



## Project Summary

# Sensitive Parameter Evaluation for a Vadose Zone Fate and Transport Model

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The full report presents information pertaining to quantitative evaluation of the potential impact of selected parameters on output of vadose zone transport and fate models used to describe the behavior of hazardous chemicals in soil. The Vadose Zone Interactive Processes (VIP) model was selected as the test model for this study.

Laboratory and field experiments were conducted to evaluate the effect of sensitive soil and model parameters on the degradation and soil partitioning of hazardous chemicals. Laboratory experiments were conducted to determine the effect of temperature, soil moisture and soil type on the degradation rate. Field-scale experiments were conducted to evaluate oxygen dynamics, through depth and time, for petroleum waste applied to soil.

Results of laboratory experiments demonstrated that the sensitivity of the degradation rate to changes in temperature and soil moisture was generally greater for low molecular weight compounds and less for high molecular weight compounds. For the two soil types evaluated, soil type was more significant with regard to immobilization. Soil type was not found to have an effect on degradation kinetics for the majority of chemicals evaluated.

The effect of oxygen concentration on chemical degradation as predicted by the test model was found to depend upon the magnitude of the oxygen half-saturation constant. Oxygen-limited degradation would be

anticipated to occur shortly after the addition of chemicals to soil and during active microbial metabolism of chemicals.

Model output results for temperature dependent reactions indicated that depth-concentration profiles would be sensitive to, and directly related to the temperature correction coefficient ( $\theta$ ) for each chemical. Model outputs would be very sensitive to soil temperature when values for  $\theta$  were 1.04 or greater.

Results from laboratory and short-term field studies indicated that sensitive model parameters of a site-specific nature need to be addressed in modeling the fate and behavior of hazardous chemicals in the unsaturated zone of a soil system.

*This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).*

### Introduction

A mathematical description of the soil/waste system establishes a unifying framework for evaluation of laboratory screening and field data that is useful for determination of treatment potential for a waste in soil. Mathematical models provide an approach for integration of the simultaneous processes of degradation and partitioning in soil systems so that an assessment can be made of the presence of hazardous substances in leach-

ate, soil and air. Models provide an estimate of the potential for groundwater and air contamination through a determination of the rate and extent of contaminant transport and degradation in soil as related to specific soil and compound characteristics for a particular site. Description of quantitative fate and transport of chemicals in soil systems also allows for identification of those chemicals that require management through control of mass transport and/or treatment to reduce or eliminate their hazardous potential. Thus, mathematical models represent powerful tools for ranking design, operation, and management alternatives, as well as for the design of monitoring programs for soil treatment systems.

The Regulatory and Investigative Treatment Zone (RITZ) model, was developed at the Robert S. Kerr Environmental Research Laboratory (RSKERL), Ada, Oklahoma, for use in evaluating volatilization-corrected degradation and partitioning of organic constituents in land treatment systems (USEPA, 1988). The RITZ model incorporates factors involved in soil treatment at a land treatment facility, including site, soil, and waste characteristics. The Vadose Zone Interactive Processes (VIP) model was developed as an enhancement of the RITZ model to allow for prediction of the dynamic behavior of hazardous substances in unsaturated soil systems under conditions of variable precipitation, temperature, and waste application (Grenney et al. 1987; Yan 1988). These models simulate vadose zone processes including volatilization, degradation, sorption/desorption, advection, and dispersion. The VIP model, Version 3.0 (Stevens et al., 1988) was used as the test model in this study.

Rational mathematical models of soil treatment are based upon conceptual models of soil treatment processes. The degradation process represents an important destructive mechanism for organic substances in soil systems. Important variables that may affect the degradation of organic chemicals in soil include temperature, oxygen concentration, moisture, and soil type. Therefore, these variables are anticipated to influence the degradation rate of a hazardous substance. Quantitative relationships for temperature and oxygen concentration were incorporated into the current version of the test model to allow for determination of the effects of sensitive parameters on model predictions of chemical fate and transport.

The overall objective of this research project was to determine the effect of sensitive model and soil parameters on soil treatment and on model outputs.

Specific objectives of this research project were to:

1. Select and modify a vadose zone transport and fate model to simulate the oxygen transport mechanism in the unsaturated zone, including transport in air, water, and free hydrocarbon phases with exchange between each phase and losses due to degradation,
2. Evaluate model output as a function of soil oxygen tension,
3. Evaluate model output as a function of soil temperature.
4. Evaluate the effect of soil moisture and type on degradation rates of organic substances, and
5. Compare model simulations with field subsurface oxygen measurements.

### Research Approach

Model modification — The selected test model was modified and evaluated with respect to incorporation of oxygen transport and oxygen-limited biodegradation, and with respect to the effect of temperature on degradation rate. The model describes a soil column 1.0 meter square with depth specified by the user. The column consists of a plow zone (Zone of Incorporation, ZOI) and a lower treatment zone (LTZ). The plow zone is typically defined as the top 15 cm of soil into which the substance is mixed during application. The LTZ extends below the ZOI to the bottom of the soil column and may contain substances which have been mobilized and transported downward from the ZOI.

The soil environment within the column is made up of four phases: soil grains, pore water, pore air, and pore oil. Characteristics of the soil environment may change with depth and/or time. An organic contaminant being tracked by the model may be a pure compound or a mixture of several compounds as long as the behavior of the mixture can be adequately described by composite constituent parameters. A waste can be applied and incorporated into the plow zone at loading rates and frequencies specified by the user.

These types of models simulate the fate of hazardous organic substances in unsaturated soil systems. The fate of a constituent in the soil is influenced by mobilization, volatilization, and decompo-

sition processes. The test model also simulates oxygen transport in the vadose zone by air, water, and free hydrocarbon phases with exchange between each phase and losses due to degradation of the hazardous waste constituents within the soil column.

