DRAFT ÉBAUCHE

CANADIAN ENVIRONMENTAL PROTECTION ACT

PRIORITY SUBSTANCES LIST

SUPPORTING DOCUMENT

BIS(CHLOROMETHYL) ETHER
AND
CHLOROMETHYL METHYL ETHER

Government of Canada
Environment Canada
National Health and Welfare

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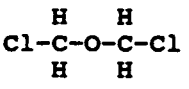
1.0 IDENTITY OF SUBSTANCE

1.1 Name and Characteristics of Substance

Bis(chloromethyl)ether (BCME) and chloromethyl(methyl)ether (CMME) are included in a large class of chemical substances known as the chloroalkyl ethers. A list of the data bases used for literature searches is presented in Appendix I.

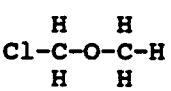
Bis (Chloromethyl)Ether

Bis(chloromethyl) ether (BCME) is a colourless liquid (CCINFO 1991) with a suffocating odour (Sittig 1981). BCME has a molecular formula of $C_2H_4Cl_2O$ and a molecular weight of 114.96 (Verschueren 1983). The Chemical Abstracts Service (CAS) registry number for BCME is 542-88-1 (CCINFO 1991). A list of synonyms for BCME is presented in Table 1-1. The most common synonyms are oxybis(chloromethane), chloromethyl ether, and bichloromethyl ether. The molecular structure for BCME is shown below.



Chloromethyl methyl ether

CMME is a colourless liquid (Verschueren 1983) with an "irritating" odour (CCINFO 1991). Freshly produced CMME contains a minimum of 95% of the pure compound (CCINFO 1991). CMME has a molecular formula of C_2H_5ClO and a molecular weight of 80.52 (Verschueren 1983). The Chemical Abstracts Service (CAS) registry number for CMME is 107-30-2 (CCINFO 1991). A list of synonyms for chloromethyl methyl ether is presented in Table 1-2. Methyl chloromethyl ether and chloromethoxymethane are commonly used synonyms. Notably, technical (industrial) grade CMME contains between 1% to 8% BCME as a contaminant (Travenius 1982). The molecular structure for CMME is shown below.



1.2 Analytical Methodology

Bis(chloromethyl)ether

Considerable information is available regarding analytical methodologies concerning the sampling and analysis of BCME for monitoring low microgram-per-cubic metre ($ug.m^{-3}$) levels of BCME in ambient workplace air (Collier 1972, Evans *et al.* 1975, Frankel and Black 1976, Parkes *et al.* 1976, Kallos 1981, Muller *et al.* 1981, Galvin and House 1988, Blease *et al.* 1989). Typically, air

samples are drawn into a sorption tube, thermally eluted, and analyzed by gas chromatography and mass spectrometry. Two methods are also described that utilize BCME vapour from air with subsequent analysis by gas chromatography (Sawicki *et al.* 1976, Langelaan and Nielen 1989). Methods of sampling and analyzing for BCME in water or soil were not identified.

Collier (1972), Frankel and Black (1976) and Galvin and House (1988) reported a detection limit of 470 $ng \cdot m^{-3}$ for BCME in air, while Evans *et al.* (1975) and Langelmaan and Nielen (1989) achieved detection limits as low as 50 $ng \cdot m^{-3}$ and 14 $ng \cdot m^{-3}$, respectively. Muller *et al.* (1981) did not report a detection limit, but quantified a BCME concentration of 2.35 $ug \cdot m^{-3}$ in air. The methods described by Sawicki *et al.*(1976) and Parkes *et al.*(1976) have a detection limit of 2.35 $ug \cdot m^{-3}$. A detection limit of approximately 4.7 $ng \cdot m^{-3}$ was established for the technique reported by Blease *et al.* (1989) for measuring BCME in air.

Chloromethyl methyl ether

Available information regarding analytical methodologies for sampling and analyzing CMME is limited to techniques developed for monitoring low $ug \cdot m^{-3}$ levels in ambient workplace air. Four methodologies are described which utilize CMME vapour and subsequent analysis by gas chromatography (Sawicki *et al.* 1976, Kallos *et al.* 1977, Langhorst *et al.* 1981, Langelaan and Nielen 1989). The reported detection limits for these methodologies are 49 $ng \cdot m^{-3}$ (Langelaan and Nielen 1989); 1.65 $ug.m^{-3}$ (Sawicki *et al.* 1976, Langhorst *et al.* 1981) to 3.29 $ug.m^{-3}$ (Kallos *et al.* 1977). Methods of sampling and analysis for CMME in water or soil were not identified.

2.0 PHYSICAL AND CHEMICAL PROPERTIES

Bis (Chloromethyl)Ether

The physical and chemical properties of BCME are reported in Table 2-1. A melting point of -41.5°C has been reported for BCME (Mabey *et al.* 1982). Reported boiling points range from 104 to 106°C (CCINFO 1991).

The reported water solubility (22,000 $mg \cdot L^{-1}$; Mabey *et al.* 1982) indicates that BCME is moderately soluble in water, however, it cannot be ascertained whether this value was calculated or estimated. The solubility of BCME in water has little real environmental significance since it undergoes rapid hydrolysis in water, with half-lives ranging from 0.12 to 4.7 min (7 to 280 sec) (U.S. EPA 1980a) and rate constants ranging from 0.15 to 6 min^{-1} (0.0025 to 0.1 sec^{-1}) (Tou *et al.* 1974). Reported half-lives for the hydrolysis of BCME in a 3:1 water:dimethylformamide solution range from 0.068 min at 45°C to 9.5 min at 0°C (Nichols and Merritt 1973). The rate constants for BCME in this medium range from 2.8×10^{-3} min^{-1} (1.70×10^{-1} sec^{-1}) to more than 3.5×10^{-1} min^{-1} (Van Duuren *et al.* 1972, Nichols and Merritt 1973).

The Henry's law constant (21.2 $Pa \cdot m^3 \cdot mol^{-1}$) and high vapour pressure (4 kPa @ 22°C) indicates that BCME has the characteristics of a volatile compound (Mabey *et al.* 1982). However, owing to its rapid hydrolysis in water, the volatilization is likely to be insignificant.

A half-life of more than 25 hours is reported for the hydrolysis of gaseous BCME in an atmosphere of water vapour (Tou and Kallos 1974a). Reported rate constants range from 0.00047 to 0.53 min^{-1} for this reaction (Tou and Kallos 1974a, 1976).

Reported half-lives for the indirect photolysis of gaseous BCME range from 1.36 to 48 hours (Clement Associates 1989). Rate constants for this reaction in water range from 0.05 to <6 $mol^{-1} \cdot min^{-1}$ (3 to <360 $mol^{-1} \cdot h^{-1}$) (Mabey *et al.* 1982).

Mabey *et al.* (1982) calculated a log octanol/water partition coefficient (log K_{ow}) for BCME of 2.4 and a sorption partition coefficient, normalized for organic carbon content (log K_{oc}) of 1.2 (Mabey *et al.* 1982).

Chloromethyl methyl ether

Physical and chemical properties of CMME are reported in Table 2-2. Reported melting points range from -103.5 to -104°C (Verschueren 1983, CCINFO 1991), while reported boiling points range from 55 to 61°C (CCINFO 1991, Durkin *et al.* 1975). A vapour pressure of 122 mm Hg at 20°C has been reported for CMME (CCINFO 1991). A Henry's law constant has not been reported for CMME.

The reported half-life of CMME in water ranges from <1.17×10^{-4} to <0.017 min (<0.007 to <1 sec) (Tou and Kallos 1974a, Radding *et al.* 1977). A single rate constant of >5400 min^{-1} (>90 sec^{-1}) has been calculated for the hydrolysis of CMME in water at 25 °C (Radding *et al.* 1977). Van Duuren *et al.* (1972) reported a rate constant of >3.5×10^{-1} min^{-1} for the hydrolysis of CMME in a 3:1 water: dimethylformamide solution at 0°C. The corresponding half-life for this reaction is <2 min (Van Duuren *et al.* 1972).

Reported half-lives for the hydrolysis of CMME in air range from 3.5 min to >390 min (>6.5 h) (Nichols and Merritt 1973, Tou and Kallos 1974a). A single rate constant of 0.0018 min^{-1} is reported for the hydrolysis of CMME in air at a relative humidity of 39% (Tou and Kallos 1974a).

A single, calculated half-life of 230 hours (13,800 minutes) is reported for the indirect photolysis of CMME (Radding *et al.* 1977).

Radding *et al.* (1977) reported a calculated log octanol/water partition coefficient (log K_{ow}) of -0.21. Information was not found regarding the partitioning of CMME between sediment and water (i.e. sorption partition coefficient, normalized for organic carbon content, or log K_{oc}).

3.0 SOURCES AND RELEASES TO THE ENVIRONMENT

3.1 Natural Sources

No natural sources of BCME or CMME have been identified.

3.2 Anthropogenic Sources

3.2.1 Manufacturing processes

bis (Chloromethyl) ether

BCME is formed when formaldehyde reacts with chloride ions in an acidic medium (Travenius 1982). Specific synthesis reactions include the reaction between paraformaldehyde and chlorosulfonic acid (Durkin *et al.* 1975) and the saturation of a paraformaldehyde solution in cold sulfuric acid with hydrogen chloride (U.S. EPA 1980a). As well, the decomposition products of commercial forms of chloromethyl methyl ether can combine to produce 1-8% BCME as an impurity (Travenius 1982). Small amounts of BCME (several percent) are also produced during the synthesis of chloromethyl methyl ether from gaseous hydrogen chloride and heated methanol and formaldehyde (Durkin *et al.* 1975).

Because of occupational concerns, considerable attention has been given to the possible spontaneous formation of BCME from formaldehyde and hydrogen chloride, two compounds that are widely used in industry and possibly present in the ambient, workplace air (Kallos and Solomon 1973, Frankel *et al.* 1974, Tou and Kallos 1974b, Travenius 1982). Investigators have studied the formation of BCME from formaldehyde and chloride salts (Tou and Kallos 1976, Travenius 1982), from formaldehyde resins and chloride salts (Travenius 1982), and from dimethyl ether and chlorine gas (Kallos and Tou 1977). Typically, these studies indicate that moderate to high concentrations (in the $mg \cdot L^{-1}$ or $mg \cdot m^{-3}$ range) of the reactants are required to produce low concentrations (in the $ug \cdot m^{-3}$ range) of BCME. While these reactions may be of significance in an occupational setting, they are not likely to have any environmental significance because the required concentrations of formaldehyde and hydrogen chloride do not occur in ambient air.

Chloromethyl methyl ether

CMME can be produced by the reaction of anhydrous hydrogen chloride, methanol and formaldehyde (Fishbein 1979) and by direct chlorination of dimethyl ether (Durkin *et al.* 1975). These formation reactions are illustrated in Figures 3-1 and 3-2. Small amounts of bis(chloromethyl) ether (several percent) are produced in the latter process (Durkin *et al.* 1975). Technical grade CMME is reported to contain 1 to 8% bis(chloromethyl) ether as an impurity, formed from the formaldehyde and hydrogen chloride produced as a result of CMME decomposition (Travenius 1982). The formation of the bis(chloromethyl) ether contaminant by this process is illustrated in Figure 3-3. An additional method has been reported (CCINFO 1991) which is designed to produce CMME that is free of bis(chloromethyl) ether impurities and ready for most uses without further purification. The method involves the addition of actinium chloride to a slight excess of anhydrous dimethoxymethane at room temperature.

3.2.2 Canadian Consumption

To ascertain the extent to which BCME and CMME are used in Canada, a Notice under subsection 16(1) of the Canadian Environmental Protection Act was published in the Canada Gazette (in 1991) and sent to 9 companies and 9 trade associations considered most likely to be involved in commercial activities involving either BCME or CMME (Canada Gazette Part I, 1991). The Notice required them to report

any commercial activity involving more than one kilogram of either compound, whether alone, in a mixture, or as a contaminant of any other commercially used material. The responses revealed that neither of these substances was used or produced in Canada in amounts greater than 1 kg in 1990 or 1991 (Environment Canada 1992). Both BCME and CMME were reported to be used in Canada between 1984 and 1986 (Canada Gazette 1991). This information was verified and was proved to be erroneous for CMME. BCME was used as an intermediate in a highly specific and closely monitored reaction sequence by one company in the early 1980's, but this process was discontinued in 1985. No BCME was present in their final product.

3.2.3 Uses

Bis (Chloromethyl)Ether

During World War I, the efficacy of BCME as a poisonous gas was investigated with minimal success (Travenius 1982). In later years, primary industrial uses of BCME were as chloromethylating agents in the preparation of ion exchange resins, water repellants and other textile treating agents, the manufacture of polymers, and a solvent for polymerization reactions (Fishbein 1979). However, BCME is no longer used as an intermediate in the production of ion exchange resins (U.S. EPA 1987). Specific minor uses of BCME have included: crosslinking of cellulose; preparation of three-block styrene-butadiene-styrene polymers; and surface treatment of vulcanized rubber to increase adhesion of epoxy resin and polyurethane elastomers (Durkin *et al.* 1975).

The use of BCME in industrial processes in the U.S. has become greatly restricted as a result of concerns about its carcinogenic action in occupational exposure. Since the early 1980's the use of BCME has been restricted to specfic chloromethylation reactions (locations not provided) (Travenius 1982). BCME is not commercially available in the United States nor it it manufactured in Canada (HSDB 1990). BCME has been removed from the toxic pollutant list in the United States (U.S. EPA, 1980b, 1981) due to insignificant production or use, lack of persistence in water, low adsorption on solid particles, low bioaccumulation and lack of toxicity when organisms ingest water or aquatic organisms exposed to it.

Chloromethyl methyl ether

CMME has been used as an intermediate in the production of chloromethyl derivatives, which are subsequently converted to amine compounds for use as ion exchange resins, water repellents and other industrial polymers (CCINFO 1991). It has also been used as a solvent for polymerization reactions (Fishbein 1979). Other minor uses of CMME have included: synthesis of methoxymethyl ethers of phenols; crosslinking of polystyrene; and surface treatment of vulcanized rubber to increase adhesion of epoxy resin or polyurethane elastomers (Durkin *et al.* 1975).

The use of CMME in industrial processes has become greatly restricted as a result of concerns about occupational exposures. However, CMME is still used at unspecified facilities for difficult chloromethylation reactions (Travenius 1982).

3.2.4 Releases

There is no known release of BCME or CMME into the Canadian environment.

According to the Toxic Release Inventory (TRI) (U.S. EPA 1990), in the United States, the total estimated aerial releases of BCME in 1989 was 1.4 kg/yr (from two chemical plants) and for CMME totalled 59 kg/yr (from three chemical plants). No release to either water or land was reported. CMME is not manufactured at these facilities but is used in the production and formulation of other chemical products.

Given that atmospheric degradation is rapid (a half-life of less than 3 and 4 days for BCME and CMME respectively), it is unlikely that even small amounts of BCME and CMME could be transported to Canada from the United States through long-range transport.

4.0 ENVIRONMENTAL TRANSPORT, TRANSFORMATION AND LEVELS

A limited amount of information was found in the literature regarding the environmental transport and transformation of BCME. Most of this information deals with the hydrolysis and, to a lesser degree, the indirect photolysis of BCME. Typically, the alpha-haloethers are highly reactive compounds as a result of the bonding of two electronegative atoms, oxygen and chlorine, to the same carbon (Durkin *et al.* 1975). Cupitt (1980) predicted the atmospheric residence time for BCME to be 0.02-2.9 days and for CMME to be 0.004-3.9 days.

4.1 Hydrolysis

bis(Chloromethyl)ether

Hydrolysis is the predominant factor affecting the environmental fate of BCME. While Alvarez and Rosen (1976) report that BCME does not readily decompose in water or aqueous base, experimental data indicates that BCME can undergo rapid hydrolysis in water (Tou and Kallos 1974b, Tou *et al.* 1974). The rate of BCME hydrolysis in water (with an acetone carrier) was found to increase with increasing temperature and was described as a nucleophilic reaction (Tou *et al.* 1974). BCME hydrolysis was also faster in alkaline than in acidic solutions (Tou *et al.* 1974). The headspace in sealed reaction vessels during these experiments was eliminated to prevent volatilization of BCME from solution. Thus, the hydrolysis rate constants (0.0025, 0.018, and 0.10 sec^{-1} for 0°C, 20°C and 40°C, respectively) obtained by Tou *et al.* (1974) may be higher than would be observed in natural open waters.

In the literature, hydrolysis rate constants for BCME were investigated in deionized water and various solutions of hydrogen chloride and formaldehyde. The hydrolysis rate (0.050 $seconds^{-1}$) was independent of hydrogen chloride and formaldehyde concentrations. BCME hydrolysis was described as a pseudo-unimolecular reaction (Tou and Kallos 1974b).

The reported half-lives for BCME hydrolysis in water were 280, 38 and 7 seconds at 0°C, 20°C and 40°C, respectively (U.S. EPA 1980). These were calculated from rate constants measured by Tou *et al.* (1974).

Rate constants for BCME hydrolysis in a 3:1 water: dimethylformamide

solution range from >$3.5x10^{-1}$ to $1.02x10^{1}$ $minutes^{-1}$ ($1.70x\ 10^{-1}$ $seconds^{-1}$). The lower limit of this range is a measured rate constant for BCME hydrolysis at 0°C (Van Duuren *et al.* 1972). The upper limit of the range is an extrapolation to 45°C of the rate constant measured by Van Duuren *et al.* (1972) at 0°C (Nichols and Merritt 1973). It is not known what effect dimethylformamide has on the rate of BCME hydrolysis in water. Reported half-lives for BCME hydrolysis in a 3:1 water:dimethylformamide solution range from 0.068 minutes (4.1 seconds) to 9.5 minutes (Van Duuren *et al.* 1972, Nichols and Merritt 1973). The upper and lower limits of this range were calculated for 45 and 0°C, respectively, by Nichols and Merritt (1973) from the data produced by Van Duuren *et al.* (1972).

Experimental data indicate that atmospheric hydrolysis of BCME is likely to occur at a slower rate than in aqueous solution. The rate of BCME hydrolysis in the headspace of a stirred reaction vessel, with both gaseous and aqueous phases in equilibrium, was found to range from 0.16 to 0.53 $minutes^{-1}$. An increase in the stirring rate increased the rate of BCME hydrolysis in the gaseous phase (Tou and Kallos 1976). In a study undertaken by Tou and Kallos (1974a) the rate of gaseous BCME hydrolysis was strongly affected by the container surface (i.e. surface catalysis) and was dependent on the reaction vessel material (i.e. ferric oxidecoated Saran > glass > fused ground glass). The rate of BCME hydrolysis in the gas phase (0.00047 $minutes^{-1}$ at 81% relative humidity) was concluded to be slower than the rate measured in the aqueous phase in the fused ground glass vessel. The corresponding half-life was >25 hours (Tou and Kallos 1974a). Collier (1972) found BCME to be stable in air (70% relative humidity) for at least 18 hours.

Chloromethyl methyl ether

Hydrolysis is probably the dominant factor affecting the environmental fate of CMME. Although measured rate constants were not found, CMME apparently hydrolyses rapidly in water, forming hydrogen chloride, methanol and formaldehyde (CCINFO 1991). A single rate constant of >90 $seconds^{-1}$ and half-life of <0.007 seconds have been calculated for the hydrolysis of CMME in water at 25°C and pH 7 (Radding *et al.* 1977). The rate constant of >$3.5x10^{-1}$ $minutes^{-1}$ corresponding to a half-life of < 2 minutes was measured during an investigation of the reactivity of CMME as an alkylating agent in biological tissues. The reaction was allowed to proceed at 0°C, using 25% dimethylformamide in water as a solvent for CMME (Van Duuren *et al.* 1972). The effect of dimethylformamide on the rate of CMME hydrolysis is not known.

A review of the hydrolysis of CMME in various aqueous solutions of high organic solvent concentrations (i.e. >90%) is reported by Durkin *et al.* (1975). These data are not discussed here since they are not considered to be applicable to ambient environmental conditions.

The half-life of CMME in aqueous solution cannot be directly measured with accuracy (U.S. EPA 1980). Reported half-lives for the hydrolysis of CMME in water range from <0.007 seconds to < 1 seconds (Radding *et al.* 1977, Tou and Kallos 1974a). The latter value was extrapolated by Tou and Kallos (1974a) from rate constants measured by Jones and Thorton (1967) for solvolysis of CMME in a series of solvents and solvent mixtures. As well, Van Duuren *et al.* (1972) reported a rate constant of >$3.5x10^{-1}$ $minutes^{-1}$ and half-life of <2 minutes for the hydrolysis of CMME in a 3:1 water:dimethylformamide solution. This mixture was used since many of the compounds tested in the

experiment had limited solubility in water.

Atmospheric hydrolysis of CMME probably occurs at a slower rate than in aqueous solution. In an investigation by Tou and Kallos (1974a) the hydrolysis of gaseous CMME was found to be surface catalyzed, and the measured reaction rate was strongly dependent on the surface materials of the reaction vessels (i.e. ferric oxide-coated Saran > glass > Teflon > Saran). The results also indicate that the rate of hydrolysis increased with increasing relative humidity (RH). The investigators concluded that the rate of CMME hydrolysis in the gas phase was slower than, or comparable to, the rate determined for the reaction in the Saran vessel (reported upper limit of 0.0018 $minutes^{-1}$ at 39% RH and 29°C). Durkin *et al.* (1975) suggests that CMME may persist in the atmosphere for extended periods of time. However, reported half-lives for CMME hydrolysis in the gaseous phase range from 3.5 minutes at 25°C and 70% relative humidity to >390 minutes (>6.5 hours) at 29°C and 39% relative humidity (Nichols and Merritt 1973, Tou and Kallos 1974a).

4.2 Photolysis

BCME and CMME are unlikely to undergo direct photolysis since alkyl ethers, even halogenated ones, are not strong absorbers of ultraviolet (UV) light (Durkin *et al.* 1975). If alkyl ethers are to undergo photochemical reactions, they must derive energy from light indirectly (Durkin *et al.* 1975). For purposes of this discussion, the oxidation of BCME and CMME by photochemically-generated radicals is referred to as indirect photolysis.

bis(Chloromethyl)ether

BCME reacts with photochemically-generated hydroxyl radicals to produce chloromethyl formate, chloroform, formaldehyde and hydrogen chloride (Cupitt 1980). In water at 25°C, rate constants of 0.05 $mol^{-1}minute^{-1}$ and <6 $mol^{-1}minute^{-1}$ have been calculated for indirect BCME photolysis by peroxy radicals and singlet oxygen, respectively (Mabey *et al.* 1982).

Chloromethyl methyl ether

A single, calculated half-life of 230 hours (13,800 min) is reported for the indirect photolysis of CMME vapour (Radding *et al.* 1977) (with a rate constant of 6.0×10^{-9} $mol^{-1}minute^{-1}$).

4.3 Volatilization

Both BCME and CMME are volatile compounds as indicated by their vapor pressures (4 kPa @ 22°C and 16.3 kPa @ 20°C for BCME and CMME, respectively), although rapid hydrolysis in water might preclude this. Studies quantifying the volatility were not found.

4.4 Adsorption/Desorption

The low log K_{oc} (1.2) calculated by Mabey *et al.* (1982) indicates that BCME has a minimal soil or sediment-adsorption potential. Confirming data

were not found. BCME and CMME would be unlikely to be mobile in soil as they would hydrolyse in the presence of water.

4.5 Biodegradation/Bioconcentration

Information regarding BCME biodegradation and bioconcentration in the environment were not identified. The rapid hydrolysis of BCME in aqueous media prevents its biodegradation potential from being realized. Available data regarding the partitioning of BCME to biological media indicate that the compound is unlikely to bioconcentrate. The calculated log K_{ow} for BCME is 2.4 (Mabey *et al.* 1982).

Although information on CMME biodegradation and bioconcentration in the environment were not identified, the rapid rate of CMME hydrolysis suggests that processes such as biodegradation, adsorption and persistence are not environmentally significant and that concentrations in the natural environment are not a concern.

4.6 Environmental Concentrations

Since no more than one kilogram of BCME and CMME are currently used in Canada and both compounds rapidly hydrolyse in aqueous media, it is improbable that these substances would be detected in various environmental media in Canada. No data were found on levels of BCME or CMME in the Canadian environment, or in foodstuffs produced in Canada.

The STORET database indicated that 14 of 977 samples of industrial effluent in the United States had detectable BCME concentrations (detection limit not reported) with a median concentration of <1.0 $ug \cdot L^{-1}$ (Staples *et al.* 1985). The validity of this information is questionable, however, since industrial effluents are likely to be comprised primarily of water and any BCME present is probably rapidly hydrolysed (U.S. EPA 1980). The STORET information indicates that BCME was not detected in any samples of U.S. ambient water, sediment or biota.

4.1.6 Predictions of environmental fate using computer modelling

As there are no data on the environmental concentration and behaviour of BCME or CMME in the Canadian environment, the fate of these compounds was predicted using a Level III Fugacity Model (Mackay and Paterson 1991). A worst-case scenario was used based on the total U.S. TRI estimates of release into each environmental compartment. Except for underground injections, which were excluded, it was assumed that the total estimated release in the U.S., 0.00136 and 0.059 tonnes/yr of BCME and CMME, respectively, was released in southern Ontario in the following proportions: air 100%, water 0% and soil 0%. For BCME the predicted environmental concentrations at equilibrium were: 1.13×10^{-10} $\mu g/m^3$ in air, 5.71×10^{-14} ng/L in surface water, 3.14×10^{-19} $\mu g/g$ in soil and 2.95×10^{-23} $\mu g/g$ in sediment. For CMME the predicted environmental concentrations at equilibrium were: 4.44×10^{-7} $\mu g/m^3$ in air, 1.15×10^{-10} ng/L in surface water, 8.7×10^{-16} $\mu g/g$ in soil and 5.99×10^{-20} $\mu g/g$ in sediment. The model shows that it is the atmospheric fate which is of primary concern for both BCME and CMME. The full computer program output is attached in Appendix II.

5.0 POPULATION EXPOSURES

5.1 Exposure of Wildlife Populations

Wildlife populations are potentially exposed to contaminants via drinking water, food and inhaled air. While evidence does not exist for the presence of BCME or CMME in the atmosphere (U.S. EPA 1980), the atmospheric half-lives for both compounds is less than 4 days. As a result of concerns for human health, restrictions in place in the U.S. concerning the release of BCME to the atmosphere also protects wildlife.

Exposure of wildlife populations to contaminated water impacted by industrial effluents is unlikely given the unstable nature of BCME and CMME in water. Exposure of herbivores to these two compounds via ingestion would depend upon their uptake from soil and their translocation to the edible portion of the plants. Information concerning the fate of either BCME or CMME in soil and uptake by plants was not found. The ease with which BCME and CMME hydrolyse should allow soil moisture to degrade this compound. Plant uptake and translocation is also unlikely due to the anticipated rapid hydrolysis of BCME and CMME in biological fluids. This same fate also prevents their uptake from contaminated animals by predators.

In addition to the difficulty related to the persistence of BCME and CMME as they travel the various pathways from source to interceptor organism (i.e. wildlife), the lack of sources in Canada make the probability of any wildlife exposure extremely remote.

5.2 Exposure of the General Human Population

Owing to their rapid hydrolysis and lack of identified information on concentrations in the environment, it is not possible to quantitatively estimate the total daily intake of BCME or CMME by the general population in Canada. In view of the lack of commercial activity in Canada reported for these compounds and their rapid hydrolysis in the environment, estimation of intake on the basis of fugacity modelling was also considered inappropriate.

6.0 KINETICS AND METABOLISM

No quantitative information was identified on the absorption, distribution, metabolism or elimination of BCME or CMME in humans or experimental animals. Exposure to of BCME and CMME to laboratory animals by dermal contact (Van Duuren *et al.* 1968, 1969) and inhalation (Laskin *et al.* 1971) indicate that they are easily absorbed via these routes. Within living tissue, it is anticipated that BCME and CMME would be rapidly hydrolysed in the aqueous environment of tissues, forming formaldehyde and hydrogen chloride, and methanol, formaldehyde and hydrogen chloride, respectively. The formaldehyde and methanol could be oxidized (to formic acid) which would be excreted in the urine (Croy and DeVoto 1991).

7.0 MAMMALIAN TOXICITY

7.1 Acute Toxicity

Studies on the acute toxicity of BCME and CMME are summarized in Table 7-1. Reported LC_{50} values for the exposure (by inhalation) of rats to BCME were 7 and 10.3 ppm (33 and 48 mg/m^3) (Drew et al. 1975, Union Carbide, 1968); LC_{50} values of 5.3 ppm (25 mg/m^3) (Leong et al. 1971) and 7 ppm (33 mg/m^3) (Drew et al. 1975) have been reported for mice and hamsters, respectively. LD_{50} values of 0.21 ml/kg b.w. (278 mg/kg b.w.) for the oral administration of BCME to rats, and 0.28 ml/kg b.w. (370 mg/kg b.w.) for the dermal exposure of rabbits to BCME have been reported (Union Carbide 1968). The acute exposure (via inhalation) of animals to BCME produced severe irritation of the eyes and respiratory tract (congestion, edema and haemorrhage (mainly of the lungs) and acute necrotizing bronchitis (U.S. EPA 1980, Drew et al. 1975). Application of BCME to the skin of rabbits produced erythema and necrosis, while exposure of the eye (rabbit) to this substance produced severe corneal necrosis (Union Carbide 1968 cited in ATDSR 1989).

The median life span of rats exposed (by inhalation) to 0, 0.7, 2.1, 6.9 and 9.5 ppm (0, 3.3, 9.9, 32.4 and 44.7 mg/m^3) BCME was 462, 420, 36, 2 and 2 days, respectively; for hamsters exposed (by inhalation) to these concentrations of BCME the median life span was 675, 657, 68, 16 and 4 days, respectively (Drew et al. 1975). Exposure to 2.1 ppm (9.9 mg/m^3) BCME for 7 hours increased the incidence of tracheal and bronchial hyperplasia 2- to 3-fold in rats and 4- to 5-fold in hamsters compared to unexposed controls (Drew et al. 1975).

LC_{50} values of 55 ppm (182 mg/m^3) and 65 ppm (215 mg/m^3) for the exposure (by inhalation for 7 hours) of rats and hamsters to CMME, were reported by Drew et al. (1975). Exposure to these concentrations of CMME produced pulmonary congestion, edema, haemorrhage, and acute necrotizing bronchitis (Drew et al. 1975). It should be noted that the toxic effects produced by CMME may be due, at least in part, to BCME.

7.2 Short-term and Sub-chronic Toxicity

The toxicological effects produced by the short-term repeated exposure (by inhalation) of experimental animals to BCME and CMME are summarized in Table 7-2. The exposure of male Sprague-Dawley rats or male Golden Syrian hamsters to 1 ppm (4.7 mg/m^3) BCME for 6 hours/day for 1, 3, 10 and 30 days produced a marked reduction in survival and an increased incidence of hyperplastic changes within the trachea and bronchus, compared to unexposed controls (Drew et al. 1975). Evidence of subarachnoid haemorrhage was observed in 24% of the rats and 8% of the hamsters which received 30 6-hour exposures to 1 ppm (4.7 mg/m^3) BCME (Drew et al. 1975).

The repeated exposure (presumably for 6 hours each) of male Sprague-Dawley rats to 10 ppm (33 mg/m^3) CMME reduced survival in addition to producing alterations in lung/body weight ratios and regenerative hyperplasia of the bronchial epithelium (Drew et al. 1975) compared to controls; exposure of these animals to 1 ppm (3.3 mg/m^3) CMME produced a slight reduction in survival as well as regenerative hyperplasia of the bronchial epithelium (Drew et al. 1975).

7.3 Chronic Toxicity and Carcinogenicity

Bis(chloromethyl)ether

Studies on the toxicological effects produced by long-term exposure (by inhalation) to BCME have been restricted primarily to limited carcinogenesis bioassays (summarized in Table 7-3). The exposure (by inhalation) of male A/Heston mice to 5 mg/m^3 BCME for 6 hours/day, 5 days/week for a period of 82 days produced a marked reduction in survival and an increase in the number of pulmonary tumors (adenomas) (20/49 and 26/47 in unexposed and BCME-exposed mice, respectively), though the statistical significance was not specified (Leong et al. 1971).

The exposure (by inhalation) of male Ha/ICR mice to concentrations of BCME of 1, 10 or 100 ppb (0.0047 to 0.47 mg/m^3) for 6 hours/day, 5 days/week for a period of 6 months, produced a reduction in survival; however all mice developed an ascending urinary tract infection (Leong et al. 1981). No difference in mortality (>90%) was observed between the control and BCME-exposed groups after 24 months. After 6 months, a significant ($p < 0.05$) increase in the incidence of pulmonary adenomas was observed only in surviving mice exposed to 100 ppb (0.47 mg/m^3); the 6-month survival of mice exposed to 0, 1, 10, 100 ppb (0, 0.0047, 0.047, 0.47 mg/m^3) BCME was 55%, 35%, 25% and 18%, respectively (Leong et al. 1981).

The exposure (by inhalation) of male (Specific Pathogen-Free) Sprague-Dawley rats to 100 ppb (0.47 mg/m^3) BCME for 6 hours/day, 5 days/week for a period of 6 months, produced a marked reduction in survival and an increase in the incidence of "tumors of the respiratory tract" (102/111 in BCME-exposed group versus 0/112 in the controls), 94% of which were tumors of the olfactory neuroepithelium-esthesioneuroepitheliomas (Leong et al. 1981). Notably, survival and the incidence of "tumors of the respiratory tract" in rats exposed to 1 and 10 ppb (0.0047 and 0.047 mg/m^3) BCME for 6 hours/day, 5 days/week for a period of 6 months, were no different than in the controls.

Kuschner et al. (1975) exposed (by inhalation) male Sprague-Dawley rats to 0.1 ppm (0.47 mg/m^3) BCME for 6 hours/day, 5 days/week for 2, 4, 8, 12, 16, and 20 weeks (10, 20, 40, 60, 80 and 100 exposures). In addition to reduced survival (the time at which 50% mortality was reached was reduced approximately 24% in animals receiving 80 or 100 exposures to BCME), the incidence of nasal esthesioneuroepitheliomas and squamous cell carcinomas of the lung increased with more exposures to BCME (the incidence of squamous cell carcinomas of the lung was 2/20, 3/50 and 8/30, after 60, 80 and 100 exposures, respectively).

It is possible that the carcinogenic activity of BCME within the respiratory system of experimental animals may be partially due to formaldehyde (produced in the respiratory tract upon hydrolysis of BCME) which has been shown to increase the incidence of squamous cell carcinomas within the nasal cavity of rats (Albert et al. 1982, Sellakumar et al. 1985).

The carcinogenicity of BCME has also been examined following subcutaneous injection of this substance into rats and mice. Groups of 20 female Sprague-Dawley rats (weighing between 120 and 125 g) were injected subcutaneously once per week with 3 mg BCME (dissolved in 0.1 ml Nujol) or vehicle alone for approximately 300 days (van Duuren et al. 1969). (Because of the corrosive effects produced by BCME, after 114 days the dose was reduced to 1 mg, and injections performed only three times per month; however because of severe weight

loss of the animals, the injections were terminated after 300 days). In the controls administered vehicle alone, no tumors were observed at the site of injection; there was a fibroadenoma and an adenocarcinoma (of the breast) observed elsewhere. In the group of animals administered BCME, two fibromas and 5 fibrosarcomas were observed at the site of injection, as well as one fibroadenoma (of the breast) found elsewhere (van Duuren et al. 1969).

The potential of BCME to increase the incidence of spontaneous lung tumors in mice was assessed by Gargus et al. (1969). A group of 50 female and 50 male newborn ICR Swiss mice received a single subcutaneous injection of 12.5 µl/kg b.w. (16.6 mg/kg b.w.) BCME (dissolved in peanut oil) and the animals were observed for a period of six months, after which time the survivors were necropsied and the number of lung tumors (adenomas, based on histopathological analysis) quantified. A group of control animals (20 females and 30 males) received a single subcutaneous injection of vehicle alone. The numbers of female mice with pulmonary adenomas in the BCME-exposed and control (vehicle) groups were 20/50 and 5/20, respectively. The numbers of male mice with pulmonary adenomas in the BCME-exposed and control (vehicle) groups were 25/50 and 2/30, respectively. The administration of BCME had no effect upon growth or survival of the mice.

Zajdela et al. (1980) assessed the carcinogenicity of BCME following repeated subcutaneous injection in male and female XVIInc/Z mice. Groups of 30 males and 30 females received 32 injections of 0.3 mg BCME (dissolved in Nujol) over a period of 42 weeks. The control group consisted of 30 male mice injected with vehicle alone. After 110 days (when the first sarcoma was observed), survival in the control, male and female BCME-exposed groups was 100%, 90% and 80%, respectively. The number of animals with tumors (mainly fibrosarcomas) at the site of injection was 0/30, 12/27 and 10/24 in the control, male and female BCME-exposed animals, respectively ($p < 0.0001$). The incidence of tumors at locations other than the site of injection was not different (statistical significance not specified) in the control and BCME-exposed groups. The incidence of pulmonary adenomas in the BCME-exposed and control groups was 7/30 and 2/30, respectively; this difference was not statistically significant (Zajdela et al. 1980).

The incidence of squamous cell carcinomas of the skin in female ICR/Ha mice that received 2 mg BCME (applied dermally) or solvent (i.e., benzene) alone (controls) thrice weekly for 325 days was 12/20 and 0/20, respectively (van Duuren et al. 1969). In two-stage skin tumour carcinogenesis bioassays in which a number of substances were examined, BCME had "weak" tumour initiating activity (Table 7-4) (van Duuren et al. 1969, Zajdela et al. 1980).

Chloromethyl(methyl)ether

Studies on the toxicological effects produced by long-term exposure (by inhalation) to CMME have been restricted primarily to limited carcinogenesis bioassays in mice, rats and hamsters (summarized in Table 7-3). It should be noted however, that since industrial grade CMME was used in these studies, the observed effects could be due to the presence of contaminating BCME.

There was no significant effect upon the incidence of pulmonary tumors in male A/Heston mice exposed (by inhalation for 6 hours/day, 5 days/week) to 2 ppm (6.6 mg/m^3) CMME for 101 days; the average number of pulmonary tumors/animal among tumour-bearing mice was 3.1 and 2.2 for the CMME-exposed and control groups, respectively (Leong et al. 1971).

The exposure (by inhalation for 6 hours/day, 5 days/week) of male Sprague-Dawley rats to 1 ppm (3.3 mg/m^3) CMME for virtually their entire lives increased the incidence of tracheal metaplasia and bronchial hyperplasia compared to unexposed controls; tumors of the respiratory tract (an esthesioneuroepithelioma and lung squamous cell carcinoma) were observed in CMME-exposed animals, while (presumably) none was found in unexposed controls (Laskin et al. 1975). The exposure (6 hours/day, 5 days/week) of male hamsters to 1 ppm (3.3 mg/m^3) CMME for virtually their entire lives increased the incidence of tracheal metaplasia and bronchial hyperplasia compared to unexposed controls; one lung adenocarcinoma and a tracheal squamous papilloma were observed in two animals exposed to CMME, while (presumably) none was found in unexposed controls (Laskin et al. 1975).

The carcinogenicity of purified CMME has also been examined following subcutaneous injection of this substance into rats and mice. Groups of 20 female Sprague-Dawley rats (weighing between 120 and 125 g) were injected once per week with 3 mg (laboratory purified) CMME (dissolved in 0.1 ml Nujol) or vehicle alone for approximately 300 days; because of moderate corrosive effects, the injections were terminated after this time (van Duuren et al. 1969). In controls administered vehicle alone, no tumors were observed at the site of injection; there was a fibroadenoma and an adenocarcinoma (of the breast) found elsewhere. In animals administered (laboratory purified) CMME, a fibrosarcoma (at the site of injection) in one animal was the only tumour described.

van Duuren et al. (1972) subcutaneously injected (laboratory purified) CMME (dissolved in 0.05 Nujol; 300 μg/animal; once per week) to a group of 30 female ICR/Ha Swiss mice for their entire lives; a similarly sized group of controls received vehicle alone. Median survival time was 643 days and 496 days, and the number of mice with sarcomas at the site of injection was 0 and 10, in the control and (laboratory purified) CMME-exposed groups, respectively.

The potential of CMME (containing BCME) to increase the incidence of spontaneous lung tumors in mice was assessed by Gargus et al. (1969). A group of 48 female and 51 male newborn ICR Swiss mice received a single subcutaneous injection of 125 μl/kg b.w. (132.5 mg/kg b.w.) CMME dissolved in peanut oil; the animals were observed for a period of six months, after which time the survivors were necropsied and the number of lung tumors (adenomas, based on histopathological analysis) quantified. Controls (20 females and 30 males) received a single subcutaneous injection of vehicle alone. The numbers of female mice with adenomas in the control (vehicle) and CMME-exposed groups were 5/20 and 8/48 females, respectively. The numbers of male mice with adenomas in the control (vehicle) and CMME-exposed groups were 2/30 and 9/51, respectively.

Laboratory purified CMME was not carcinogenic when applied thrice weekly (2 mg/animal for 325 days) to the skin of female ICR/Ha Swiss mice; however this substance did have "weak" tumour initiating activity (Table 7-4) (van Duuren et al., 1969).

7.4 Mutagenicity and Related End-Points

The genotoxicity of BCME and CMME has been examined in a variety of limited and generally poorly documented studies. Bis(chloromethyl)ether (at a maximum concentration of 20 μg/plate) was mutagenic in the presence of an exogenous microsomal activating system in *S. typhymurium* strain TA100, based on a 3-fold increase in the frequency of revertants above control levels; however similar results were not observed in *S. typhymurium* strains TA1535, TA1538 and TA98

(Anderson and Styles 1978). Bis(chloromethyl)ether was also reported to be mutagenic in various strains of *E. coli* and *S. typhymurium*, but no experimental details or results were provided (Mukai and Hawryluk 1973).

Bis(chloromethyl)ether (at concentrations as low as 0.16 µg/ml) was reported to increase DNA repair (unscheduled DNA synthesis) in human skin fibroblasts, although no quantitative results were provided (Agrelo and Severn 1981). In *in vitro* assays with BHK-21 and human WI-38 cells, concentrations of BCME between 0.008 and 25 mg/ml (in the presence of an exogenous microsomal activating system) increased the frequency of transformed cells approximately 6.6- and 11-fold, respectively, (Styles 1978). The exposure (*in vitro*) of human neonatal foreskin fibroblasts to BCME (between 0.1 and 8 µg/ml) produced a 3- to 14-fold increase in the frequency of anchorage-independent (transformed) cells (Kurian et al. 1990).

Bis(chloromethyl)ether was reported to directly alkylate DNA (at guanine and adenine residues), when the two substances were incubated together in an *in vitro* assay (Goldschmidt et al. 1975), although a portion of the DNA damage was likely caused by the formaldehyde formed from the hydrolysis of BCME in aqueous medium (Batten et al. 1987). Bis(chloromethyl)ether was reported to damage RNA within bacteriophage R17, however the result was attributed to formaldehyde produced from the hydrolysis of BCME (Shooter 1975).

Chloromethyl(methyl)ether was reported to be mutagenic in various strains of *E. coli* and *S. typhymurium*; however no experimental details or results were provided (Mukai and Hawryluk 1973). In the presence of an exogenous microsomal activating system, 1 and 10 mM CMME increased unscheduled DNA synthesis in human lymphocytes approximately 30% and 100%, respectively (Perocco et al. 1983). The weight of evidence from these investigations in which a range of endpoints were examined indicates that both BCME and CMME are genotoxic, though available studies are limited and generally poorly documented.

7.5 Other Toxicity Studies

The exposure (by inhalation) of male Sprague-Dawley rats to 100 ppb (0.47 mg/m^3) BCME for 6 hours/day, 5 days/week for a period of six months had no observable effect upon the nervous or reproductive systems, based on gross and microscopic analysis (Leong et al. 1981). No other relevant information was identified regarding the reproductive, developmental, immunological, or neurological toxicity of BCME or CMME.

8.0 EFFECTS ON HUMANS

In a number epidemiological studies mortality and the incidence of cancer in workers occupationally exposed to BCME and CMME have been examined. No relevant studies were identified concerning the neurological, immunological, developmental or reproductive effects of BCME or CMME in humans.

8.1 Case Reports

An anecdotal report (cited in Durkin et al. 1975) indicated that workers exposed to "rather high" concentrations of CMME experienced respiratory difficulty, sore throat, fever and chills.

Sakabe (1973) reported that 5 of 32 Japanese males employed in dyestuffs factories who had been exposed to BCME died of "lung cancer" (between 1963 and 1969). Small (oat) cell carcinoma was identified in only one of the cases. No quantitative information on exposure was provided in this published account and these individuals were exposed to a number of chemical substances in addition to BCME (smoking habits could not be confirmed). However, because a large proportion (approximately 16%) of the individuals exposed to BCME developed lung cancer, and those exposed to chemicals other than BCME did not, the authors attributed the occurrence of these pulmonary tumors to exposure to BCME.

Reznick et al. (1977) reported the case of a 45-year old male chemist who had died of a slightly differentiated adenocarcinoma of the lung. Twelve years earlier this individual had been exposed to BCME and CMME over a period of two years. Although no quantitative information on exposure was presented (and the individual was also exposed to vinyl chloride), the lung adenocarcinoma was attributed to his exposure to BCME and CMME.

Roe (1985) reported the case of three males (between 35 and 40 years of age) who had died of lung cancer (small (oat) cell and squamous cell carcinomas) after having been occupationally exposed to BCME. Although no quantitative or qualitative information on exposure was provided, and the individuals had been smokers, the relatively young age at which these individuals died was attributed to their exposure to BCME.

8.2 Epidemiological Studies

Epidemiological studies concerning the effects on human health produced by exposure to BCME and CMME have been restricted to occupationally exposed populations. Lemen et al. (1976) examined the incidence of lung cancer in a group of workers employed in a chemical plant in California, where BCME was used in the production of ion-exchange resins. The authors identified 136 individuals who had been employed for at least 5 years between 1955 and 1972. The number of cases of lung cancer (5) was significantly higher ($p < 0.01$) than the number expected (0.54) (based on age-respiratory cancer-specific incidence rates for white males in the state of Connecticut in 1960-1962). Notably, 80% of the tumors were small cell undifferentiated cancers[1]. Individuals (80% were smokers) with cancer averaged 47 years of age, and the average latency period was approximately 10 years. No quantitative or qualitative information on exposure was provided in this published account. The incidence of metaplastic and atypical cells in the sputum of workers exposed to BCME was greater than controls (uranium miners), based on cytological analysis.

Nishimura et al. (1990) examined the incidence of lung cancer in a group of Japanese workers employed in two dyestuff factories where BCME was used. The study group consisted of 35 males employed at these plants between 1955 and 1970. The number of cases (13) of lung cancer (some of which occurred in smokers) was significantly ($p < 0.001$) higher than the number expected (0.62). Tumors from eight of the individuals were examined histopathologically; four were diagnosed as small cell undifferentiated carcinomas, two were adenocarcinomas and one a large cell carcinoma; in one individual, both a small cell carcinoma and an

[1] Importantly, lung tumors in populations occupationally exposed to BCME and CMME are predominately small (oat) cell carcinomas (Weiss 1976, Pasternack et al. 1977). The occurrence of this type of lung cancer in these individuals is quite distinct from that caused by tobacco, one of the potential confounders in such studies, where the lung tumors are predominantly squamous cell carcinomas (Weiss 1976, Pasternack et al. 1977).

adenocarcinoma were found. The average age at which individuals with lung cancer died was 46 years, and the latency period was approximately 13.5 years. The average duration of exposure to BCME was approximately 7.2 years, although no other quantitative or qualitative information on exposure was provided.

Technical grade CMME contains between 1% and 8% BCME (Travenius 1982). Consequently, in epidemiological studies in which mortality and the incidence of cancer in workers exposed to CMME were examined, the effects may have been due (at least in part) to BCME.

Weiss (1976) reported the results of a 10-year prospective study (1963-1973) in which 125 male employees of a chemical plant in the United States who had been occupationally exposed to CMME (BCME), were examined with respect to the "incidence" of pulmonary cancer. No quantitative or qualitative information on exposure was provided; however an exposure index (low, medium and high) based on type and duration of job associated with potential exposure to CMME (BCME) was developed. Eleven cases of lung cancer were reported in 49 individuals with medium or high exposure to CMME (BCME); no "incidence" of lung cancer was reported in 76 workers with none or low exposure to CMME (BCME). The number of deaths (16) during this period was 2.7-fold greater than the number expected (5.9), based on a comparison with death rates for white males in the United States. All of the excess deaths (10) were attributable to lung cancer, 100% of which were small cell carcinomas which developed in individuals less than 55 years of age. The latency period for these cancers ranged from 10 to 24 years. Among individuals exposed to CMME (BCME) the "incidence" of pulmonary tumors was inversely related to their use of tobacco (Weiss 1980). In a subsequent follow-up study of these workers, the number of deaths (13) due to lung cancer (which were attributable to either moderate or heavy exposure to CMME (BCME)), was 19.5-fold greater than the number (0.66) expected, based on lung cancer mortality rates in the surrounding municipality (Philadelphia) (Weiss 1982). The standardized mortality ratio for deaths due to lung cancer which peaked 15 to 19 years from the onset of exposure, declined during the subsequent 20 to 29 year period.

Maher and Defonso (1987) examined mortality in a group of workers exposed to CMME (BCME). (This report represented an update and extension of a previous investigation on death due to lung cancer performed by these authors (Defonso and Kelton 1976)). The study population consisted of a group of 737 "exposed" and 2,120 "unexposed" white male workers (who comprised 97% of the labour force) employed for any length of time at a chemical plant in the United States between 1948 and 1971. The vital status of 90% of the group was determined up to 1982. No quantitative information on exposure was provided; however an exposure rating (from 0-6) was developed based on the type of work, proximity of exposure to CMME (BCME) and production methods. Cumulative exposure was calculated based on the exposure rating and duration of employment at a particular job. The expected number of deaths for each type of cancer was calculated using cause-specific death rates for white males residing in the surrounding municipality (Philadelphia). Information on smoking habits was incomplete but "*No marked differences between smoking habits of exposed and unexposed workers were noted*" (Maher and DeFonso 1987).

Among the workers exposed to CMME (BCME), the number of deaths (32) due to cancer of the "respiratory tract" was significantly ($p < 0.01$) higher than the number expected (11.5). For those individuals not exposed to CMME (BCME), the number of deaths (25) due to respiratory tract cancer was similar to those expected (23.8). In the CMME (BCME)-exposed group the number of deaths due to

cancer of the digestive, genito-urinary, hematopoetic, lymphatic and central nervous systems was not significantly greater than expected. The greatest increase in deaths due to cancer of the respiratory tract occurred approximately 10 to 20 years after the first exposure to CMME (BCME). Among workers exposed to CMME (BCME), the ratio of observed/expected number of deaths due to lung cancer was lower between 1975-1981, than for the period between 1960-1974, this being attributed to a reduction in the level of exposure to CMME (BCME) in 1971 as a result of the implementation of stringent engineering controls on the use of this substance Maher and Defonso (1987).

Collingwood et al. (1987) assessed mortality due to respiratory cancer in a group of workers employed at seven industrial facilities in which CMME (BCME) was produced or utilized. (This report represented a follow-up and extension of a previous study by two of these authors (Pasternack et al. 1977)). The study group (97% white, 96% male) comprised 2,460 CMME (BCME)-exposed and 3,692 unexposed workers employed between 1948 and 1980. Only limited information on smoking habits was available. No quantitative or qualitative information on exposure was provided, but an exposure index (taking into account type of job, frequency of work and potential exposure to CMME (BCME)) was developed. Cumulative exposure was calculated on the basis of the exposure index and duration of employment at a particular job. The number of expected deaths was calculated from death rates in the United States specific for age, cause, sex, race and calendar year. Among workers exposed to CMME (BCME), the standardized mortality ratio (SMR) for death due to respiratory cancers was significantly increased (SMR = 3.01; 95% CI = 2.24-3.98); this was attributed to excess deaths at two companies (where the ratio of observed to expected deaths due to lung cancer among exposed workers was 32/7.4 and 9/1.5). In the entire study group, there were 90 deaths due to respiratory cancer, 52 and 38 in the CMME (BCME)-exposed and unexposed groups, respectively. In those cases with verifiable histology, 12/32 (38%) cases in the exposed group had small (oat) cell carcinomas while 6/20 (30%) cases in the unexposed group had adenocarcinomas. The relative risk of death due to lung cancer was found to be related to total cumulative exposure based on a regression model.

Sram et al. (1983) reported that the proportion (3.73% ± 0.2%) of peripheral lymphocytes with chromosomal aberrations (breaks, exchanges) isolated from 77 workers exposed to BCME and CMME was higher than that observed in lymphocytes isolated from 25 non-exposed controls (1.64% ± 0.21%). Other than information on whether the workers were smokers (which did not influence the results), no other relevant information was provided in this published account.

9.0 EFFECTS ON THE ECOSYSTEM

Information concerning the effects of either BCME or CMME on aquatic or terrestrial ecosystems was not found. Highly reactive compounds such as these cannot be maintained in the natural environment at concentrations or for periods of time which constitute an environmental threat (Nichols and Merritt 1973).

10.0 OTHER PERTINENT DATA

No other pertinent data were obtained.

11.0 CURRENT REGULATIONS, GUIDELINES AND STANDARDS

Bis(chloromethyl)ether and CMME are considered to be "carcinogenic to humans" in the classification schemes of IARC (Group 1) (IARC 1987) and the U.S. Environmental Protection Agency (Group A) (U.S. EPA 1991). The cancer risk, estimated by the U.S. Environmental Protection Agency based on extrapolation by the linear multi-stage model of tumour incidence in male rats exposed (by inhalation) to BCME (Kuschner et al. 1975) is 6.2×10^{-3} per $\mu g/litre$ for ingestion (via drinking water) and 6.2×10^{-2} per $\mu g/m^3$ for inhalation (U.S. EPA 1991); quantitative estimates of cancer risk from exposure to CMME are not available (U.S. EPA 1991). In the United States, regulations require that manufacturing processes using BCME be strictly contained in order to prevent its fugitive release into the environment (HSDB 1991, ATSDR 1989).

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TABLE 1-1: SYNONYMS FOR BIS(CHLOROMETHYL) ETHER

Chloro(chloromethoxy) methane (1)
Dichlordimethylaether (German) (1)
Sym-dichloro-dimethyl ether (1)
Dimethyl-1,1-dichloroether (1)
Oxybis(chloromethane) (1)
Bis-CME (2)
BCME (2)
Chloromethyl ether (2)
Sym-dichloromethyl ether (2)
Bichloromethyl ether (3)
Dichloromethyl ether (3)
Dichloro-dimethyl ether (3)
1,1'-dichlorodimethyl ether (4)
Dichlorodimethyl ether symmetrical (4)
Methane, oxybis(chloro) (4)
Oxyde de dichlorodimethyle symetrique (French) (4)
1' ether de bis(chloromethyle) (French) (4)

(1) Sax 1984
(2) RTECS 1991
(3) Verschueren 1983
(4) CCINFO 1991

TABLE 1-2: SYNONYMS FOR CHLOROMETHYL METHYL ETHER

Chlordimethylether (Czech) (1)
Dimethylchloroether (1)
Ether methylique monochlore (French) (1)
Methyl chloromethyl ether, anhydrous (1)
CMME (2)
Ether, dimethyl chloro (2)
Chloromethoxymethane (3)
Monochlorodimethylether (3)
Chloromethyl ether (3)
Methyl chloromethyl ether (4)
Monochloromethyl ether (4)
Methoxymethyl chloride (5)
Methane, chloromethoxy- (5)
Methyl(chloromethyl) ether (5)
Chloromethoxy, methane (5)
Chlorodimethyl ether (5)

(1) Sax 1984
(2) RTECS 1991
(3) Verschueren 1983
(4) