ENVIRONMENTAL FATE ASSESSMENT OF, METHYLMERCURY FROM COAL-FIRED POWER PLANTS IN OKLAHOMA

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CHAPTER I

INTRODUCTION

As of the year 2000, coal fired power plants generated more than 50 percent of the electricity generated in the United States. For nearly a decade, the United States Environmental Protection Agency has laid emphasis on regulating mercury especially from coal fired power plants, having recognized that source as the largest remaining source of mercury emissions in the country (EPA, 2009).

The U.S, Centre for Disease Control and Prevention, the National Research Council of the National Academy of Sciences and the World Health Organization all agree that mercury can pose unacceptable public health risks to some segment of population. Mercury in the atmosphere comes from two sources, human activities (anthropogenic) and natural activities i.e. volcanic activities. In the U.S, coal fired power plants are the largest unregulated source of mercury emissions accounting for about 40 percent of the country’s industrial emission (EPA, 2009).

1.1 Motivation

When the Clean Air Act was amended in 1990, EPA was given the authority to control mercury and other hazardous air pollutants from major sources of emissions to the air. For fossil fuel-fired power plants, the amendments required EPA to conduct a study of hazardous air pollutant emissions. The Administrator was required to consider the study and other information and to make a finding as to whether regulation was appropriate and necessary. Standards of control were to be issued if a positive finding was made. In 2000, the EPA Administrator found that regulation of hazardous air pollutants, including mercury, from coal and oil-fired power plants was appropriate and necessary, (EPA, 2009).

This was however justified, having discovered the hazardous effect of mercury on environment and the threat it pose to human health and the ecosystem.

The results of the survey conducted by CDC and released in 2003 shows that one in 12 (eight percent) of American women of childbearing age had mercury in their blood above the threshold that CDC considered safe. The implication of this is that 4.7 million women of childbearing age had already an excessive mercury level in their blood; which that implies that 322,000 newborns might be at risk for neurological problems. Secondly, current studies also show that exposure to mercury can also leads to cardiovascular defects in adult (EPA, 2003).

1.2 Objectives

The basic objective of this research is to determine the environmental fate of mercury and its most toxic compound methylmercury in a multimedia environment using various computer models.

The specifics of this research are to;

- Examine the physical and chemical properties of methylmercury,
- Predict the behavior of methylmercury as it partition to multiple media in the environment,
- Determine the fate of the chemicals of concern in multimedia environment using a general fate model.

The general fate model to be adapted in this research utilizes the data from chemical and physical properties of the chemicals of concern, the emission rate, degradation rates and various reactivity constants. The model can be used to predict the fate and risk assessment of the chemical.

1.3Thesis outline

This thesis report has five major chapters. Chapter one introduces the topic and the justification for the research .Chapter two reviews existing literature and the properties of the chemicals of concern, mercury and methylmercury, and the identifiable risks associated with them. Chapter three addresses the methodology involved in using the models for the fate and risk assessment. Chapter four includes discussion and analysis of the results obtained from chapter three. Chapter five includes the conclusions and recommendations from the previous chapters; appendices follow chapter five.

CHAPTER II

REVIEW OF LITERATURE

2.1 Introduction

This chapter describes the environmental fate of mercury as it relates to the present study. The release of mercury to the atmosphere and the resulting effect of the exposure to human and wildlife from inhalation and ingestion pathways are discussed. The chapter discussed the mercury cycle and speciation in the environment.

2.2 Mercury in the Environment

Mercury enters the environment by two processes, natural and anthropogenic. The behavior of mercury which enables it to partition into different media is due to its chemical properties; this process can simply be referred to as the mercury cycle.

2.2.1 How mercury enters the environment

Mercury is released into the air by human activities, otherwise known as “anthropogenic” source through manufacturing or burning coal for fuel, and from “natural” sources, such as volcanoes. According to Tom Atkeson and Paul Parks, (2002), there are three basic forms in which mercury can exist in the atmosphere and these are;

- Elemental mercury, which can travel a long distance and which may remain in the atmosphere for up to a year before any change can occur to it.

- Particulate mercury, otherwise called particle-bond mercury, which might easily undergo transformation having traveled a considerable distance.
- Oxidized mercury also called ionic or reactive gas mercury (RGM); found predominantly in water soluble forms which can be deposited at a range of distances depending on topography, and metereologic downwind conditions of a source.

Upon mercury emission into the environment, the fate of mercury in the environment will however depend on the following factors:

- The form of mercury emitted,
- The location of the emission source,
- How high above the landscape the mercury is released (i.e. stack height)
- The surrounding terrain
- The weather

“Depending on these factors, atmospheric mercury can be transported over a range of distances before it is deposited, potentially resulting in deposition on local, regional, continental and/or global scales. Mercury that remains in the air for prolonged periods of time and travels across continents is said to be in the "global cycle." Recent emissions estimates of annual global mercury emissions from all sources, natural and anthropogenic (human-generated), which are highly uncertain, are about 4800-8300 tons per year” (EPA, 2009).

"U.S. anthropogenic mercury emissions are estimated to account for roughly three percent of the total global emissions, and the U.S. power sector is estimated to account for about one percent the total global emissions. EPA has estimated that about one third of U.S. emissions are deposited within the contiguous U.S., and the remainder enters the global cycle. Current estimates are that less than half of all mercury deposition within the U.S. comes from U.S. sources, although deposition varies by geographic location. For example, compared to the country as a whole, U.S. sources represent a greater fraction of the total deposition in parts of the Northeast because of the direction of the prevailing winds".

2.3 State- of -the art of mercury emission from coal-fired power plants

On May 18, 2005, the U.S. Environmental Protection Agency (EPA) promulgated the first national standards for mercury emissions from coal-fired electric power plants.EPA's reasons for the standard are:

1. "Mercury is a potent neurotoxin that can cause adverse health effects (principally delayed development, neurological defects, and lower IQ in fetuses and children) at very low concentrations.
2. The principal route of exposure to mercury is through consumption of fish. Mercury enters water bodies, often through air emissions, and is taken up through the food chain, ultimately affecting humans as a result of fish consumption. According to the Environmental Protection Agency (EPA), as of December 2004, 44 states had issued fish consumption advisories due to mercury.
3. Twenty-one states (primarily in the Midwest and Northeast) have issued advisories for mercury in all their freshwater lakes and/or rivers.

4. Twelve states in the Southeast and New England have advisories for mercury statewide in their coastal waters, and Hawaii has a state wide advisory for mercury in marine fish “. (EPA,2004)

EPA gives the following rationale for the standards

“Mercury reaches water bodies from many sources, including combustion of fuels containing the substance in trace amounts. In the United States, coal-fired power plants are the largest emission source, accounting for 42% of total mercury emissions according to EPA. EPA’s 2005 regulations, referred to as Clean Air Mercury Rule (CAMR), establish a cap-and-trade program for power plant mercury that will take effect in 2010. CAMR will have little impact on emissions before 2018; however the conclusion regarding the rule’s lack of impact is based on EPA’s analysis. The rule establishes a cap of 38 tons of emissions from affected units between 2010 and 2017, but the agency estimates that actual emissions will be reduced to 31 tons in 2010 as the result of pollution controls installed under other (non-mercury) regulatory programs. Emissions will continue to decline, according to EPA, reaching 28 tons in 2015, while the cap remains at 38 tons. Thus, the CAMR rule’s cap in the period 2010-2017 serves primarily to generate credits that will be used to delay full compliance with the 69% reduction otherwise required beginning in 2018. Full compliance with the 69% reduction, according to EPA’s analysis at that time, the regulations call for a 69% reduction in emissions as compared to the1999 level.

In setting the limit so far in the future, EPA stated, in part, that mercury control technologies are not now commercially available, and will not be generally available until after 2010, even though many observers disagree with that conclusion, including a growing number of states.” (EPA, 2005)

2.4 Chemistry of Mercury

According to EPA (1997), describes the chemistry of mercury as follows:

“Elemental mercury is a heavy, silvery-white liquid metal at typical ambient temperatures and pressures. The vapor pressure of mercury metal is strongly dependent upon temperature, and it vaporizes readily under ambient conditions. Its saturation vapor pressure of 14 mg/m^3 greatly exceeds the average permissible concentrations for occupational (0.05 mg/m^3) or continuous environmental exposure (0.015mg/m^3). Elemental mercury partitions strongly to air in the environment and is not found in nature as a pure, confined liquid. Most of the mercury encountered in the atmosphere is elemental mercury vapor”. (Nriagu, 1979; WHO, 1976).

“Mercury can exist in three oxidation states: Hg^0 (metallic), Hg^{2+} (mercurous), and Hg^{+2} (mercuric-Hg (II)). The properties and chemical behavior of mercury strongly depend on the oxidation state. Mercurous and mercuric mercury can form numerous inorganic and organic chemical compounds; however, mercurous mercury is rarely stable under ordinary environmental conditions. Mercury is unusual among metals because it tends to form covalent rather than ionic bonds. Most of the mercury encountered in water/soil/sediments/biota (all environmental media except the atmosphere) is in the form of inorganic mercuric salts and organomercurics. Organomercurics are defined by the presence of a covalent C-Hg bond. The presence of a covalent C-Hg bond differentiates organomercurics from inorganic mercury compounds that merely associate with the organic material in the environment but do not have the C-Hg bond. The compounds most likely to be found under environmental conditions are these, the mercuric salts HgCl, Hg(OH) and HgS; the methylmercury compounds, methylmercury 2, 2 chloride (CH HgCl) and methylmercury hydroxide (CH HgOH); and, in small fractions, other 3 3 organomercurics (i.e., dimethylmercury and phenylmercury).

Mercury compounds in the aqueous phase often remain as undisassociated molecules, and the reported solubility values reflect this. Solubility values for mercury compounds which do not disassociate are not based on the ionic product. Most organomercurics are not soluble and do not react with weak acids or bases due to the low affinity of the mercury for oxygen bonded to carbon. Methylmercury hydroxide (CH HgOH), however, is highly soluble due to the strong hydrogen bonding capability of the hydroxide 3 group. The mercuric salts vary widely in solubility. For example HgCl is readily soluble in water, and HgS is as unreactive as the organomercurics due to the high affinity of mercury for sulfur” (Mason et al, 1994).

2.4.1 The Mercury Cycle

EPA describes the mercury cycle as follows:“Given the present understanding of the mercury cycle, the flux of mercury from the atmosphere to land or water at any one location is comprised of contributions from: The natural global cycle, the global cycle perturbed by human activities, regional sources, and local sources. Recent advances allow for a general understanding of the global mercury cycle and the impact of anthropogenic sources. It is more difficult to make accurate generalizations of the fluxes on a regional or local scale due to the site-specific nature of emission and deposition processes”. (Mason et al, 1994).

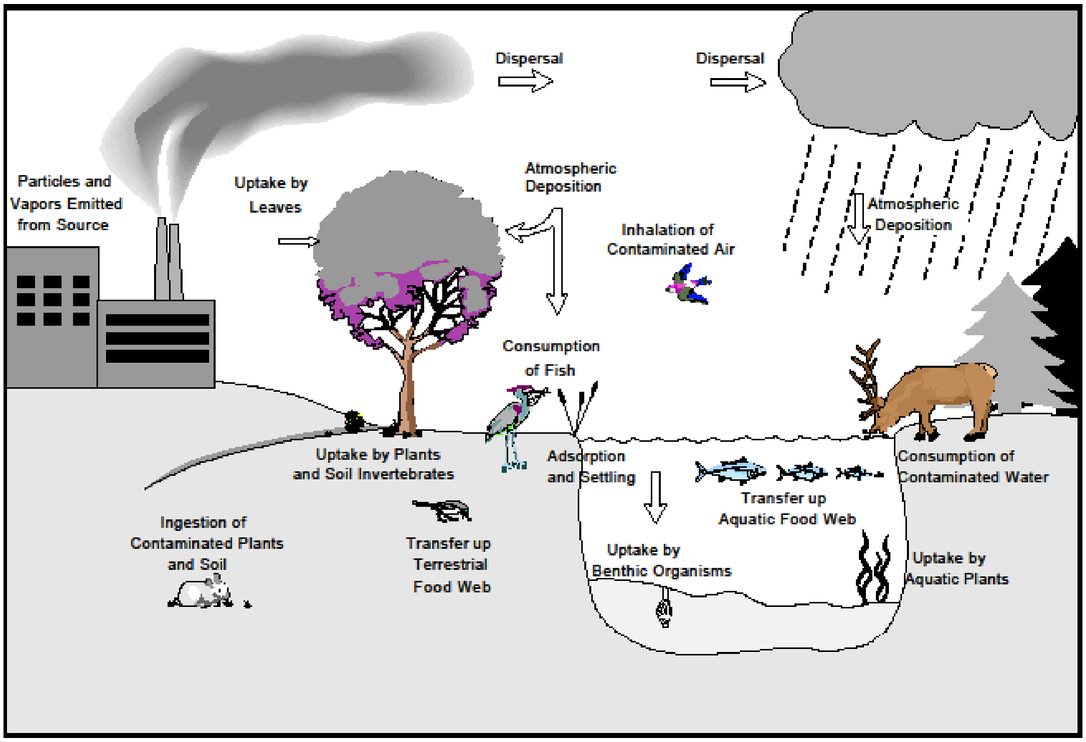


Fig 2.0; Mercury cycle, (Hoffman, 2002)

2.4.2 The Global Mercury Cycle

According to EPA (1997) “As a naturally occurring element, mercury is present throughout the environment in both environmental media and biota. Nriagu (1979) estimated the global distribution of mercury, and concluded that by far the largest repository is ocean sediments. Nriagu estimated that the ocean sediments may contain about 1017 g of mercury, mainly as HgS. Nriagu also estimated that ocean waters contain around 1013 g soils and freshwater sediments 1013 g, the biosphere 1011 g (mostly in land biota), the atmosphere 108 g and freshwater on the order of 107 g though this account does not includes mercury in mines and other subterranean repositories. A more recent estimate of the global atmospheric repository by Fitzgerald (1994) is 25 Mmol or approximately 5×10^{9} g. The estimate of Fitzgerald (1994) is about 50 times the previous estimate of Nriagu (1979) and illustrates how rapidly the scientific understanding of environmental mercury has changed in recent years.”

“Several authors have used a number of different techniques to estimate the pre-industrial mercury concentrations in environmental media before anthropogenic emissions became a part of the global mercury cycle. It is difficult to separate current mercury concentrations by origin (i.e. anthropogenic or natural) because of the continuous cycling of the element in the environment. For example, anthropogenic releases of elemental mercury may be oxidized and deposit as divalent mercury far from the source; the deposited mercury may be reduced and re-emitted as elemental mercury only to be deposited again continents away. Not surprisingly, there is a broad range of estimates and a great deal of uncertainty with each. When the estimates are combined, they indicate that between 40 and 75 percent of the current atmospheric mercury concentrations are the result of anthropogenic releases”

“The Expert Panel on Mercury Atmospheric Processes, (1994) concluded that pre-industrial atmospheric concentrations constitute approximately one-third of the current atmospheric concentrations. The panel estimated that anthropogenic emissions may currently account for 50 - 75 percent of the total annual input to the global atmosphere (Expert Panel on Mercury Atmospheric Processes, (1994). The estimates of the panel are corroborated by Lindqvist et al., (1991), who estimated that 60 percent of the current atmospheric concentrations are the result of anthropogenic emissions and by Porcella (1994), who estimated that this fraction was 50 percent. Horvat et al., (1993b) assessed the anthropogenic fraction as constituting 40 to 50 percent of the current total. This overall range appears to be in agreement with the several fold increase noted in inferred deposition rates (Swain et al., 1992; Engstrom et al., 1994; Benoit et al., 1994). The percentage of current total atmospheric mercury which is of anthropogenic origin may be much higher near mercury emissions sources. Better understanding of the relative contribution of mercury from anthropogenic sources is limited by substantial remaining uncertainties regarding the level of natural emissions as well as the amount of mercury that is re-emitted to the atmosphere from soils, watersheds, and ocean waters. Recent estimates indicate that of the approximately 200,000 tons of mercury emitted to the atmosphere since 1890, about 95 percent resides in terrestrial soils, about 3 percent in the ocean surface waters, and 2 percent in the atmosphere (Expert Panel, 1994).

“More study is needed before it is possible to accurately differentiate natural fluxes from these soils, watersheds, and ocean waters from reemissions of mercury which originated from anthropogenic sources. For instance, approximately one third of total current global mercury emissions are thought to cycle from the oceans to the atmosphere and back again to the oceans, but a major fraction of the emissions from oceans consists of recycled anthropogenic mercury. According to the Expert Panel on Mercury Atmospheric Processes (1994) 20 to 30 percent of the current oceanic emissions are from mercury originally mobilized by natural sources (Fitzgerald and Mason, 1996). Similarly, a potentially large fraction of terrestrial and vegetative emissions consists of recycled mercury from previously deposited anthropogenic and natural emissions, (Expert Panel, 1994).

“Comparisons of contemporary (within the last 15-20 years) measurements and historical records indicate that the total global atmospheric mercury burden has increased since the beginning of the industrialized period by a factor of between two and five. For example, analysis of sediments from Swedish lakes shows mercury concentrations in the upper layers that are two to five times higher than those associated with pre-industrialized times. In Minnesota and Wisconsin, an investigation of whole-lake mercury accumulation indicates that the annual deposition of atmospheric mercury has increased by a factor of three to four since pre-industrial times. Similar increases have been noted in other studies of lake and peat cores from this region, and results from remote lakes in southeast Alaska also show an increase, though somewhat lower than found in the upper Midwest U.S. (Expert Panel, 1994)”.

“Although it is accepted that atmospheric mercury burdens have increased substantially since the preindustrial period, it is uncertain whether overall atmospheric mercury levels are currently increasing, decreasing, or remaining stable. Measurements over remote areas of the Atlantic Ocean show increasing levels up until 1990 and a decrease for the period 1990-1994 (Slemr, 1996). Measurements of deposition rates suggest decreased deposition at some localities formerly subject to local or regional deposition .However, other measurements at remote sites in northern Canada and Alaska show deposition rates that continue to increase (Lucotte et al., 1995; Engstrom and Swain, 1997). Since these sites are subject to global long-range sources and few regional sources, these measurements may indicate a still increasing global atmospheric burden. More research is necessary; a multi-year, worldwide atmospheric mercury measurement program may help to better determine current global trends (Fitzgerald, 1995).” (EPA, 1997)

2.4.3 Regional and Local Mercury Cycles

EPA mercury study report to congress (EPA,1997) states that “According to one estimate, about half of total anthropogenic mercury emissions eventually enter the global atmospheric cycle (Mason et al., 1994); the remainder is removed through local or regional cycles. An estimated 5 to 10 percent of primary Hg(II) emissions are deposited within 100 km of the point of emission and a larger fraction on a regional scale. Hg (0) that is emitted may be removed on a local and regional scale to the extent that it is oxidized to Hg (II). Some Hg (0) may also be taken up directly by foliage; most Hg (0) that is not oxidized will undergo long-range transport due to the insolubility of Hg (0) in water. In general, primary Hg (II) emissions will be deposited on a local and regional scale to the degree that wet deposition processes remove the soluble Hg(II). Dry deposition may also account for some removal of atmospheric Hg(II). Assuming constant emission rates, the quantity of mercury deposited on a regional and local scale can vary depending on source characteristics (especially the species of mercury emitted), meteorological and topographical attributes, and other factors (Expert Panel, 1994). For example, deposition rates at some locations have been correlated with wind trajectories and precipitation amounts (Jensen and Iverfeldt, 1994; Dvonch et al., 1995).

Although these variations prohibit generalizations of local and regional cycles, such cycles may be established for specific locations. For example, unique mercury cycles have been defined for Siberia on a regional scale (Sukhenko and Vasiliev, 1996) and for the area downwind of a German chlor-alkali plant on a local scale (Ebinghaus and Kruger, 1996). Mercury cycles dependent on local and regional sources have also been established for the Upper Great Lakes region (Glass et al., 1991; Lamborg et al., 1995) and the Nordic countries (Jensen and Iverfeldt, 1994)”.

While the overall trend in the global mercury burden since pre-industrial times appears to be increasing, there is some evidence that mercury concentrations in the environment in certain locations have been stable or decreasing over the past few decades.

For example, preliminary results for eastern red cedar growing near industrial sources (chlor-alkali, nuclear weapons production) show peak mercury concentrations in wood formed in the 1950s and 1960s, with stable or decreasing concentrations in the past decade (Expert Panel, 1994). Some results from peat cores and lake sediment cores also suggest that peak mercury deposition in some regions occurred prior to 1970 and may now be decreasing (Swainet al., 1992; Benoit et al., 1994; Engstrom et al., 1994; Engstrom and Swain, 1997). Data collected over 25 years from many locations in the United Kingdom on liver mercury concentrations in two raptor species and a fish-eating grey heron indicate that peak concentrations occurred prior to 1970. The sharp decline in liver mercury concentrations in the early 1970s suggests that local sources, such as agricultural uses of fungicides, may have led to elevated mercury levels two to three decades ago (Newton et al.,1993). Similar trends have been noted for mercury levels in eggs of the common loon collected from New York and New Hampshire (McIntyre et al., 1993)”. (EPA, 1997)

2.5 Atmospheric Processes

Basic processes involved in the atmospheric fate and transport of mercury include, emissions to the atmosphere, transformation and transport in the atmosphere, deposition from the air; and then re-emission to the atmosphere. Each of these processes is briefly described below.

2.5.1 Emissions of Mercury

EPA (1997) states that, “mercury is emitted to the atmosphere through both naturally occurring and anthropogenic processes. Natural processes include volatilization of mercury in marine and aquatic environments, volatilization from vegetation, degassing of geologic materials (e.g., soils) and volcanic emissions. The natural emissions are thought to be primarily in the elemental mercury form. Conceptually, the current natural emissions can arise from two components: mercury present as part of the pre-industrial equilibrium and mercury mobilized from deep geologic deposits and added to the global cycle by human activity. Based on estimates of the total annual global input to the atmosphere from all sources (i.e., 5000 Mg from anthropogenic, natural, and oceanic emissions), U.S. sources are estimated to contribute about 3 percent, based on 1995 emissions result. (Lindqvist et al., 1991).

“Anthropogenic mercury releases are thought to be dominated on the national scale by industrial processes and combustion sources that release mercury into the atmosphere.

Stack emissions are thought to include both gaseous and particulate forms of mercury. Gaseous mercury emissions are thought to include both elemental and oxidized chemical forms, while particulate mercury emissions are thought to be composed primarily of oxidized compounds due to the relatively high vapor pressure of elemental mercury.

The analytic methods for mercury speciation of exit gasses and emission plumes are being refined, and there is still controversy in this field. Chemical reactions occurring in the emission plume are also possible. The speciation of mercury emissions is thought to depend on the fuel used (e.g., coal, oil, municipal waste), flue gas cleaning and operating temperature. The exit stream is thought to range from almost all divalent mercury to nearly all elemental mercury. Most of the mercury emitted at the stack outlet is found in the gas phase although exit streams containing soot can bind up some fraction of the mercury. The divalent fraction is split between gaseous and particle bound phases (Lindqvist et al., 1991). Much of this divalent mercury is thought to be HgCl (Michigan Environmental Science Board, 1993). An emission factor-based approach was used to develop the nationwide emission estimates for the source categories presented in Table 2.1.

Table 2.1 (Annual estimates of mercury release by various combustion and manufacturing source)

Source	**Annual mercury emission rate**
Combustion source type	125.2 Mg/yr (137/9 tons/yr)
Electric utilities	-
Oil and gas fired	0.2 Mg/yr (0.2 tons/yr)
Coal-fired	46.9 Mg/yr (51.6tons/yr)
Incinerator	-
Municipal waste combustor	26.9Mg/yr (29.6 tons/yr)
Medical waste incinerator	14.6 Mg/yr(16.0 tons/yr)
Commercial /industrial boiler	25.8 Mg/yr (28.4 tons/yr)
Chloro –alkali production	6.5Mg/yr (7.1 tons/yr)
Primary lead smelting	0.1 Mg/yr (0.1 tons/yr)
Primary copper smelting	0.06 Mg/yr (0.06 tons/yr)
Other combustion sources	10.8 Mg/yr (11.9 tons/yr)
Other sources	12.1 Mg/yr (13.3 tons/yr)

(EPA, 1997)

EPA (1997) states that “the emission factors presented are estimates based on ratios of mass mercury emissions to measures of source activities and nation-wide source activity levels. It is estimated that the mercury content of typical lakes and rivers has been increased by a factor of two to four since the onset of the industrial age (Nriagu, 1979). More recently, researchers in Sweden estimate that mercury concentrations in soil, water and lake sediments have increased by a factor of four to seven in southern Sweden and two to three in northern Sweden in the 20th century (Swedish EPA 1991). It is estimated that present day mercury deposition is two to five times greater now than in preindustrial times (Lindqvist et al., 1991).”(EPA, 1997)

2.5.2 Mercury Transformation and Transport

“Elemental (Hg (0)) has an average residence time in the atmosphere of about one year and will thus be distributed fairly evenly in the troposphere. Oxidized mercury (Hg (II)) may be deposited relatively quickly by wet and dry deposition processes, leading to a residence time of hours to months. Longer residence times are possible as well; the atmospheric residence time for some Hg(II) associated with fine particles may approach that of Hg0 (Porcella et al., 1996).

The transformation of Hg0(g) to Hg(II)(aq) and Hg(II)(p) in cloud water demonstrates a possible mechanism by which natural and anthropogenic sources of Hg0 to air can result in mercury deposition to land and water. This deposition can occur far from the source due to the slow rate of Hg0 (g) uptake in cloud water. It has been suggested that this mechanism is important in a global sense for mercury pollution, while direct wet deposition of anthropogenic Hg(II) is the most important locally (Fitzgerald,1994; Lindqvist et al., 1991). Gaseous Hg (II) is expected to deposit at a faster rate after release than particulate Hg (II) assuming that most of the particulate matter is less than 1 μm in diameter.

“An atmospheric residence time of ½ - 2 years for elemental mercury compared to as little as hours for some Hg(II) species (Lindqvist and Rodhe, 1985) is expected. This behavior is observed in the modeling results presented in this effort as well. It is possible that dry deposition of Hg0 can occur from ozone mediated oxidation of elemental mercury taking place on wet surfaces, but this is not expected to be comparable in magnitude to the cloud droplet mediated processes.

“This great disparity in atmospheric residence time between Hg0 and the other mercury species leads to very much larger scales of transport and deposition for Hg0. Generally, air emissions of Hg0 from anthropogenic sources, fluxes of Hg0 from contaminated soils and water bodies and natural fluxes of Hg0 all contribute to a global atmospheric mercury reservoir with a holding time of ½ to 2 years. Global atmospheric circulation systems can take Hg0 emissions from their point of origin and carry them anywhere on the globe before transformation and deposition occur. Emissions of all other forms of mercury are likely to be deposited to the earth's surface before they thoroughly dilute into the global atmosphere. Continental-scale atmospheric modeling, such as that performed for the study using the Relative Mapping Triangulation (RELMAP) program, can explicitly simulate the atmospheric lifetime of gaseous and particulate Hg(II) species, but not Hg0. Although Hg0 is included as a modeled species in the RELMAP analysis, the vast majority of Hg0 emitted in the simulation transports outside the spatial model domain without depositing, and the same is generally thought to happen in the real atmosphere. Natural Hg0 emissions and anthropogenic Hg0 emissions from outside the model domain are simulated in the form of a constant background Hg0 concentration of 1.6 g/m^{-3}, approximating conditions observed in remote oceanic regions (Fitzgerald, 1994).

"This background Hg0 concentration is subject to simulated wet deposition by the same process as explicitly modeled anthropogenic sources of Hg0 within the model domain. Explicit numerical models of global-scale atmospheric mercury transport and deposition have not yet been developed .The understanding of the global nature of atmospheric mercury pollution develop, numerical global-scale atmospheric models will surely follow. Deposition of mercury the divalent species emitted, either in the vapor or particulate phase, are thought to be subject to much faster atmospheric removal than elemental mercury (Lindberg et al., 1991, Shannon and Voldner, 1994). Both particulate and gaseous divalent mercury are assumed to dry deposit (this is defined as deposition in the absence of precipitation) at significant rates when and where measurable concentrations of these mercury species exist. The deposition velocity of particulate mercury is dependent on atmospheric conditions and particle size. Particulate mercury is also assumed to be subject to wet deposition due to scavenging by cloud microphysics and precipitation. The gaseous divalent mercury emitted is also expected to be scavenged readily by precipitation. Divalent mercury species have much lower Henry's law constants than elemental mercury, and thus are assumed to partition strongly to the water phase. Dry deposition of gas phase divalent mercury is thought to be significant due to its reactivity with surface material. Overall, gas phase divalent mercury is more rapidly and effectively removed by both dry and wet deposition than particulate divalent mercury (Lindberg et al., 1992; Petersen et al., 1995; Shannon and Voldner, 1994), a result of the reactivity and water solubility of gaseous divalent mercury. In contrast, elemental mercury vapor is not thought to be susceptible to any major process of direct deposition to the earth's surface due to its relatively high vapor pressure and low water solubility.

“On non-assimilating surfaces elemental mercury deposition appears negligible (Lindberg et al., 1992), and though elemental mercury can be formed in soil and water due to the reduction of divalent mercury species by various mechanisms, this elemental mercury is expected to volatilize into the atmosphere (Expert Panel on Mercury Atmospheric Processes 1994).

“In fact, it has been suggested that *in-situ* production and afflux of elemental mercury could provide a buffering role in aqueous systems, as this would limit the amount of divalent mercury available for methylation (Fitzgerald, 1994). Water does contain an amount of dissolved gaseous elemental mercury (Fitzgerald et al., 1991), but it is minor in comparison to the dissolved-oxidized and particulate mercury content. There appears to be a potential for deposition of elemental mercury via plant-leaf uptake. Lindberg et. al. (1992) indicated that forest canopies could accumulate elemental mercury vapor, via gas exchange at the leaf surface followed by mercury assimilation in the leaf interior during the daylight hours. This process causes a downward flux of elemental mercury from the atmosphere, resulting in a deposition velocity. Recent evidence (Hanson et al., 1994) indicates that this does occur but only when air concentrations of elemental mercury are above an equilibrium level for the local forest ecosystem.

“At lower air concentration levels, the forest appears to act as a source of elemental mercury to the atmosphere, with the measured mercury flux in the upward direction.

Lindberg et. al. (1991) noted this may be explained by the volatilization of elemental mercury from the canopy/soil system, most likely the soil. Hanson et al. (1994) stated that dry foliar surfaces in terrestrial forest landscapes may not be a net sink for atmospheric elemental mercury, but rather a dynamic exchange surface that can function as a source or sink dependent on current mercury vapor concentrations, leaf temperatures, surface condition (wet versus dry) and level of atmospheric oxidants. Similarly, Mosbaek et al. (1988) showed that most of the mercury in leafy plants is due to air-leaf transfer, but that for a given period of time the amount of elemental mercury released from the plant-soil system greatly exceeds the amount collected from the air by the plants. It is also likely that many plant/soil systems accumulate airborne elemental mercury when air concentrations are higher than the long-term average for the particular location, and release elemental mercury when air concentrations fall below the local long-term average. On regional and global scales, dry deposition of elemental mercury does not appear to be a significant pathway for removal of atmospheric mercury, although approximately 95% or more of atmospheric mercury is elemental mercury (Fitzgerald, 1994).

“There is an indirect pathway, however, by which elemental mercury vapor released into the Atmosphere may be removed and deposited to the earth's surface. Chemical reactions occur in the aqueous phase (cloud droplets) that both oxidize elemental mercury to divalent mercury and reduce the divalent mercury to elemental mercury. The most important reactions in this aqueous reduction oxidation balance are thought to be oxidation of elemental mercury with ozone, reduction of divalent mercury by sulfite (SO) ions or complexation of divalent mercury with soot to form particulate 3-2divalent mercury: Hg0 (g) Fitzgerald, 1994).” (EPA, 1997)

2.6 Mercury Air Concentrations

EPA (1997) states that “anthropogenic emissions are currently thought to account for between 40-75% of the total annual input to the global atmosphere (Expert Panel, 1994; Hovart et al., 1993b). Current air concentrations are thought to be 2 - 3 times preindustrial levels. This is in agreement with the several fold increase noted in inferred deposition rates (Swain et al., 1992; Engstrom et al., 1994; Benoit et al., 1994)”. A summary of atmospheric mercury concentration is shown in Tables 2.2 and 2.3

Table 2.2 (Summary of measured mercury concentration in the atmosphere)

Total atmospheric mercury (ng/m^3)	**% Hg (II)**	**% Methylmercury**
Rural areas ; 1-4	1-25%	0-215
Urban areas ; 10 – 170		

(EPA, 1993)

Table 2.3 (vapor and particulate-phase atmospheric mercury concentration measured)

Site	**Vapor phase mercury concentration in ng/m3**	**Particulate phase mercury concentration in ng/m^3**	**References**
Chicago ,IL	8.7 (1.8-62.7)	0.098(0.022-0.52)	Keeler et al.1994
Lake Michigan	2.3(1.3-4.9)	0.028 (0.009-0.054)	Keeler et al 1994
South haven	2.0 (1.8-4.3)	0.019 (0.009-0.029)	Keeler eta al1994
		0.022(max 0.086)	Keeler et al 1995
Ann Arbor MI	2.0 (max 4.4)	0.10 (max 0.21)	Keeler eta al1994
		0.022 (max 0.0770	Keeler et al 1995
Detroit MI	40.8 (max 70.4)	0.34 9 (max 1.09)	Keeler eta a,l1994
		0.094 (0.022-0.23)	Keeler et al, 1995
Detroit MI site B	3.7 (max 8.5)	0.3 (max 1.23)	Keeler et al.1994
Pellston MI		0.011 (max 0.32)	Keeler et al 1995
Broward county FI	1.8	0.034	Dvonch et al, 1995
Broward county FI site 2	3.3	0.051	Dvonch et al, 1995
Little rock WI	1.6 (1.0 -2.5)	0.022 (0.007-0.062)	Fitzgerald et al, 1991
Long island CT	1.4 – 5.3	0.0062 (0.005-0.18)	Fitzgerald et al, 1991
Crab lake WI	1.7	Winter 0.006 Summer 0.014	Lamborg et al , (in press)
Underhill VT	2.0 (1.2-4.2)	0.011 (0.001-0.043)	Burke et al, 1995

(EPA, 1997)

EPA (1997) states that “measured U.S. atmospheric mercury concentrations are generally very low. The dominant form in the atmosphere is vapor-phase elemental mercury, although close to emission sources, higher concentrations of the divalent form may be present. Small fractions of particulate mercury and methylmercury may also be measured in ambient air. In rural areas, airborne particulate mercury is typically 4% or less of the total (particulate + gas phase) mercury in air (U.S. EPA, 1993; WHO, 1990). Particulate mercury comprises a greater fraction of the total in urban areas (U.S.EPA, 1993), and will consist primarily of bound Hg (II) compounds.

