated by linear interpolation between the third and fourth largest values by TABLE20. EXAMS II modeling was conducted for fate and transport analysis in surface water.

The application data for propazine used in this assessment are presented in Table 1.The chemical parameters used in the fate and transport modeling are summarized in Table 2. All applications were assumed to be made by aerial spray.

Table 1. Usage Practice for Modeling Propazine

Chemical	Crop	Application Method	Application Rate, lb/acre	Max. Annual Applications
Propazine	sorghum	Aerial	1.2	1

Table 2. Environmental Chemical Parameters

Parameter	Value	Source
Molecular Weight	229.71 g/mole	EFED One-Liner
Water Solubility (20 ^{0}C)	8.6 mg/L	EFED One-Liner
Vapor Pressure	2.90E-8 Torr	EFED One-Liner
Henry's Law Constant	1.02E-9 atm.-m^3/mole	EFED One-Liner
Soil Adsorption Coefficient (Koc)	110 L/kg	Ave. Koc-EFED One-Liner
Hydrolysis Half-life (pH5, 7, and 9)	Stable	EFED One-liner
Aerobic Soil Metabolism $t_{1/2*}$	315 days**	EFED One-Liner (see footnote)
Anaerobic Soil Metabolism $t_{1/2}$*	56 days	EFED One-Liner
Aerobic Aquatic Metabolism $t_{1/2*}$	not available	
Anaerobic Aquatic Metabolism $t_{1/2*}$	not available	

*$t_{1/2}$ = half-life

** 315 days was derived by multipying 105 days by 3 to account for the uncertainty in the meaurement of aerobic soil metabolism half-life when a single value is available. The derived value of 315 days is comparable or generally similar to 289 days reported in a study on aerobic soil metabolism of propazine submitted by the registrant. A cursory review of this study has been undertaken. Final review of this study will be completed later.

3.3 Modeling Results

The EECs have been calculated so that in any given year, there is a 10% probability that the maximum average concentration of that duration in that year will equal or exceed the EEC at the site. The Tier II upper tenth percentile EEEcs are presented in Table 3. The maximum surface water concentration is 30.5 ug/L. The overall upper 90% confidence bound on the mean concentrations of propazine is 9.5 ug/L. The upper 90% confidence limit on mean is the best value to use in cancer risk assessments because it is the best estimate of lifetime mean concentration.

Table 3. Tier II Upper Tenth Percentile EECs for Propazine Use on Grain Sorghum.

Crop	Aerobic Soil Metabolism Half-life	EEC's (ug/L)		
		Max	Mean of Annual Values	Upper 90% Confidence Bound on the Overall Mean
Sorghum	315 days	85	54	57

3.4 Limitations of the Analysis

There are several factors which limit the accuracy and precision of this analysis including the selection of the high-end exposure scenarios, the quality of the data, the ability of the model to represent the real world, and the number of years that were modeled. There are additional limitations on the use of these numbers as an estimate of drinking water exposure.

Scenarios that are selected for use in Tier II calculations are ones that are likely to produce large concentrations in the aquatic environment. It should represent a site that actually exists and is likely to have the pesticide applied. It should be extreme enough to provide conservative estimates of the EEC, but not so extreme that the model cannot properly simulate the fate and transport processes at the site. Currently, sites are chosen by best professional judgement to represent sites which generally produce EECs larger than 90% of all sites used for that crop. The EECs in this analysis are accurate only to the extent that the sites represent the hypothetical high exposure sites. The most limiting aspect of the site selection is the use of the standard pond with no outlet. Obviously, a Georgia pond , even with appropriately modified temperature data is not the most appropriate water body for use in Texas. It should be remembered that while the standard pond would be expected to generate higher EECs than most water bodies, some water bodies would likely have higher concentrations. These would be shallow bodies near agricultural fields that receive most of their water as runoff from the cropped field.

The quality of the analysis is directly related to the quality of the input parameters. In general, the chemical and fate parameters for propazine are considered good. The measured metabolism data lacked sufficient measuring points to accurately establish the half-life. However, the use of range data in the analysis would be sufficient to capture the probable estimated environmental concentration had a single measured value been available.

The models themselves represent a limitation on the analysis quality. While the models are among the best environmental fate estimation tools available, they have sufficient limitations in their ability to represent some processes. Spray drift is estimated as a straight 1% of the application rate reaching the pond for each ground application. The actual value may vary with each application from zero to perhaps as high as 15%. A second major limitation of the models is the lack of validation at the field level for pesticide runoff. while several of the algorithms (volume of runoff water, eroded sediment mass) are well validated and well understood, no adequate validation has yet been made of PRZM 3.1 for the amount of pesticide transported in runoff event. Other limitations on the models used is the inability to handle within site variation (spatial variability), no crop growth algorithms, and an overly simple soil water transport algorithm (the "tipping bucket" method).