Once applied to the land and mixed into the soil, the constituent and oxygen may be mobilized by three mechanisms: advection, dispersion, and migration between phases.

Dispersion — Mobilization of the constituent and oxygen by dispersion of the phase within the soil column is only included in the vapor phase.

Advection — The advection mechanism for the constituent and oxygen is used for the water and vapor phases only. This version of the test model constrains the oil to the zone of application and mixing.

Sorption/desorption — This term represents migration of the constituent or oxygen between phases. This mass flux of the constituents or oxygen among phases is modeled as a linear sorption mechanism. This term is applied between the water phase and each of the other phases for the constituent, and between the air phase and water or oil phases for oxygen.

Volatilization is represented in the model by two processes: mass flux into the air phase and advection/dispersion. The constituent is transported with the air phase by advection and/or dispersion, and may leave the system through the top or bottom boundaries of the control volume.

Degradation is represented by biochemical, photochemical or hydrolytic processes. Field and laboratory studies have indicated that the use of first order kinetics provides a reasonable approximation for the degradation of many hazardous substances in soil systems. Others have found that the microbial metabolism can be limited by a lack of either substrate (carbon and energy source), oxygen (electron acceptor) or both simultaneously. The degradation expression in version 3.0 of the VIP model combines the first order kinetics of the previous version with a modified Monod function. Because the constituent may degrade at different rates in different phases, separate rate and half-saturation coefficients are provided for each phase in the model. The apparent degradation rate coefficients also are permitted to vary with depth.

Effect of soil oxygen tension — The effect of oxygen tension on constituent

degradation was evaluated by conducting a series of model simulations using different values of the oxygen half-saturation coefficient,  $K_0$ .

**Effect of soil temperature** — Temperature is an important climatic factor influencing rates of decomposition in soils. Laboratory scale experiments using glass beakers were conducted for 16 PAH compounds representative of hazardous chemicals of concern to the U.S. Environmental Protection Agency. Experiments were conducted at three temperatures (10°C, 20°C, and 30°C) using a Kidman sandy loam soil. Details of these experiments have been reported by Coover, 1987.

A form of the Arrhenius expression,  $\mu_T = \mu_{T_0} \theta^{(T-T_0)}$ , was used in the test model to evaluate the effect of temperature on the rate of degradation of several hazardous constituents in the soil. Here  $\mu_T$  and  $\mu_{T_0}$  are the first order rate constants at temperatures  $T$  and  $T_0$ , respectively, and  $\theta$  is the temperature correction factor. The method of non-linear least squares was used to establish the degradation rate at 20°C and the temperature correction coefficient values ( $\theta$ ) for a subset of the hazardous substances given in Table 1, fluorene, benzo[b]fluoranthene, and chrysene. The parameter estimates were then used in the VIP model to predict the degradation of fluorene, benzo[b]fluoranthene, and chrysene in a soil system at 10°, 20°, and 30°C. The sensitivity of the output of the model was evaluated with respect to the effect of temperature on degradation rate for these three PAH compounds.

**Effect of soil moisture** — Soil water serves an important function as a transport medium through which nutrients are transported and through which waste products are removed from the microbial cell surface. Under saturation or near-saturation conditions the diffusion of gases through the soil is severely restricted, oxygen is consumed and the soil becomes anaerobic, and major shifts in microbial metabolic activity occur.

Experiments were conducted to determine the effect of soil moisture on the rate of apparent degradation of a subset of hazardous substances. Soil moisture levels of -0.33, -1.0, and -5.0 bars matric potential were used. Temperature was maintained at 20°C, and glass beaker reactors containing 200 g sandy loam soil were incubated in the dark to prevent photodegradation. Periodically through time triplicate sets of reactors containing each soil type were removed from incubation, solvent extracted with dichloro-

romethane, and analyzed by HPLC analysis of the soil extracts.

**Effect of soil type** — Soil texture and clay mineralogy are also important factors affecting soil microbial processes, controlling factors such as swelling, cation exchange capacity, buffer capacity, and sorption of organic compounds and inorganic ions. Soil organic matter content plays an important role in sorption as well as degradation, controlling availability for microbial metabolism and transformation. Soil pH is important for controlling competition between fungi, that are effective at pH < 5, and other microorganisms whose optimum pH is between 6.5 and 8.5. The effect of pH in soils is less clear than in aqueous systems, however, because the buffer capacity of clay and humic materials affects the concentration of protons at the microsite scale.

Two soil types, a McLaurin sandy loam and a Kidman sandy loam, were evaluated with regard to degradation and immobilization, or partitioning, of a subset of hazardous substances. For biodegradation rate determination, selected substances were mixed with the two soils and incubated in glass beaker reactors at 20°C and constant -0.33 bar matric potential in the dark. Periodically through time triplicate sets of reactors containing each soil type were removed from incubation, solvent extracted with dichloromethane, and analyzed by HPLC analysis of the soil extracts. Details of these experiments have been reported by Coover (1987) and Park (1987).

**Field verification of oxygen dynamics** — A field-scale experiment was conducted to evaluate the spatial and temporal variability of oxygen in soil after a petroleum waste was applied to the top six inches of soil. Air phase oxygen sensors were installed in the soil at 6 inches, 12 inches, and 24 inches below the site, and a continuous record of air phase oxygen content was kept before, during, and after waste application. Measurements from the test plots were compared with VIP model predictions.