“There is a substantial body of recent data pertaining to the atmospheric concentrations and deposition rates of atmospheric mercury collected at specific sites across the U.S. Most of the collected deposition data are from sites located some distance from large emission sources. The data have been collected by several different groups of researchers. Keeler et al., (1994) measured vapor- and particulate-phase atmospheric mercury concentrations from a site in Chicago, IL, two sites in Detroit, MI and a Lake Michigan site. The mean values are presented along with the range of measurement data. The collection period for these sites was generally less than one month; for example, the Detroit data were collected during a 10-day period. Keeler et al., (1995) reported the results of several short-term atmospheric particulate mercury measurements in Detroit, Michigan and longer-term (1-year) particulate measurements at rural sites in Michigan and Vermont. In the Detroit measurements the particulates sampled were divided into two categories: fine (<2.5 μm) and coarse (>2.5 μm). The average size of the fine particles was 0.68 μm, and the average size of the coarse particles was 3.78 μm. Most (mean = 88%) of the particulate mercury at the Detroit, MI site was measured on fine particles; the range for individual samples was 60-100% of total particulate.

Fitzgerald et al., (1991) reported measured mercury concentrations at Little Rock Lake, WI from May of 1988 through September of 1989 and particulate mercury concentrations at Long Island Sound (Avery Point, CT)." (EPA, 1997)

2.7 Mercury Concentrations in Soil/Sediment

EPA (1997) reports that Soil mercury levels are usually less than 200 ng/g in the top soil layer, but values exceeding this level are not uncommon, especially in areas affected by anthropogenic activities. Soil mercury levels vary greatly with depth, with nearly all the mercury found in the top 20 cm of soil. Mercury levels are also positively correlated with the percentage of organic matter in soil (Nriagu, 1979).Top soil mercury concentrations are estimated to be a factor of 4-6 (Swedish EPA, 1991) higher now as compared to pre-industrial concentrations. Methylmercury percentages in soil are typically on the order of a few percent. Soil mercury levels are continuing to rise (Fitzgerald 1994), and most (up to 95%) of the anthropogenic mercury released over the past 100 years resides in surface soil (Fitzgerald, 1994; Expert Panel on Mercury Atmospheric Processes, 1994).

"Mercury from soil provides in most cases (depending on watershed characteristics) the main source of mercury to water bodies and fish. Mercury is very slowly removed from soil, and long after anthropogenic emissions are reduced, soil and water concentrations can be expected to remain elevated. Sediment mercury levels are typically higher than soil levels, and concentrations exceeding 200 ng/g are not unusual. Sediment mercury levels follow the same trends as soil in regards to depth, humic matter, and historical increases, and methylmercury percentage. There is some evidence suggesting that the methylmercury percentage increases with increasing total mercury contamination (Parks et al, 1989). “Two large-scale monitoring projects have measured mercury levels in coastal sediments: the National Oceanic and Atmospheric Administration’s (NOAA’s) National Status and Trends (NS&T) Program and EPA’s Environmental Monitoring and Assessment Program (EMAP) for estuaries. These programs and their findings are discussed below.

2.8 Chemical and physical properties of Methylmercury

EPA (1997) states that “a commonly occurring form of methyl mercury is methyl mercuric chloride ($CH3Hg^+Cl^-$), a stable salt form that exists as a white crystal. This compound is often used in laboratory dosing experiments investigating the toxicological properties of methylmercury. Because methylmercury exists as a free ion only in minute quantities (Prager, 1997), the chemical and physical data provided below are for the chloride salt. The table below presents available chemical and physical data for methylmercury chloride.

Table 2.4 (Chemical and physical properties of Methyl mercuric chloride)

Methylmercury	**Value**
Chemical formula	CH_3HgCl
Chemical structure	CH3-Hg-Cl-
Molecular weight	251.10 g/mol
Physical state (25°C)	White crystals
Boiling point (at 25 mm Hg)	No data
Melting point	170C
Density (25°C)	4.06 g/mL
Vapor pressure (25°C)	0.0085 mmHg
Water solubility (21°C)	100 mg/l
Log octanol/Water partition coeff	No data
Odor threshold (air)	No data
Conversion facto air (1ppm)	10.27 mg/m^3

(ATSDR, 1999; Kaufman, 1969).

2.9 Methylmercury Bioaccumulation.

According to EPA (1997) “methylmercury is a chemical that bioaccumulates and biomagnifies in aquatic food webs. The fates of mercury and methylmercury in the environment are complex. The processes are affected by numerous biotic and abiotic factors that are subjects of ongoing research. Methylation of mercury is a key step in the entrance of mercury into food chains. The biotransformation of inorganic mercury forms to methylated organic forms in water bodies can occur in the sediment and the water column. Inorganic mercury can be absorbed by aquatic organisms but is generally taken up at a slower rate and with lower efficiency than is methylmercury. Methylmercury continues to accumulate in fish as they age. Predatory organisms at the top of aquatic and terrestrial food webs generally have higher methylmercury concentrations because methylmercury is typically not completely eliminated by organisms and is M transferred up the food chain. Nearly 100% of the mercury that bioaccumulates in upper trophic level fish (predator) tissue is methylmercury.

“Numerous factors can influence the bioaccumulation of mercury in aquatic biota. These include, but are not limited to, the acidity (pH) of the water, length of the aquatic food chain, temperature, and dissolved organic material. (Dutton, 1998) Physical and chemical characteristics of a watershed, such as soil type and erosion or proportion of area that is wetlands, can affect the amount of mercury that is transported from soils to water bodies. Interrelationships among these factors are poorly understood and are likely to be site-specific. No single factor (including pH) has been correlated with extent of mercury bioaccumulation in all cases examined. Two lakes that are similar biologically, physically, and chemically can have different methylmercury concentrations in water, fish, and other aquatic organism (Dutton, 1998).

“After mercury is deposited from the atmosphere, its greatest adverse impact occurs in the aquatic ecosystem. In a series of chemical reactions, mercury can be converted by bacteria in the sediments to methylmercury, a form that is especially toxic to humans and wildlife. Fish absorb methylmercury from the water as it passes over their gills and as they feed on other organisms. As larger fish eat smaller ones, methylmercury concentrations increase in the bigger fish, a process known as bioaccumulation. Consequently, larger predator fish usually have higher concentrations of methylmercury from eating contaminated prey. Humans, birds and other wildlife that eat fish are exposed to methylmercury in this way.

“Women of child bearing age (i.e. 15 to 44 years of age) and pregnant women are of special concern in terms of methylmercury exposure Methylmercury exposure prior to pregnancy can also place the developing fetus at risk because methylmercury persists in body tissue and is slowly excreted from the body .As a result, the fetus maybe exposed to methylmercury concentrations of concern as a result of maternal exposure prior to pregnancy. Infants may ingest methylmercury from breastfeeding, thereby making them susceptible to greater risk than adults since breast feeding is the primary source of the infant diet”. (EPA, 1997)

2.10 Government Standards and Guidance of Methylmercury Exposure

Many government and international agencies have developed health standards for methylmercury exposure. These standards are utilized in the risk assessment, regulatory development and in issuing fish advisories. There is substantial agreement among these agencies on a safe level in terms of exposure to methylmercury. As a result of different uncertainty factors to provide the public with an ample margin of safety, however there is some difference in published advisory levels as shown in table 2.5

Table 2.5 (Methylmercury exposure assessment)

Population group	Highest acceptable level of mercury in maternal hair (PPM)	Uncertainty factor	Amount of methylmercury that can be safely consumed on daily bases over a lifetime without adverse effect
Women of Reproductive Age, pregnant women and children			
U.S EPA reference dose (RFD)	12	10	0.1 µg/kg/d
ATSDR minimal risk level	15.3	4.5	0.3 µg/kg/d
Canada provisional tolerable daily intake (PTDI)	10	5	0.2 µg/kg/d
Joint FAO/WHO Expert committee on food additives	14	6.4	0.23 µg/kg/d
Adults			
FDA TDI	NA	NA	0.47µg/kg/d

(NESCAUM, 2003**)**

2.13.1 Legal requirement to regulate Mercury emission from power plants.

2.13.1.1 Federal Requirement

Section 122(n)(1)(A) of the Clean Air Act of 1990 required EPA to conduct a study of hazardous air pollutant (HAP) emissions from electric utility steam generating units by 1993, and after considering the result of that study, to determine whether regulation limiting those emissions was appropriate and necessary. Exactly eight years after EPA documented the result of hazardous air pollutant emissions from the electric utility steam generating units, the final report was submitted by EPA to Congress.

The report states, that for the utility industry, mercury from coal fired power plants units was the greatest concern, as it endangers public health in a multiple ways however the report did not include a regulatory determination that was deferred to later date. Some environmental groups sued to require to required the agency to do the following;

- Collect additional information and control technologies
- Issue a regulatory finding by December 15, 2003
- Issue a propose regulation in the case of positive regulatory determination by December15, 2003
- Issue a final regulation by December15, 2004 (EPA, 2003)

2.13.1.2 State Requirement

As of June 2006, seven states have established more stringent emission limits that will take effect sooner than will EPA's, and ten other states are developing regulations that would do so. The states with regulations already promulgated (or laws enacted) are generally small and/or have few coal-fired power plants; they are Connecticut, Maryland, Massachusetts, Minnesota, New Hampshire, New Jersey, and Virginia. Together, these states have 42 coal-fired power plants, with a total of 86 electric generating units. The combined generation capacity of these units is estimated at 19,016 megawatts (Mw), 6% of total U.S. coal-fired electric generation. The states that have proposed but not yet finalized mercury standards, on the other hand, are generally larger and/or have a significant share of the nation's coal-fired generation capacity. These ten states are: Delaware, Florida, Georgia, Illinois, Michigan, Montana, New York, North Carolina, Pennsylvania, and Washington. They have 149 plants, with a total of 380 units. Their combined generation capacity is estimated at 94,008 Mw, about 31% of total U.S. coal-fired generation. At least 13 of the 17 state programs will require reductions of 80% to 90% in mercury emissions when fully implemented. The effective dates range from 2007 at the earliest to 2015, with most of the programs imposing at least a first phase reduction by 2010. The Clean Air Mercury Rule (CAMR) as noted earlier, also imposes a cap in 2010, but it calls for a 22% reduction in that year, whereas most of the state requirements call for 80% to 90% reductions by then. In general, the programs provide some flexibility by measuring compliance as a rolling 12-month average of emissions, rather than setting an emission limit to be met at all times. (EPA, 2009)

CAMR is even more flexible, allowing utilities to exceed the standard at individual facilities and even company-wide, provided that they obtain allowances for each pound of mercury emitted. Unlike the CAMR program, a key feature of which is the trading of emission allowances, the state programs generally prohibit interstate trading of mercury credits; many prohibit in-state trading, as well. These prohibitions address the concern that mercury hot spots might persist if individual plants could avoid installing controls by buying credits. Also, the states that prohibit interstate trading are insuring that emission reductions within their state not generate credits that could be used to delay reductions by plants in other states (i.e., states participating in the CAMR program) (EPA, 1997).

2.13.1.3 Oklahoma state and mercury ruling

The members of Oklahoma's Air Quality Council still have not decided whether to wait on the Federal Environmental Protection Agency to create new rules or adopt stricter standards proposed by national air quality interest group .The later rules would require mercury emission reductions of 90 percent by coal-fired power plants. The U.S.

Court of Appeals for the District of Columbia ruled that the EPA violated the Clean Air Act when it created a cap and trade systems for mercury emissions from coal-fired plants. The cap and trade system would have allowed power companies violating the emission standards to meet them by buying credits from other companies that were emitting less than permitted. The system gradually would have lowered mercury emissions nationally from 48 tons annually to about 15 tons about a 70 percent reduction by 2018, according to EPA. (EPA, 2009)

Oklahoma's Air Quality Council met in January 2008 to consider its options, environmentalists urged the group to adopt the stricter standard, saying that Oklahoma had some of the highest mercury contamination in the nation and that the emissions cause health problems for pregnant women, women of child-bearing age and children .

Any rules ultimately adopted by the council must be approved by the Environmental Quality Board of Oklahoma's Department of Environmental Quality and Oklahoma's Legislature. The DEQ director for the Air Quality Division in Oklahoma however agreed that he was not surprised that the agency's Air Quality Council will have another chance to make a decision about the proposed rules when it meets again in April. Representatives of Oklahoma's major utility companies described the court's ruling as a setback (Jack Money, 2008)

2.11 ATMOSPHERIC FATE AND TRANSPORT MODELING RESULTS

This section summarizes the results of the atmospheric fate and transport modeling of mercury using the long-range and local models.

2.11.1 Oklahoma state Emission inventories from eGRID.

The US EPA just launched an emission inventory database for the nation called eGRID where data for all emission inventories for all kinds of emissions can be accessed. The Emissions & Generation Resource Integrated Database (eGRID) is a comprehensive source of data on the environmental characteristics of almost all electric power generated in the United States, the eGRID web displays eGRID data in a user friendly way and allows the user to export data selected the current version of eGRID is eGRID2007 Version 1.1, which contains:

- Year 2005 information configured to reflect the electric power industry’s current structure as of December 31, 2007, including plant ownership and operators, parent company affiliations, company mergers, and grid configurations;
- Year 2004 data; and
- Years 2004 and 2005 State import-export and U.S. generation and consumption data.

State: **Oklahoma**

- 2004 2005

Capacity (MW): 21,126.7
Net Generation (MWh): 60,641,219.9
Heat Input (MMBtu): 613,186,712.9

Table 2.6 (emission inventories for power plants in Oklahoma for the year 2004)

Pollutant	**Emissions**	**Units**	**Output Emission Rates**	**Units**	**Input Emission Rates**	**Units**
Annual CO_2	52,334,634.9	tons	1,726.04	lb/MWh	170.70	lb/MMBtu
Annual SO_2	105,404.86	tons	3.4760	lb/MWh	0.3440	lb/MMBtu
Annual NO_x	83,122.34	tons	2.7410	lb/MWh	0.2710	lb/MMBtu
Ozone Season NO_x	37,214.52	tons	2.5560	lb/MWh	0.2530	lb/MMBtu
Annual Hg	**2,800.52**	**lbs**	**0.0462**	**lb/GWh**	**0.0046**	**lb/BBtu**
Annual CH_4	N/A		N/A		N/A	
Annual N_2O	N/A		N/A		N/A	

(eGRID- US-EPA, 2009)

State: **Oklahoma**

Data Year

● 2005

Capacity (MW): 21,796.6
Net Generation (MWh): 70,283,511.1
Heat Input (MMBtu): 640,617,403.1

Table 2.7 (emission inventories for power plants in Oklahoma for the year 2005)

Pollutant	Emissions	Units	Output Emission Rates	Units	Input Emission Rates	Units
Annual CO_2	54,918,161.6	tons	1,562.76	lb/MWh	171.45	lb/MMBtu
Annual SO_2	108,741.39	tons	3.0944	lb/MWh	0.3395	lb/MMBtu
Annual NO_x	87,234.01	tons	2.4823	lb/MWh	0.2723	lb/MMBtu
Ozone Season NO_x	41,141.98	tons	2.3163	lb/MWh	0.2545	lb/MMBtu
Annual Hg	**1,949.63**	**lbs**	**0.0277**	**lb/GWh**	**0.0030**	**lb/BBtu**
Annual CH_4	1,522,726.5	lbs	21.67	lb/GWh	N/A	
Annual N_2O	1,436,581.1	lbs	20.44	lb/GWh	N/A	

(eGRID- US-EPA, 2009)

Table 2.7 and 2.8 shows the annual mercury emission total to be 4749.63 lbs which is 2158.92kg for the year 2004 and 2005. Therefore, the average mercury emission on a yearly basis is approximated to 1079 kg/yr. It is assumed that with the decrease in 2005 mercury emissions, it is most reasonable to consider an average value of 1000 kg/yr mercury emission which will be used in the computer model to be used for the environmental fate assessment of this research work.

2.12 Assessment method to estimate environmental fate of chemicals

To know the fate of a chemical substance after it has been discharged into the environment, several mathematical modeling can be used, Numerous software programs have been developed that are able to compute and predict the concentrations of a substance to which organisms in any environmental medium might be exposed. With the aid of these models predictions can be made on how the substance behaves in the environment. The subsequent health risk assessments associated with it can be investigated. Scientists from the Institute for Environmental Studies at the University of Toronto, Ontario, Canada, have been working on this issue for many years, and have developed a model to predict the environmental fate of chemical substances.

The model they have proposed consists on five-stage process (Mackay, et al., 1996). These stages are developed to understand the fate of a substance after it has been discharged to the environment. These five stages are as follows:

- Stage 1 - Substance classification by its chemical type, and based on its type, the appropriate physical, chemical, and reactivity data is collected
- Stage 2 – compilation of discharge and background concentration data
- Stage 3 – evaluative or generic assessment of fate to determine the general features of the substance’s behavior

- Stage 4 – regional or far-field evaluation, using regional climatic and geographic conditions, to determine the impact of environmental conditions on the chemical’s behavior, and estimate average regional concentrations

- Stage 5 – local or near-field evaluation on points of entry and other potentially impacted sites to predict the exposure concentrations.

The first stage of an assessment is to determine the type of a chemical substance, which is one of the most important parts of an assessment. Hence, for the appropriate model to be used, the classification of a chemical of interest into one of five types is required. Description of these chemical types is summarized in Table 2.10 below

Table 2.8(Chemical classification and properties)

Chemical category	**Criteria**	**Partitioning data required**
Type 1	Substances that partition into all phases	Water, fat or lipids solubility, vapor pressure. Henry's law constant, octanol water partitioning coefficient.
Type 2	Substances that does not partition into the air	Partition coefficient into the solid surface and to organic carbon, solubility in water and fat.
Type 3	Substances that does not partition into the water	Partition coefficient into solids from air or a pure phase
Type 4	Substances does not partition into air and water or with negligible solubility	Sorptive properties from a pure phase to various solids
Type 5	Speciation chemicals	Partition data for all species

(Mackay, et al., 1996)

In the second stage of the computer model, the rates at which chemical substances are discharged into the environment media are determined. The third stage of the process involves the assessment itself. In this stage the fate assessment focuses on figuring out how the different properties of the chemical control its fate, its partitioning, how is it transported and transformed within environmental media, and its general persistence. This model predicts the substance itself, not its degradation products and metabolites. There are three reasons for conducting an evaluative fate assessment. First, it predicts the general features of chemical behavior, based on the most important characteristics of the chemical itself, not the environment. Secondly, by this assessment the level of concern warranted can be determined. Finally, the assessment can be undertaken, compared and communicated internationally. The most important information obtained from this stage of the fate assessment is the tendency for intermedia transport, such as evaporation, as well as for the persistence of the substance in the environment. This stage of the assessment involves four levels of the multimedia models, which are described in Table 2.9 below. Each of these levels provides the estimation of a chemical substance behavior in the environment (Mackay et al., 1996).

Table 2.9 Levels of multimedia fate models (Mackay, et al., 1996)

Model level	**Conditions evaluated**	**Fate information obtained**
Level I	Equilibrium partitioning under steady state	Environmental media to which the substance is partition. Substance concentration in these compartments.
Level II	Same as in level I plus losses through advective transport and degrading reactions	Residence time/persistence in the environment, major mechanism of loss by the reaction and advection tendency to transport
Level III	Non equilibrium since includes intermedia transport processes, steady state	The fate affect by media discharge, which of the intermedia transport processes are most important, which processes account for contamination in media besides receiving that receiving the discharge persistence
Level IV	Same as level III but unsteady state	Time needed to build up to recover from a initial concentration

(Mackay, et al., 1996)

Having conceptualized the relationship between the chemical properties and their significance in predicting the fate of the chemical using the model, the effects of the characteristics of the specific regional environment can also be determined. The fourth stage of the fate assessment is designated for this purpose, where the effects of environmental characteristics, such as changes in temperature, hydrology, meteorology, and the proportions and compositions of water and soil are estimated. (Mackay, et al., 1996). Moreover, if reliable discharge data are known, average concentrations for each medium can be determined. But if such data are unavailable, the general characteristics of chemical fate, like persistence, tendency for intermedia transport, and relative concentrations, can be evaluated. Therefore, the purpose of this stage is to assess the difference of the chemical's fate under regional environmental characteristics from the chemical's fate, determined for the generic environment (Mackay et al., 1996).

The fifth stage conducts the local or near-field evaluation on points of entry and other potentially impacted sites to predict the exposure concentrations (Mackay et al., 1996).

2.13. Assessment of environmental fate of chemicals for the generic environment Using the EQC Model

Mackay and others proposed the fifth stage of the process (1996) to estimate the environmental fate of chemicals. After all five stages have been examined; the effects of chemicals on environment and risk can be evaluated. The Equilibrium Criterion (EQC) Model addresses stage 3 of this assessment process. This model has been successfully used for the assessment of environmental fate of different type chemicals in generic environments (CEMC, 2003).

The purpose of the EQC Model is to evaluate the chemical behavior in the environment. However, this computer modeling software estimates an environmental fate of a chemical in a generic or hypothetical environment, which means that the behavior of a substance is estimated, based on its chemical properties, but no particular environmental parameters are taken into consideration in this stage of the assessment.

Generally, this model establishes the general characteristics of chemical behavior, such as into which media the chemical will tend to partition, the major loss mechanisms, an intermedia transport tendency, and its persistence features.

2.13.1 The principle of work of the EQC Model

Since the EQC model is designed to estimate environmental fate of a chemical substance in a generic environment, the standard default parameters of the hypothetical environment were established by Mackay et al. (1996). The evaluative environment set in the EQC Model has an area of 100,000 km^2, and the compartment dimensions and properties are given in the article (Mackay et al., 1996a). The model runs through a sequence of levels I, II, and III. These levels of the model calculate the chemical's partitioning, susceptibility to transformation and transport, environmental process and chemical characteristics that affect chemical fate. Figure 2-1 is a schematic diagram, representing a sequence of model calculations. Currently Level IV is not included in the program as the model currently is undergoing some updates to accommodate for the level IV which is the non steady state.

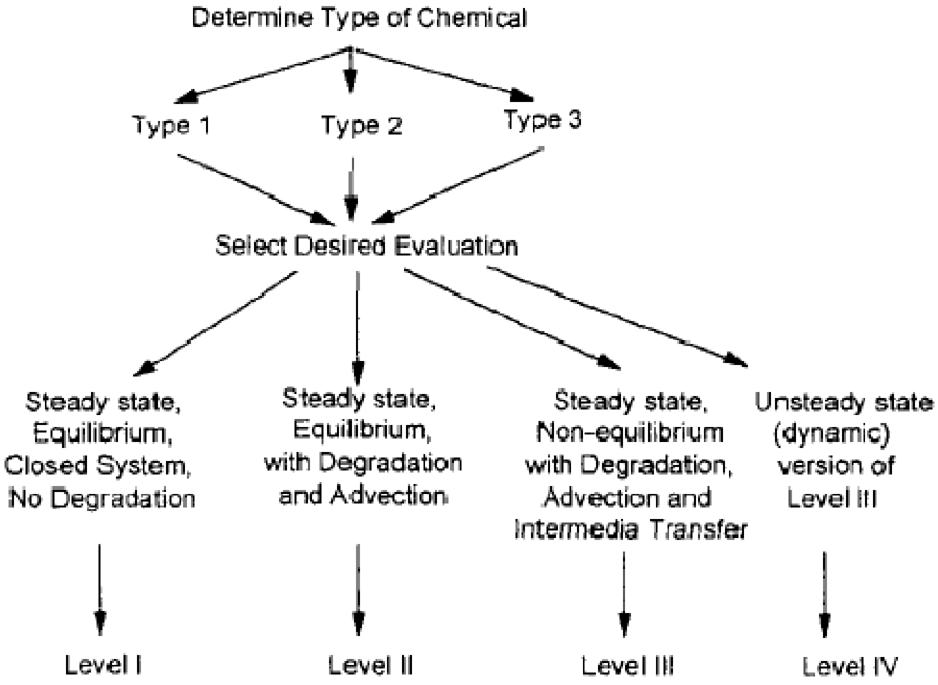


Figure 2.1, Block diagram of the variety of simulations possible with the EQC Model (Mackay et al., 1996a)

One of the first things to do to run the EQC Model is to determine the category the chemical. This model simulates chemicals, which fall into three categories:

Type 1 – chemical able to partition into all environmental media

Type 2 – chemical is involatile substance

Type 3 – substance is insoluble in water.

This software program treats only first three types of chemicals.

- Type 4 (involatile and insoluble chemicals), and
- Type 5 (multispecies substances), described earlier, are not modeled in this software.

For any types of chemicals, partitioning characteristics are described as Z values (fugacity capacities), expressing the affinity of a chemical to each environmental phase, such as air, water, soil, and sediment. Zero value of Z for a certain environmental phase indicates the zero or negligible tendency of a chemical to partition into this phase. The ratio of two Z values of different phases represents a partition coefficient between these phases (Mackay et al., 1996). Figure 2-2 represents a schematic diagram of partitioning relationships between various environmental phases.

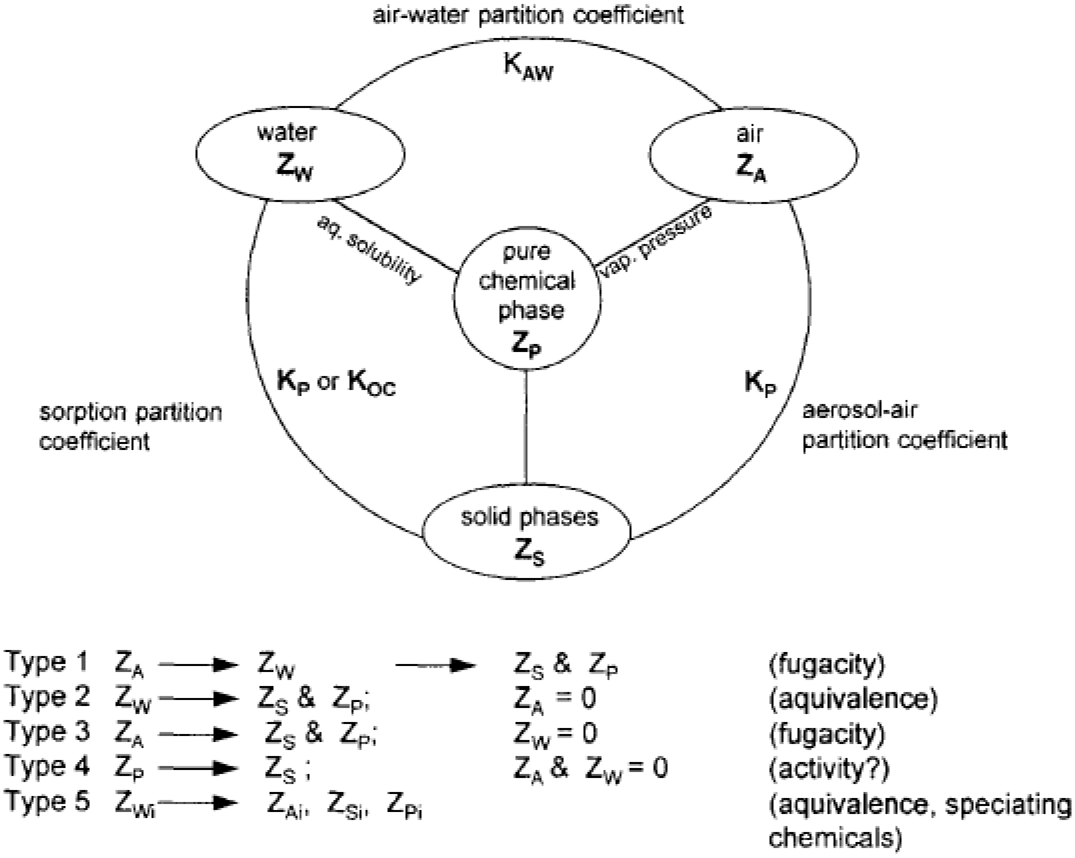


Figure 2.2, Schematic diagram of partitioning relationships

After Z values are calculated, the next stage of the model takes place – Level I, II ,and III calculations. Level I describe a scenario at which a fixed quantity of conserved (i.e. non-reacting) chemical is discharged in a closed system, under steady-state and equilibrium conditions. The information obtained from this estimation gives an idea of to which environmental phases does a chemical tend to partition, and it also computes relative concentrations of a substance that remain in each medium. The bio-concentration tendency is also estimated (Mackay et al., 1996a). Level II describes a situation where a chemical is continuously discharged into various environmental phases at constant rates, and achieves a steady-state and equilibrium condition, where input and output rates are equal. Here the degradation and advection rates are calculated from half-life rates. Intermedia transport processes are not considered in this part of the model. In a result of this level calculation, an overall environmental persistence of the chemical is estimated (Mackay et al., 1996a).

Level III calculates distribution of the chemical in an environment at steady-state conditions, not at equilibrium (between phases). Again, as in Level II, the chemical is assumed to be continuously discharged into a chosen environmental media at a constant rate, and achieves a steady-state condition, where input and output rates are equal. Intermedia transport processes, such as evaporation, sedimentation, are included. Here, the media receiving the emissions are very crucial, since the overall fate of the chemical depends on it (Mackay et al., 1996a).

When all three levels have been calculated, output data are generated in the form of graphs, charts and tables, giving a complete and easy to interpret picture of the chemical’s fate in an evaluative or generic environment (Mackay et al., 1996a).

2.14 ChemCAN software model

The more detailed assessment of environmental fate of chemicals can be done in stage IV and V of the five-stage assessment method. The fourth stage of an assessment can be accomplished by using ChemCAN v. 6 model (Webster et al., 2003), which is designed to estimate the multimedia behavior and fate of chemicals in certain environments with particular properties of the media. This software program is developed for the 24 regions of Canada. However, it may also be applied to an evaluative environment, or other regions of interest, where properties of the environment are defined by the user, (Webster et al. 2003).

ChemCAN version 6 model was also developed by the scientists of the Institute for Environmental Studies, University of Toronto, and was described in details by Mackay and others (Mackay et al., 1996b), and by Webster and others (Webster et al., 2003).

This model applies information on properties of chemicals and the environment to estimate a substance’s fate by computing partitioning, intermedia transport, and persistence of a chemical under certain environmental conditions. In this program, for the partitioning, transport, and transformation processes estimation, similar equations to those used in EQC Model are employed. The difference between these two models is that the ChemCAN estimates the behavior of a substance at some particular circumstance of some particular environment. Furthermore, this program estimates concentrations in fish, vegetation, groundwater, and coastal waters. Output characteristics are presented in tabular and graphical format, similar to the EQC Model.

CHAPTER III

METHODOLOGY

3.1 Introduction

This chapter gives a detailed description of the computer models that were used for the project. The basic physical and chemical property of methylmercury chloride as methylmercury is presented in Table 2.4. Table 4.1 listed the available results of the physical and chemical properties utilized in this project. The table 2.4 shows that the data published by the sources are not consistent with data predicted by the EPI model. These differences can be attributed to the uncertainty regarding the conditions and circumstances under which those values were measured. Therefore, in this research project it was decided not to use literature published data on chemical and physical parameters for the modeling process. Instead, it was decided to use a reliable software program which could be able to estimate and provide the data, needed for the fate modeling project.

For this purpose, to obtain a consistent data set on chemical and physical properties of substances, the EPI-EPA model was used in this work.(Estimation Program Interface (EPI) ™ Suite, v. 3.20 (U.S. EPA, 2007))

The EPI-EPA Suite program is used to overcome variations of data obtained from numerous literature observed in this work The EPI-EPA model is able to provide all the values to be applied for the modeling of the environmental fate of methylmercury.

Moreover, this program was accepted as a reliable source to use, since it was released by the U.S. Environmental Protection Agency. After producing the necessary parameters from the EPI Suite program, other programs were employed to predict the environmental fate of methylmercury compounds, the models including

Equilibrium Criterion (EQC) ™ Model, v. 2.02;

ChemCAN™, v. 6.0.

These two software programs are based on the work of Mackay and others (1996) on the five-stage assessment of chemical fate in the environment, described previously.

The EQC Model represents the third stage of the evaluation process, where the behavior of a chemical in an environment is simulated based on physical and chemical properties of a substance during a continuous input. The ChemCAN program corresponds to the fourth stage of an assessment, which describes the environmental fate of a chemical within a particular environment. This program was run to predict the fate of chemicals in Oklahoma, and to observe the behavior of chemicals under specified environmental conditions.

3.2 Description of Estimation Program Interface (EPI) Suite™ 3.20

Estimation Program Interface (EPI) Suite™ is a Windows® based suite, developed by the U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, along with Syracuse Research Corporation (SRC). EPI Suite™ and models, included in this software, are trademarks owned by the U.S. Environmental Protection Agency. Permission is granted to download and use this software for personal and business purposes. Software EPI Suite™ version 3.20 is available on the official web site of the U.S EPA.

3.2.1 Basic Functions of EPI software

EPI Suite™ v. 3.20 computer model is designed to estimate physical and chemical properties, and environmental fate of chemical substances. This software consists of the following estimation models:

- MPBPWIN: estimates the melting point, boiling point and vapor pressure
- WSKOWWIN: computes an octanol-water partitioning coefficient, and using this data estimates a chemical’s water solubility
- WATERN: water solubility estimation, using a “fragment constant” method
- ECOSAR: aquatic toxicity (LD_{50}, LC_{50}) estimation
- HENRYWIN: Henry’s Low constant (air/water partitioning coefficient)
- KOAWIN: octanol-air partitioning coefficient estimation, using the ratio of the octanol-water partitioning coefficient from KOWWIN, and the Henry’s Law constant from HENRYWIN
- KOWWIN: the log octanol-water partitioning coefficient estimation tool, using an Atom/fragment contribution method
- BIOWIN: an aerobic and anaerobic biodegradation probability of organic chemicals estimation
- BIOHCWIN: biodegradation half-life estimation for compounds, containing only carbon and hydrogen
- PCKOCWIN: soil adsorption coefficient (K_{oc}) estimation, i.e. the ability of a chemical to sorbs to soil and sediment

- HYDROWIN: estimation of hydrolysis rates (acid-base-catalyzed) for specific organic classes
- BCFWIN: estimation of the Bioconcentration Factor and its logarithm from the low K_{ow}
- STPWIN: the removal of chemical in a Sewage Treatment Plant prediction, using outputs from EPI Suite; values are given for the total removal and three contributing processes, which are: biodegradation, sorption to sludge, and stripping to air;
- LEV3EPI: the level III fugacity model predicts partitioning of chemicals between air, soil, sediment, and water under steady state conditions for a default model “environment
- AOPWIN: computes the atmospheric oxidation rates.

EPI Suite™ provides screening level evaluations of physical and chemical properties of chemical compounds, and their environmental fate properties. This modeling software is simple and easy to use, and does not require a lot of inputs to run.

EPI Suite is facilitated by a database of more than 40,000 chemicals (EPA, 2007) therefore, to run this computer program, only one input parameter is required – the chemical structure in SMILES notation, which means “Simplified Molecular Input Line Entry System”. SMILES can be entered via a linked file of CAS numbers, included within the EPI Suite. So, only the chemical name and CAS number are needed to be known to find out the chemical structure in SMILES notation (EPA, 2008b). As soon as SMILES of a chemical compound is input into the system, physical properties of the chemical can be obtained from the program’s database, which then can be transferred as the input parameters. After that, the program is ready to run the calculations. Results are then provided in the form of a report with tables and include the chemical structure of an evaluated substance. EPI Suite software was successfully run for this research project to estimate the properties of methylmercury. Results of these calculations will be presented and discussed in Chapter 4 of the report.

3.3 Equilibrium Criterion (EQC) ™ Model

Equilibrium Criterion (EQC) Model, a Visual Basic™ for Windows™ computer model, was developed by a group of Canadian scientists from the Institute for Environmental Studies, University of Toronto, Ontario. This model is designed to quantify a chemical's behavior in an evaluative environment, including air, water, soil, sediment, aerosol, and suspended sediments (CEMC, 2003). The EQC™ version 2.02 software is owned by Trent University, Canadian Environmental Modeling Center, and protected by Canadian copyright laws, (CEMC, 2003).

3.3.1 EQC Model description

The EQC Model uses the physical-chemical properties of a substance to quantify its behavior in a hypothetical environment. As was described in section 2.16.3 of the report, this model consists of three levels of complexity, Level I, Level II, Level III. The first two levels, I and II, assume that thermodynamic equilibrium is achieved. Level II also includes advective and reaction process; Level III estimates a chemical's fate in the environment at non-equilibrium, steady state conditions (CEMC, 2003). Here the common temperature of the environment is set to be 25 ^{0}C. The data of an evaluative area of 105 Km^2 with 10% of the area being covered with water was suggested by Mackay et al. (1996a).

3.3.2 EQC™ Model input parameters

The model is designed to evaluate different types of chemicals, and different parameters are required as input depending upon the type of chemical. This model classifies chemicals into three types. Table 2-10 summarized criteria for each of the types. Hence, Type 1 includes chemicals partitioning into all media; Type 2 includes involatile chemicals; and Type 3 includes chemicals with zero, or close to zero solubility.

According to the published data, methylmercury is sparingly miscible with water and able to evaporate into air the phase, but not partition into the soil phase (Schmidt, 2001; WHO, 2002).According to Table 2-10 this chemicals can be classified as Type 1 chemicals. The chemical property values of methylmercury shown in table 3.1 below:

Table 3.1(Chemical properties to determine the type of EQC)

Chemical property	**Methylmercury**
Solubility in water (g/m3)	3.125×10^{4}
Vapor pressure (Pa)	1.2×10^{4}

(EPI software, 2009)

According to Mackay et al. (1996a), if a chemical's vapor pressure is greater than 10^{-7} Pa and solubility in water is more than 10^{-6} g/m^3, this chemical belongs in a Type 1 chemical of the EQC model.

The required input data for the Type 1 chemicals in the EQC model are as follows:

- Chemical name;
- Molecular mass, g/mol;
- Reaction half-lives in each of air, water, soil, and sediment, hr;
- Data collection temperature, ^{o}C;
- Melting point, ^{o}C;
- Water solubility, g/m^3;
- Vapor pressure, Pa;
- Log Kow.

As explained in the introduction to this chapter, it was decided to use as input to the fate model values for physical and chemical properties produced by the EPIsuite model. The input data derived from the EPI Suite program are presented in Table 3.2 below.

Table 3.2 (Input data for EQC model determined)

Chemical Name	**Methylmercury**
Molecular weight (g/mol)	215.63
Data collection temperature ^{O}C	25
Melting point ^{O}C	60
Water solubility (g/m^3)	31250
Vapor pressure (Pa)	12000
Log Kow	0.08
Air	100000
Water	360
Soil	720
Sediment	3240

(EPI software, 2009)

The partitioning in the level III model is greatly influenced by the compartment receiving the emissions. It was recommended by Mackay et al. (1996), to run the level III model for emissions of 1,000 kg/hr into air, water, and soil first individually, and then in total. Because the equations are linear, the total case is the sum of first three cases (individual discharge into each phase). This method will indicate which emission is primarily responsible for the chemical substance present in each compartment (Mackay et al., 1996a). Input data of this is given in Table 3-3 below.

Table 3.3 (Emission rates for input for EQC model)

Emission	**Unit**	**Methylmercury**
Level I	Kg	100,000
Level II	Kg/hr	1000
Level III		1000
Air	Kg/hr	1000
Water	Kg/hr	0
Soil	Kg/hr	0
Sediment	Kg/hr	0
Level III		2nd case scenario
Air	Kg/hr	0
Water	Kg/hr	1000
Soil	Kg/hr	0
Sediment	Kg/hr	0
Level III		3rdcase scenario
Air	Kg/hr	0
Water	Kg/hr	0
Soil	Kg/hr	1000
Sediment	Kg/hr	0
Level III		4th case scenario
Air	Kg/hr	1000
Water	Kg/hr	1000
Soil	Kg/hr	1000
Sediment	Kg/hr	0

Table 3.3 above shows the four different scenarios that were run with the level III model (EQC) to predict the environmental fate of methylmercury in multimedia phases.

- The first case scenario considers 1000 kg/hr of methylmercury emitted through the air phase alone while other media are consider insignificant.
- The second case scenario involves methylmercury emission into the aqueous (water) phase alone, considering other media to have negligible emissions.
- The third case involves 1000 kg/hr of methyl mercury emitted or released into the soil phase, considering emission into other media negligible.

- The fourth case scenario involves running the model with 1000kg/hr of methyl mercury emitted into each phase of the media, air, water and soil, that's 3000 kg/hr for total.

3.4 ChemCAN Model description

ChemCAN v. 6.00 is a level III fugacity model of regional fate of chemicals, and was developed and released in September 2003 by the Institute for Environmental Studies, University of Toronto; Ontario. The Copyright belongs to Trent University. This program, as well as EQC Model v. 2.02 are provided by the Canadian Environmental Modeling Center, Trent University, and can be downloaded from the following web address http://www.trentu.ca/academic/aminss/envmodel/models/CC600.html.

3.4.1 ChemCAN v. 6.0 input parameters

ChemCAN v. 6.0 is designed to estimate the fate of different chemicals. Certain parameters must be input to run this program. As in the EQC Model, this model classifies chemicals into three types, and accordingly, for each type of chemical, certain input data are required. Previously, in section 3.3 of the report, the chemical type to which methylmercury belongs, was determined and justified. This substances falls into the type1 category. For this type of chemical, the following input data are required in this program.

Input data:

- Chemical name;
- Molecular mass, (g/mol);
- Any 2 out of 3 partition coefficients
- log K_{OW} (octanol-water), log K_{OA} (octanol-air), K_{AW} (air-water)

- Temperature dependence coefficients to adjust partition coefficient to region temperature
- Delta H KAW - Delta H KOW + Delta H KOA = 0, (J/mol)
- Reaction half-lives in each of air, water, soil, and sediment, (hr);
- Data collection temperature, (^{0}C);
- Coefficient to estimate aerosol partitioning.

The manual states that K_{AW} value can be entered as a measured value, in terms of Henry's law constant, or as water solubility and vapor pressure. In the case of the current study, KAW was entered through water solubility and vapor pressure parameters.

Temperature dependence coefficients to adjust partition coefficient to region temperature, Delta H KAW, Delta H KOW, and Delta H KOA, are not readily available for the methylmercury compounds. Hence, the default values were used, which are represented in Table 3-4 below.

Input data to run the ChemCAN model to predict the fate of methyl mercury in the Oklahoma region, are shown in Table 3.4 below. Chemical properties used as Input data for this model were derived from EPI Suite outputs.

Table 3.4 (Input data for ChemCAN model)

Chemical Name	**Methylmercury**
Molecular weight (g/mol)	215.63
Data collection temperature ^{O}C	11.4
Melting point ^{O}C	60
Water solubility (g/m^3)	31250
Vapor pressure (Pa)	12000
Log Kow	0.08
Temperature dependence coefficient	
ΔH for K_{ow}	-
ΔH for K_{ow}	-
ΔH for K_{oa}	-
Coefficient to estimate aerosol partitioning coefficient	
Air	31.46
Water	360
Soil	720
Sediment	3240

(EPI software, 2009)

The other input parameters, required by this software program are “regional properties”, which include data on environmental properties for a given region. For the purpose of this work, the regional data obtained and incorporated with this model is include the total area of the land for Oklahoma (181,195 km^2) and the percentage covered by water (1.8%)(http://www.ers.usda.gov/statefacts/ok.htm, 06/11/2009). These were the only two parameter required for the model.

However, the ChemCAN model requires a pollutant’s discharge input rate in terms of kg per year. No data currently exist for the 2006-2009 emission inventories on the eGRID –EPA data base, therefore the 1000 kg/yr estimated for the 2004-2005 emission data will be used as input into the ChemCAN model. Therefore, in this

The output data on the rate of methylmercury degradations in different media were taken. Table 3-5 displays input parameters of emission rates of Methylmercury.

Table 3.5 (Input Emission rates of methyl mercury chemical in Oklahoma (kg/yr))

Environmental phase	**Methylmercury**
Air	1000
Water	1000
Soil	1000
Sediment	0

(eGRID-EPA, 2009)

CHAPTER IV

FINDINGS

4.1 Introduction

This chapter present the analysis of results obtained from the various computer models described in chapter 3.

4.2 EPI model result

The chemical properties of Methylmercury calculated by the EPI modeling program are summarized in Table 4.1.

4.2.1 EPI Suite results for methylmercury modeling

The chemical properties estimated for methylmercury by the EPI model show that the basic properties, such as molecular weight, boiling point, melting point, water solubility, and vapor pressure cannot be directly compared as literature predict the properties of methylmercury chloride as methylmercury while the EPI suite utilizes the methylmercury predictions without the chloride and so this brings about variation in the basic properties from each other. Therefore, it is however appropriate to use the values estimated by EPI software to this study.

Partitioning coefficients such as Log KAW (air-water) and log KOA (octanol-air) were estimated by the program but were not available in the literature. The soil adsorption coefficient, log KOC, and bioaccumulation coefficient, log BCF, were obtained only by the EPI software. The half-live in air, water and sediment compartments were estimated. Here, the half-life for methylmercury in the air phase was estimated to be 31.46 hrs, whereas the half-life rate of this substance cannot be found in the literature.

For the water phase, the half-life rate estimated is 900 hours. The published data on half-life time for the chemical in soil phase also cannot be found. The estimated half-life by computer modeling gave 1800 hrs. Concerning the half-life time in sediments, there are no data available in the literature, and the estimated value by the EPI Suite is 8100 hrs.

Table 4.1 (Chemical and physical properties of Methylmercury)

Methylmercury	**Units**	**Value**	**Source/citation**
Molecular formula		CH3Hg	EPI-EPA model
CAS Number		016056-34-1	EPI-EPA model
Molecular weight	g/mol	215.63	EPI-EPA model
Melting point	Deg C	-69.49	EPI-EPA model
Vapor pressure	mmHg	89.8	EPI-EPA model
Boiling point	Deg C	82.97	EPI-EPA model
Log Kow	KowWin est	0.08	EPI-EPA model
Henry's law constant at 25C	Atm-m3/mole	7.22E-003	EPI-EPA model
logKoa	Atm-m3/mole	0.610	EPI-EPA model
			EPI-EPA model
Half-lives	Hrs		EPI-EPA model
Air	Hrs	31.46	EPI-EPA model
Water	Hrs	900	EPI-EPA model
Soil	Hrs	1800	EPI-EPA model
sediment	Hrs	8100	EPI-EPA model
			EPI-EPA model
Advection	Hrs		EPI-EPA model
Air	Hrs	100	EPI-EPA model
Water	Hrs	1000	EPI-EPA model
sediment	Hrs	5E+004	EPI-EPA model

(EPI software, 2009)

4.3 EQC Model results

The EQC Model was run for a Type 1 chemical compound for methylmercury. This section of the report represents the results obtained by using this software program. Tabular output data will be presented in appendices

4.3.1 EQC Model result for Methylmercury modeling

4.3.1.1 Level I outputs

The level I of EQC Model shows the general tendency of the pollutant to partition into various pure phases present in the environment. In this level, a fixed amount of chemical, 100,000 kg, is discharged in a closed system, under steady state conditions, and at equilibrium values are calculated with no reaction or advection loss processes.

Figure 4-1 represents the level I model diagram, depicting the general affinity of the methylmercury for the various phases present in the environment.

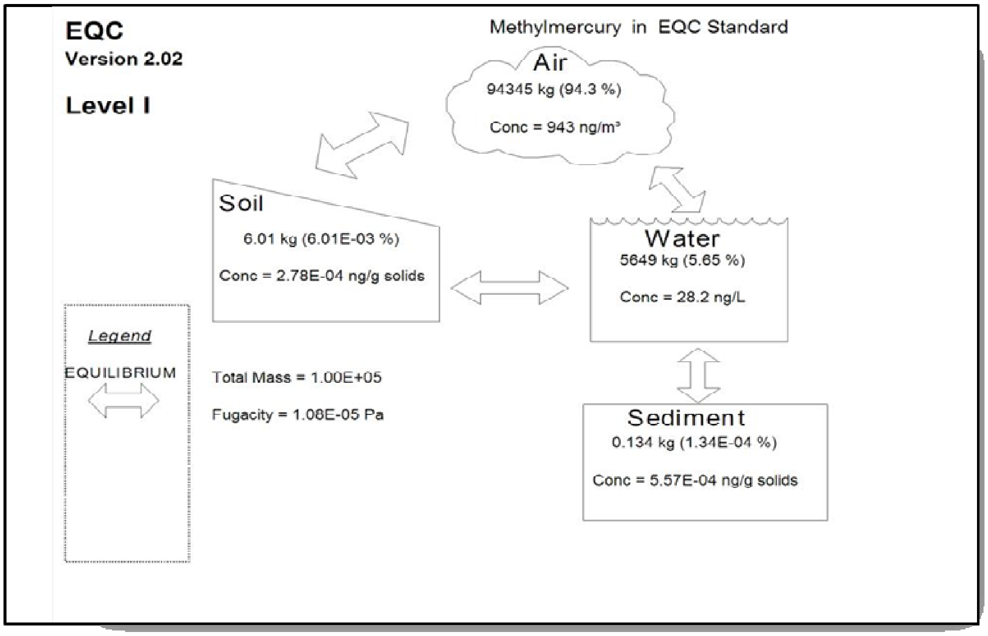


Fig 4.1 EQC level I result for Methylmercury emission

The above represented diagram, Figure 4.1, gives a general impression of how the chemical will most likely partition. Relative concentrations in each medium are also presented. According to Figure 4.1 above, most methylmercury, 94.3% tends to partition into the air. The rest of its amount, about 5.65%, partitions into water, and just about $6.01*10^{-3}$% partitions into soil compartment. Negligible amounts are found in sediment particles, (1.34*10^{-4}%) which are negligible. Thus most of the chemical will remain in the atmosphere while a small amount will dissolved in the aqueous phase methylmercury can then biaccumulate and enter the ecosystem.

4.3.1.2 Level II outputs

Level II describes a situation where a chemical is continuously introduced into environment at a constant rate, 1,000 kg/hr, and achieves a steady state and equilibrium condition, when input and output rates are equal. Here, the rates of degradation and advection are calculated. So, the initial emissions are balanced by reaction and advection losses in this system.

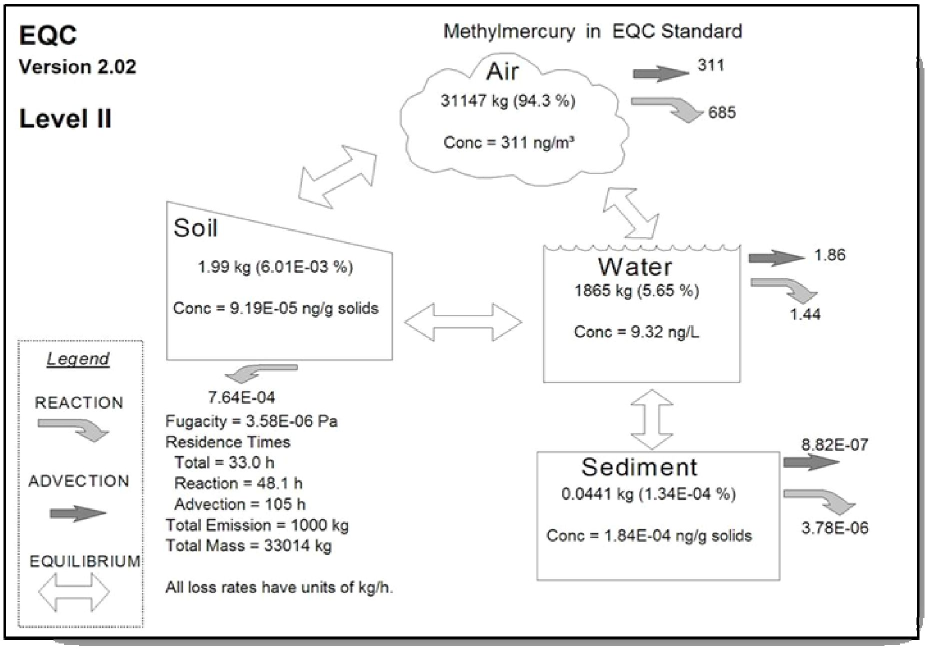


Fig 4.2 EQC level II result for methylmercury emission

The Level II model estimates the overall environmental persistence of the substance, and shows the most important removal processes going on in this system for the chemical of concern, methylmercury.

The Level II diagram in Figure 4-2, pictures relative partitioning of methylmercury in the environmental system, identical to Level I. However, decay reactions are included in this Level II modeling. According to the Figure 4-2, most of the methylmercury partition into the air (about 94.3%). There is about 311g of the contaminant removed from the air phase by advection flows, which is insignificant. In the water compartment, about 5.65% of the chemical while about 1.86 kg is taken away by advection. Sediment loss processes are very low and can be neglected, as well as the losses in the soil phase.

Figures 4-1 and 4-2 show the correlation between the chemical partitioning and deposition into the various media (air, water, soil and sediment). While about 94.3% of the chemical will remain in the air phase (312.86 kg) are been removed by advection 686.44 kg of the chemical is reacted. The overall residence time of the chemical is about 33 hours, meaning that there is about 33 hours inventory of chemical in the system. When the system reaches equilibrium, the total mass remaining in the environment is 33014 kg. The residence time of methylmercury in the system before it is removed by advection (ignoring reactions) is 105 hours, or 4.4 days. The residence time of the methylmercury remaining in the environment until reacting with other substances is 48.1 hours, which is about 2 days.

Therefore, the chemical has a tendency to largely remain in the atmosphere while about 6% of it remains in the water phase with insignificant amounts dissolving in water phase with low degradation rates. There is a negligible concentration of methyl mercury remaining in soil compartment, with slow degradation rates, which can be explained by the tendency of the substance to migrate from soil phase into the water compartment and evaporate into the air phase.

4.3.1.3 First case scenario - release into air

Figure 4-3 gives the more complex level III diagram, which shows non equilibrium, steady-state conditions, with emission rates of 1,000 kg/hr of methylmercury into the air phase only. The four compartments in this level model are not at equilibrium because of the resistances for intermedia transport processes. The level III output for methylmercury discharge shows that the about 96.8% of the chemical will partition to the air phase. The transfer rates from the air compartment to water and soil phases are low: approximately 3.06% of the initial chemical amount ends up in the water phase, and the rest of 0.172% remains in soil compartment, while about 5.95E-03% ends up in the sediment.

The major part of the substance mass is, contained in air phase, (68.7%) approximately 686kg/hr of the contaminant is removed by reaction process while 312 kg/hr is removed by advection. Therefore, the ratio of degradation in the air phase between the advection and the reaction is about 1:2.

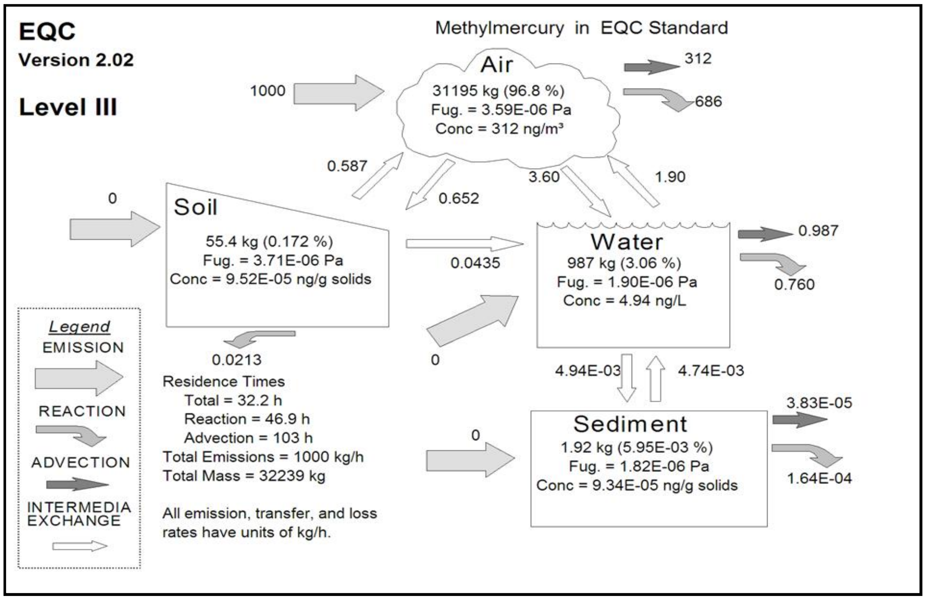


Fig 4.3a EQC level III result for methylmercury emission into air

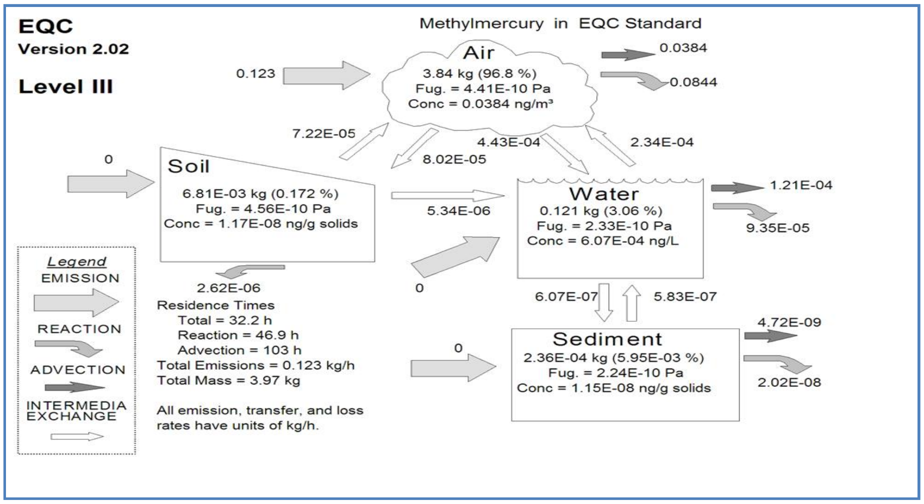


Fig 4.3b EQC level III result for methylmercury emission into air

As it can be seen from the diagram, there is intermedia transfer from soil to water, but not from water to soil, which again, confirms the mobility of the substance and resistance or partitioning of it into particles. In the soil phase methyl mercury migrates to the water compartment and thereby potentially increases the bioaccumulation. Very little of it degrades in this medium, and the rest remains. Degradation and advection rates in the aqueous phase are very low. Some small amount the chemical evaporates into air, and transfers into sediment particles. The total residence time of the chemical in the environment is about one and half days (32.2hrs). An advection persistence time is about four days, and reaction residence time is about two days. Hence, according to these estimations, out of the total mass of 32239 kg, accumulated in the system, 31195kg will persist in the atmosphere, 987 kg in water, and 55.4 kg in soil phases.

4.3.1.4 Second case scenario - discharge into water media

The results obtained for this case scenario are represented in Figures 4-4. In this simulation, when the contaminant is emitted only to water, almost all of the methylmercury, 94.2%, partitions into the aqueous phase, and some small amount transfers into the air phase (5.64%), while 0.183% is found in the sediment and a negligible amount is found in the soil phase.

The major removal mechanism in this case is the reaction process in water phase, removing about 43.6 % of the initial amount introduced into the media, and about 56.4 % of the methylmercury is advected in this phase. The evaporation rate of the substance from water to the atmosphere is estimated as 522 kg/hr, most of which reacts in this phase, and very little of it is advected by air flows. Methylmercury partitioned from air to soil can be neglected due to very small transfer rates, from which part of it dissolves in water, evaporates into the atmosphere, and degrades in this compartment. The mass of the chemical transferred from water to sediment particles is partly degraded and very little of it is removed by advection mechanisms.

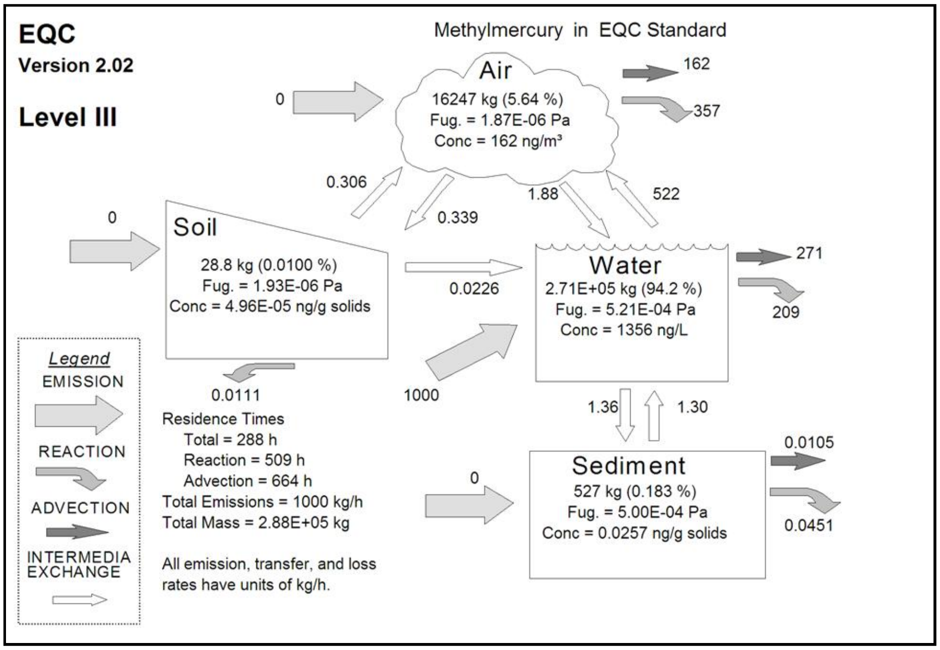


Fig 4.4a EQC level III result for methylmercury emission into water

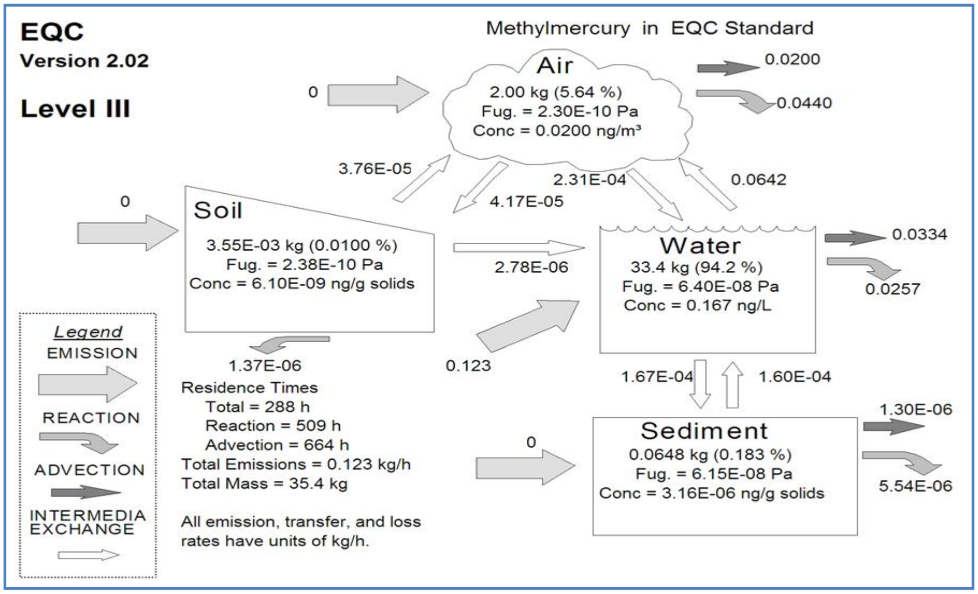


Fig 4.4 EQC level III result for methylmercury emission into water

Figure 4.4 shows the Level III estimation for the methylmercury discharged into water media. The total residence time of methylmercury in the system is 228 hours, or about two weeks is 509 hours, or 20 days, and the time while the chemical is not removed by the advection is 664 hours, or about 28 days. During this residence time the chemical is building up in the system, and the total mass, accumulated in the environment is 288,000 kg, most of which remains in the aqueous phase.

Hence, the outputs of the EQC Model show that methylmercury, if discharged directly into the aqueous phase, mostly dissolves there, and very little of it evaporates or is deposited in sediment. Even though the main removal process of the substance occurs in water media by reaction with other substances, significant mass accumulates in this media, due to high residence time. Therefore water contamination by methylmercury should be of the most concern in this case, since it is the primary and major source of exposure to methylmercury since methylmercury biaccumulates in the water phase and the aquatic organisms eventually become an exposure pathway to humans.

4.3.1.5 Third case scenario - spillage into soil

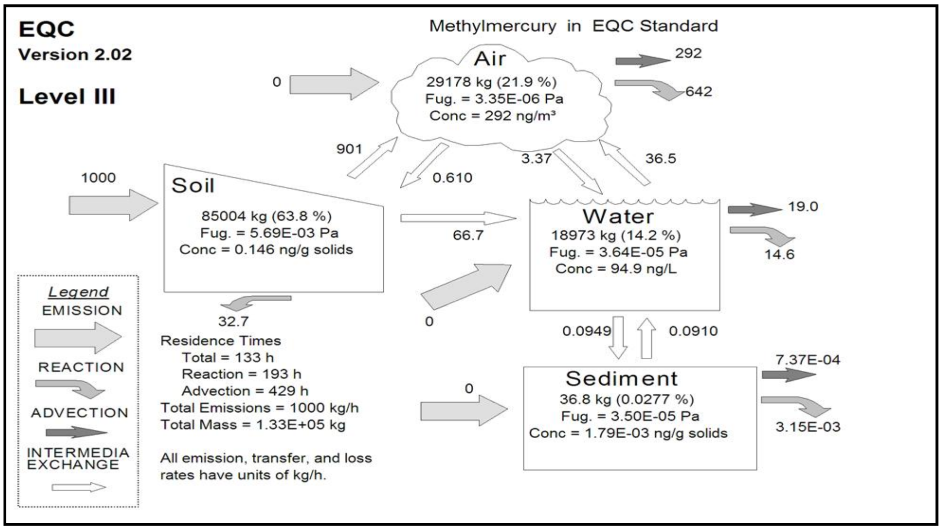


Fig 4.5a EQC level III result for Methylmercury emission into Soil

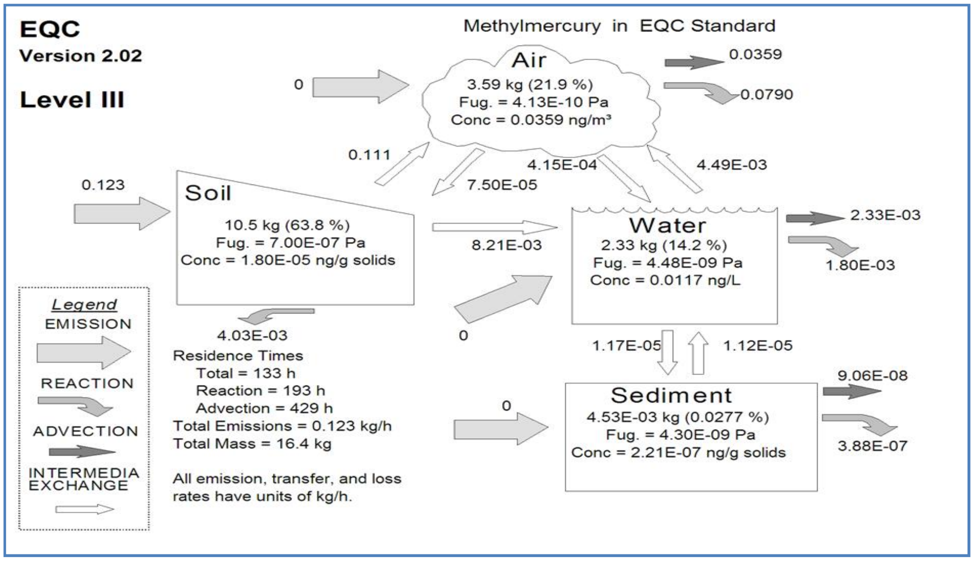


Fig 4.5b EQC level III result for Methylmercury emission into Soil

Figure 4.5 show that methylmercury discharged into the soil compartment is partitions into the phase of its release, approximately 63.8% of the amount introduced into the compartment. The remainder about 14.2 %, migrates to the aqueous phase. A considerable amount, 21.9 %, of initial concentration evaporates into atmosphere, and 0.0277 % ends up in sediment particles.

In this process, the main removal mechanism of methylmercury occurs in form of evaporation in which about 90.1% of the chemical is transported to the atmosphere. A considerable amount of the chemical, 66.7kg/hr, migrates into water phase, where its degradation rate is estimated at 14.6 kg/hr, or about 0.15% of initial discharge concentration. In the aqueous phase, about 13% of methylmercury is removed by advection flows at a rate of 16 kg/hr the contaminant evaporates into the atmosphere.

Small concentrations are transmitted from the atmosphere to soil and water. There is also a small mass of the chemical transferred from water to sediments, where it is degraded and advected as well.

The total residence time for methylmercury in the environment, before it starts to degrade is 133 hours, which is about 6 days. Due to such a long residence time, a large amount of the methylmercury accumulates in the environment, with a total mass of 1,300,000 kg. Most of it remains in the soil compartment (850004 kg), and in the aqueous phase, 18973kg. A smaller amount of 29178 kg remain in the atmosphere, while 36.8 kg stays in sediment particles.

Hence, it may be concluded that in case of methylmercury spillage into the soil the media, the methylmercury will remain in the environment for a long period of time, and a large amount of it will build up in soil and water phases. In other words, the most contaminated media will be soil and water, and the less polluted will be atmosphere.

4.3.1.6 Fourth case scenario - discharge into all three environmental phases: Air, soil, and water.

The results obtained for this case scenario are represented in Figures 4.6.

In the fourth scenario, the total discharge of 1,000 kg/hr into air, soil and water at the same time shows that approximately equal partitions of methylmercury between air and soil phases, 16.9% and 18.8% respectively, with a large amount of methylmercury partitioning into water, while insignificant percentage is bound with the sediment compartments.

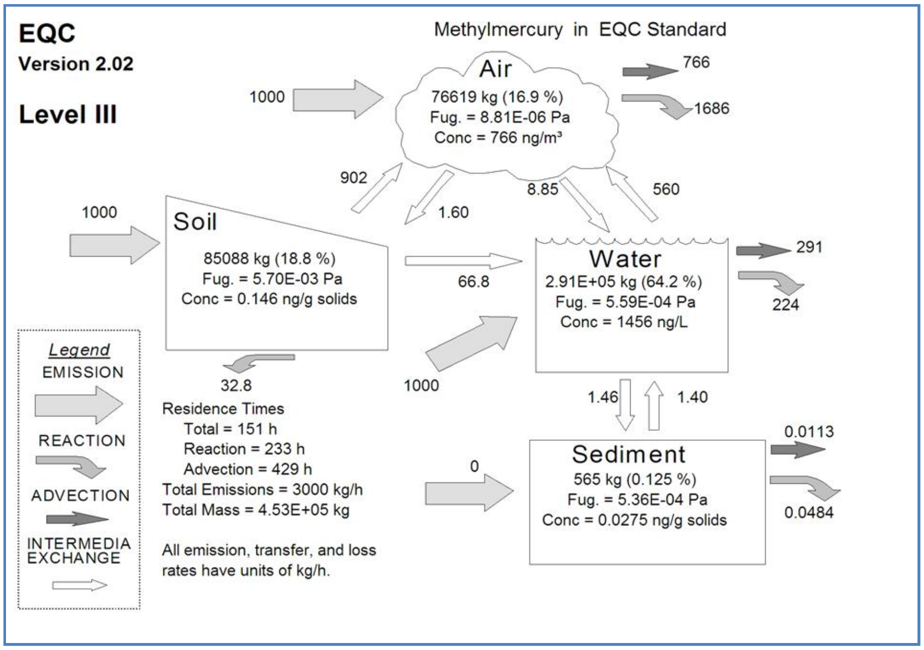


Fig 4.6a EQC level III result for Methylmercury emission into Air, Water and Soil

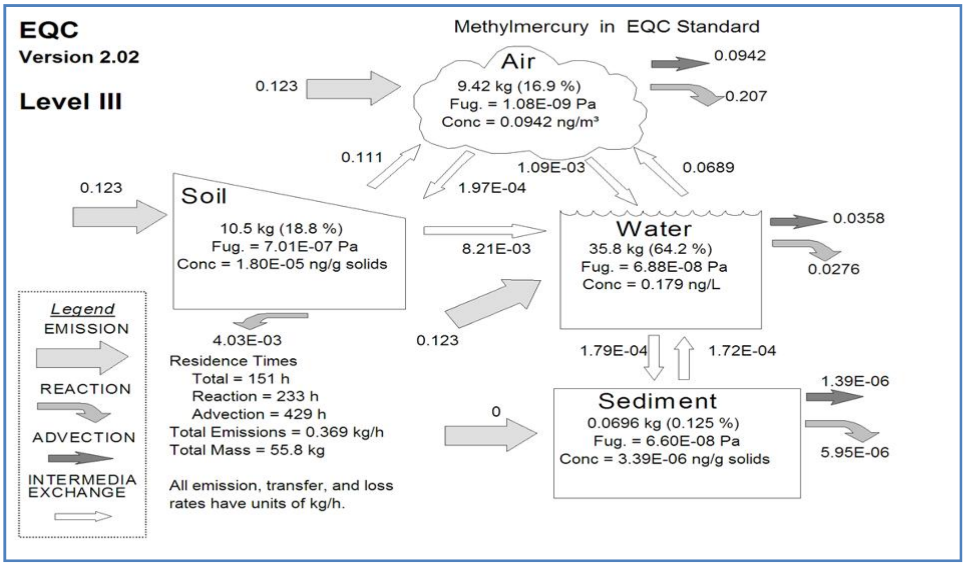


Fig 4.6b EQC level III result for Methylmercury emission into Air, water and Soil

Figure 4-6 the Level III estimation shows impact of the methyl mercury discharge into air, soil, and water. The major removal mechanism takes place in atmosphere, where approximately 81.7 % of the total initial concentration, introduced into all compartment, is removed by reaction and advection processes. In the air phase, about 60% of the contaminant from the aqueous and soil phases comes into the atmosphere via vaporization of the contaminant in aqueous and soil phase, 560 kg/hr and 902 kg/hr respectively, thereby increasing the mass emission in the air phase to about 82% which is 2462 kg/hr of total of 3000 kg/hr emitted. Of the 82% partitioning into the atmosphere, about 99.6% of the contaminant is removed as a result of reaction or advection processes. Approximately 766 kg/hr, which is about 31.5%, is taken away by advection, while 1686kg/hr that is 68.76% of the contaminant is reacted. Therefore the total percentage reduction of the contaminant in the air phase is 99.6%. Media transport of the contaminant from the air phase to the soil and aqueous phase is very insignificant (0.36%).

In the aqueous phase, also called the water or liquid phase, a total of 1000 kg/hr of the contaminant is released into the phase and about 53% of the total emission undergoes media transport (560kg/hr) into the air phase while 1.46kg/hr goes to sediment phase. About 47.8% of the contaminant released undergoes degradation with 56.5% of the losses through advection and 43.4 % through reaction, this equates to 224kg/hr of the contaminant taken away by reaction and 291kg/hr taken away by advection. Media transport of the contaminant to the aqueous phase from soil and air phase is about 7% 66.8kg/hr is transported from the soil (6.2%) and 8.85kg/hr is transported from the air phase while 1.40kg/hr is transported from the sediment. In the soil phase, a total of 1000kg/hr of the contaminant is considered to have been released, out of which 90.2% (902kg/hr) of the contaminant vaporized into the atmosphere while 66.8kg/hr migrates to the aqueous phase. About 96.8% of the contaminant released into the soil phase undergoing media transport. Degradation only occurs in the soil phase by reaction of the contaminant with 32.8 kg/hr of the emission is reacting which is just exactly about (3.28%) of the contaminant released.

The total residence time is about 6 days and 8 hours and advection persistence time is about 18 days while reaction residence time is 10 days. The total mass of methylmercury accumulated in the system is 453000 kg. Most of the contaminant mass partition into the water, (64.2%) while 16.9% partitions into the air and 18.8% partitions into the soil. The sediment retains the smallest partition approximately 0.125%. The concentration in the media is also estimated by the model with water (aqueous phase) having 1456 ng/l , the air phase 766 ng/m^3 , soil phase 0.146 ng/g, while sediment has 0.0275 ng/g.

According to all above discussed results, it can be concluded that the environmental fate of the contaminant (methylmercury) depends not just on its chemical properties, but also on the medium to which it is discharged. In this case the most critical is the water phase, since this is the most common exposure route by which the contaminant gets into the ecosystem and the human body.

4.3.1.8 Conclusions for methylmercury fate estimation with EQC Model

From the results of the EQC Model estimation of the environmental fate of methylmercury, it can be concluded that the medium into which discharge occurs affects the distribution characteristics in the environment. If the emission coming from the power plant is strictly from the stack the model shows that most of the methylmercury will remain in the air phase only minor amount of the contaminant partitioning into the water phase ,the soil and sediment phase.

Hence, in general, it can be concluded that methylmercury from power plant stack emission is most likely to partition into the atmosphere and the residence time is long.

4.4 ChemCAN™ Model simulation results

4.4.1 ChemCAN modeling results for methylmercury fates in Oklahoma region.

The ChemCAN Model v. 6.00 was run to estimate the behavior of methylmercury for the environmental conditions in Oklahoma. The model incorporates specific regional characteristics (temperature, weather, etc.) coupled with dynamic modeling from the EQC model. As explained in Chapter 3, it assumes a 1000 kg/year input to the air under the release column. The table 4.1 below shows the regional specific data incorporated into the ChemCAN model.

Table 4.2 (Specific regional properties for Oklahoma)

Regional parameters for Oklahoma	**Values**	**Source**
Temperature - Winter	36^o F	Oklahoma weather report, 2009.localweather-forecast.com
Spring	40^oF	Oklahoma weather report, 2009.localweather-forecast.com
Summer	82^oF	Oklahoma weather report, 2009.localweather-forecast.com
Wind speed	10.35 mph S	Oklahoma weather report, 2009.localweather-forecast.com
Total land area	181195 km^2	Oklahoma quick fact from bureau of US census,2009
Surface covered by water	1.8%	Oklahoma quick fact from bureau of US census,2009
Residence time	0.60 day	Estimated

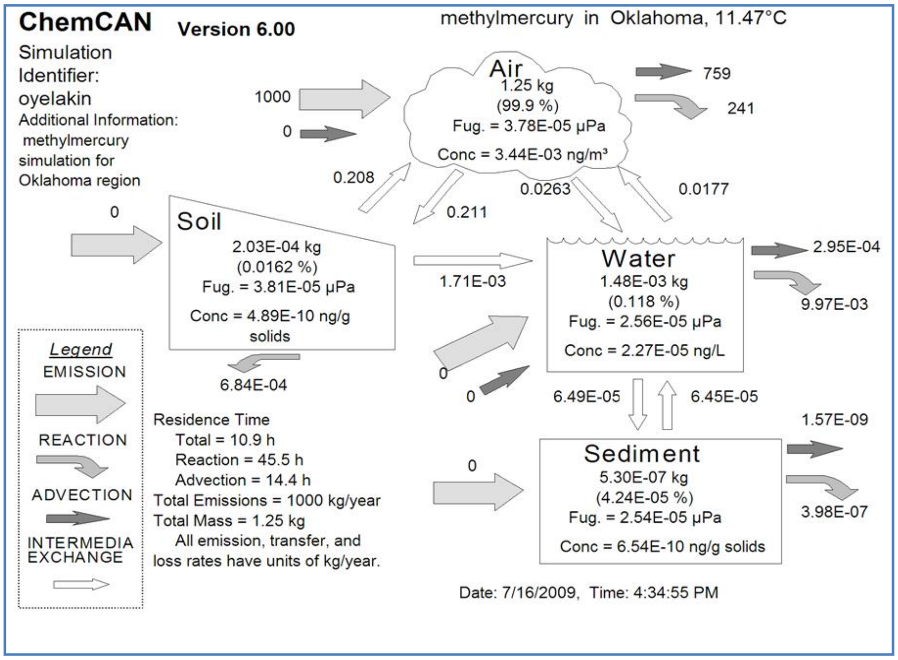


Fig 4.7 ChemCAN result for methylmercury emission into air phase

Figure 4.7 shows that 99.9% of the contaminant is release into the air phase. 1.25kg of the total mass emitted remains after equilibrium, 0.118% of the contaminant migrates to water phase while 0.00148 kg is left in the media after equilibrium. The concentration in the aqueous phase is critical to this study, so as to know the methylmercury concentration in Oklahoma fish. However the result of the ChemCAN model predicted 2.27 * 10^{-5}ng/L as the aqueous methylmercury concentration and so bioaccumulation factor is required.

The Department of Environmental Quality, report on Oklahoma fish consumption advisory level of mercury simply implies that mercury concentration in fish that is less than 0.5 µg/g is considered to be safe (Oklahoma DEQ, 2005). While Electric Power Research Institute (EPRI) from a research on Atmospheric Mercury Research Updates released in 2004,shows two different ranges of methylmercury bioaccumulation factor , that it 2500000 and 5200000 (EPRI,2004).

The methylmercury concentration in Oklahoma fish using the bioaccumulation factors obtained from the EPRI and the ChemCAN model aqueous concentration from fig 4.7 are therefore, 56.76 µg /g and 118.04µg/g.

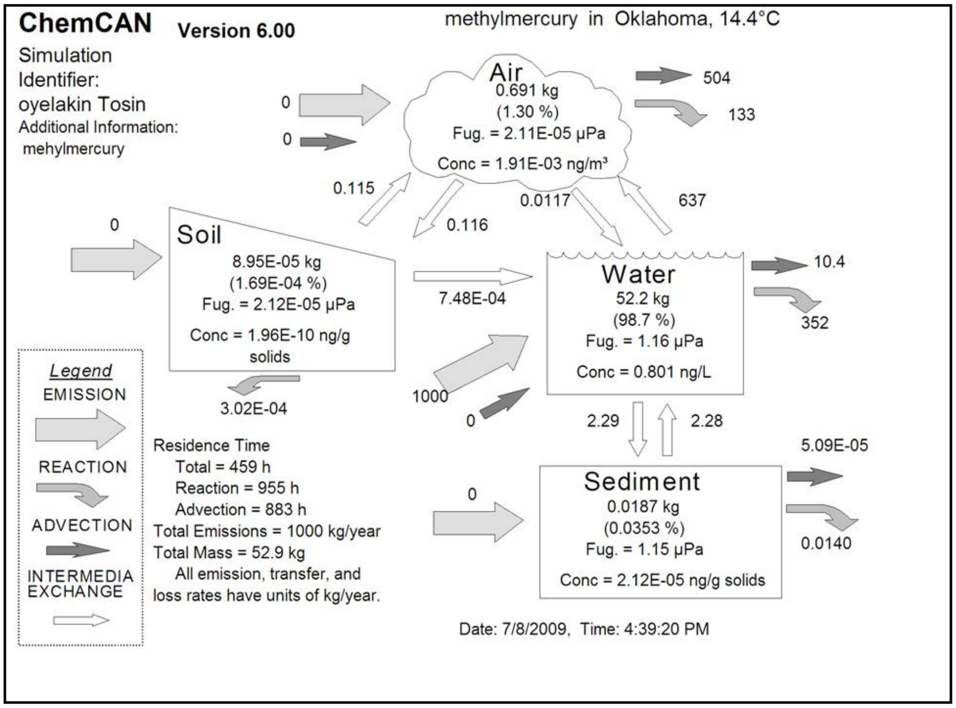


Fig 4.8 ChemCAN result for methylmercury emission into water phase

The second stage introduced when the entire emission into the water phase. The results show that 39kg/year of the contaminant comes into the water phase by advection approximately 66.6% of the total released into the water phase eventually evaporates into the atmosphere, while about 378 kg of the remaining mass undergoes degradation. About 97.4% of the total contaminant remaining in the water phase reacts while about 3% of the contaminant is taken away by advection.

4.4.2 Conclusions Methylmercury fates in Oklahoma region

The impact of mercury emissions from coal fired power plants in Oklahoma appears to be minimal under current conditions. The most common route of exposure through is water and modeling shows only a minor methylmercury enters into the water phase.

Overall, this software model estimation shows that as continuous emission of the mercury compounds from the coal-fired power plants in Oklahoma region considering the data for the 2004 and 2005 used in the model which the averaged is 1000 kg/year.

Based on this, the amount of methylmercury left in the environment is likely to be very low in air, soil, and sediment compartments. This perhaps could be the reason why EPA suspended the monitoring of mercury emissions.

CHAPTER V

CONCLUSION

5.1 Conclusion

The research study described herein provided an analysis of the environmental fate methylmercury, such that these data can be used in a risk assessment for humans. The main focus of this research effort includes the following:

1. Determination of chemical properties of methylmercury;
2. Based on chemical properties, estimation of the general environmental fate of the compound; and
3. Evaluation of the behavior of these chemicals in a particular environment, in Oklahoma.

Based on results just presented, conclusions can be made regarding the chemical properties and environmental fates of the methylmercury. These are listed below:

- Chemical properties of methylmercury can be estimated with EPI Suite model. Many of these calculated values do not agree well with experimentally determined values published in the literature because methylmercury properties are studied as methylmercury chloride in literature.
- Additional chemical properties for methylmercury, not available in published data, were also estimated with the EPI Suite, including the following:

- Partition coefficient air-water, log K_{AW} = -0.530
  - Partition coefficient octanol-air, log K_{OA} = 0.610
  - Half-life in air = 31.46 hrs
  - Half-life in water = 900 hrs
  - Half-life in soil = 1800 hrs
  - Half-life in sediment = 8100 hrs

1. Application of the EQC Model yielded estimates of methylmercury environmental fate. Conclusions from this model include:

- Distribution characteristics of the chemicals in the environment depend not only on the chemical properties but also on the media of discharge.
- The methylmercury concentration prediction in Oklahoma river is found to be far beyond the safe level, however these maybe due to various limiting factors such incorporated by the ChemCAN model
- Methylmercury is most likely to partition into the atmosphere.

2. Result of the ChemCAN Model evaluation of the environmental fate of a release of mercury emissions model as methylmercury from coal fired power plants into atmosphere include the following:

- Minimal concentration in the atmosphere or soil is expected for the conditions tested.
- Methylmercury tends to degrade in the air and water phase,

5.2 Recommendations for further research

Based on the current literature for the environmental fate of methylmercury as well as the results obtained from this study, the following list of recommended studies should be addressed. The losses of methylmercury through advection and reaction may be investigated to know if there is a possible potential risk associated that is not covered by this study, such as conclusion to the mercuric salts HgCl, Hg (OH) and HgS; the methylmercury compounds, methylmercury 2, 2 chloride (CH HgCl) and methylmercury hydroxide (CH HgOH); and, in small fractions, other 3, 3 organomercurics (i.e., dimethylmercury and phenylmercury).

- It is however recommended for future study that the advective inflow rate of mercury from neighboring states around Oklahoma region should be known for accurate fate study of methylmercury.
- It is also important to know the methylmercury concentration in Oklahoma river to be able to obtain a better degree of accuracy of methylmercury assessment in the future.

REFERENCES

1. Aberg, B., L. Ekman, R. Falk, U. Greitz, G. Persson, and J. Snihs. 1969. Metabolism of methyl mercury (Hg) compounds in man: excretion and distribution. Arch. Environ. Health 19:478-484.

2. Aschner, M., and J.L. Aschner. 1990. Mercury neurotoxicity: mechanisms of blood-brain barrier transport. Neurosci. Biobehav. Rev. 14(2):169-176.

3. ATSDR (Agency for Toxic Substances Disease Registry). 1999. Toxicological profile for mercury. Update. Atlanta, GA: ATSDR.

4. Bakir, F., S. Damluji, L. Amin-Zaki, et al. 1973. Methylmercury poisoning in Iraq. Science 181:230-241.

5. Ballatori, E. Miles and T. W. Clarkson Am J Physiol Regulatory Integrative Comp Physiol 252:842-847, 1987

6. Benoit, J.M., W.F. Fitzgerald and A.W.H. Damman (1994) Historical Atmospheric Mercury Deposition in the Mid-Continental U.S. as Recorded in an Ombrotrophic Peat Bog. Pp. 187-202 in Watras, C.J. and J.W. Huckabee eds. Mercury Pollution Integration and Synthesis.

7. Bernard, S., and P. Purdue. 1984. Metabolic models for methyl and inorganic mercury. Health Phys.46 (3):695-699.

8. Dvonch, J.T., A.F. Vette, G.J. Keeler, G. Evans and R. Stevens (1995) An intensive Multi-site Pilot Study Investigating Atmospheric Mercury in Broward County, Florida. Water, Air, and Soil Pollution 80: 169-178.

9. Ebinghaus, R., and O. Kruger (1996) Emission and Local Deposition Estimates of Atmospheric Mercury in North-Western and Central Europe. Pp. 135-159 in Baeyens, W., R. Ebinghaus, and O. Vasiliev, eds. Global and Regional Mercury Cycles: Sources, Fluxes and Mass Balances

10. Expert Panel on Mercury Atmospheric Processes (1994) Mercury Atmospheric Processes: A Synthesis Report. Report No. TR-104214.

11. Engstrom D.R., E.B. Swain, T.A. Henning, M.E. Brigham and P.L. Brezonick (1994) Atmospheric Mercury Deposition to Lakes and Watersheds: A Quantitative Reconstruction from Multiple Sediment Cores. Pp. 33-66 in L.A. Baker (ed). Environmental Chemistry of Lakes and Reservoirs. American Chemical Society.

12. Engstrom, D. R., and E. B. Swain (1997) Recent Declines in Atmospheric Mercury Deposition in the Upper Midwest. Environmental Science and Technology 31: 960-967.

13. Farris, F.F., R.L. Derrick, P.V. Allen, J.C. Smith. 1993. Physiological model for the pharmacokinetics of methyl mercury in the growing rat. Toxicol. Appl. Pharmacol. 119:74-90

14. Fang, S.C. 1980. Comparative study of uptake and tissue distribution of methyl mercury in female rats by inhalation and oral routes of administration. Bull. Environ. Contam. Toxicol. 24:65-72.

15. Fängström et al. (2000) Effects of developmental co-exposure to methylmercury and 2,2′,4,4′,5,5′-hexachlorobiphenyl (PCB153) on cholinergic muscarinic receptors in rat brain. NeuroToxicology 27 (2006) 468–47

16. Fitzgerald, W. F., and R. P. Mason (1996) The Global Mercury Cycle: Oceanic and Anthropogenic Aspects. Pp. 85-108 in Baeyens, W., R. Ebinghaus, and O. Vasiliev, eds., Global and Regional Mercury Cycles: Sources, Fluxes and Mass Balances

17. Ganther, H.E. 1978. Modification of methyl mercury toxicity and metabolism by selenium and vitamin E: possible mechanisms. Environ. Health Perspect. 25:71-76.

18. Glass, G., J. Sorensen, K. Schmidt, G. Rapp, D. Yap, and D. Fraser (1991) Mercury Deposition and sources for the Upper Great Lakes Region. Water, Air and Soil Pollution. 56:235-249.

19. Greenwood, M.R., T.W. Clarkson, R.A. Doherty, et al. 1978. Blood clearance half-times in lactating and nonlactating members of a population exposed to methyl mercury. Environ. Res. 16:48-54.

20. Hansen, J. 1988. Blood mercury concentrations in birth giving Greenlandic women. Arctic. Med. Res.47 (1):175-178.

21. Hansen, J., E. Reske-Nielsen, O. Thorlacius-Ussing, et al. 1989. Distribution of dietary mercury in a dog.Quantitation and localization of total mercury in organs and central nervous system. Sci. Total Environ.78:23-43.R-10 Methylmercury Water Quality Criterion 1/3/01

22. Hansen, J.E., U. Tarp, and J. Bohm. 1990. Prenatal exposure to methyl mercury among Greenlandic Polar Inuits. Arch. Environ. Health 45:355-358.

23. Harada, M. 1995. Minamata disease: Methylmercury poisoning in Japan caused by environmental pollution. Crit. Rev. Toxicol. 25(1):1-24.

24. Harada, M., H. Akagi, T. Tsuda, T. Kizaki, and H. Ohno. 1999. Methylmercury level in umbilical cords from patients with congenital Minamata disease. Sci. Total Environ. 234(1-3):59-62.

25. Hanson, P.J., S.E. Lindberg, T.A. Tabberer, J.G. Owens and K.-H. Kim (1995) foliar exchange of mercury vapor: Evidence for a compensation point. Water, Air and Soil Pollution 80:373-382.

26. Harada, M., J. Nakanishi, S. Konuma, K. Ohno, T. Kimura, H. Yamaguchi, K. Tsuruta, T. Kizaki, T.Ookawara, and H. Ohno. 1998. The present mercury contents of scalp hair and clinical symptoms in inhabitants of the Minamata area. Environ. Res. Section A 77:160-164.

27. Hollins, J., R. Willes, F. Bryce, et al. 1975. The whole body retention and tissue distribution of 203Hg methylmercury in adult cats. Toxicol. Appl. Pharmacol. 33:438-449.

28. Hovart, M., L. Liang, N. S. Bloom (1993b) Comparison of distillation with other current isolation methods for the determination of methylmercury compounds in low level environmental samples. Part II: Water. Analytica Chimica Acta, 282:153-168.

29. Hoffman**,** G.L., 2002.Environmental cycling and fate of mercury in the Arctic.RGM in ambient air is mercuric chloride vapor. Atmospheric Environment 37 (2003) 2551–2555

30. Jack Money, (2008). Mercury ruling hits coal plants in state, NewsOK.com

31. Jensen, A., and A. Iverfeldt (1994) Atmospheric Bulk Deposition of Mercury to the Southern Baltic Sea Area. Pp. 221-229 in Watras, C. J., and J. W. Huckabee eds. Mercury Pollution: Integration and Synthesis.

32. Keeler, G., M. Hoyer, and C. Lamborg (1994) Measurements of Atmospheric Mercury in the Great Lakes Basin. Pp. 231-241 in Watras, C.J. and J.W. Huckabee eds. Mercury Pollution Integration and Synthesis.

33. Keeler, G., G. Glinsorn and N. Pirrone (1995) Particulate Mercury in the Atmosphere: Its Significance, Transport, Transformation and Sources. Water, Air and Soil Pollution 80:159-168.

34. Keeler, G. J. (1997) Lake Michigan mass balance study atmospheric mercury data report. Submitted to the U. S. Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois, for Grant No. GL995569-01

35. Korogi, Y., M. Takahashi, T. Hirai, I. Ikushima, M. Kitajima, T. Sugahara, Y. Shigematsu, T. Okajima,and K. Mukuno. 1997. Representation of the visual field in the striate cortex: comparison of MR findings with visual field deficits in organic mercury poisoning (Minamata Disease). AJNR Am J. Neuroradiol.18:1127-1130

36. Lindberg, S. E., R. R. Turner, T. P. Meyers, G. E. Taylor, and W. H. Schroeder (1991) Atmospheric Concentrations and Deposition of Hg to a Deciduous Forest at Walker Branch Watershed, Tennessee,USA. Water, Air and Soil Poll. 56:577-594. Lindberg, S. E., T. P. Meyers, G. E. Taylor, R. R. Turner, and W. H. Schroeder (1992)

37. Lindqvist, O., and H. Rodhe. 1985. Atmospheric mercury: a review. Tellus 37B:136-159

38. Lindqvist, O. 1991. Mercury in the Swedish environment. Recent research on causes, consequences and corrective measures. Water Air Soil Pollut. 55:1-261.

39. Lindqvist, O., K. Johansson, M. Aastrup, A. Andersson, L. Bringmark, G. Hovsenius, L. Hakanson, A. Iverfeldt, M. Meili, and B. Timm (1991) Mercury in the Swedish Environment - Recent Research on Causes, Consequences and Corrective Methods. Water, Air and Soil Poll. 55:(all chapters)

40. Mackay D., Paterson, S., Kicsi, G., Di Guardo, A., Gowan, C.E. (1996). Assessing the Fate of chemicalsNew and Existing Chemicals: a five-stage process. Environmental Toxicology and Chemistry, Vol. 15, No. 9, pp. 1618-1626.

41. Mackay D., Pateson, S., Di Guardo, A., Cowan, C.E. (1996a). Evaluating the environmental fate of a variety of types of chemicals using the EQC Model. Environmental Toxicology and Chemistry, Vol. 15, No.9, pp. 1627-1637.

42. Mason, R.P., W.F. Fitzgerald, and F.M.M. Morel (1994). The Biogeochemical Cycling of Elemental Mercury: Anthropogenic Influences. Geochemical et Cosmochimica Acta, 58(15):3191-3198.

43. Mason, R.P., and K.A. Sullivan. 1997. Mercury in Lake Michigan. Environ. Sci. Technol. 31:942-947.

44. Mason, R. P., and K. A. Sullivan. 1998. Mercury and methylmercury transport through an urban water shed. Water Res. 32:321-330.

45. Mason, R.P., W.F. Fitzgerald, and F.M.M. Morel. 1994. The biogeochemical cycling of elemental mercury: anthropogenic influences. Geochim. Cosmochim. Acta. 58(15):3191-3198.

46. McIntyre, J.W., J.T. Hickey, K. Karwowski, C.L. Holmquist, and K. Carr (1993) In Proceedings fo the 1992 Conference on the Loon and its Ecosystem Status. Edited by L. Morse and M. Pokras. Concord,NH. U.S. Fish and Wildlife Service, pp. 73-91.

47. Michigan Environmental Science Board (1993) Mercury in Michigan's Environment: Environmental and Human Health Concerns. Report to Gov. John Engler.

48. Miettinen, J.K., T. Rahola, T. Hattula, K. Rissanen, and M. Tillander. 1971. Elimination of Hg methylmercury in man. Ann. Clin. Res. 3:116-122.

49. Mitsumori, K., K. Maita, and Y. Shirasu. 1984. Chronic toxicity of methyl mercury chloride in rats: Pathological study. Jpn. J. Vet. Sci. 46(4):549-557.

50. Nakamura, I., K. Hosokawa, H. Tamra, et al. 1977. Reduced mercury excretion with feces in germfree mice after oral administration of methyl mercury chloride. Bull. Environ. Contam. Toxicol. 17:528-533.

51. Newton, I., I. Wyllie, and A. Asher (1993) Long-term trends in organochlorine and mercury residues in some predatory virds in Britain. Environ. Pollut. 79:143-151.

52. Northeast States for Coordinated Air Use Management (NESCAUM), 2003 Mercury Emissions From coal -fired power plants Norseth T., and T.W. Clarkson. 1970. Studies on the biotransformation of 203Hg-labeled methyl mercurychloride in rats. Arch. Environ. Health 21:717-727 (as cited in Gray, 1995).

53. Nriagu, J.O. (1979). The Biogeochemistry of Mercury in the Environment. Elsevier/North Holland. Biomedical Press: New York.

54. Ostlund, K. 1969. Studies on the metabolism of methylmercury in mice. Acta Pharmacol. Toxicol.27 (Suppl.1):1-132.

55. Petersen, G., Å. Iverfeldt and J. Munthe, (1995) Atmospheric mercury species over Central and Northern Europe. Model calculations and comparison with observations from the Nordic Air and Precipitation Network for 1987 and 1988. Atmospheric Environment 29:47-68.

56. Porcella, D. B. 1994. Mercury in the environment, in Mercury Pollution: Integration and Synthesis, C.J.Watras and J.W. Huckabee, Eds. New York: Lewis Publishers. 727 pp.

57. Porcella, D.B., C.J. Watras, and N.S. Bloom. 1991. Mercury species in lake water. In: Verry, S., and S.J.Vermette. The deposition and fate of trace metals in our environment. Gen. Tech. Rep. NC-150. St. Paul,MN: U.S. Dept. Agric., Forest Service, North Central Forest Exp. Station, pp. 127-138.

58. Rowland, I., M. Davies, and J. Evans. 1980. Tissue content of mercury in rats given methyl mercury chloride orally: influence of intestinal flora. Arch. Environ. Health. 35:155-160.

59. Rice, D.C., D. Krewski, B.T. Collins, and R.F. Willes. 1989. Pharmacokinetics of methylmercury in the blood of monkeys (Macaca fascicularis). Fundam. Appl. Toxicol. 12:23-33.

60. Shannon, J. D., and E. C. Voldner (1994) Modeling Atmospheric Concentrations and Deposition of Mercury to the Great Lakes. Presented at the DOE/FDA/EPA

Workshop on Methylmercury and Human Health, Bethesda, MD March 22-23 1994.

61. Skerfving, S. 1988. Mercury in women exposed to methylmercury through fish consumption, and in their newborn babies and breast milk. Bull. Environ. Contam. Toxicol. 41(4):475-482

62. Suda, I., and H. Takahashi. 1986. Enhanced and inhibited biotransformation of methyl mercury in the rat spleen. Toxicol. Appl. Pharmacol. 82:45-52.

63. Sundberg, J., and A. Oskarsson. 1992. Placental and lactational transfer of mercury from rats exposed to methyl mercury in their diet: Speciation of mercury in the offspring. J. Trace Elem. Exp. Med. 5 (1):47- 56

64. Sukhenko, S. A., and O. F. Vasiliev (1996) A Regional Mercury Budget for Siberia and the Role of the Region in Global Cycling of the Metal. Pp. 123-133 in Baeyens, W., R. Ebinghaus, and O. Vasiliev,eds., Global and Regional Mercury Cycles: Sources, Fluxes and Mass Balances.

65. Suzuki, T., J. Yonemoto, H. Satoh, A. Naganuma, N. Imura, and T. Kigama. Normal organic and
66. Inorganic mercury levels in the human feto-placental system. J. Appl. Toxicol. 4(5):249-252.

67. Swain, E. B., D. A. Engstrom, M. E. Brigham, T. A. Henning, and P. L. Brezonik. (1992) Increasing Rates of Atmospheric Mercury Deposition in Midcontinent North America. *Science* 257:784-787

68. Swedish EPA (1991) Mercury in the Environment: Problems and Remedial Measures in Sweden. ISBN 91-620-1105-7.

69. Takeuchi, T., and K. Eto. 1975. Minamata disease. Chronic occurrence from pathological view points. In: Studies on the Health Effects of Alkyl mercury in Japan. Tokyo, Japan Environment Agency

70. The Canadian Centre for Environmental Modelling and Chemistry,EQC Modelhttp://www.trentu.ca/academic/aminss/envmodel/models/EQC2.html

71. Thomas, D., H. Fisher, L. Hall, et al. 1982. Effects of age and sex on retention of mercury by methylmercury-treated rats. Toxicol. Appl. Pharmacol. 62:445-454.

72. Thomas, D., H. Fisher, M. Sumler, et al. 1986. Sexual differences in the distribution and retention of organic and inorganic mercury in methylmercury-treated rats. Environ. Res. 41:219-234.

73. Thomas, D.J., H.L. Fisher, M.R. Sumler, et al. 1988. Distribution and retention of organic and inorganic mercury in methyl mercury-treated neonatal rats. Environ. Res. 47:59-71.

74. U.S. EPA. 1997a. Mercury study report to Congress. Vol. I. Executive summary. U.S. Environmental Protection Agency. December, 1997.

75. U.S. EPA. 1997b. Mercury study report to Congress. Vol. III. Fate and transport of mercury in the environment. U.S. Environmental Protection Agency. December 1997. EPA-452/R97-005.

76. U.S. EPA. 1997c. Mercury study report to Congress. Vol. IV. An assessment of exposure to mercury in the United States. U.S. EPA, Office of Air Quality Planning and Standards and Office of Research and Development. EPA/452/R-97-006.(http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm).

77. U.S. EPA. 1997e. Mercury study report to Congress. Vol. V. Health effects of mercury and mercury compounds. U.S. Environmental Protection Agency. December, 1997.

78. U.S. EPA. 1997f. Mercury study report to Congress. Vol. VI. An Ecological assessment for anthropogenic mercury emissions in the United States. U.S. Environmental Protection Agency. December 1997.

79. U.S. EPA. 1997g. Mercury study report to Congress. Vol. VII. Characterization of human health and wildlife risks from mercury exposure in the United States. U.S. Environmental Protection Agency. December 1997.

80. U.S Environmental protection Agency (2001) Water Quality Criterion for the Protection of Human Health: Methylmercury EPA-823-R-01-001;Washington D.C
81. U.S Environmental protection Agency **(**2003). Progress Report: Mercury Transformations in Coal Combustion Flue Gas .R827649C009.October,2003

82. U.S. EPA. 2004. Mercury emission from coal-fired Electric utility boiler. U.S. Environmental Protection Agency,NC. December, 2004

83. U.S. EPA. 2005. Mercury emission from coal-fired Electric utility boiler. U.S. Environmental Protection Agency, NC. December, 2005

84. US Environmental Protection Agency. (2007a). Estimation Programs Interface Suite™ for Microsoft® Windows, v3.20. United States Environmental Protection Agency, Washington,DC, http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

85. U.S. Environmental Protection Agency (2009). Estimation Program Interface Suite (EPI).http://www.epa.gov/opptintr/exposure/pubs/episuite.htm Found on March 2009

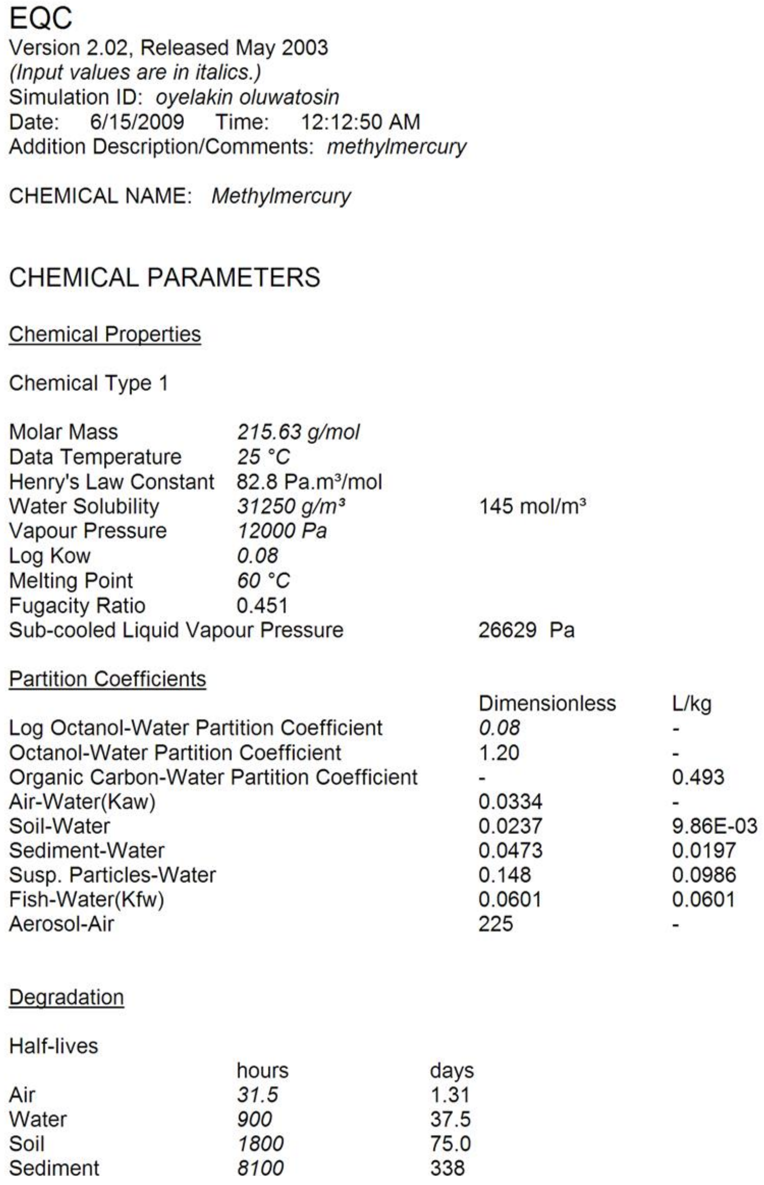
86. U.S. Environmental Protection Agency (2009).Human Exposure to methylmercury http://www.epa.gov/mercury/exposure.htm 31/03/2009

87. U.S. Environmental Protection Agency (2009).Air Toxic, technology transfer networks www.epa.gov/ttn/atw/utility/hgwhitepaperfinal.pdf 31/03/2009

88. Webster, E., Mackay, D., Di Guardo, A., Kane, D., Woofine D. (2003). Regional differences in chemical fate model outcome. Chemosphere 55 (2004) 1361-1376.

APPENDICES-A

First case scenario (Air)



EQC

Version 2.02, Released May 2003
(Input values are in italics.)
Simulation ID: *oyelakin oluwatosin*
Date: 6/15/2009 Time: 12:12:50 AM
Addition Description/Comments: *methylmercury*

CHEMICAL NAME: *Methylmercury*

CHEMICAL PARAMETERS

Chemical Properties

Chemical Type 1

Molar Mass	*215.63 g/mol*	
Data Temperature	*25 °C*	
Henry's Law Constant	82.8 Pa.m³/mol	
Water Solubility	*31250 g/m³*	145 mol/m³
Vapour Pressure	*12000 Pa*	
Log Kow	*0.08*	
Melting Point	*60 °C*	
Fugacity Ratio	0.451	
Sub-cooled Liquid Vapour Pressure		26629 Pa

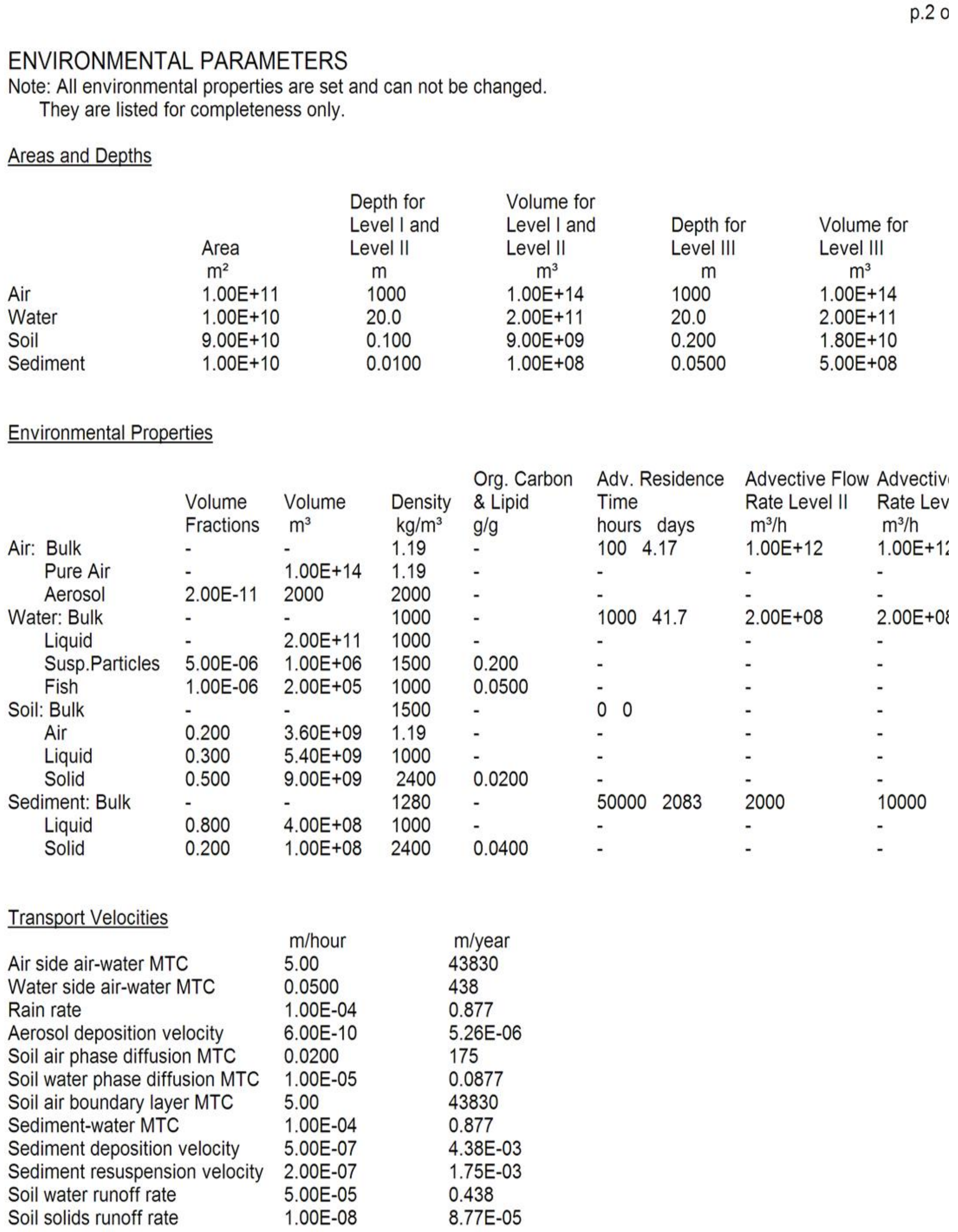
Partition Coefficients

	Dimensionless	L/kg
Log Octanol-Water Partition Coefficient	*0.08*	-
Octanol-Water Partition Coefficient	1.20	-
Organic Carbon-Water Partition Coefficient	-	0.493
Air-Water(Kaw)	0.0334	-
Soil-Water	0.0237	9.86E-03
Sediment-Water	0.0473	0.0197
Susp. Particles-Water	0.148	0.0986
Fish-Water(Kfw)	0.0601	0.0601
Aerosol-Air	225	-

Degradation

Half-lives

	hours	days
Air	*31.5*	1.31
Water	*900*	37.5
Soil	*1800*	75.0
Sediment	*8100*	338



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ENVIRONMENTAL PARAMETERS

Note: All environmental properties are set and can not be changed.
They are listed for completeness only.

Areas and Depths

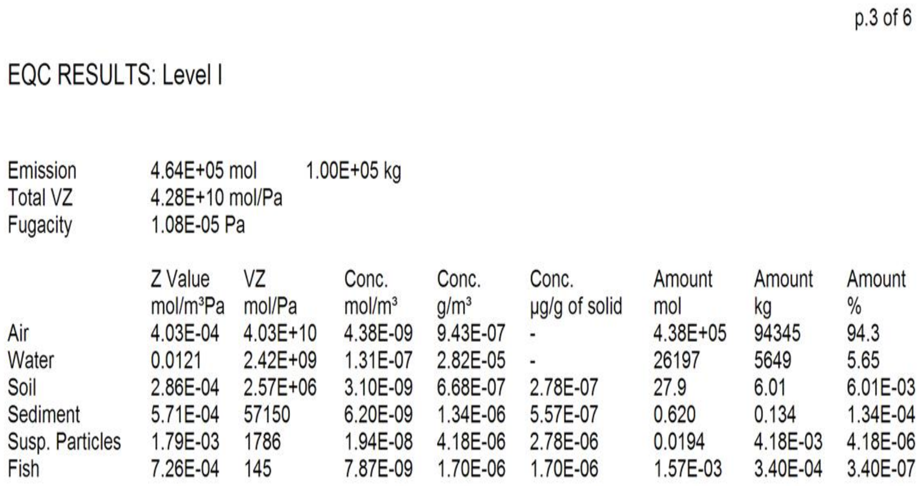
	Area m²	Depth for Level I and Level II m	Volume for Level I and Level II m³	Depth for Level III m	Volume for Level III m³
Air	1.00E+11	1000	1.00E+14	1000	1.00E+14
Water	1.00E+10	20.0	2.00E+11	20.0	2.00E+11
Soil	9.00E+10	0.100	9.00E+09	0.200	1.80E+10
Sediment	1.00E+10	0.0100	1.00E+08	0.0500	5.00E+08

Environmental Properties

	Volume Fractions	Volume m³	Density kg/m³	Org. Carbon & Lipid g/g	Adv. Residence Time hours	days	Advective Flow Rate Level II m³/h	Advectiv Rate Lev m³/h
Air: Bulk	-	-	1.19	-	100	4.17	1.00E+12	1.00E+1
Pure Air	-	1.00E+14	1.19	-	-		-	-
Aerosol	2.00E-11	2000	2000	-	-		-	-
Water: Bulk	-	-	1000	-	1000	41.7	2.00E+08	2.00E+0
Liquid	-	2.00E+11	1000	-	-		-	-
Susp.Particles	5.00E-06	1.00E+06	1500	0.200	-		-	-
Fish	1.00E-06	2.00E+05	1000	0.0500	-		-	-
Soil: Bulk	-	-	1500	-	0	0	-	-
Air	0.200	3.60E+09	1.19	-	-		-	-
Liquid	0.300	5.40E+09	1000	-	-		-	-
Solid	0.500	9.00E+09	2400	0.0200	-		-	-
Sediment: Bulk	-	-	1280	-	50000	2083	2000	10000
Liquid	0.800	4.00E+08	1000	-	-		-	-
Solid	0.200	1.00E+08	2400	0.0400	-		-	-

Transport Velocities

	m/hour	m/year
Air side air-water MTC	5.00	43830
Water side air-water MTC	0.0500	438
Rain rate	1.00E-04	0.877
Aerosol deposition velocity	6.00E-10	5.26E-06
Soil air phase diffusion MTC	0.0200	175
Soil water phase diffusion MTC	1.00E-05	0.0877
Soil air boundary layer MTC	5.00	43830
Sediment-water MTC	1.00E-04	0.877
Sediment deposition velocity	5.00E-07	4.38E-03
Sediment resuspension velocity	2.00E-07	1.75E-03
Soil water runoff rate	5.00E-05	0.438
Soil solids runoff rate	1.00E-08	8.77E-05



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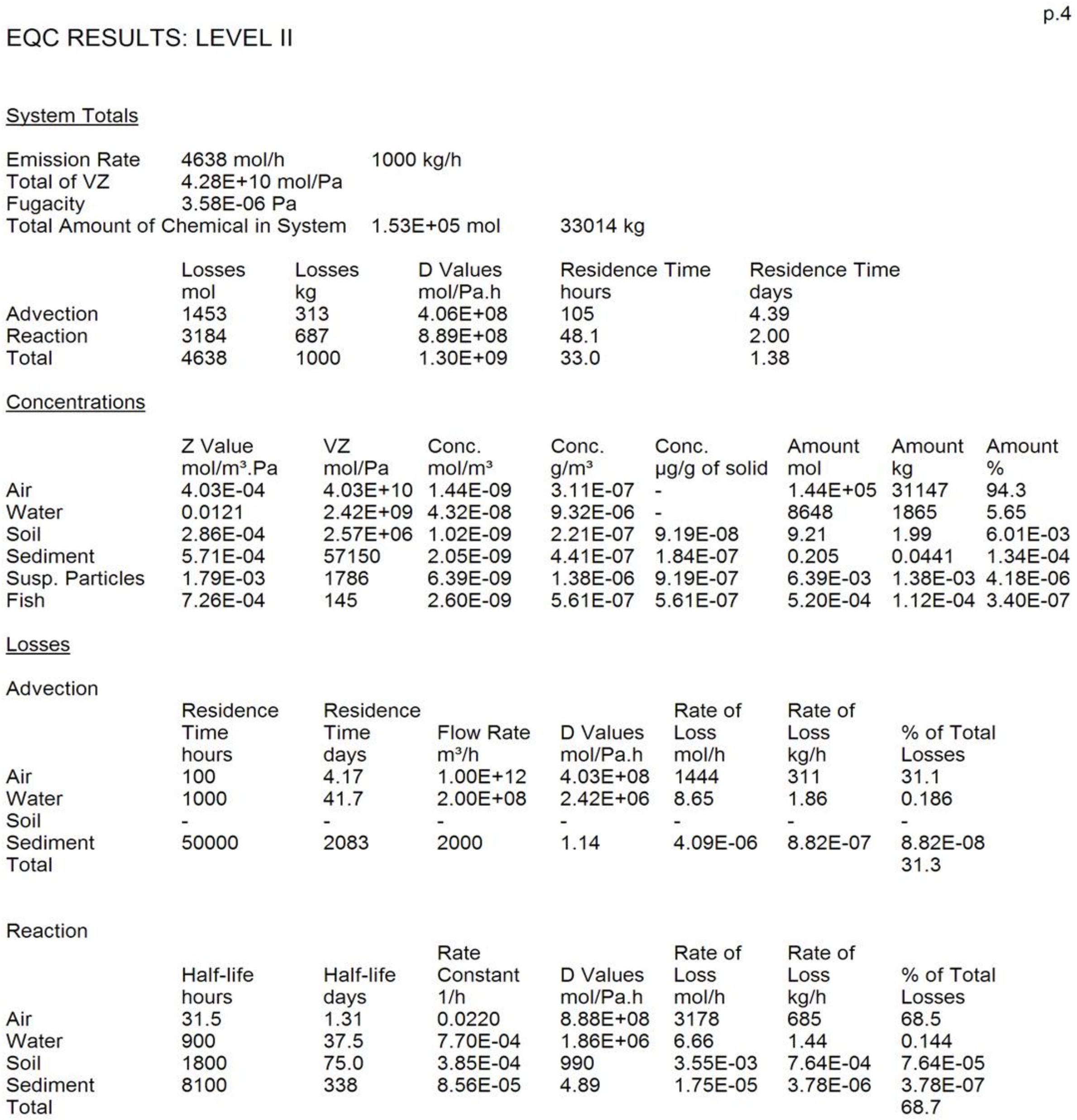
EQC RESULTS: Level I

Emission	4.64E+05 mol	1.00E+05 kg
Total VZ	4.28E+10 mol/Pa	
Fugacity	1.08E-05 Pa	

	Z Value mol/m³Pa	VZ mol/Pa	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	4.38E-09	9.43E-07	-	4.38E+05	94345	94.3
Water	0.0121	2.42E+09	1.31E-07	2.82E-05	-	26197	5649	5.65
Soil	2.86E-04	2.57E+06	3.10E-09	6.68E-07	2.78E-07	27.9	6.01	6.01E-03
Sediment	5.71E-04	57150	6.20E-09	1.34E-06	5.57E-07	0.620	0.134	1.34E-04
Susp. Particles	1.79E-03	1786	1.94E-08	4.18E-06	2.78E-06	0.0194	4.18E-03	4.18E-06
Fish	7.26E-04	145	7.87E-09	1.70E-06	1.70E-06	1.57E-03	3.40E-04	3.40E-07



p.4

EQC RESULTS: LEVEL II

System Totals

Emission Rate	4638 mol/h	1000 kg/h	
Total of VZ	4.28E+10 mol/Pa		
Fugacity	3.58E-06 Pa		
Total Amount of Chemical in System		1.53E+05 mol	33014 kg

	Losses mol	Losses kg	D Values mol/Pa.h	Residence Time hours	Residence Time days
Advection	1453	313	4.06E+08	105	4.39
Reaction	3184	687	8.89E+08	48.1	2.00
Total	4638	1000	1.30E+09	33.0	1.38

Concentrations

	Z Value mol/m^3.Pa	VZ mol/Pa	Conc. mol/m^3	Conc. g/m^3	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	1.44E-09	3.11E-07	-	1.44E+05	31147	94.3
Water	0.0121	2.42E+09	4.32E-08	9.32E-06	-	8648	1865	5.65
Soil	2.86E-04	2.57E+06	1.02E-09	2.21E-07	9.19E-08	9.21	1.99	6.01E-03
Sediment	5.71E-04	57150	2.05E-09	4.41E-07	1.84E-07	0.205	0.0441	1.34E-04
Susp. Particles	1.79E-03	1786	6.39E-09	1.38E-06	9.19E-07	6.39E-03	1.38E-03	4.18E-06
Fish	7.26E-04	145	2.60E-09	5.61E-07	5.61E-07	5.20E-04	1.12E-04	3.40E-07

Losses

Advection

	Residence Time hours	Residence Time days	Flow Rate m^3/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	1444	311	31.1
Water	1000	41.7	2.00E+08	2.42E+06	8.65	1.86	0.186
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	2000	1.14	4.09E-06	8.82E-07	8.82E-08
Total							31.3

Reaction

	Half-life hours	Half-life days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	31.5	1.31	0.0220	8.88E+08	3178	685	68.5
Water	900	37.5	7.70E-04	1.86E+06	6.66	1.44	0.144
Soil	1800	75.0	3.85E-04	990	3.55E-03	7.64E-04	7.64E-05
Sediment	8100	338	8.56E-05	4.89	1.75E-05	3.78E-06	3.78E-07
Total							68.7

EQC RESULTS: LEVEL III

Mass Balance

	Emission mol/h	Emission kg/h	Fugacity Pa	VZ mol/Pa
Air	4638	*1000*	3.59E-06	4.03E+10
Water	0	*0*	1.90E-06	2.42E+09
Soil	0	*0*	3.71E-06	6.92E+07
Sediment	0	*0*	1.82E-06	4.89E+06
Total	4638	1000		

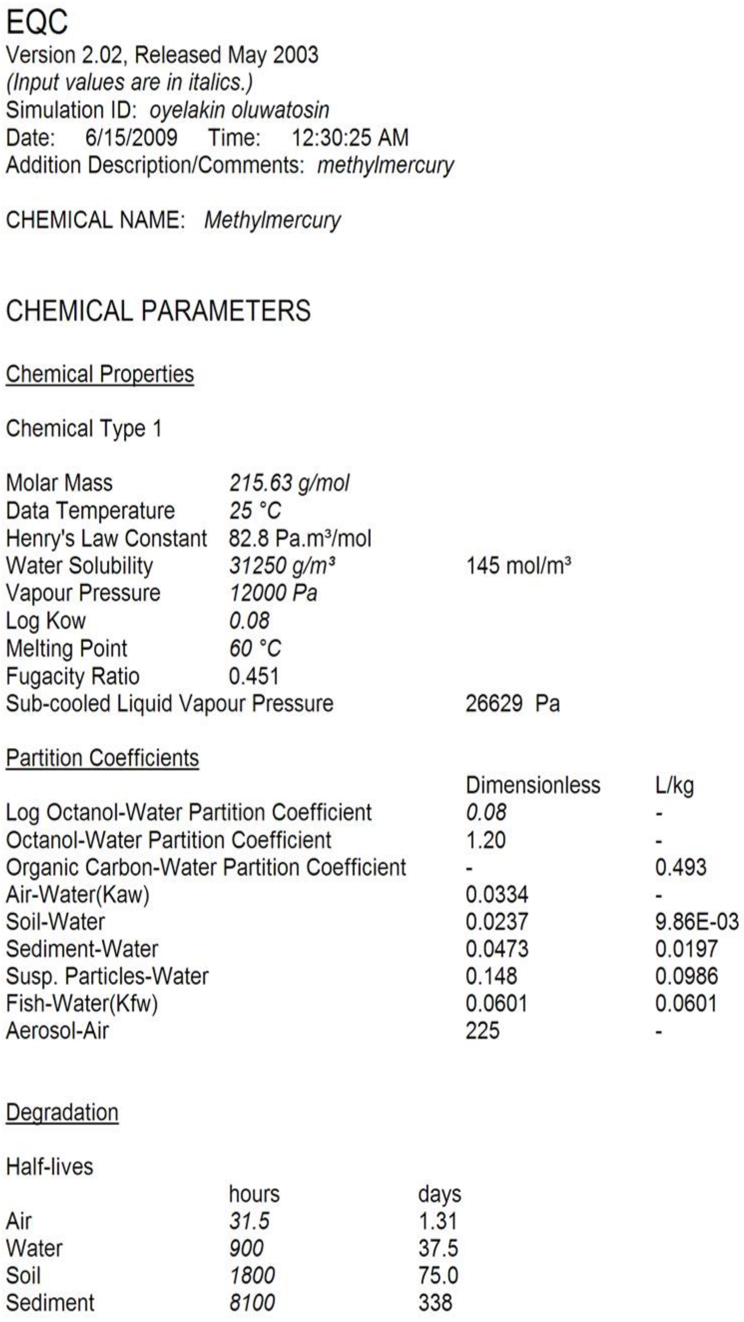
	Loss Rate mol/h	Loss Rate kg/h	Residence Time hours	Residence Time days
Advection	1451	313	103	4.29
Reaction	3186	687	46.9	1.96
Overall	4638	1000	32.2	1.34

Amount of Chemical in Environment 1.50E+05 mol 32239 kg

Phase Properties

	Z Value mol/m^{3}Pa	Amount mol	Amount kg	Amount %	Conc. mol/m^3	Conc. g/m^3	Conc. µg/g of solids
Air: Bulk	4.03E-04	1.45E+05	31195	96.8	1.45E-09	3.12E-07	
Vapour	4.03E-04	1.45E+05	31195	96.8	1.45E-09	3.12E-07	
Aerosol	0.0909	6.52E-04	1.41E-04	4.36E-07	3.26E-07	7.03E-05	3.51E-05
Water: Bulk	0.0121	4577	987	3.06	2.29E-08	4.94E-06	
Liquid	0.0121	4577	987	3.06	2.29E-08	4.94E-06	
Susp. Part.	1.79E-03	3.38E-03	7.30E-04	2.26E-06	3.38E-09	7.30E-07	4.87E-07
Fish	7.26E-04	2.75E-04	5.93E-05	1.84E-07	1.38E-09	2.97E-07	
Soil: Bulk	3.85E-03	257	55.4	0.172	1.43E-08	3.08E-06	
Air	4.03E-04	5.39	1.16	3.60E-03	1.50E-09	3.23E-07	
Liquid	0.0121	242	52.1	0.162	4.48E-08	9.66E-06	
Solid	2.86E-04	9.54	2.06	6.38E-03	1.06E-09	2.28E-07	9.52E-08
Sediment: Bulk	9.78E-03	8.89	1.92	5.95E-03	1.78E-08	3.83E-06	
Water	0.0121	8.79	1.89	5.88E-03	2.20E-08	4.74E-06	
Solid	5.71E-04	0.104	0.0224	6.95E-05	1.04E-09	2.24E-07	9.34E-08

Second case scenario (water)



EQC

Version 2.02, Released May 2003
(Input values are in italics.)
Simulation ID: *oyelakin oluwatosin*
Date: 6/15/2009 Time: 12:30:25 AM
Addition Description/Comments: *methylmercury*

CHEMICAL NAME: *Methylmercury*

CHEMICAL PARAMETERS

Chemical Properties

Chemical Type 1

Molar Mass	*215.63 g/mol*	
Data Temperature	*25 °C*	
Henry's Law Constant	82.8 Pa.m³/mol	
Water Solubility	*31250 g/m³*	145 mol/m³
Vapour Pressure	*12000 Pa*	
Log Kow	*0.08*	
Melting Point	*60 °C*	
Fugacity Ratio	0.451	
Sub-cooled Liquid Vapour Pressure		26629 Pa

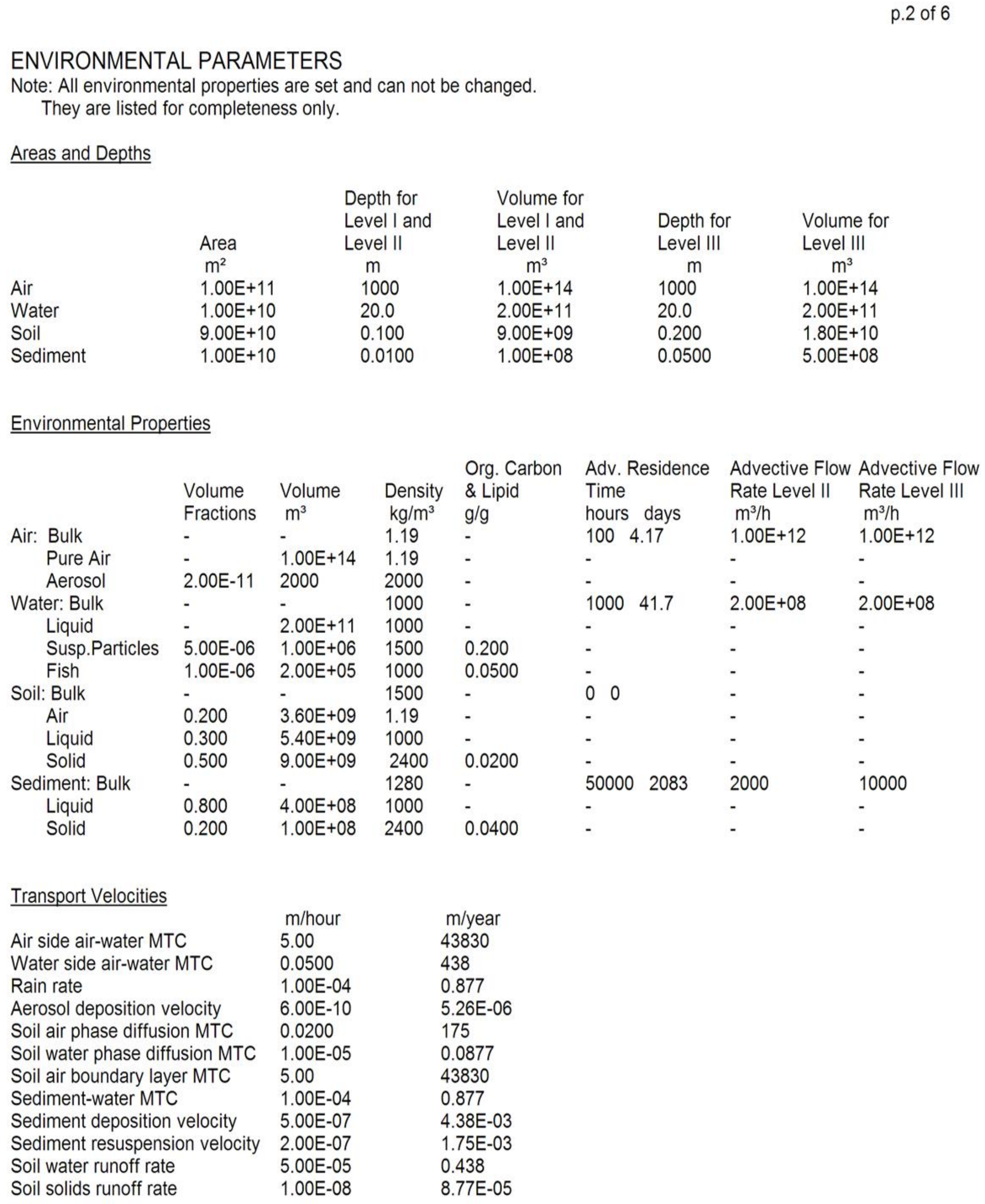
Partition Coefficients

	Dimensionless	L/kg
Log Octanol-Water Partition Coefficient	*0.08*	-
Octanol-Water Partition Coefficient	1.20	-
Organic Carbon-Water Partition Coefficient	-	0.493
Air-Water(Kaw)	0.0334	-
Soil-Water	0.0237	9.86E-03
Sediment-Water	0.0473	0.0197
Susp. Particles-Water	0.148	0.0986
Fish-Water(Kfw)	0.0601	0.0601
Aerosol-Air	225	-

Degradation

Half-lives

	hours	days
Air	*31.5*	1.31
Water	*900*	37.5
Soil	*1800*	75.0
Sediment	*8100*	338



ENVIRONMENTAL PARAMETERS

Note: All environmental properties are set and can not be changed.
They are listed for completeness only.

Areas and Depths

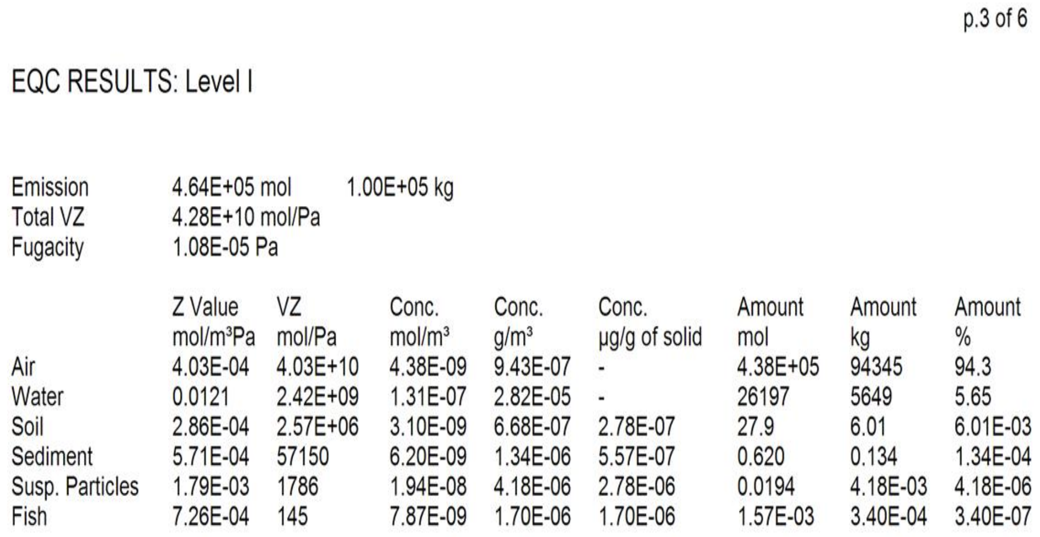
	Area m²	Depth for Level I and Level II m	Volume for Level I and Level II m³	Depth for Level III m	Volume for Level III m³
Air	1.00E+11	1000	1.00E+14	1000	1.00E+14
Water	1.00E+10	20.0	2.00E+11	20.0	2.00E+11
Soil	9.00E+10	0.100	9.00E+09	0.200	1.80E+10
Sediment	1.00E+10	0.0100	1.00E+08	0.0500	5.00E+08

Environmental Properties

	Volume Fractions	Volume m³	Density kg/m³	Org. Carbon & Lipid g/g	Adv. Residence Time hours days	Advective Flow Rate Level II m³/h	Advective Flow Rate Level III m³/h
Air: Bulk	-	-	1.19	-	100 4.17	1.00E+12	1.00E+12
Pure Air	-	1.00E+14	1.19	-	-	-	-
Aerosol	2.00E-11	2000	2000	-	-	-	-
Water: Bulk	-	-	1000	-	1000 41.7	2.00E+08	2.00E+08
Liquid	-	2.00E+11	1000	-	-	-	-
Susp.Particles	5.00E-06	1.00E+06	1500	0.200	-	-	-
Fish	1.00E-06	2.00E+05	1000	0.0500	-	-	-
Soil: Bulk	-	-	1500	-	0 0	-	-
Air	0.200	3.60E+09	1.19	-	-	-	-
Liquid	0.300	5.40E+09	1000	-	-	-	-
Solid	0.500	9.00E+09	2400	0.0200	-	-	-
Sediment: Bulk	-	-	1280	-	50000 2083	2000	10000
Liquid	0.800	4.00E+08	1000	-	-	-	-
Solid	0.200	1.00E+08	2400	0.0400	-	-	-

Transport Velocities

	m/hour	m/year
Air side air-water MTC	5.00	43830
Water side air-water MTC	0.0500	438
Rain rate	1.00E-04	0.877
Aerosol deposition velocity	6.00E-10	5.26E-06
Soil air phase diffusion MTC	0.0200	175
Soil water phase diffusion MTC	1.00E-05	0.0877
Soil air boundary layer MTC	5.00	43830
Sediment-water MTC	1.00E-04	0.877
Sediment deposition velocity	5.00E-07	4.38E-03
Sediment resuspension velocity	2.00E-07	1.75E-03
Soil water runoff rate	5.00E-05	0.438
Soil solids runoff rate	1.00E-08	8.77E-05

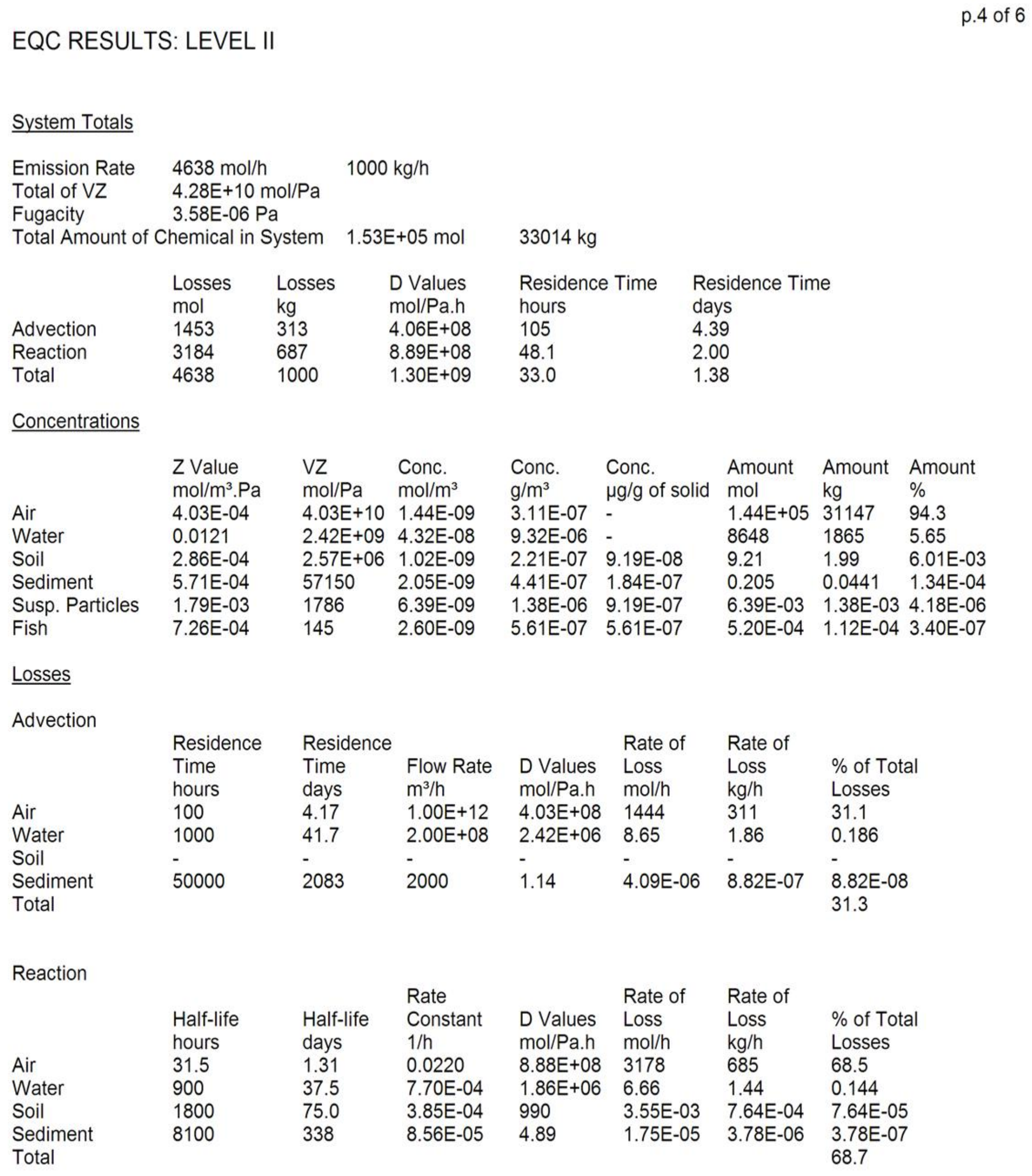


p.3 of 6

EQC RESULTS: Level I

Emission 4.64E+05 mol 1.00E+05 kg
Total VZ 4.28E+10 mol/Pa
Fugacity 1.08E-05 Pa

	Z Value mol/m³Pa	VZ mol/Pa	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	4.38E-09	9.43E-07	-	4.38E+05	94345	94.3
Water	0.0121	2.42E+09	1.31E-07	2.82E-05	-	26197	5649	5.65
Soil	2.86E-04	2.57E+06	3.10E-09	6.68E-07	2.78E-07	27.9	6.01	6.01E-03
Sediment	5.71E-04	57150	6.20E-09	1.34E-06	5.57E-07	0.620	0.134	1.34E-04
Susp. Particles	1.79E-03	1786	1.94E-08	4.18E-06	2.78E-06	0.0194	4.18E-03	4.18E-06
Fish	7.26E-04	145	7.87E-09	1.70E-06	1.70E-06	1.57E-03	3.40E-04	3.40E-07



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EQC RESULTS: LEVEL II

System Totals

Emission Rate	4638 mol/h	1000 kg/h		
Total of VZ	4.28E+10 mol/Pa			
Fugacity	3.58E-06 Pa			
Total Amount of Chemical in System		1.53E+05 mol	33014 kg	

	Losses mol	Losses kg	D Values mol/Pa.h	Residence Time hours	Residence Time days
Advection	1453	313	4.06E+08	105	4.39
Reaction	3184	687	8.89E+08	48.1	2.00
Total	4638	1000	1.30E+09	33.0	1.38

Concentrations

	Z Value mol/m³.Pa	VZ mol/Pa	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	1.44E-09	3.11E-07	-	1.44E+05	31147	94.3
Water	0.0121	2.42E+09	4.32E-08	9.32E-06	-	8648	1865	5.65
Soil	2.86E-04	2.57E+06	1.02E-09	2.21E-07	9.19E-08	9.21	1.99	6.01E-03
Sediment	5.71E-04	57150	2.05E-09	4.41E-07	1.84E-07	0.205	0.0441	1.34E-04
Susp. Particles	1.79E-03	1786	6.39E-09	1.38E-06	9.19E-07	6.39E-03	1.38E-03	4.18E-06
Fish	7.26E-04	145	2.60E-09	5.61E-07	5.61E-07	5.20E-04	1.12E-04	3.40E-07

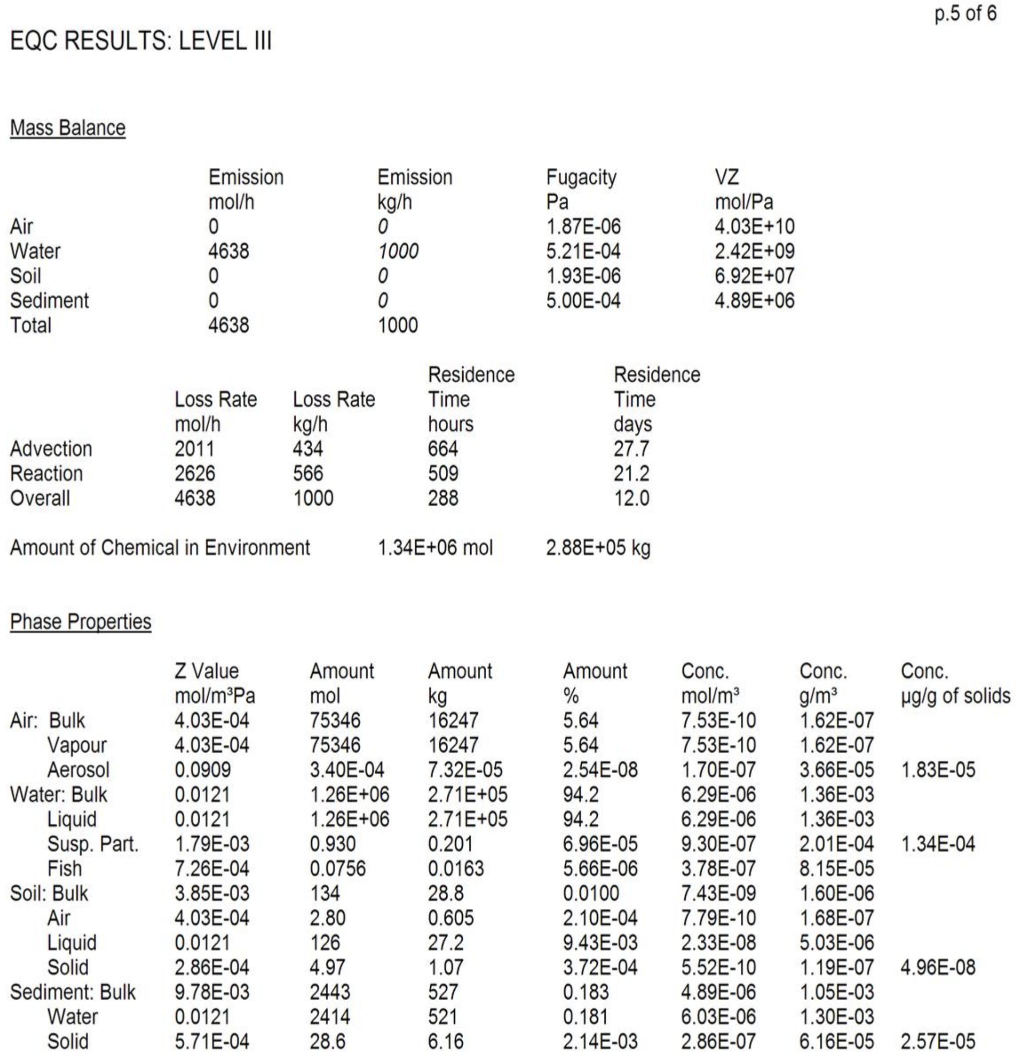
Losses

Advection

	Residence Time hours	Residence Time days	Flow Rate m³/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	1444	311	31.1
Water	1000	41.7	2.00E+08	2.42E+06	8.65	1.86	0.186
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	2000	1.14	4.09E-06	8.82E-07	8.82E-08
Total							31.3

Reaction

	Half-life hours	Half-life days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	31.5	1.31	0.0220	8.88E+08	3178	685	68.5
Water	900	37.5	7.70E-04	1.86E+06	6.66	1.44	0.144
Soil	1800	75.0	3.85E-04	990	3.55E-03	7.64E-04	7.64E-05
Sediment	8100	338	8.56E-05	4.89	1.75E-05	3.78E-06	3.78E-07
Total							68.7



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EQC RESULTS: LEVEL III

Mass Balance

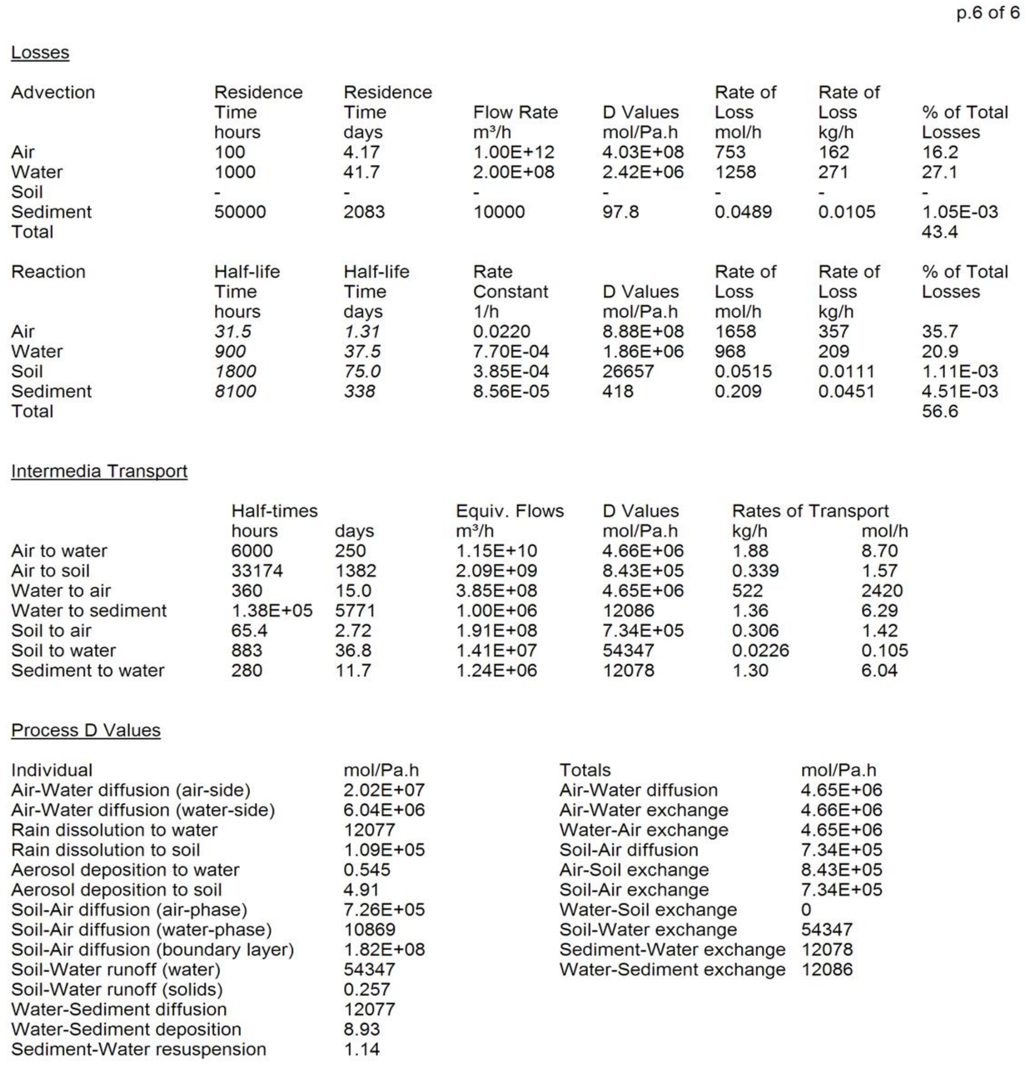
	Emission mol/h	Emission kg/h	Fugacity Pa	VZ mol/Pa
Air	0	*0*	1.87E-06	4.03E+10
Water	4638	*1000*	5.21E-04	2.42E+09
Soil	0	*0*	1.93E-06	6.92E+07
Sediment	0	*0*	5.00E-04	4.89E+06
Total	4638	1000		

	Loss Rate mol/h	Loss Rate kg/h	Residence Time hours	Residence Time days
Advection	2011	434	664	27.7
Reaction	2626	566	509	21.2
Overall	4638	1000	288	12.0

Amount of Chemical in Environment 1.34E+06 mol 2.88E+05 kg

Phase Properties

	Z Value mol/m³Pa	Amount mol	Amount kg	Amount %	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solids
Air: Bulk	4.03E-04	75346	16247	5.64	7.53E-10	1.62E-07	
Vapour	4.03E-04	75346	16247	5.64	7.53E-10	1.62E-07	
Aerosol	0.0909	3.40E-04	7.32E-05	2.54E-08	1.70E-07	3.66E-05	1.83E-05
Water: Bulk	0.0121	1.26E+06	2.71E+05	94.2	6.29E-06	1.36E-03	
Liquid	0.0121	1.26E+06	2.71E+05	94.2	6.29E-06	1.36E-03	
Susp. Part.	1.79E-03	0.930	0.201	6.96E-05	9.30E-07	2.01E-04	1.34E-04
Fish	7.26E-04	0.0756	0.0163	5.66E-06	3.78E-07	8.15E-05	
Soil: Bulk	3.85E-03	134	28.8	0.0100	7.43E-09	1.60E-06	
Air	4.03E-04	2.80	0.605	2.10E-04	7.79E-10	1.68E-07	
Liquid	0.0121	126	27.2	9.43E-03	2.33E-08	5.03E-06	
Solid	2.86E-04	4.97	1.07	3.72E-04	5.52E-10	1.19E-07	4.96E-08
Sediment: Bulk	9.78E-03	2443	527	0.183	4.89E-06	1.05E-03	
Water	0.0121	2414	521	0.181	6.03E-06	1.30E-03	
Solid	5.71E-04	28.6	6.16	2.14E-03	2.86E-07	6.16E-05	2.57E-05



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Losses

Advection	Residence Time hours	Residence Time days	Flow Rate m³/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	753	162	16.2
Water	1000	41.7	2.00E+08	2.42E+06	1258	271	27.1
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	10000	97.8	0.0489	0.0105	1.05E-03
Total							43.4

Reaction	Half-life Time hours	Half-life Time days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	*31.5*	*1.31*	0.0220	8.88E+08	1658	357	35.7
Water	*900*	*37.5*	7.70E-04	1.86E+06	968	209	20.9
Soil	*1800*	*75.0*	3.85E-04	26657	0.0515	0.0111	1.11E-03
Sediment	*8100*	*338*	8.56E-05	418	0.209	0.0451	4.51E-03
Total							56.6

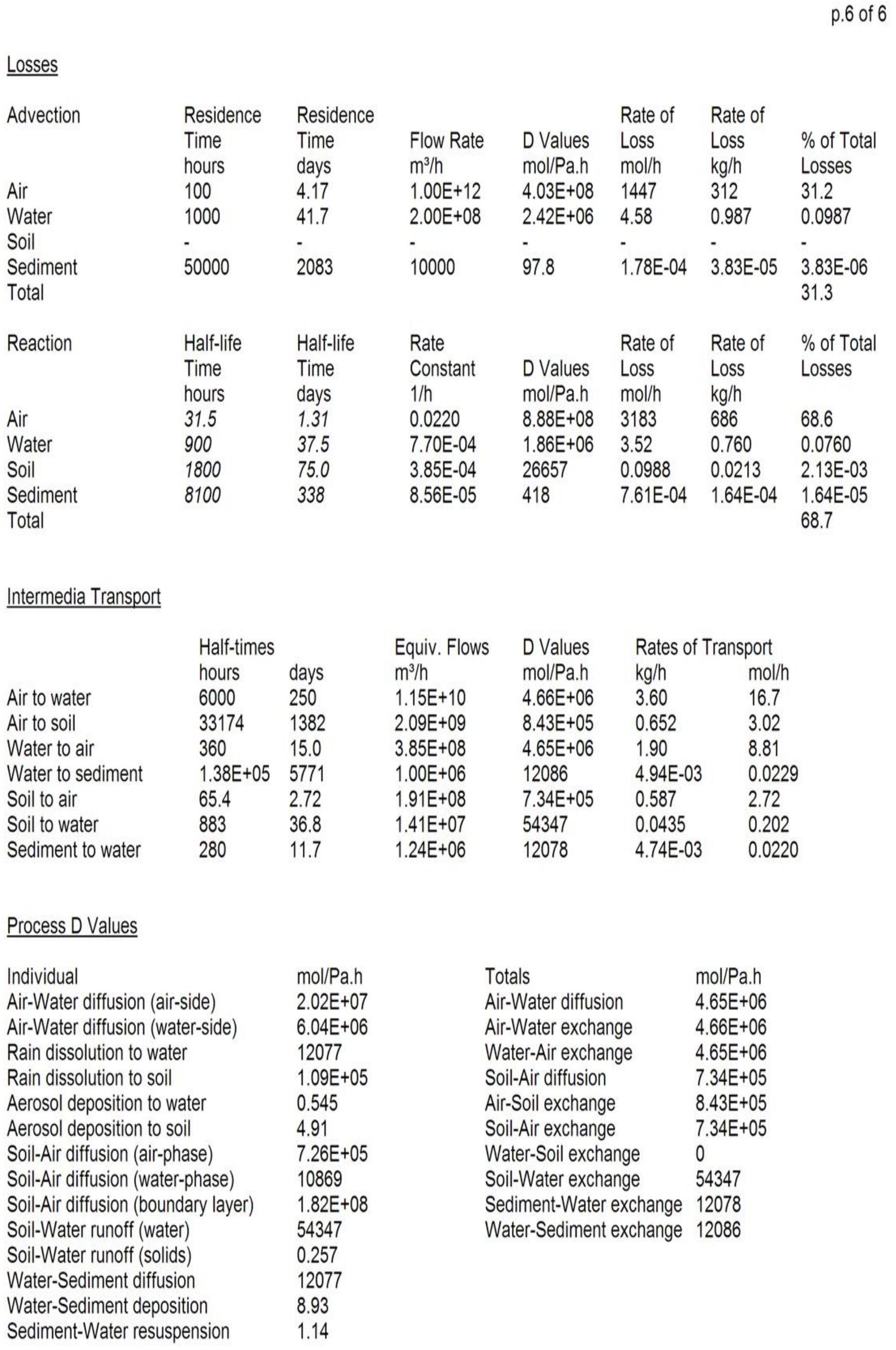
Intermedia Transport

	Half-times hours	days	Equiv. Flows m³/h	D Values mol/Pa.h	Rates of Transport kg/h	mol/h
Air to water	6000	250	1.15E+10	4.66E+06	1.88	8.70
Air to soil	33174	1382	2.09E+09	8.43E+05	0.339	1.57
Water to air	360	15.0	3.85E+08	4.65E+06	522	2420
Water to sediment	1.38E+05	5771	1.00E+06	12086	1.36	6.29
Soil to air	65.4	2.72	1.91E+08	7.34E+05	0.306	1.42
Soil to water	883	36.8	1.41E+07	54347	0.0226	0.105
Sediment to water	280	11.7	1.24E+06	12078	1.30	6.04

Process D Values

Individual	mol/Pa.h
Air-Water diffusion (air-side)	2.02E+07
Air-Water diffusion (water-side)	6.04E+06
Rain dissolution to water	12077
Rain dissolution to soil	1.09E+05
Aerosol deposition to water	0.545
Aerosol deposition to soil	4.91
Soil-Air diffusion (air-phase)	7.26E+05
Soil-Air diffusion (water-phase)	10869
Soil-Air diffusion (boundary layer)	1.82E+08
Soil-Water runoff (water)	54347
Soil-Water runoff (solids)	0.257
Water-Sediment diffusion	12077
Water-Sediment deposition	8.93
Sediment-Water resuspension	1.14

Totals	mol/Pa.h
Air-Water diffusion	4.65E+06
Air-Water exchange	4.66E+06
Water-Air exchange	4.65E+06
Soil-Air diffusion	7.34E+05
Air-Soil exchange	8.43E+05
Soil-Air exchange	7.34E+05
Water-Soil exchange	0
Soil-Water exchange	54347
Sediment-Water exchange	12078
Water-Sediment exchange	12086



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Losses

Advection	Residence Time hours	Residence Time days	Flow Rate m³/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	1447	312	31.2
Water	1000	41.7	2.00E+08	2.42E+06	4.58	0.987	0.0987
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	10000	97.8	1.78E-04	3.83E-05	3.83E-06
Total							31.3

Reaction	Half-life Time hours	Half-life Time days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	*31.5*	*1.31*	0.0220	8.88E+08	3183	686	68.6
Water	*900*	*37.5*	7.70E-04	1.86E+06	3.52	0.760	0.0760
Soil	*1800*	*75.0*	3.85E-04	26657	0.0988	0.0213	2.13E-03
Sediment	*8100*	*338*	8.56E-05	418	7.61E-04	1.64E-04	1.64E-05
Total							68.7

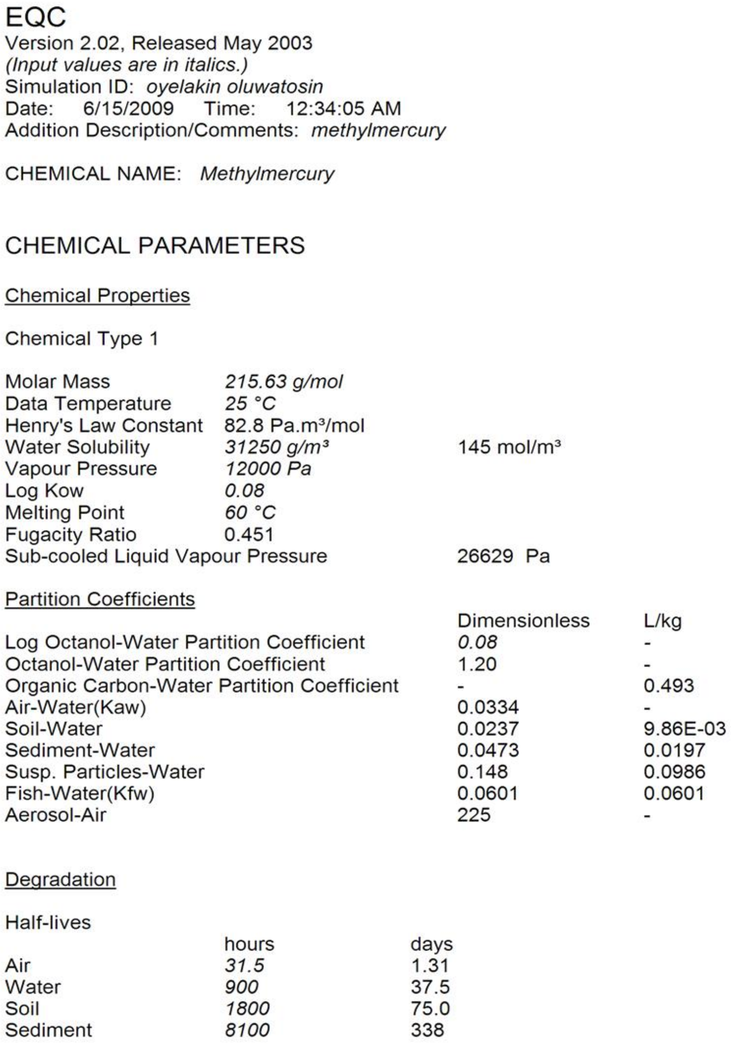
Intermedia Transport

	Half-times hours	days	Equiv. Flows m³/h	D Values mol/Pa.h	Rates of Transport kg/h	mol/h
Air to water	6000	250	1.15E+10	4.66E+06	3.60	16.7
Air to soil	33174	1382	2.09E+09	8.43E+05	0.652	3.02
Water to air	360	15.0	3.85E+08	4.65E+06	1.90	8.81
Water to sediment	1.38E+05	5771	1.00E+06	12086	4.94E-03	0.0229
Soil to air	65.4	2.72	1.91E+08	7.34E+05	0.587	2.72
Soil to water	883	36.8	1.41E+07	54347	0.0435	0.202
Sediment to water	280	11.7	1.24E+06	12078	4.74E-03	0.0220

Process D Values

Individual	mol/Pa.h	Totals	mol/Pa.h
Air-Water diffusion (air-side)	2.02E+07	Air-Water diffusion	4.65E+06
Air-Water diffusion (water-side)	6.04E+06	Air-Water exchange	4.66E+06
Rain dissolution to water	12077	Water-Air exchange	4.65E+06
Rain dissolution to soil	1.09E+05	Soil-Air diffusion	7.34E+05
Aerosol deposition to water	0.545	Air-Soil exchange	8.43E+05
Aerosol deposition to soil	4.91	Soil-Air exchange	7.34E+05
Soil-Air diffusion (air-phase)	7.26E+05	Water-Soil exchange	0
Soil-Air diffusion (water-phase)	10869	Soil-Water exchange	54347
Soil-Air diffusion (boundary layer)	1.82E+08	Sediment-Water exchange	12078
Soil-Water runoff (water)	54347	Water-Sediment exchange	12086
Soil-Water runoff (solids)	0.257		
Water-Sediment diffusion	12077		
Water-Sediment deposition	8.93		
Sediment-Water resuspension	1.14		

Third case scenario (soil)



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EQC
Version 2.02, Released May 2003
(Input values are in italics.)
Simulation ID:  oyelakin oluwatosin
Date:    6/15/2009    Time:    12:34:05 AM
Addition Description/Comments:  methylmercury

CHEMICAL NAME:   Methylmercury


CHEMICAL PARAMETERS

Chemical Properties

Chemical Type 1

Molar Mass              215.63 g/mol
Data Temperature        25 °C
Henry's Law Constant    82.8 Pa.m³/mol
Water Solubility        31250 g/m³              145 mol/m³
Vapour Pressure         12000 Pa
Log Kow                 0.08
Melting Point           60 °C
Fugacity Ratio          0.451
Sub-cooled Liquid Vapour Pressure               26629  Pa

Partition Coefficients
                                                Dimensionless    L/kg
Log Octanol-Water Partition Coefficient         0.08             -
Octanol-Water Partition Coefficient             1.20             -
Organic Carbon-Water Partition Coefficient      -                0.493
Air-Water(Kaw)                                  0.0334           -
Soil-Water                                      0.0237           9.86E-03
Sediment-Water                                  0.0473           0.0197
Susp. Particles-Water                           0.148            0.0986
Fish-Water(Kfw)                                 0.0601           0.0601
Aerosol-Air                                     225              -


Degradation

Half-lives
                        hours           days
Air                     31.5            1.31
Water                   900             37.5
Soil                    1800            75.0
Sediment                8100            338
```

ENVIRONMENTAL PARAMETERS

Note: All environmental properties are set and can not be changed.
They are listed for completeness only.

Areas and Depths

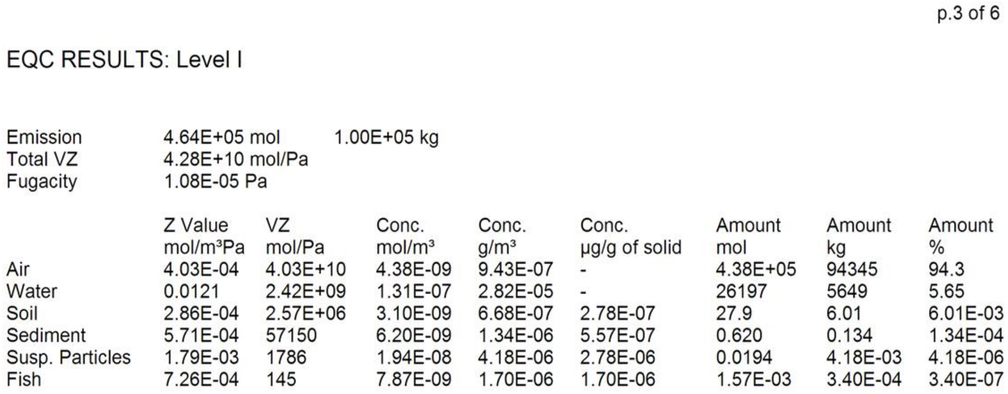
	Area m²	Depth for Level I and Level II m	Volume for Level I and Level II m³	Depth for Level III m	Volume for Level III m³
Air	1.00E+11	1000	1.00E+14	1000	1.00E+14
Water	1.00E+10	20.0	2.00E+11	20.0	2.00E+11
Soil	9.00E+10	0.100	9.00E+09	0.200	1.80E+10
Sediment	1.00E+10	0.0100	1.00E+08	0.0500	5.00E+08

Environmental Properties

	Volume Fractions	Volume m³	Density kg/m³	Org. Carbon & Lipid g/g	Adv. Residence Time hours	days	Advective Flow Rate Level II m³/h	Advective Flow Rate Level III m³/h
Air: Bulk	-	-	1.19	-	100	4.17	1.00E+12	1.00E+12
Pure Air	-	1.00E+14	1.19	-	-		-	-
Aerosol	2.00E-11	2000	2000	-	-		-	-
Water: Bulk	-	-	1000	-	1000	41.7	2.00E+08	2.00E+08
Liquid	-	2.00E+11	1000	-	-		-	-
Susp.Particles	5.00E-06	1.00E+06	1500	0.200	-		-	-
Fish	1.00E-06	2.00E+05	1000	0.0500	-		-	-
Soil: Bulk	-	-	1500	-	0	0	-	-
Air	0.200	3.60E+09	1.19	-	-		-	-
Liquid	0.300	5.40E+09	1000	-	-		-	-
Solid	0.500	9.00E+09	2400	0.0200	-		-	-
Sediment: Bulk	-	-	1280	-	50000	2083	2000	10000
Liquid	0.800	4.00E+08	1000	-	-		-	-
Solid	0.200	1.00E+08	2400	0.0400	-		-	-

Transport Velocities

	m/hour	m/year
Air side air-water MTC	5.00	43830
Water side air-water MTC	0.0500	438
Rain rate	1.00E-04	0.877
Aerosol deposition velocity	6.00E-10	5.26E-06
Soil air phase diffusion MTC	0.0200	175
Soil water phase diffusion MTC	1.00E-05	0.0877
Soil air boundary layer MTC	5.00	43830
Sediment-water MTC	1.00E-04	0.877
Sediment deposition velocity	5.00E-07	4.38E-03
Sediment resuspension velocity	2.00E-07	1.75E-03
Soil water runoff rate	5.00E-05	0.438
Soil solids runoff rate	1.00E-08	8.77E-05



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EQC RESULTS: Level I


Emission         4.64E+05 mol       1.00E+05 kg
Total VZ         4.28E+10 mol/Pa
Fugacity         1.08E-05 Pa

                 Z Value     VZ          Conc.       Conc.       Conc.            Amount      Amount      Amount
                 mol/m³Pa    mol/Pa      mol/m³      g/m³        µg/g of solid    mol         kg          %
Air              4.03E-04    4.03E+10    4.38E-09    9.43E-07    -                4.38E+05    94345       94.3
Water            0.0121      2.42E+09    1.31E-07    2.82E-05    -                26197       5649        5.65
Soil             2.86E-04    2.57E+06    3.10E-09    6.68E-07    2.78E-07         27.9        6.01        6.01E-03
Sediment         5.71E-04    57150       6.20E-09    1.34E-06    5.57E-07         0.620       0.134       1.34E-04
Susp. Particles  1.79E-03    1786        1.94E-08    4.18E-06    2.78E-06         0.0194      4.18E-03    4.18E-06
Fish             7.26E-04    145         7.87E-09    1.70E-06    1.70E-06         1.57E-03    3.40E-04    3.40E-07
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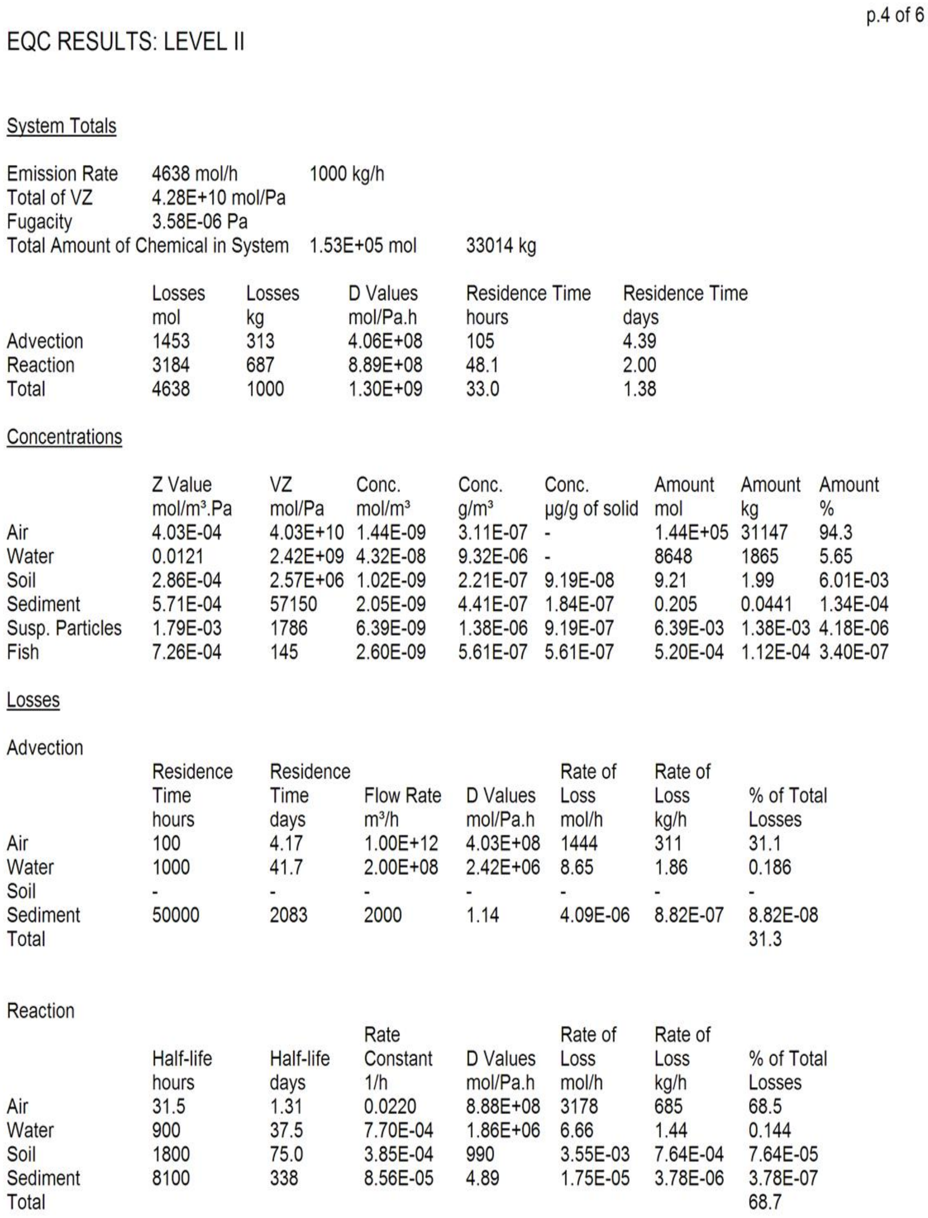

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EQC RESULTS: LEVEL II

System Totals

Emission Rate	4638 mol/h	1000 kg/h	
Total of VZ	4.28E+10 mol/Pa		
Fugacity	3.58E-06 Pa		
Total Amount of Chemical in System		1.53E+05 mol	33014 kg

	Losses mol	Losses kg	D Values mol/Pa.h	Residence Time hours	Residence Time days
Advection	1453	313	4.06E+08	105	4.39
Reaction	3184	687	8.89E+08	48.1	2.00
Total	4638	1000	1.30E+09	33.0	1.38

Concentrations

	Z Value mol/m^3.Pa	VZ mol/Pa	Conc. mol/m^3	Conc. g/m^3	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	1.44E-09	3.11E-07	-	1.44E+05	31147	94.3
Water	0.0121	2.42E+09	4.32E-08	9.32E-06	-	8648	1865	5.65
Soil	2.86E-04	2.57E+06	1.02E-09	2.21E-07	9.19E-08	9.21	1.99	6.01E-03
Sediment	5.71E-04	57150	2.05E-09	4.41E-07	1.84E-07	0.205	0.0441	1.34E-04
Susp. Particles	1.79E-03	1786	6.39E-09	1.38E-06	9.19E-07	6.39E-03	1.38E-03	4.18E-06
Fish	7.26E-04	145	2.60E-09	5.61E-07	5.61E-07	5.20E-04	1.12E-04	3.40E-07

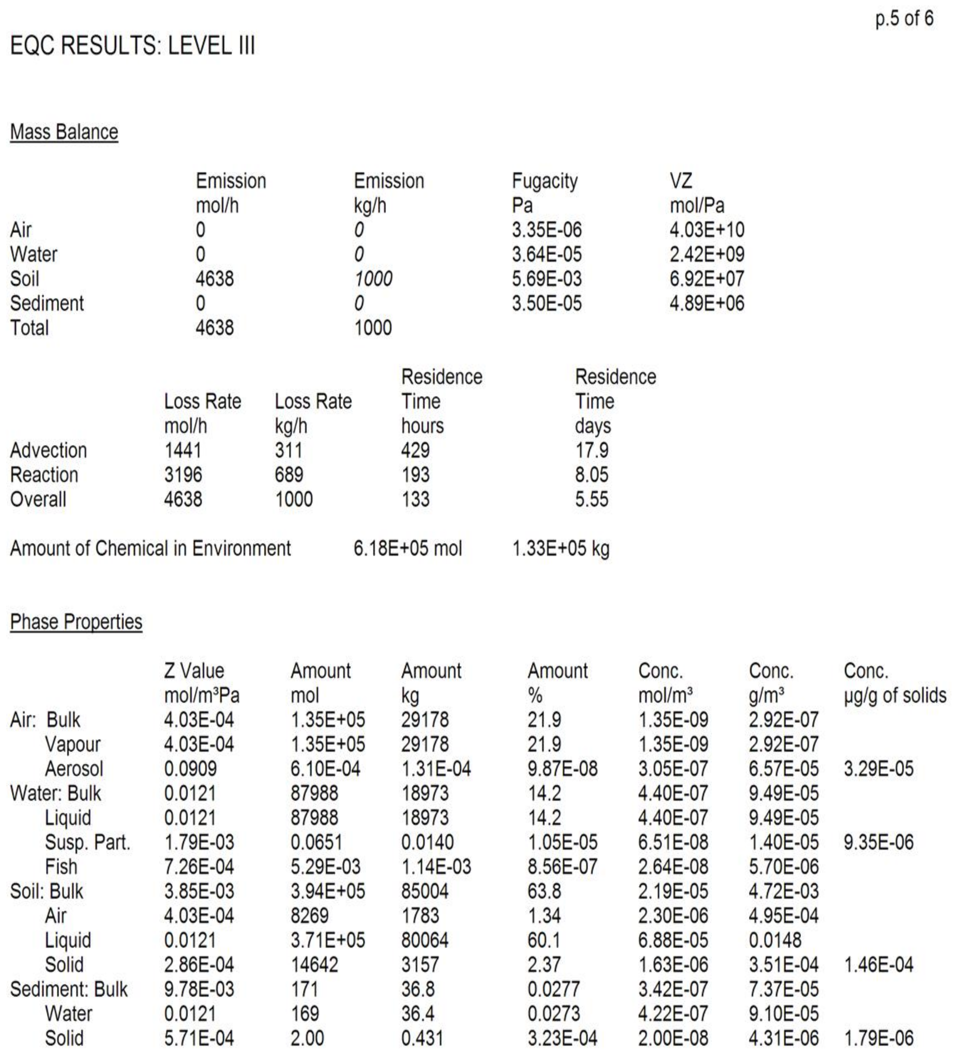
Losses

Advection

	Residence Time hours	Residence Time days	Flow Rate m^3/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	1444	311	31.1
Water	1000	41.7	2.00E+08	2.42E+06	8.65	1.86	0.186
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	2000	1.14	4.09E-06	8.82E-07	8.82E-08
Total							31.3

Reaction

	Half-life hours	Half-life days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	31.5	1.31	0.0220	8.88E+08	3178	685	68.5
Water	900	37.5	7.70E-04	1.86E+06	6.66	1.44	0.144
Soil	1800	75.0	3.85E-04	990	3.55E-03	7.64E-04	7.64E-05
Sediment	8100	338	8.56E-05	4.89	1.75E-05	3.78E-06	3.78E-07
Total							68.7



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EQC RESULTS: LEVEL III

Mass Balance

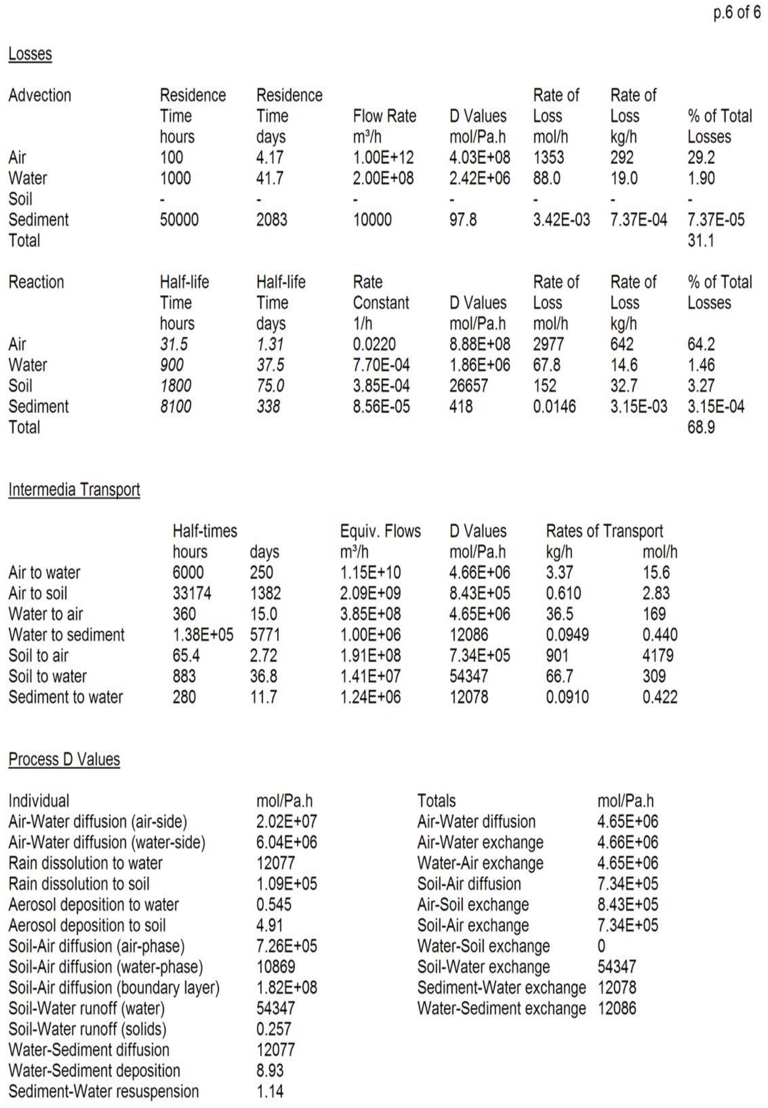
	Emission mol/h	Emission kg/h	Fugacity Pa	VZ mol/Pa
Air	0	*0*	3.35E-06	4.03E+10
Water	0	*0*	3.64E-05	2.42E+09
Soil	4638	*1000*	5.69E-03	6.92E+07
Sediment	0	*0*	3.50E-05	4.89E+06
Total	4638	1000		

	Loss Rate mol/h	Loss Rate kg/h	Residence Time hours	Residence Time days
Advection	1441	311	429	17.9
Reaction	3196	689	193	8.05
Overall	4638	1000	133	5.55

Amount of Chemical in Environment 6.18E+05 mol 1.33E+05 kg

Phase Properties

	Z Value mol/m³Pa	Amount mol	Amount kg	Amount %	Conc. mol/m³	Conc. g/m³	Conc. μg/g of solids
Air: Bulk	4.03E-04	1.35E+05	29178	21.9	1.35E-09	2.92E-07	
Vapour	4.03E-04	1.35E+05	29178	21.9	1.35E-09	2.92E-07	
Aerosol	0.0909	6.10E-04	1.31E-04	9.87E-08	3.05E-07	6.57E-05	3.29E-05
Water: Bulk	0.0121	87988	18973	14.2	4.40E-07	9.49E-05	
Liquid	0.0121	87988	18973	14.2	4.40E-07	9.49E-05	
Susp. Part.	1.79E-03	0.0651	0.0140	1.05E-05	6.51E-08	1.40E-05	9.35E-06
Fish	7.26E-04	5.29E-03	1.14E-03	8.56E-07	2.64E-08	5.70E-06	
Soil: Bulk	3.85E-03	3.94E+05	85004	63.8	2.19E-05	4.72E-03	
Air	4.03E-04	8269	1783	1.34	2.30E-06	4.95E-04	
Liquid	0.0121	3.71E+05	80064	60.1	6.88E-05	0.0148	
Solid	2.86E-04	14642	3157	2.37	1.63E-06	3.51E-04	1.46E-04
Sediment: Bulk	9.78E-03	171	36.8	0.0277	3.42E-07	7.37E-05	
Water	0.0121	169	36.4	0.0273	4.22E-07	9.10E-05	
Solid	5.71E-04	2.00	0.431	3.23E-04	2.00E-08	4.31E-06	1.79E-06



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Losses

Advection	Residence Time hours	Residence Time days	Flow Rate m³/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	1353	292	29.2
Water	1000	41.7	2.00E+08	2.42E+06	88.0	19.0	1.90
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	10000	97.8	3.42E-03	7.37E-04	7.37E-05
Total							31.1

Reaction	Half-life Time hours	Half-life Time days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	*31.5*	*1.31*	0.0220	8.88E+08	2977	642	64.2
Water	*900*	*37.5*	7.70E-04	1.86E+06	67.8	14.6	1.46
Soil	*1800*	*75.0*	3.85E-04	26657	152	32.7	3.27
Sediment	*8100*	*338*	8.56E-05	418	0.0146	3.15E-03	3.15E-04
Total							68.9

Intermedia Transport

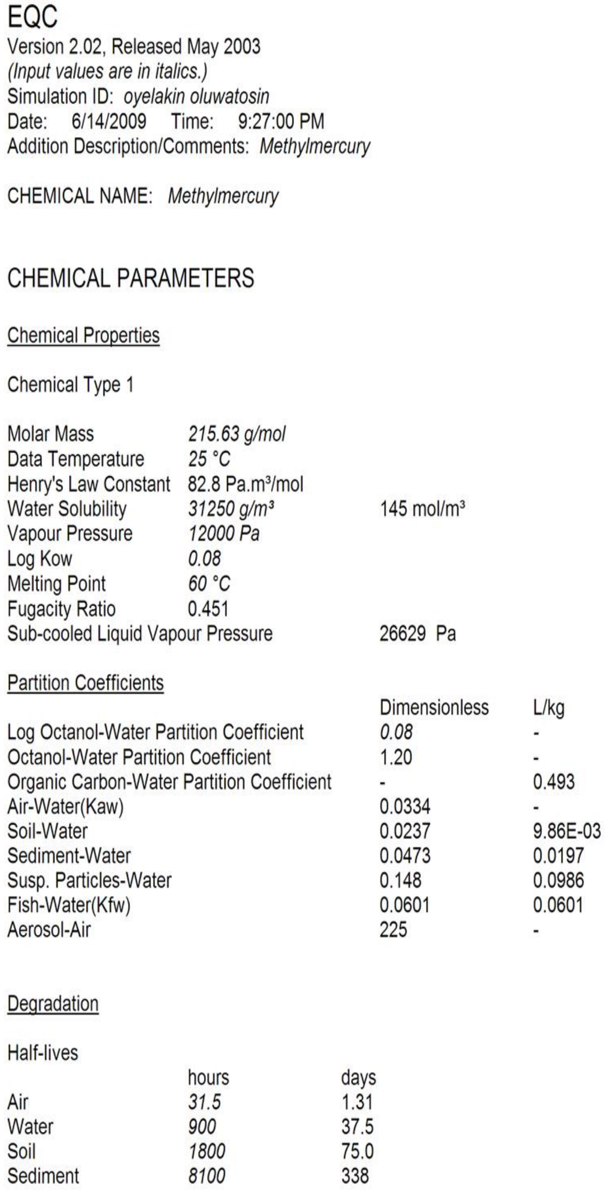
	Half-times hours	days	Equiv. Flows m³/h	D Values mol/Pa.h	Rates of Transport kg/h	mol/h
Air to water	6000	250	1.15E+10	4.66E+06	3.37	15.6
Air to soil	33174	1382	2.09E+09	8.43E+05	0.610	2.83
Water to air	360	15.0	3.85E+08	4.65E+06	36.5	169
Water to sediment	1.38E+05	5771	1.00E+06	12086	0.0949	0.440
Soil to air	65.4	2.72	1.91E+08	7.34E+05	901	4179
Soil to water	883	36.8	1.41E+07	54347	66.7	309
Sediment to water	280	11.7	1.24E+06	12078	0.0910	0.422

Process D Values

Individual	mol/Pa.h
Air-Water diffusion (air-side)	2.02E+07
Air-Water diffusion (water-side)	6.04E+06
Rain dissolution to water	12077
Rain dissolution to soil	1.09E+05
Aerosol deposition to water	0.545
Aerosol deposition to soil	4.91
Soil-Air diffusion (air-phase)	7.26E+05
Soil-Air diffusion (water-phase)	10869
Soil-Air diffusion (boundary layer)	1.82E+08
Soil-Water runoff (water)	54347
Soil-Water runoff (solids)	0.257
Water-Sediment diffusion	12077
Water-Sediment deposition	8.93
Sediment-Water resuspension	1.14

Totals	mol/Pa.h
Air-Water diffusion	4.65E+06
Air-Water exchange	4.66E+06
Water-Air exchange	4.65E+06
Soil-Air diffusion	7.34E+05
Air-Soil exchange	8.43E+05
Soil-Air exchange	7.34E+05
Water-Soil exchange	0
Soil-Water exchange	54347
Sediment-Water exchange	12078
Water-Sediment exchange	12086

Fourth case scenario (release into the three media)



EQC

Version 2.02, Released May 2003
(Input values are in italics.)
Simulation ID: *oyelakin oluwatosin*
Date: 6/14/2009 Time: 9:27:00 PM
Addition Description/Comments: *Methylmercury*

CHEMICAL NAME: *Methylmercury*

CHEMICAL PARAMETERS

Chemical Properties

Chemical Type 1

Molar Mass	*215.63 g/mol*	
Data Temperature	*25 °C*	
Henry's Law Constant	82.8 Pa.m³/mol	
Water Solubility	*31250 g/m³*	145 mol/m³
Vapour Pressure	*12000 Pa*	
Log Kow	*0.08*	
Melting Point	*60 °C*	
Fugacity Ratio	0.451	
Sub-cooled Liquid Vapour Pressure		26629 Pa

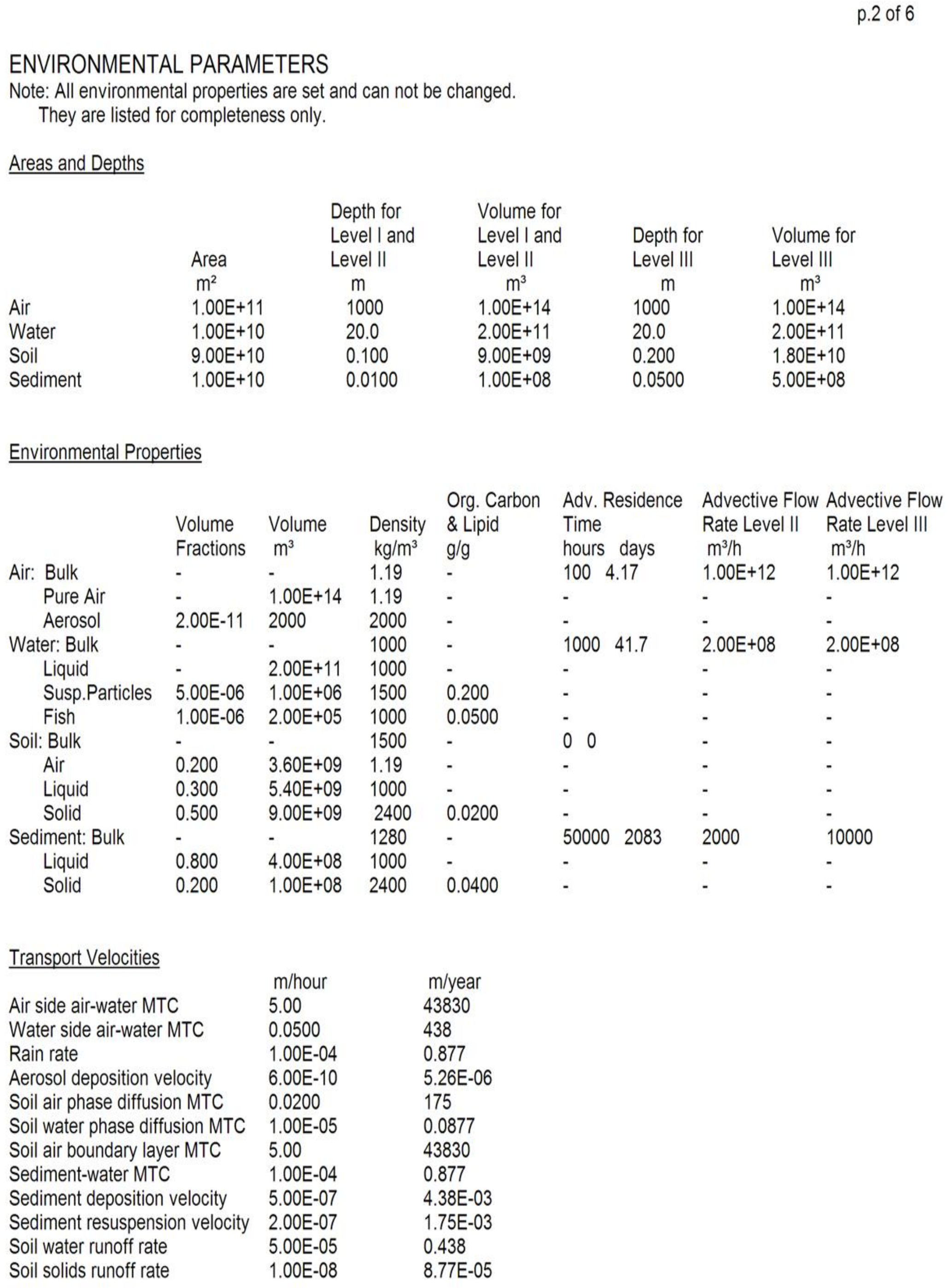
Partition Coefficients

	Dimensionless	L/kg
Log Octanol-Water Partition Coefficient	*0.08*	-
Octanol-Water Partition Coefficient	1.20	-
Organic Carbon-Water Partition Coefficient	-	0.493
Air-Water(Kaw)	0.0334	-
Soil-Water	0.0237	9.86E-03
Sediment-Water	0.0473	0.0197
Susp. Particles-Water	0.148	0.0986
Fish-Water(Kfw)	0.0601	0.0601
Aerosol-Air	225	-

Degradation

Half-lives

	hours	days
Air	*31.5*	1.31
Water	*900*	37.5
Soil	*1800*	75.0
Sediment	*8100*	338



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ENVIRONMENTAL PARAMETERS

Note: All environmental properties are set and can not be changed.
They are listed for completeness only.

Areas and Depths

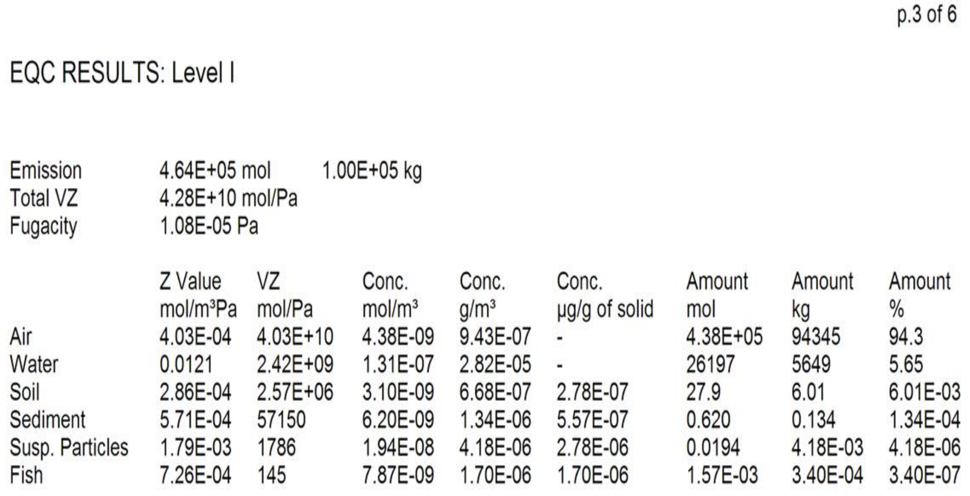
	Area m²	Depth for Level I and Level II m	Volume for Level I and Level II m³	Depth for Level III m	Volume for Level III m³
Air	1.00E+11	1000	1.00E+14	1000	1.00E+14
Water	1.00E+10	20.0	2.00E+11	20.0	2.00E+11
Soil	9.00E+10	0.100	9.00E+09	0.200	1.80E+10
Sediment	1.00E+10	0.0100	1.00E+08	0.0500	5.00E+08

Environmental Properties

	Volume Fractions	Volume m³	Density kg/m³	Org. Carbon & Lipid g/g	Adv. Residence Time hours	days	Advective Flow Rate Level II m³/h	Advective Flow Rate Level III m³/h
Air: Bulk	-	-	1.19	-	100	4.17	1.00E+12	1.00E+12
Pure Air	-	1.00E+14	1.19	-	-		-	-
Aerosol	2.00E-11	2000	2000	-	-		-	-
Water: Bulk	-	-	1000	-	1000	41.7	2.00E+08	2.00E+08
Liquid	-	2.00E+11	1000	-	-		-	-
Susp.Particles	5.00E-06	1.00E+06	1500	0.200	-		-	-
Fish	1.00E-06	2.00E+05	1000	0.0500	-		-	-
Soil: Bulk	-	-	1500	-	0	0	-	-
Air	0.200	3.60E+09	1.19	-	-		-	-
Liquid	0.300	5.40E+09	1000	-	-		-	-
Solid	0.500	9.00E+09	2400	0.0200	-		-	-
Sediment: Bulk	-	-	1280	-	50000	2083	2000	10000
Liquid	0.800	4.00E+08	1000	-	-		-	-
Solid	0.200	1.00E+08	2400	0.0400	-		-	-

Transport Velocities

	m/hour	m/year
Air side air-water MTC	5.00	43830
Water side air-water MTC	0.0500	438
Rain rate	1.00E-04	0.877
Aerosol deposition velocity	6.00E-10	5.26E-06
Soil air phase diffusion MTC	0.0200	175
Soil water phase diffusion MTC	1.00E-05	0.0877
Soil air boundary layer MTC	5.00	43830
Sediment-water MTC	1.00E-04	0.877
Sediment deposition velocity	5.00E-07	4.38E-03
Sediment resuspension velocity	2.00E-07	1.75E-03
Soil water runoff rate	5.00E-05	0.438
Soil solids runoff rate	1.00E-08	8.77E-05



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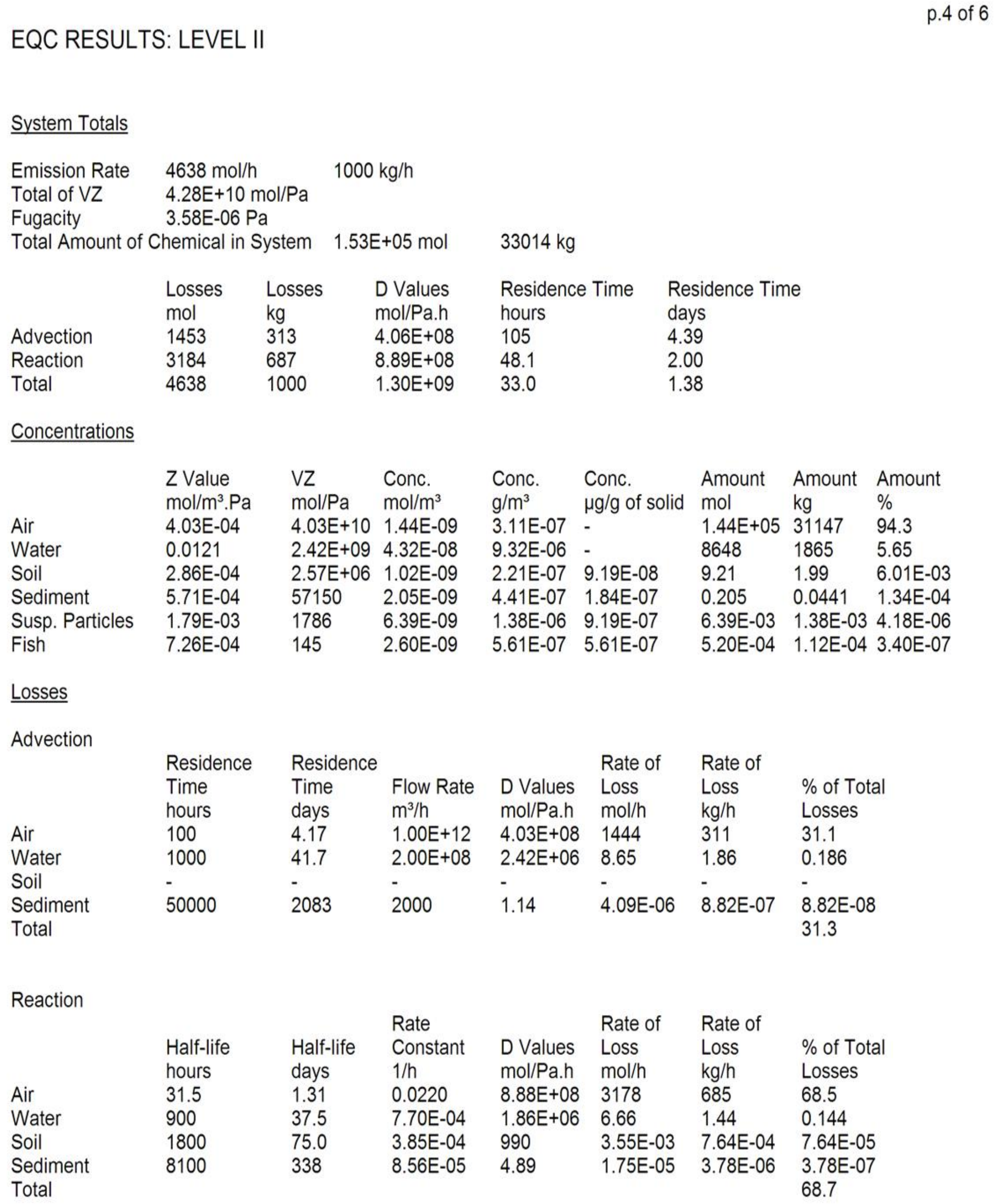
EQC RESULTS: Level I

Emission	4.64E+05 mol	1.00E+05 kg
Total VZ	4.28E+10 mol/Pa	
Fugacity	1.08E-05 Pa	

	Z Value mol/m³Pa	VZ mol/Pa	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	4.38E-09	9.43E-07	-	4.38E+05	94345	94.3
Water	0.0121	2.42E+09	1.31E-07	2.82E-05	-	26197	5649	5.65
Soil	2.86E-04	2.57E+06	3.10E-09	6.68E-07	2.78E-07	27.9	6.01	6.01E-03
Sediment	5.71E-04	57150	6.20E-09	1.34E-06	5.57E-07	0.620	0.134	1.34E-04
Susp. Particles	1.79E-03	1786	1.94E-08	4.18E-06	2.78E-06	0.0194	4.18E-03	4.18E-06
Fish	7.26E-04	145	7.87E-09	1.70E-06	1.70E-06	1.57E-03	3.40E-04	3.40E-07



p.4 of 6

EQC RESULTS: LEVEL II

System Totals

Emission Rate	4638 mol/h	1000 kg/h	
Total of VZ	4.28E+10 mol/Pa		
Fugacity	3.58E-06 Pa		
Total Amount of Chemical in System		1.53E+05 mol	33014 kg

	Losses mol	Losses kg	D Values mol/Pa.h	Residence Time hours	Residence Time days
Advection	1453	313	4.06E+08	105	4.39
Reaction	3184	687	8.89E+08	48.1	2.00
Total	4638	1000	1.30E+09	33.0	1.38

Concentrations

	Z Value mol/m³.Pa	VZ mol/Pa	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solid	Amount mol	Amount kg	Amount %
Air	4.03E-04	4.03E+10	1.44E-09	3.11E-07	-	1.44E+05	31147	94.3
Water	0.0121	2.42E+09	4.32E-08	9.32E-06	-	8648	1865	5.65
Soil	2.86E-04	2.57E+06	1.02E-09	2.21E-07	9.19E-08	9.21	1.99	6.01E-03
Sediment	5.71E-04	57150	2.05E-09	4.41E-07	1.84E-07	0.205	0.0441	1.34E-04
Susp. Particles	1.79E-03	1786	6.39E-09	1.38E-06	9.19E-07	6.39E-03	1.38E-03	4.18E-06
Fish	7.26E-04	145	2.60E-09	5.61E-07	5.61E-07	5.20E-04	1.12E-04	3.40E-07

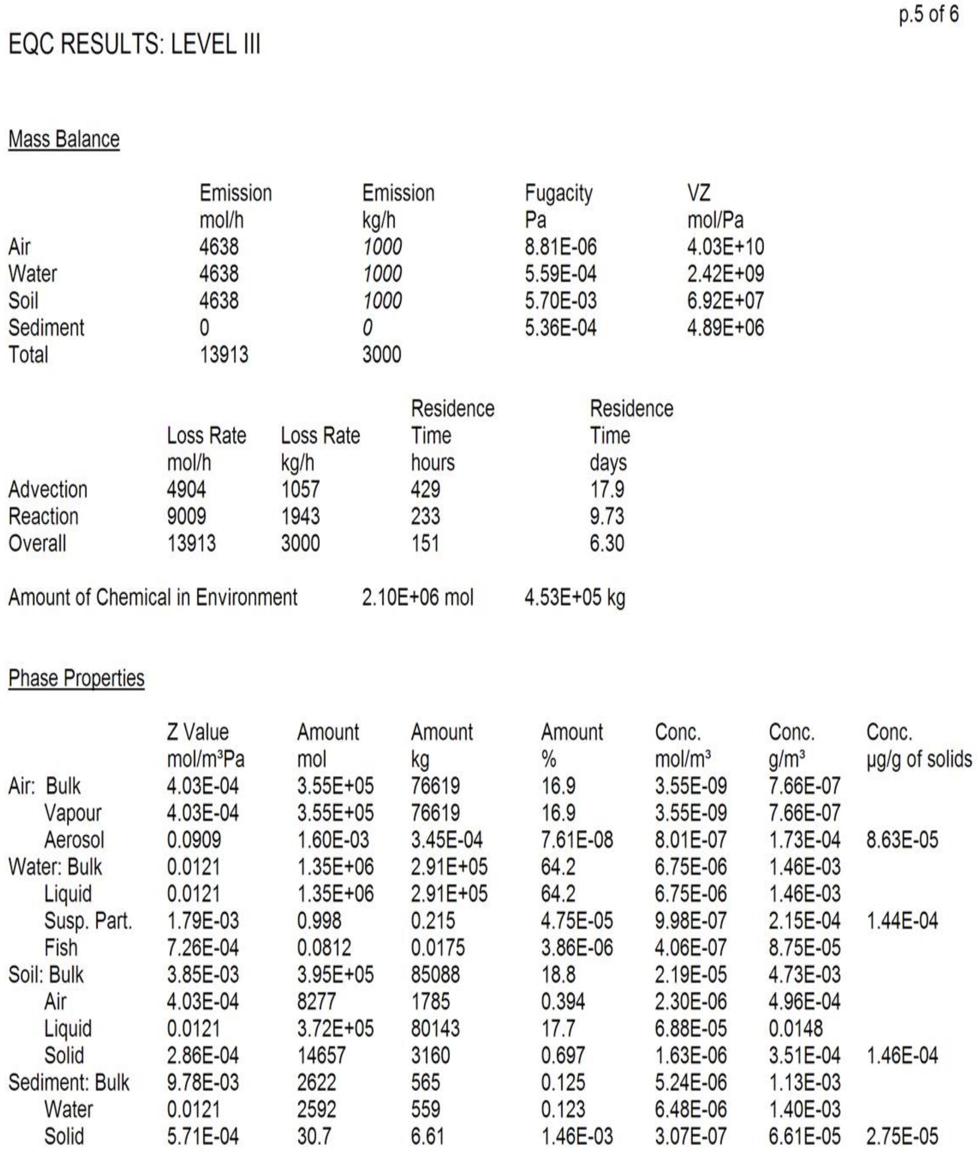
Losses

Advection

	Residence Time hours	Residence Time days	Flow Rate m³/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	1444	311	31.1
Water	1000	41.7	2.00E+08	2.42E+06	8.65	1.86	0.186
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	2000	1.14	4.09E-06	8.82E-07	8.82E-08
Total							31.3

Reaction

	Half-life hours	Half-life days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	31.5	1.31	0.0220	8.88E+08	3178	685	68.5
Water	900	37.5	7.70E-04	1.86E+06	6.66	1.44	0.144
Soil	1800	75.0	3.85E-04	990	3.55E-03	7.64E-04	7.64E-05
Sediment	8100	338	8.56E-05	4.89	1.75E-05	3.78E-06	3.78E-07
Total							68.7



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EQC RESULTS: LEVEL III

Mass Balance

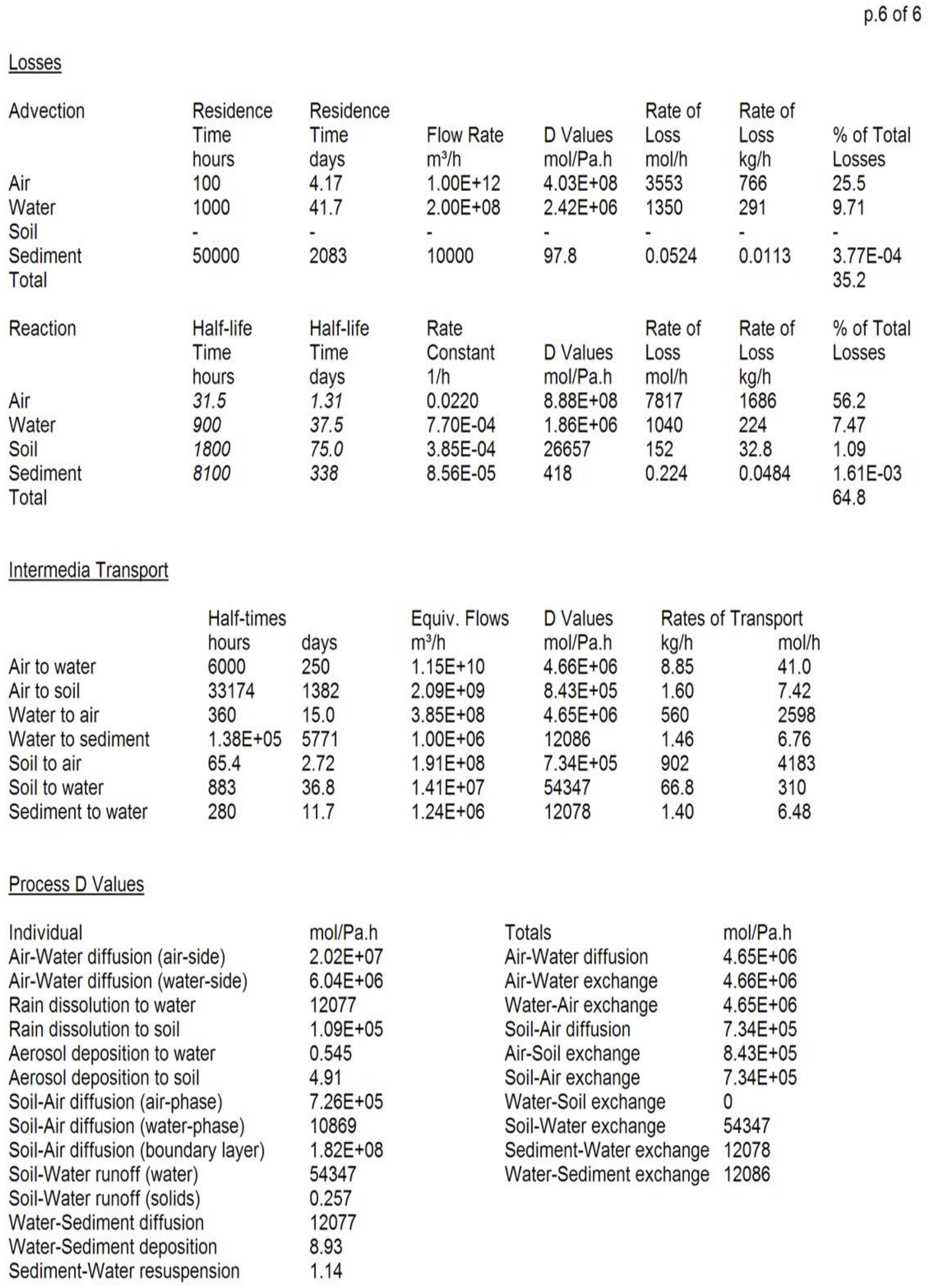
	Emission mol/h	Emission kg/h	Fugacity Pa	VZ mol/Pa
Air	4638	*1000*	8.81E-06	4.03E+10
Water	4638	*1000*	5.59E-04	2.42E+09
Soil	4638	*1000*	5.70E-03	6.92E+07
Sediment	0	*0*	5.36E-04	4.89E+06
Total	13913	3000		

	Loss Rate mol/h	Loss Rate kg/h	Residence Time hours	Residence Time days
Advection	4904	1057	429	17.9
Reaction	9009	1943	233	9.73
Overall	13913	3000	151	6.30

Amount of Chemical in Environment 2.10E+06 mol 4.53E+05 kg

Phase Properties

	Z Value mol/m³Pa	Amount mol	Amount kg	Amount %	Conc. mol/m³	Conc. g/m³	Conc. µg/g of solids
Air: Bulk	4.03E-04	3.55E+05	76619	16.9	3.55E-09	7.66E-07	
Vapour	4.03E-04	3.55E+05	76619	16.9	3.55E-09	7.66E-07	
Aerosol	0.0909	1.60E-03	3.45E-04	7.61E-08	8.01E-07	1.73E-04	8.63E-05
Water: Bulk	0.0121	1.35E+06	2.91E+05	64.2	6.75E-06	1.46E-03	
Liquid	0.0121	1.35E+06	2.91E+05	64.2	6.75E-06	1.46E-03	
Susp. Part.	1.79E-03	0.998	0.215	4.75E-05	9.98E-07	2.15E-04	1.44E-04
Fish	7.26E-04	0.0812	0.0175	3.86E-06	4.06E-07	8.75E-05	
Soil: Bulk	3.85E-03	3.95E+05	85088	18.8	2.19E-05	4.73E-03	
Air	4.03E-04	8277	1785	0.394	2.30E-06	4.96E-04	
Liquid	0.0121	3.72E+05	80143	17.7	6.88E-05	0.0148	
Solid	2.86E-04	14657	3160	0.697	1.63E-06	3.51E-04	1.46E-04
Sediment: Bulk	9.78E-03	2622	565	0.125	5.24E-06	1.13E-03	
Water	0.0121	2592	559	0.123	6.48E-06	1.40E-03	
Solid	5.71E-04	30.7	6.61	1.46E-03	3.07E-07	6.61E-05	2.75E-05



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Losses

Advection	Residence Time hours	Residence Time days	Flow Rate m³/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	100	4.17	1.00E+12	4.03E+08	3553	766	25.5
Water	1000	41.7	2.00E+08	2.42E+06	1350	291	9.71
Soil	-	-	-	-	-	-	-
Sediment	50000	2083	10000	97.8	0.0524	0.0113	3.77E-04
Total							35.2

Reaction	Half-life Time hours	Half-life Time days	Rate Constant 1/h	D Values mol/Pa.h	Rate of Loss mol/h	Rate of Loss kg/h	% of Total Losses
Air	*31.5*	*1.31*	0.0220	8.88E+08	7817	1686	56.2
Water	*900*	*37.5*	7.70E-04	1.86E+06	1040	224	7.47
Soil	*1800*	*75.0*	3.85E-04	26657	152	32.8	1.09
Sediment	*8100*	*338*	8.56E-05	418	0.224	0.0484	1.61E-03
Total							64.8

Intermedia Transport

	Half-times hours	days	Equiv. Flows m³/h	D Values mol/Pa.h	Rates of Transport kg/h	mol/h
Air to water	6000	250	1.15E+10	4.66E+06	8.85	41.0
Air to soil	33174	1382	2.09E+09	8.43E+05	1.60	7.42
Water to air	360	15.0	3.85E+08	4.65E+06	560	2598
Water to sediment	1.38E+05	5771	1.00E+06	12086	1.46	6.76
Soil to air	65.4	2.72	1.91E+08	7.34E+05	902	4183
Soil to water	883	36.8	1.41E+07	54347	66.8	310
Sediment to water	280	11.7	1.24E+06	12078	1.40	6.48

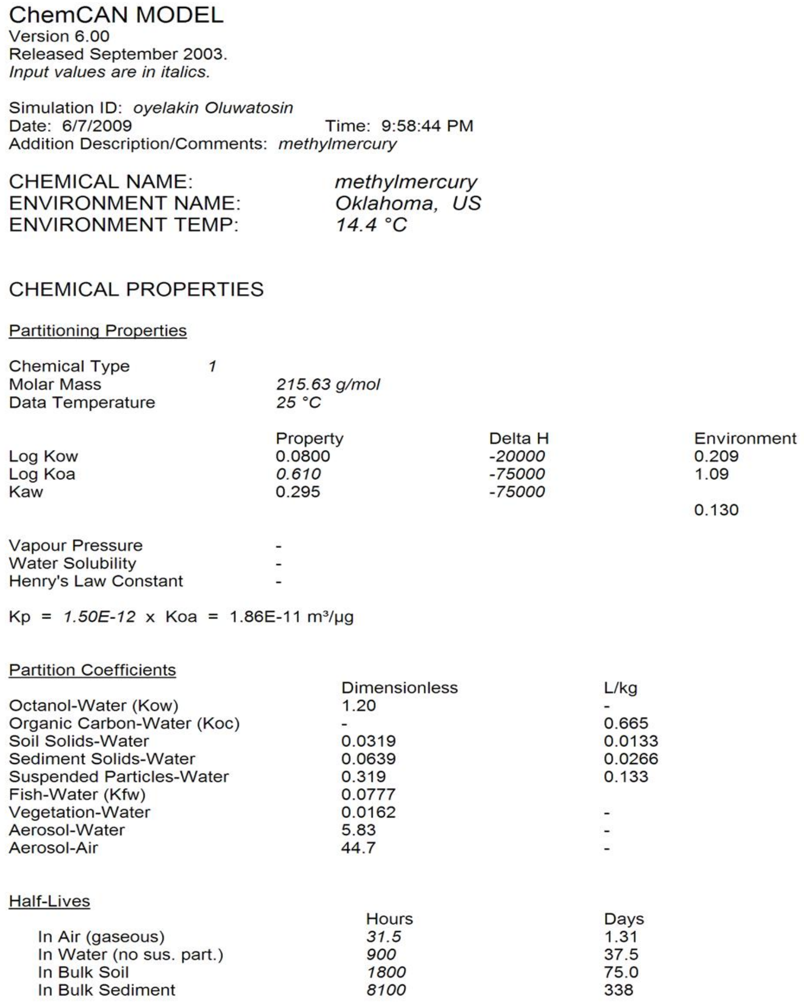
Process D Values

Individual	mol/Pa.h
Air-Water diffusion (air-side)	2.02E+07
Air-Water diffusion (water-side)	6.04E+06
Rain dissolution to water	12077
Rain dissolution to soil	1.09E+05
Aerosol deposition to water	0.545
Aerosol deposition to soil	4.91
Soil-Air diffusion (air-phase)	7.26E+05
Soil-Air diffusion (water-phase)	10869
Soil-Air diffusion (boundary layer)	1.82E+08
Soil-Water runoff (water)	54347
Soil-Water runoff (solids)	0.257
Water-Sediment diffusion	12077
Water-Sediment deposition	8.93
Sediment-Water resuspension	1.14

Totals	mol/Pa.h
Air-Water diffusion	4.65E+06
Air-Water exchange	4.66E+06
Water-Air exchange	4.65E+06
Soil-Air diffusion	7.34E+05
Air-Soil exchange	8.43E+05
Soil-Air exchange	7.34E+05
Water-Soil exchange	0
Soil-Water exchange	54347
Sediment-Water exchange	12078
Water-Sediment exchange	12086

A

APPENICES-B



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ChemCAN MODEL
Version 6.00
Released September 2003.
Input values are in italics.

Simulation ID:  oyelakin Oluwatosin
Date:  6/7/2009                          Time:  9:58:44 PM
Addition Description/Comments:  methylmercury

CHEMICAL NAME:              methylmercury
ENVIRONMENT NAME:           Oklahoma,  US
ENVIRONMENT TEMP:           14.4 °C


CHEMICAL PROPERTIES

Partitioning Properties

Chemical Type           1
Molar Mass                      215.63 g/mol
Data Temperature                25 °C

                                Property          Delta H          Environment
Log Kow                         0.0800            -20000           0.209
Log Koa                         0.610             -75000           1.09
Kaw                             0.295             -75000
                                                                   0.130

Vapour Pressure                 -
Water Solubility                -
Henry's Law Constant            -

Kp  =  1.50E-12  x  Koa  =  1.86E-11 m³/µg


Partition Coefficients
                                  Dimensionless          L/kg
Octanol-Water (Kow)               1.20                   -
Organic Carbon-Water (Koc)        -                      0.665
Soil Solids-Water                 0.0319                 0.0133
Sediment Solids-Water             0.0639                 0.0266
Suspended Particles-Water         0.319                  0.133
Fish-Water (Kfw)                  0.0777
Vegetation-Water                  0.0162                 -
Aerosol-Water                     5.83                   -
Aerosol-Air                       44.7                   -


Half-Lives
                                     Hours               Days
   In Air (gaseous)                  31.5                1.31
   In Water (no sus. part.)          900                 37.5
   In Bulk Soil                      1800                75.0
   In Bulk Sediment                  8100                338
```

ENVIRONMENTAL PROPERTIES

Dimensions

Total Surface Area	*181195 km^2*
Surface Covered by Water	*1.8 %*
Average Air Height	*2 km*
Average Water Depth	*20 m*
Average Soil Depth	*10 cm*
Average Sediment Depth	*1 cm*
Length of Coastline	*9777 km*
Average Depth of Coast	*100 m*
Average Width of Coast	*1 km*

Temperature Conditions	°C
Year round mean	*14.4*
Winter mean	*-26.5*
Summer mean	*19.7*

Organic Carbon	g/g
Particles in Water	*0.2*
Soil Solids	*0.02*
Sediment Solids	*0.04*
Fish Lipid	*0.048*

Residence Times	Days	Hours
Air	*1.67*	40.08
Water	*1830*	43920
Coastal Water	*4*	96

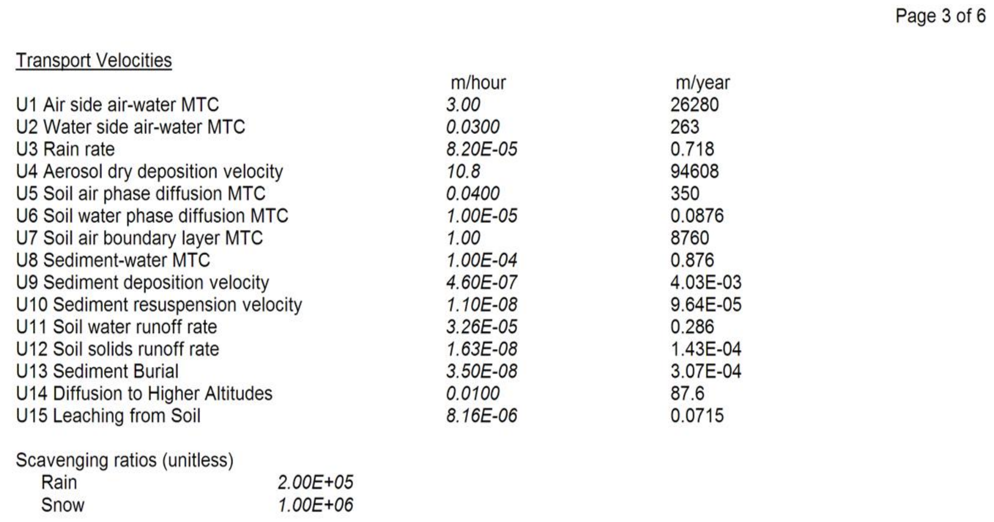
Conc in Groundwater = Conc in Soil Pore Water / (1 + Kow / *500*)

Bulk Compartments

	Volume m^3	Density kg/m^3
Air	3.62E+14	1.229
Water	6.52E+10	1000
Soil	1.78E+10	1500
Sediment	3.26E+07	1420
Groundwater	-	1000
Coastal Water	9.78E+11	1000
Terrestrial Plants	-	*900*

Sub Compartments

	Volume Fraction	Volume m^3	Density kg/m^3
Air Vapour	1.00	3.62E+14	1.229
Air Particles	*2.00E-11*	7248	*2400*
Water	1.00	6.52E+10	1000
Water Particles	*5.00E-06*	3.26E+05	*2400*
Biota	*1.00E-06*	65230	*1000*
Soil Air	*0.200*	3.56E+09	1.229
Soil Water	*0.300*	5.34E+09	1000
Soil Solids	*0.500*	8.90E+09	*2400*
Pore Water	*0.700*	2.28E+07	1000
Sediment Solids	*0.300*	9.78E+06	*2400*



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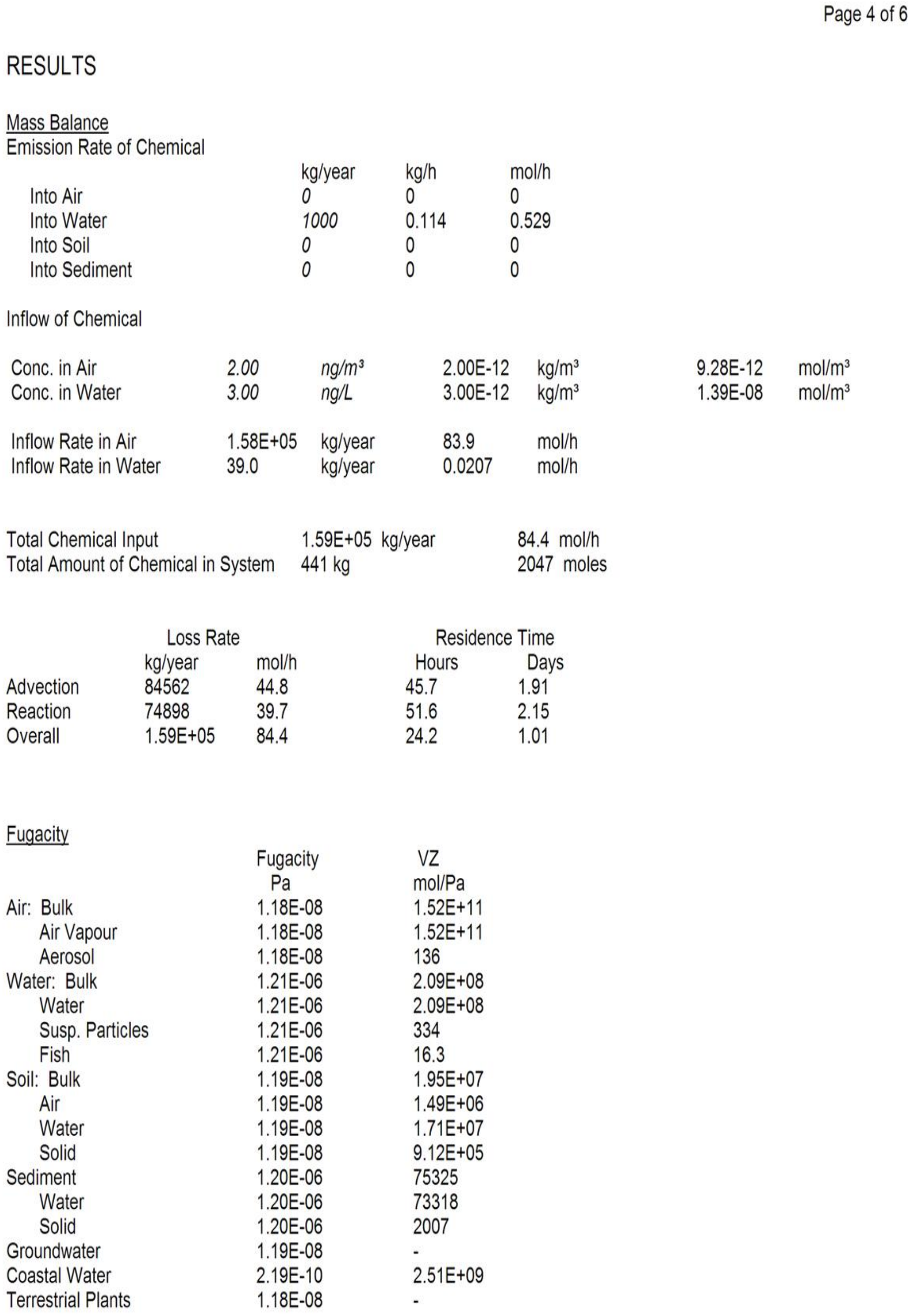
Transport Velocities

	m/hour	m/year
U1 Air side air-water MTC	*3.00*	26280
U2 Water side air-water MTC	*0.0300*	263
U3 Rain rate	*8.20E-05*	0.718
U4 Aerosol dry deposition velocity	*10.8*	94608
U5 Soil air phase diffusion MTC	*0.0400*	350
U6 Soil water phase diffusion MTC	*1.00E-05*	0.0876
U7 Soil air boundary layer MTC	*1.00*	8760
U8 Sediment-water MTC	*1.00E-04*	0.876
U9 Sediment deposition velocity	*4.60E-07*	4.03E-03
U10 Sediment resuspension velocity	*1.10E-08*	9.64E-05
U11 Soil water runoff rate	*3.26E-05*	0.286
U12 Soil solids runoff rate	*1.63E-08*	1.43E-04
U13 Sediment Burial	*3.50E-08*	3.07E-04
U14 Diffusion to Higher Altitudes	*0.0100*	87.6
U15 Leaching from Soil	*8.16E-06*	0.0715

Scavenging ratios (unitless)

Rain	*2.00E+05*
Snow	*1.00E+06*



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RESULTS

Mass Balance

Emission Rate of Chemical

	kg/year	kg/h	mol/h
Into Air	*0*	0	0
Into Water	*1000*	0.114	0.529
Into Soil	*0*	0	0
Into Sediment	*0*	0	0

Inflow of Chemical

Conc. in Air	*2.00*	*ng/m³*	2.00E-12	kg/m³	9.28E-12	mol/m³
Conc. in Water	*3.00*	*ng/L*	3.00E-12	kg/m³	1.39E-08	mol/m³

Inflow Rate in Air	1.58E+05	kg/year	83.9	mol/h
Inflow Rate in Water	39.0	kg/year	0.0207	mol/h

Total Chemical Input	1.59E+05 kg/year	84.4 mol/h
Total Amount of Chemical in System	441 kg	2047 moles

	Loss Rate		Residence Time	
	kg/year	mol/h	Hours	Days
Advection	84562	44.8	45.7	1.91
Reaction	74898	39.7	51.6	2.15
Overall	1.59E+05	84.4	24.2	1.01

Fugacity

	Fugacity Pa	VZ mol/Pa
Air: Bulk	1.18E-08	1.52E+11
Air Vapour	1.18E-08	1.52E+11
Aerosol	1.18E-08	136
Water: Bulk	1.21E-06	2.09E+08
Water	1.21E-06	2.09E+08
Susp. Particles	1.21E-06	334
Fish	1.21E-06	16.3
Soil: Bulk	1.19E-08	1.95E+07
Air	1.19E-08	1.49E+06
Water	1.19E-08	1.71E+07
Solid	1.19E-08	9.12E+05
Sediment	1.20E-06	75325
Water	1.20E-06	73318
Solid	1.20E-06	2007
Groundwater	1.19E-08	-
Coastal Water	2.19E-10	2.51E+09
Terrestrial Plants	1.18E-08	-

Phase Properties

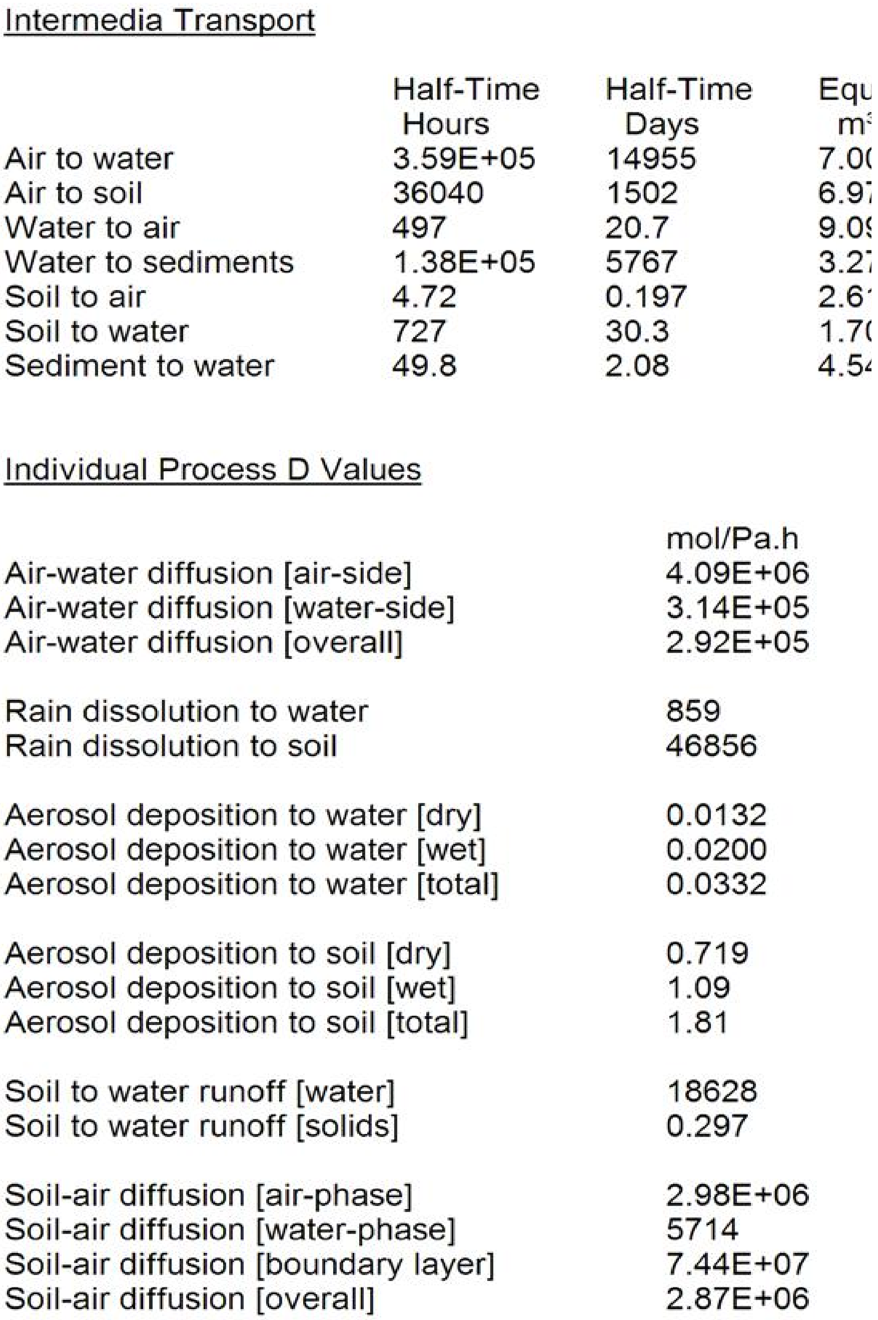
	Z Value mol/m^3.Pa	Amount kg	Amount mol	Amount %	Conc. mol/m^3	Conc. g/m^3	Conc. µg/g
Air: Bulk	4.18E-04	387	1793	87.6	4.95E-12	1.07E-09	8.68E-07
Air Vapour	4.18E-04	387	1793	87.6	4.95E-12	1.07E-09	8.68E-07
Aerosol	0.0187	3.46E-07	1.60E-06	7.84E-08	2.21E-10	4.77E-08	1.99E-08
Water: Bulk	3.21E-03	54.6	253	12.4	3.88E-09	8.37E-07	8.37E-07
Water	3.21E-03	54.6	253	12.4	3.88E-09	8.37E-07	8.37E-07
Susp. Particles	1.03E-03	8.72E-05	4.04E-04	1.98E-05	1.24E-09	2.67E-07	1.11E-07
Fish	2.50E-04	4.24E-06	1.97E-05	9.62E-07	3.02E-10	6.51E-08	6.51E-08
Soil: Bulk	1.10E-03	0.0501	0.233	0.0114	1.31E-11	2.82E-09	1.88E-09
Air	4.18E-04	3.82E-03	0.0177	8.65E-04	4.98E-12	1.07E-09	8.73E-07
Water	3.21E-03	0.0440	0.204	9.96E-03	3.82E-11	8.24E-09	8.24E-09
Solid	1.03E-04	2.34E-03	0.0109	5.30E-04	1.22E-12	2.63E-10	1.10E-10
Sediment: Bulk	2.31E-03	0.0196	0.0907	4.43E-03	2.78E-09	5.99E-07	4.22E-07
Water	3.21E-03	0.0190	0.0883	4.31E-03	3.87E-09	8.34E-07	8.34E-07
Solid	2.05E-04	5.21E-04	2.42E-03	1.18E-04	2.47E-10	5.32E-08	2.22E-08
Groundwater	3.21E-03	-	-	-	3.81E-11	8.22E-09	8.22E-09
Coastal Water	2.57E-03	-	-	-	5.63E-13	1.21E-10	1.21E-10
Terrestrial Plants	5.20E-05	-	-	-	6.15E-13	1.33E-10	1.47E-10

Advection

	Residence Time Hours	Days	Flow Rate m^3/h	D Value mol/Pa.h	Rate kg/year	Rate mol/h	% of Total Losses
Air	40.1	*1.67*	9.04E+12	3.78E+09	84523	44.7	53.0
Water	43920	*1830*	1.49E+06	4770	10.9	5.77E-03	6.83E-03
Coastal Water Flushing	96.0	*4.00*	1.02E+10	2.62E+07	10.8	5.73E-03	6.79E-03
Sediment Burial	-	-	-	0.0234	5.32E-05	2.82E-08	3.34E-08
Loss To Higher Altitudes	-	-	-	7.58E+05	16.9	8.97E-03	0.0106
Leaching To Groundwater	-	-	-	4663	0.105	5.55E-05	6.57E-05
TOTAL					84562	44.8	53.0

Reaction

	Half-Life hours	Half-Life days	Rate Const. 1/h	D Value mol/Pa.h	Rate kg/year	Rate mol/h	% of Total Losses
Air	*31.5*	1.31	0.0220	3.33E+09	74529	39.5	46.7
Water	*900*	37.5	7.70E-04	1.61E+05	368	0.195	0.231
Soil	*1800*	338	3.85E-04	7524	0.169	8.95E-05	1.06E-04
Sediment	*8100*	338	8.56E-05	6.44	0.0147	7.76E-06	9.19E-06
Coastal Water	-	-	-	1.61E+05	0.0668	3.53E-05	4.19E-05
TOTAL					74898	39.7	47.0



Intermedia Transport

	Half-Time Hours	Half-Time Days	Equ m
Air to water	3.59E+05	14955	7.0
Air to soil	36040	1502	6.9
Water to air	497	20.7	9.0
Water to sediments	1.38E+05	5767	3.2
Soil to air	4.72	0.197	2.6
Soil to water	727	30.3	1.7
Sediment to water	49.8	2.08	4.5

Individual Process D Values

	mol/Pa.h
Air-water diffusion [air-side]	4.09E+06
Air-water diffusion [water-side]	3.14E+05
Air-water diffusion [overall]	2.92E+05
Rain dissolution to water	859
Rain dissolution to soil	46856
Aerosol deposition to water [dry]	0.0132
Aerosol deposition to water [wet]	0.0200
Aerosol deposition to water [total]	0.0332
Aerosol deposition to soil [dry]	0.719
Aerosol deposition to soil [wet]	1.09
Aerosol deposition to soil [total]	1.81
Soil to water runoff [water]	18628
Soil to water runoff [solids]	0.297
Soil-air diffusion [air-phase]	2.98E+06
Soil-air diffusion [water-phase]	5714
Soil-air diffusion [boundary layer]	7.44E+07
Soil-air diffusion [overall]	2.87E+06

VITA

OYELAKIN OLUWATOSIN AKINTOYE

Candidate for the Degree of

Master of Science

Thesis: ENVIRONMENTAL FATE ASSESSMENT OF MERCURY COMPOUND, METHYLMERCURY FROM COAL-FIRED POWER PLANTS INOKLAHOMA STATE

Major Field: Environmental Engineering

Biographical:

Personal Data: Born in Shomolu- Lagos, Nigeria on July 20,1979.
The last son in the family of six.

Education: Received Bachelor of Science degree in Environmental and Agric Engineering from University of Ibadan, Nigeria in February, 2006.
Completed the requirements for the Master of Science in Environmental Engineering at Oklahoma State University, Stillwater, Oklahoma in July, 2009.

Experience: Employed by Pivot Engineering 2003 April to December as an Intern. Work with Technodev Nigerian limited as a Maintenance Engineer in the year 2004, April-October,2005, Work as an Environmental physic instructor in a Government school between 2006-September,2007 and Finally worked as Environmental lab assistant as graduate assistant in CIVE department of Oklahoma state University between January,2008-Till date.

Professional Memberships:
Chi Epsilon.
Society of Petroleum Engineers (SPE).
American Society of Agricultural and Biological Engineers (ASABE).
Nigerian Society of Engineers (NSE).
Nigerian Institute of Management (NIM).

Name: OYELAKIN OLUWATOSIN AKINTOYE Date of Degree: July, 2009

Institution: Oklahoma State University Location: Stillwater, Oklahoma

Title of Study: ENVIRONMENTAL FATE ASSESSMENT OF, METHYLMERCURY FROM COAL-FIRED POWER PLANTS IN OKLAHOMA

Pages in Study: 119 Candidate for the Degree of Master of Science

Major Field: Environmental Engineering

Scope and Method of Study:

The basic objective of this research is to determine the environmental fate of methylmercury by assuming all mercury emitted from power plants as methylmercury and by modeling the properties and the fate in a multimedia environment using various computer models such EPIsuite model, EQC and ChemCAN model.

Findings and Conclusions:

Application of the EQC Model yielded estimates of methylmercury environmental fate. Conclusions from this model include:

- Distribution characteristics of the chemicals in the environment depend not only on the chemical properties but also on the media of discharge.
- The methylmercury concentration prediction in Oklahoma river is found to be far beyond the safe level, however these maybe due to various limiting factors incorporated by the ChemCAN model
- Methylmercury is most likely to partition into the atmosphere, while minimal concentration in the atmosphere or soil is expected for the conditions tested.

ADVISER’S APPROVAL: Dr. Dee Ann Sanders