EXAMS II is primarily limited because it is a steady-state model and cannot accurately characterize the dynamic nature of water flow. A model with dynamic hydrology can more accurately reflect the changes in concentration due to pond overflow and evaporation.

Another limitation is that there were limited years of weather data that were available at this site. Consequently there is approximately 1 in 36 that the true 10% exceedance EECs are larger than the maximum EEC in the analysis. If the number of years of weather data could be increased, it would increase the level of confidence that the estimated value for the 10% exceedance EEC was close to the true value.

An additional set of limitations is imposed when Tier II EECs are used for drinking water exposure estimates. A single 10 hectare drainage basin with a 1 hectare pond does not accurately reflect the dynamics in a watershed which is large enough to support a drinking water utility. A basin of adequate size to support a drinking water utility would not be planted completely in a single crop or, for that matter, entirely of crops nor would it be treated entirely with the pesticide being modeled. Additionally, the pesticide would more than likely be applied over several days to weeks rather than on a single day. This would reduce the magnitude of the conservative concentration peaks, but also make them broader, reducing the acute exposure but perhaps increasing the chronic exposure. The final overriding concern with estimates derived from the current models is the fact that the simulated pond has no outlets which any water body in this size would at least have some flow through (rivers) or turnover (reservoirs). In spite of these limitations, A Tier II EEC can provide a reasonable upper bound on the concentration found in drinking water if not an accurate assessment of the real concentration. Risk assessment using Tier II values can adequately be used as refined screens to demonstrate that the risk is below the level of concern.

4.0 GROUNDWATER SCREENING CONCENTRATION

As previously mentioned in the introduction (section 1.0), the ground water exposure value of 3.5 ug/L was predicted from SCIGROW model in the Tier I assessment. This screening concentration represents an upper-bound estimate of the concentration that might be found in ground water due to the use of propazine on grain sorghum. SCIGROW predicts likely ground water concentrations if the pesticide is used at the maximum application rate in areas where groundwater is exceptionally vulnerable to contamination. In most cases, a large majority of the use areas will have groundwater that is less vulnerable to contamination than the areas used to derive the SCIGROW estimate.

5.0 MONITORING DATA

Readily available reports on surface and ground water monitoring data for propazine were reviewed to get an idea of the levels of the pesticide actually detected in different environmental media. The monitoring data for surface waters will be considered first, followed by those for ground water.

5.1 Surface Water

The surface water monitoring data from U.S. EPA's Office of Water STORET Data base as summarized by Nelson (1997) will be presented here. As shown in the propazine STORET data in Appendix 1 Table, a total of 8518 surface water samples were collected from 34 states. Out of these collected samples, 479 had measurements at or above the detection limits ranging form 0.05 ug/L to several ug/L. Only a few concentrations exceeded 1 ug/L and only one value exceeded 10 ug/L (13 ug/L in Pennsylvania), with some exceptions on the reported values from Kansas. There was a problem in interpreting the STORET data for Kansas. As explained by Nelson (1997), the remark code "K" in STORET is supposed to mean "actual value is known to be less than value given" and generally accompanies a detection limit. However, for Kansas, there were a substantial number of concentrations higher than 1 ug/L and a few exceeding 10 ug/L that were reported with the remark code "K". The values were higher than most detection limits and were not repeated as frequently as is the case for most detection limits. Thus, it was difficult to determine if they were detections or detection limits. Consequently, in Appendix 1 Table, two entries were provided for Kansas: Kansas (1) and Kansas (2). For Kansas (1), no values accompanied by "K" were treated as detects. For Kansas (2), values exceeding 1.2 ug/L with "K" were treated as detects.

For the five states currently considered for propazine market, there was no detection in surface water samples from Colorado and New Mexico. In Oklahoma, 3 out of 111 samples had propazine concentrations of 0.1 ug/L. In Texas, 12 out of 633 samples had maximum propazine detections ranging from 0.4 to 2.1 ug/L. Using the data for Kansas (1), 70 out of 3505 samples had maximum propazine concentrations ranging 1.1 to 5.6 ug/L. Comparatively higher detections ranging from 9.1 to 105 ug/L were reported for the case of Kansas (2). But as previously mentioned, there was a problem with the interpretation of surface water monitoring data for Kansas related to the remark code "K". Hence, these data should be used with extra caution.

5.2 Ground Water

No small-scale ground water monitoring study was reported to have been done for propazine. However, several studies conducted by counties, states, regulatory agencies, and USGS have been reported in the literature and compiled. According to the Pesticides Ground Water Database (PGWDB) of US EPA (1992), the total number of wells sampled for propazine in 12 states was 1428. The number of detections was only 15 (1.1%), with concentrations ranging from 0.1 to 0.20 ug/L, as shown in Appendix 2 Table. Propazine detections were reported for the states of Texas, Kansas, Nebraska, and Connecticut. The detections occurred only in one out of 91 wells in Texas (unknown concentration) and one out of 27 wells in Kansas (0.1 ug/L). In Connecticut, two out of 139 wells had propazine detections at 0.1 ug/L. The highest number of detections was in Nebraska, where 10 out 173 wells had propazine concentrations up to 0.11 ug/L.

6.0 COMPARATIVE EVALUATION OF MODEL OUTPUT AND MONITORING DATA

The results of the PRZM/EXAM modeling indicated that the surface water maximum (acute) estimated environmental concentration (EEC) is 85 ug/L and the long term mean (chronic) concentration is 57 ug/L. The surface water concentrations in the STORET database range from 0.1 to 105 ug/L if the Kansas (2) data are included (see Appendix 1 table). If the Kansas (2) data are excluded, the range is 0.1 to 13 ug/L. Both the model-generated maximum and long term mean concentrations are within the 0.1 - 105 ug/L range. Since the scenario is adequately defined and the pesticide application rate is known, the modeling results are recommended to be used as propazine residue levels for screening risk assessments. Confidence in the model results is higher relative to that of the available surface water monitoring data. The quality, validity, and reliability of the monitoring data could not be adequately or reasonably assessed due to the following problems: (1) information about the application dose or rate, areas of pesticide use, and farming practices involving application frequency and irrigation are insufficient or not available; (2) the monitoring data base is a collection of isolated studies because the monitoring activities were not performed in a consistently uniform manner due to differences in study designs that radically affected the results; (3) characterization of the sampling sites such as susceptibility of the watershed soils to runoff, soil index, monthly precipitation, and residence times of surface water bodies are inadequate; (4) the integrity of the sampling techniques, preservation procedures, and storage methods are questionable or sometimes not documented; (5) analytical methods and limits of detections are sometimes different in several monitoring studies, thus contributing to difficulty in data interpretation.

The above mentioned problems, except item (3), are similarly responsible for the data limitations and difficulty in evaluating the monitoring data for ground water concentrations of propazine. In addition, differences in hydrogeological features (depth to ground water table, matric and preferential flow, and types of soil) among different investigations could complicate the pesticide leaching assessment. Also, differences in well construction, depth, location and intended used (domestic, municipal, irrigation, or monitoring wells) further make the comparison of pesticide levels in ground water less reliable.

Even though the PRZM/EXAMS modeling results are recommended for use in risk assessment, the monitoring data showed detections of propazine in several states and tend to support the contamination of surface waters by propazine. It is possible that the detections of propazine in the surface waters may have been reported in some monitoring studies even with the voluntary herbicide cancellation by Ciba Geigy in 1988, and quite possibly with reduced herbicide application since then.

7.0 USE OF SCREENING ESTIMATES FOR DRINKING WATER ASSESSMENTS

The EECs predicted from PRZM/EXAM model (maximum=85 ug/L and long term mean=57 ug/L) are recommended to be used for drinking water risk assessment. The screening ground water concentration of 3.5 ug/L generated from SCIGROW model in the Tier I assessment is similarly proposed to be used for human health risk evaluation. As explained before, the quality and reliability of both the surface and ground water monitoring data considered in this report could not be assessed.Thus, due to this limitation, the monitoring data are not recommended for quantitaive risk assessment.

Screening estimates derived from models provide a screen to eliminate those chemicals that are not likely to cause concerns in drinking water. Exceedances in drinking water assessments using model estimates do not necessarily mean a risk actually exists but point to the need for better data (e.g., monitoring studies specific to use patterns and drinking water resources) on which to confirm model predictions and make a new finding. Moreover, in conducting risk assessments, the actual exposure concentrations are expected to vary depending on the nature and type of water purification and treatment techniques used for the contaminated raw surface or ground water.

The results of the current Tier II assessment for propazine are not recommended to be used for Section 3 assessment.

Literature Cited

EPA, 1992. Pesticides In Ground Water Database. Office of Prevention, Pesticides and Toxic Substances. U.S. Environmental Protection Agency. Washington, DC

Nelson, H. 1997. Review of surface water exposure portions of Griffin Corporation's response to he propazine Grassley-Allen letter and a supporting study (D224188). Surface Water Section. Environmental Fate and Ground Water Branch/EFED/OPP. Washington, DC

Appendix I Table. STORET Data for Propazine in Surface Waters

STATE	PROPAZINE DETECTS/SAMPLE	PROPAZINE DETECTION LIMITS (ug/L)	MAXIMUM PROPAZINE DETECTIONS (ug/L)
Arkansas	0/243 (0.0%)	0.01	None
California	2/153 (1.3%)	0.1	0.1, 0.1
Colorado	0/42 (0.0%)	0.1	None
Connecticut	0/64 (0.0%)	0.05, 0.1	None
Delaware	2/47 (4.3%)	0.05	0.22, 0.11
Georgia	0/8 (0.0%)	0.05, 0.1	None
Hawaii	0/3 (0.0%)	0.1	None
Iowa	0/32 (0.0%)	0.05, 20, 25	None
Idaho	0/5 (0.0%)	0	None
Illinois	26/228 (11.4%)	0.05, 0.1	0.29, 0.2, 0.2
Indiana	6/43 (13.9%)	0.05, 0.1	0.11, 0.1, 0.1
Kansas (1)	70/3505 (2.0%)	0.05, 0.1, 0.3, 1.2	5.6, 4.9, 2.6, 1.8, 1.3, 1.1
Kansas (2)	201/3505 (5.7%)	0.05, 0.1, 0.3, 1.2	105, 27, 20, 15, 13, 13, 13, 12, 11, 9.7, 9.2, 9.1
Kentucky	0/63 (0.0%)	0.1	None
Louisiana	0/243 (0.0%)	0.05, 0.1	None
Maryland	5/188 (2.7%)	0.05, 0.1	0.1, 0.09
Missouri	9/160 (5.6%)	0.05, 0.1, 0.3, 1.2	1.9, 0.8, 0.3
Mississippi	2/98 (2.0%)	0.10	0.1, 0.1
Montana	0/3 (0.0%)	0.10	None
North Carolina	0/60 (0.0%)	0.05, 0.10	None
North Dakota	0/38 (0.0%)	0.10	None
Nebraska	129/853 (15.1%)	0.05, 0.1, 0.3, 3.4, 20	3.9, 3.4, 1.1, 0.65, 0.63
New Mexico	0/21 (0.0%)	0.10	None

Appendix 1 Table. STORET Data for Propazine (cont'd)

STATE	PROPAZINE DETECTS/SAMPLE	PROPAZINE DETECTION LIMITS (ug/L)	MAXIMUM PROPAZINE DETECTIONS (ug/L)
Ohio	13/50 (26.0%)	0.05	0.57, 0.42, 0.23
Oklahoma	3/111 (2.7%)	0.05, 0.1, 0.3	0.1, 0.1, 0.1
Oregon	0/42 (0.0%)	0.1	None
Pennsylvania	68/1114 (6.1%)	0.05, 0.1, 0.2, 1	13, 2.6, 2.4, 2.3, 2.3, 2.0
South Carolina	0/5 (0.0%)	0.05	None
South Dakota	0/131 (0.0%)	0.1	None
Tennessee	0/6 (0.0%)	0.1	None
Texas	12/633 (1.9%)	0.1	2.1, 1.3, 0.4
Utah	0/6 (0.0%)	0.1	None
Virginia	0/67 (0.0%)	0.1	None
Washington	0/82 (0.0%)	0.1, 0.2, 0.25	None
Wisconsin	1/171 (0.6%)	0.05, 0.1	0.1
TOTAL (3)	479/8518(5.6%)	-	-

(1) KS (1): Excluding all "K" designations from detects
(2) KS (2): Including as detects those "K" designations that may not be detection limits.
(3) Total computed KS (2) instead of KS (1).

Appendix 2 Table. Ground Water Monitoring Data for Propazine.

STATE	Year	Propazine Detects/Sample	Concentration Range (ug/L)
California	1984-89	0 / 313	
Connecticut	1987-89	2 / 139	0.1
Hawaii	1984-85	0 / 42	
Indiana	1987-88	0 / 161	
Kansas	1984	1 / 27	0.1
Maryland	1983	0 / 30	
Mississippi	1989-90	0 / 120	
Nebraska	< 1989	10 / 173	0 - 0.11
New Jersey	1985-88	0 / 188	
Pennsylvania	1983-84	1 / 63	0.20
Texas	1988-90	1 / 91	unknown
Washington	1988	0 / 81	
TOTAL		15 / 1428	0.1 - 0.20