## Results and Discussion

**Test model** — the modular structure of the VIP model, programmed in FORTRAN and solved numerically, also provides a convenient means for evaluating the behavior of various processes by isolating the modules for independent analysis. The main solution algorithm is divided into functional modules: loading rates, degradation, oil decay, and phase transport and sorption.

**Effect of soil oxygen tension** — Comparison of the test model results with and without oxygen limits (Figure 1a) show no discernible difference between the constituent concentration profiles for the two cases. Both constituent and oxygen depth profiles are shown in Figure 1b. The oxygen concentration decreases over these depths due to the oxygen demand imposed by microbial degradation of the constituent. No microbial activity has occurred below the constituent wave front, therefore the oxygen concentration is maintained at the saturation concentration.

Breakthrough curves of the constituent and oxygen concentration in the water phase at a depth of 1.0 meter are shown in Figure 1c. The oxygen concentration decreases when the constituent passes this depth due to microbial degradation of the constituent. After the constituent slug passes a particular depth, the oxygen concentration is replenished due to the advective transport mechanism in the air and water phases. The effect of the half-saturation constant for the same input data set are shown in Figure 1d for a range of  $K_0$  from 0.01 to 10 g/m<sup>3</sup> in the air, oil, and water phases. These simulations demonstrate that, as the value of this constant increases, the oxygen-limitation of degradation increases, as would be expected.

It is recognized that, under field conditions, where  $O_2$  is replenished by dispersion/diffusion from the atmosphere, this rate limitation will be less severe over the long term, for slowly degradable substrates. However, for short term dynamics, such as immediately after a waste application in land treatment of petroleum sludges,  $O_2$  limits may be very important and warrant inclusion in the model.

**Effect of soil temperature** — The percentages of each compound remaining in the soil at the end of the 240-day incubation period are presented in Table 1. Also presented are the estimated half-lives based on a first-order kinetic model for degradation and representative half-life values obtained from the literature.

The extent and rate of apparent loss was much greater for PAHs of low molecular weight and high aqueous solubility. Substantial loss of three-ring compounds acenaphthene, fluorene, and phenanthrene was observed at all temperatures during the course of the study. Four-ring compounds, including fluoranthene, pyrene, and benz[a]anthracene demonstrated greatly reduced rates of degradation. Loss of chrysene, a four-ring compound, and the remaining five- and

**Table 1. Percentages of PAH Remaining at the End of the 240-Day Study Period and Estimated Apparent Loss Half-Lives**

Compound	Percent of PAH Remaining			Estimated Half-Life (day) <sup>a</sup>			Half-Lives reported in the literature (day)
	10°C	20°C	30°C	10°C	20°C	30°C	
Acenaphthene	5	0	0	< 60	< 10	< 10	96 <sup>b</sup> ,45 <sup>b</sup> ,0.3-4 <sup>c</sup>
Fluorene	8	3	2	60 (50-71)	47 (42-53)	32 (29-37)	64 <sup>b</sup> ,39 <sup>b</sup> ,2-39 <sup>c</sup>
Phenanthrene	36	19	2	200 (160-240)	< 60	< 60	69 <sup>b</sup> ,23 <sup>b</sup> ,26 <sup>c</sup> ,9.7 <sup>d</sup> ,14 <sup>d</sup>
Anthracene	83	51	58	460 (320-770)	260 (190-420)	200 (170-290)	28 <sup>b</sup> ,17 <sup>b</sup> ,108-175 <sup>c</sup> ,17 <sup>d</sup> ,45 <sup>d</sup>
Fluoranthene	94	71	15	f	440 (280-1000)	140 (120-180)	104 <sup>b</sup> ,29 <sup>b</sup> ,44-182 <sup>c</sup> ,39 <sup>d</sup> ,34 <sup>d</sup>
Pyrene	93	89	43	f	1900 (1100-8100)	210 (150-370)	73 <sup>b</sup> ,27 <sup>b</sup> ,3-35 <sup>c</sup> ,58 <sup>d</sup> ,48 <sup>d</sup>
Benz[a]anthracent	82	71	50	680 (520-980)	430 (360-540)	240 (200-280)	52 <sup>b</sup> ,123 <sup>b</sup> ,102-252 <sup>c</sup> ,240 <sup>d</sup> ,130 <sup>d</sup>
Chrysene	85	88	86	980 (710-1500)	1000 (750-1900)	730 (550-1100)	70 <sup>b</sup> ,42 <sup>b</sup> ,5.5-10.5 <sup>c</sup> ,328 <sup>d</sup> ,224 <sup>d</sup>
Benzo[b]fluoranthene	77	75	62	580 (400-1100)	610 (410-1200)	360 (280-510)	73-130 <sup>a</sup> ,85 <sup>b</sup> ,65 <sup>b</sup>
Benzo[k]fluoranthene	93	95	89	910 (640-1600)	1400 (840-5700)	910 (500-5310)	143 <sup>b</sup> ,74 <sup>b</sup>
Benzo[a]pyrene	73	54	53	530 (300-2230)	290 (170-860)	220 (160-380)	91 <sup>b</sup> ,69 <sup>b</sup> ,30-420 <sup>c</sup> ,347 <sup>d</sup> ,218 <sup>d</sup>
Dibenz[a,h]anthracene	88	87	83	820 (520-1920)	750 (490-1600)	940 (490-12940)	74 <sup>b</sup> ,42 <sup>b</sup> ,100-190 <sup>e</sup>
Benzo[g,h,i]perylene	81	76	75	650 (420-1300)	600 (410-1170)	590 (340-2390)	179 <sup>b</sup> ,70 <sup>b</sup>
Indeno[1,2,3-c,d]pyrene	80	77	70	600 (450-910)	730 (460-1830)	630 (350-3130)	57 <sup>b</sup> ,42 <sup>b</sup> ,200-600 <sup>e</sup>

<sup>a</sup>t<sub>1/2</sub> (95 percent confidence interval)

<sup>b</sup>Sims [1986], T=20°C

<sup>c</sup>Sims and Overcash [1983], T=15-25°C

<sup>d</sup>PACE [1985], T=20°C

<sup>e</sup>Sims [1982], T=20°C

<sup>f</sup>Least squares slope (for calculation of t<sub>1/2</sub>) = zero with 95% confidence

six-ring compounds was minimal at all three temperatures.

A series of simulations using fluorene, benzo[b]fluoranthene, and chrysene was run to evaluate the effects of soil temperature on the model prediction. The  $\theta$  values ( $\pm$  95% confidence intervals) were  $1.04 \pm 0.0075$ ,  $1.024 \pm 0.012$ , and  $1.003 \pm 0.016$ , for these compounds, respectively. For this series of runs, a high recharge rate  $3.95 \text{ (cm}^3\text{/day/cm}^3\text{)}$  was used, the mass transfer rate coefficients for the constituents and oxygen were  $1000 \text{ day}^{-1}$ , assuming the constituents and oxygen reached equilibrium very rapidly.

A summary of degradation data of the three compounds after a one year simulation in the Kidman sandy loam is presented in Table 2. The extent and rate of apparent loss due to the biochemical degradation for the higher temperature are greater than those for the lower temperature for each of the three compounds studied. However, the effect of temperature on the apparent loss from decay are quite different for each compound. At 30°C the apparent degradation loss ranged from 20 percent for chrysene to 100 percent for fluorene. Figure 2 demonstrates the depth profiles of chrysene, benzo[b]fluoranthene, and fluorene

in the water phase after one year in the Kidman sandy loam. Compared to the profiles for benzo[b]fluoranthene (Figure 2b) and fluorene (Figure 2c), the profile for chrysene shows little apparent effect of temperature. The plot for fluorene (Figure 2c) shows the largest apparent effect of temperature on the model output profiles. The effect of temperature on the degradation rate depends on the value of  $\theta$ . Higher values of  $\theta$  (1.040 for fluorene), show more sensitivity to temperature in the model prediction than that for  $\theta$  values close to 1.0 (1.003 for chrysene).

**Effect of soil moisture** — Results for the effects of soil moisture at 20°C on

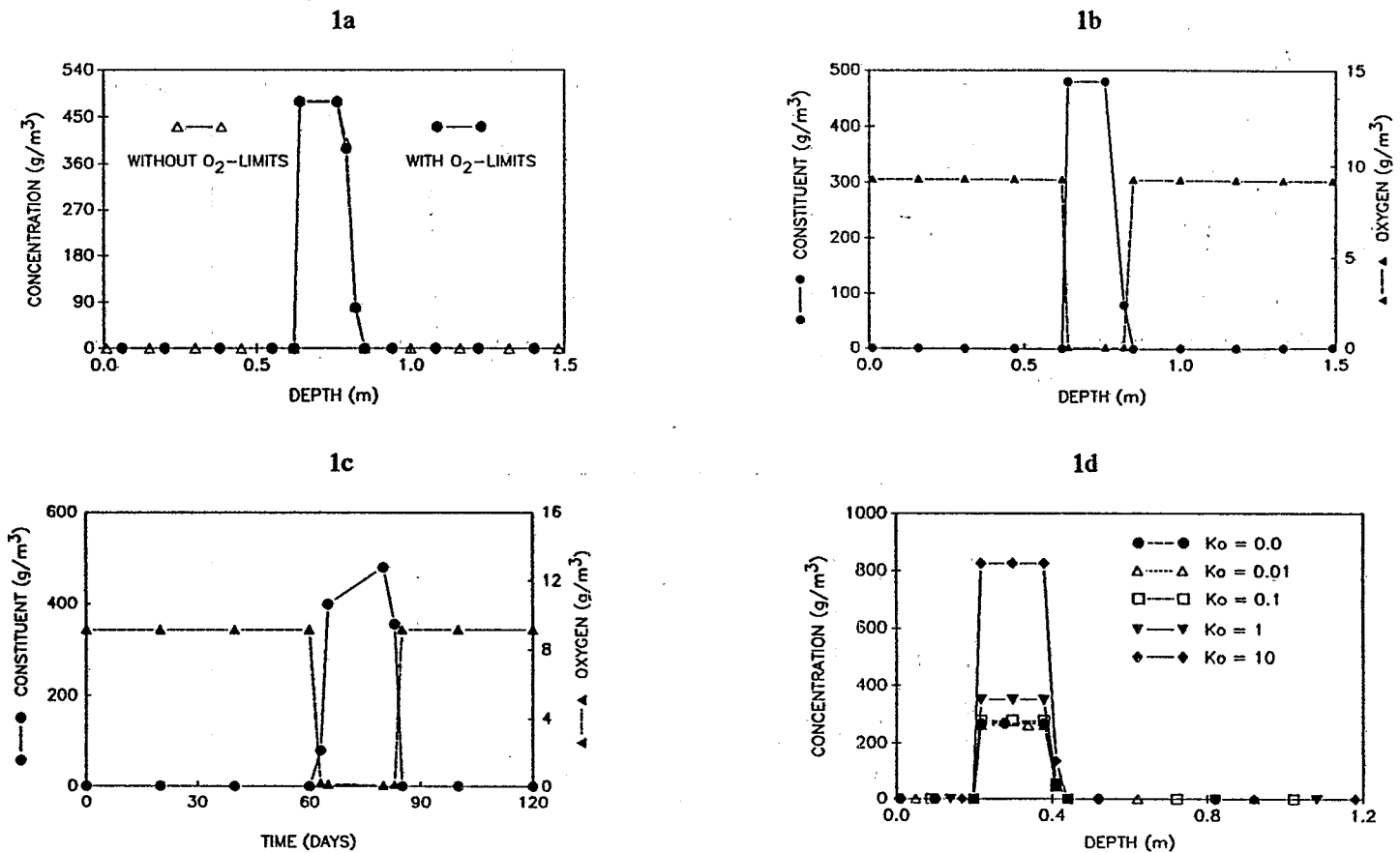


Figure 1. Effect of oxygen tension on VIP model simulation.

Table 2. Degradation Summary from Output Files

Compound	Temp. °C	% Decayed
Chrysene	10	18.6
	20	19.2
	30	19.7
Benzo[b]fluoranthene	10	37.9
	20	45.5
	30	53.4
Fluorene	10	98.3
	20	99.8
	30	100.0

the rate of degradation of a subset of PAH compounds, expressed in terms of the half-life values and their 95% confidence intervals (CI), are presented in Table 3. Half-life values were calculated based on a first-order model for PAH disappearance.

Degradation rates were significantly different at different soil moisture levels for the three-ring anthracene and the four-ring fluoranthene. No significant effect of soil moisture was evident for the naphthalene (two-ring), phenanthrene (three-ring), and pyrene (four-ring). Because of the lack of a rational quantitative relationship between soil moisture content and rate of degradation, it was not possible to evaluate the mathematical model VIP with regard to model output as a function of soil moisture.

*Effect of soil type* — Results for volatilization-corrected degradation rates as a function of soil type are presented in Table 4 for a subset of PAH compounds and pesticides incubated individually at -0.33 bar soil moisture and 20°C. Half-life values were calculated based on a first-order kinetic model for degradation; 95% confidence intervals (CI) are also given.

There was no statistically significant difference in degradation rate as a

function of soil type for the majority of PAH compounds investigated. A statistically significant difference was observed for anthracene and phenanthrene; however, the difference was not consistent for one soil type.

Eight pesticides were also evaluated (Table 4). There were statistically significant differences for degradation rates as a function of soil type for only two, aldicarb and pentachloronitrobenzene; however the differences were not consistent across the two soil types investigated. Because of the lack of a rational quantitative relationship between soil type and rate of degradation, it was not possible to evaluate the VIP model with regard to model output as a function of soil type.

*Field verification of oxygen dynamics* — The test model was run for the 5-day period of the data record. Air phase O<sub>2</sub> concentrations predicted by the model at the 6-inch, 12-inch, and 24-inch depths

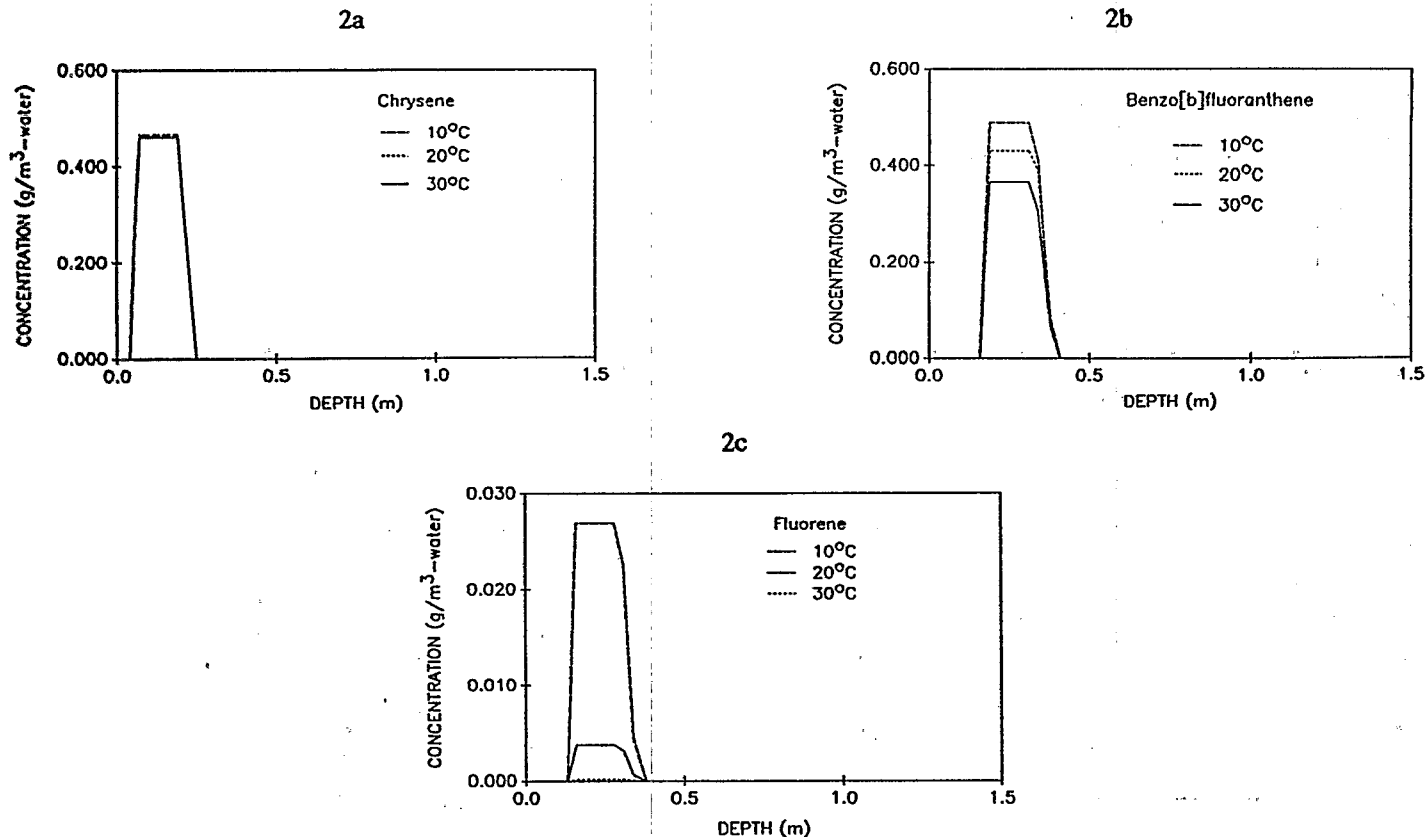


Figure 2. Simulated concentration profiles for chrysene, benzo[b]fluoranthene, and fluorene, at 10°, 29°, and 30°C.

were plotted alongside the field data. Results are given in Figure 3 for 6-inch, 12-inch, and 24-inch depths. The solid lines on the plots represent the model simulation and the dashed lines represent the field data.

The results for the 6-inch depth (Figure 3a) showed quite good agreement between the model prediction and the field data during the first 80 hours of the simulation. The model was able to track the descending leg of the data record but was unable to simulate the recovery of the  $O_2$  content at this level after 80 hours. For the 12-inch depth (Figure 3b), the model was able to predict the general behavior of the data for 60 hours but was unable to predict the recovery after this time. At a depth of 24 inches (Figure 3c), the model was able to predict the initial drop in the  $O_2$  level, but continued to descend while the field data leveled off. However, at 60 hours, when the  $O_2$  had decreased to about 25 g/m<sup>3</sup>, the model and data agreed. The model failed to predict the recovery after about 80 hours.

The inability of the test model to predict the recovery of the  $O_2$  levels after about 80 hours may be related to the boundary conditions at the bottom of the treatment zone. For the simulations presented, the treatment zone was assumed to extend to the 24-inch level. Below that level, the soil was assumed to be saturated with water, and therefore no oxygen could be transported from below. A more realistic condition for this physical system, in which the groundwater was well below the 24-inch level, is a boundary that permits free transport of vapor. This would provide an oxygen source from below and would make the  $O_2$  drop more slowly at this level, and therefore would provide an oxygen source for recovery.

#### Summary and Conclusions

The VIP model for simulating the fate and transport of organic contaminants in the vadose zone was enhanced to include dynamics of oxygen transport and oxygen-limited degradation. The model was verified against an analytical

solution for a linear, two-phase case, and used to evaluate the sensitivity of vadose zone processes to temperature, subsurface oxygen tension, soil type and moisture content. Specific conclusions based on the objectives of this research are:

1. Under field conditions with petroleum waste addition, the model successfully predicted the depth location of the decrease in the oxygen concentration in the air phase, and semi-quantitatively predicted the oxygen concentration. The model did not predict the recovery of oxygen with depth.
2. The effect of oxygen concentration on chemical degradation predicted by the test model was found to depend upon the magnitude of the oxygen half-saturation constant and the soil oxygen concentrations. Low oxygen concentrations in the soil would be expected to occur shortly after waste addition to soil and during active microbial metabolism of waste.

**Table 3.** The Effect of Soil Moisture on Degradation Rate of PAH Compounds in Sandy Loam Soil

Compound	20-40% F.C.*		40-60% F.C.		60-80% F.C.	
	$t_{1/2}$ (days)	95% CI	$t_{1/2}$ (days)	95% CI	$t_{1/2}$ (days)	95% CI
Naphthalene	30	15-93 a <sup>+</sup>	28	14-93 a	33	18-23 a
Anthracene	72	50-128 a	46	27-173 a	18	7-46 b
Phenanthrene	79	53-154 a	-	-	58	72-147 a
Fluoranthene	530	462-578 a	200	165-267 b <sup>+</sup>	230	193-289 b
Pyrene	-	-	7500	877-∞ a	5300	2500-∞ a

\*F.C. = field capacity of the soil.

<sup>+</sup>The same letter (a or b) for a compound at two moisture contents indicates no statistical difference at the 95% level based on the t-test.

**Table 4.** Degradation Rates Corrected for Volatilization for PAH Compounds and Pesticides Applied to Two Soils

Compound	Kidman Sandy Loam		McLaurin Sandy Loam	
	$t_{1/2}$ (days)	95% CI	$t_{1/2}$ (days)	95% CI
<b>PAHs:</b>				
Naphthalene	2.1	1.7-2.7 a <sup>+</sup>	2.2	1.7-3.4 a
1-Methyl-naphthalene	1.7	1.4-2.1 a	2.2	1.6-3.2 a
Anthracene	134	106-182 a	50	42-61 b <sup>+</sup>
Phenanthrene	16	13-18 a	35	27-53 b
Fluoranthene	377	277-587 a	268	173-630 a
Pyrene	260	193-408 a	199	131-408 a
Chrysene	371	289-533 a	387	257-866 a
Benz[a]anthracene	261	210-347 a	162	131-217 a
7,12-Dimethyl-				
benz[a]anthracene	20	18-24 a	28	21-41 a
Benzo[b]fluoranthene	294	231-385 a	211	169-277 a
Benzo[a]pyrene	309	239-462 a	229	178-315 a
Dibenz[a,h]anthracene	361	267-533 a	420	267-990 a
Dibenzo[a,i]pyrene	371	277-533 a	232	178-330 a
<b>Pesticides:</b>				
Phorate	32	29-85 a	24	19-35 a
Aldicarb	385	257-845 a	30	27-35 b
Pentachloronitrobenzene	17	15-21 a	51	38-74 b
Lindane	61	35-257 a	65	39-204 a
Heptachlor	58	50-70 a	63	58-76 a
Famphur	53	46-69 a	69	58-98 a
Dinoseb	103	87-128 a	92	74-124 a
Pronamidé	96	81-122 a	94	69-151 a

<sup>+</sup>The same letter (a or b) for a compound at two soil types indicates no statistical difference at the 95% level based on a t-test.

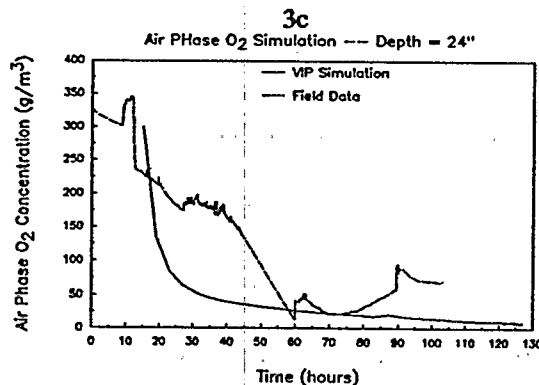
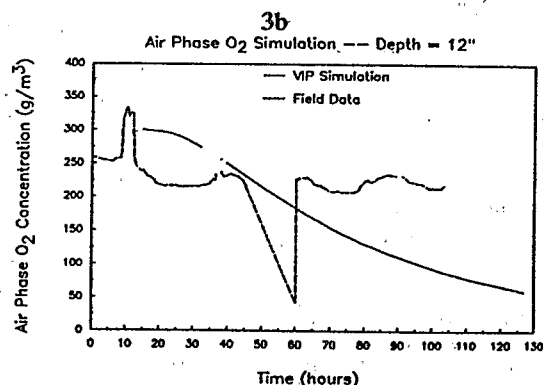
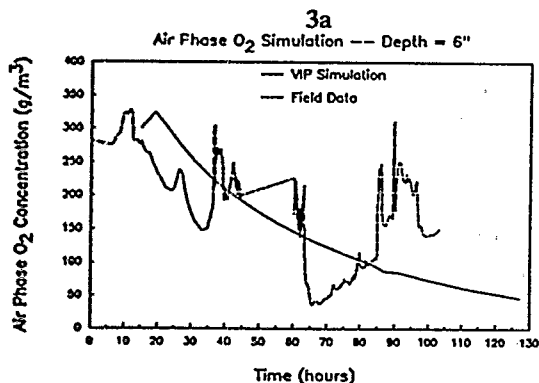


Figure 3. Field oxygen data from Nanticoke Refinery high load plot and VIP model predictions.

3. Model output results for temperature dependent reactions indicated that depth-concentration profiles were sensitive to and were directly related to the temperature correction coefficient ( $\theta$ ) for each chemical used in the model. Model outputs were very sensitive to soil temperature when values for  $\theta$  were 1.04 or greater; however, for chemicals with values for  $\theta=1.02$  or less, there was little sensitivity in the model output with respect to temperature.
4. Results of laboratory experiments demonstrated that the sensitivity of degradation rate to changes in temperature, soil moisture, and soil type was generally greater for low molecular weight compounds and less for high molecular weight compounds.

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*The complete report, entitled "Sensitive Parameter Evaluation for a Vadose Zone Fate and Transport Model," (Order No. PB 89-213 987/AS; Cost: \$15.95, subject to change) will be available only from:*

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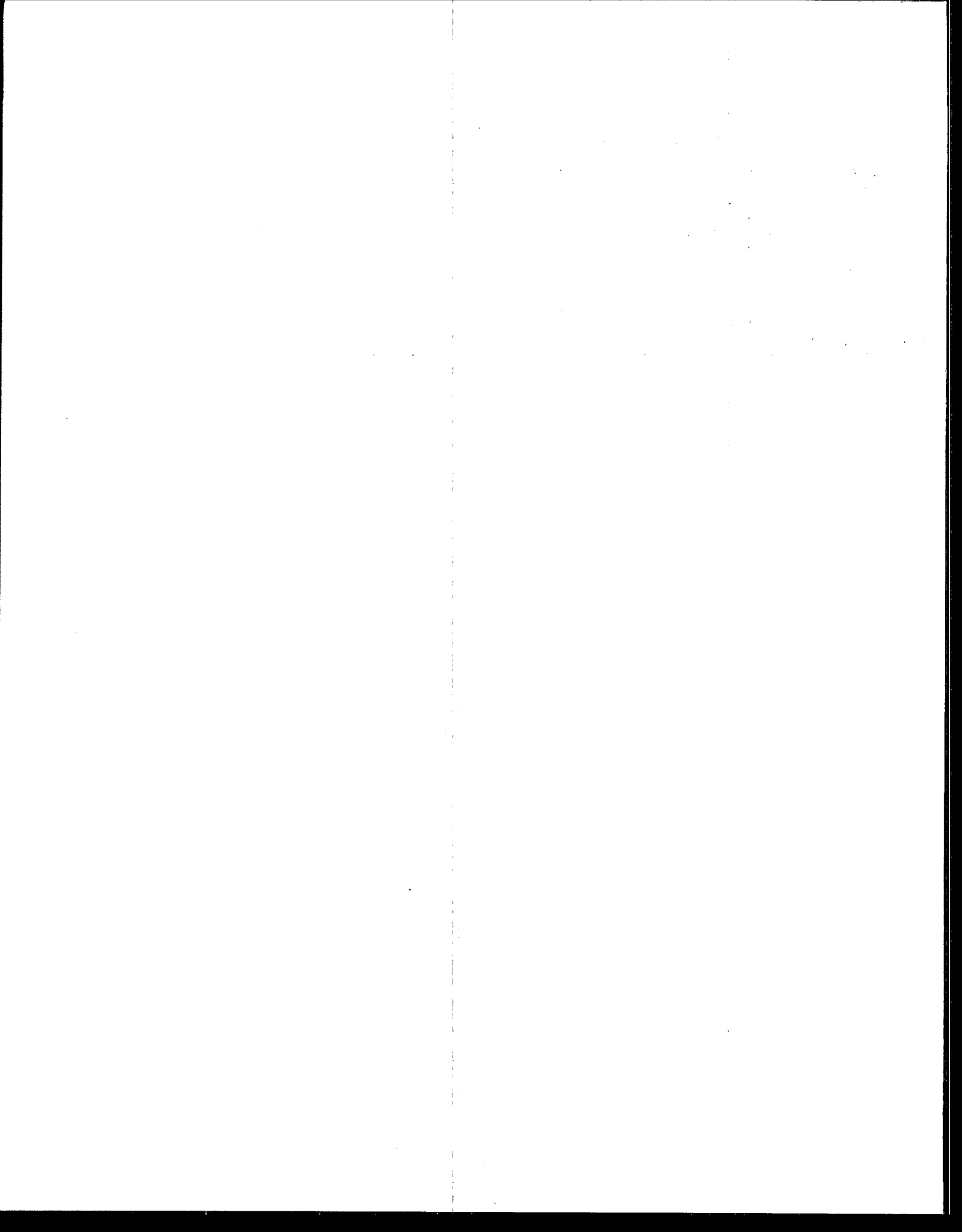
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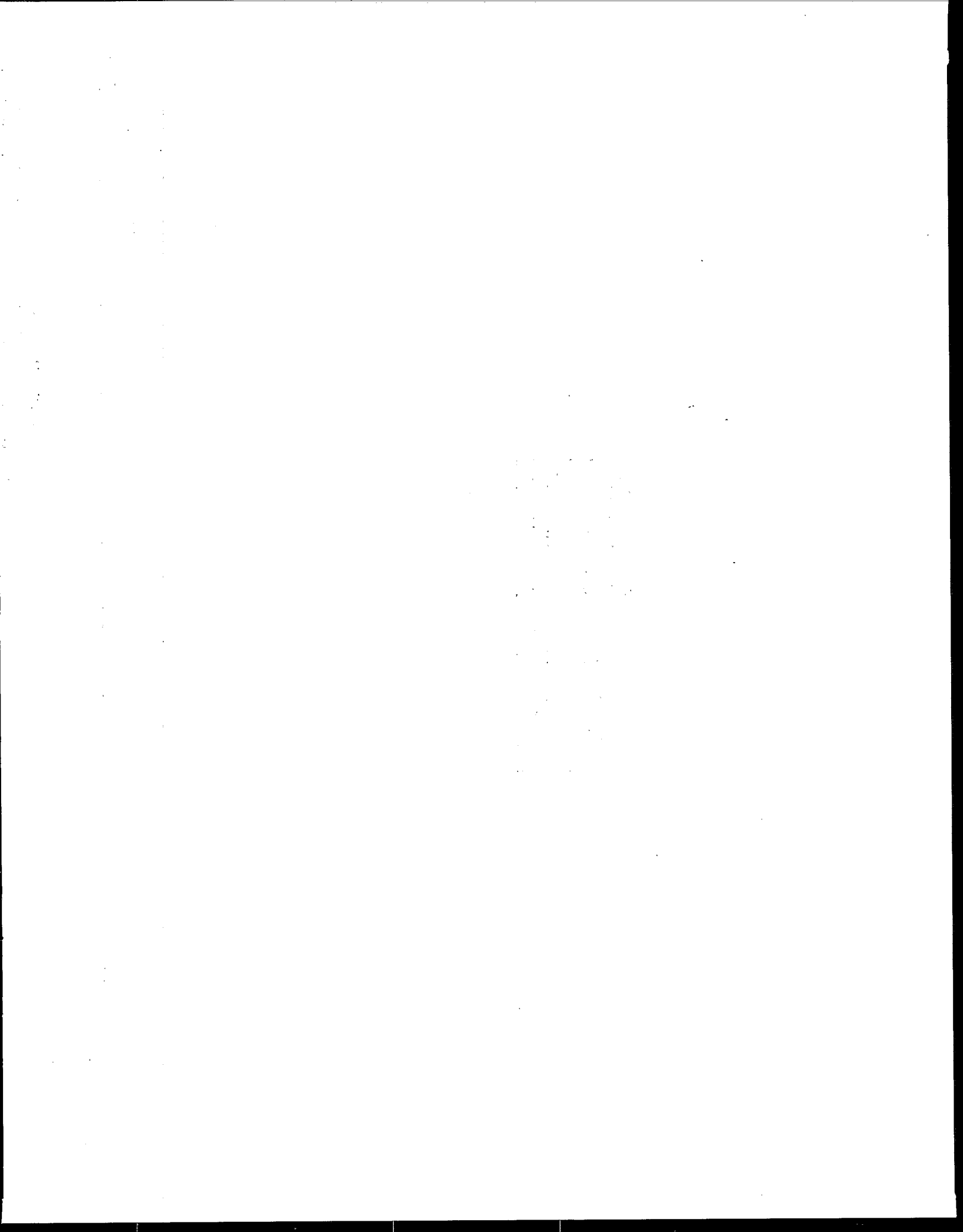
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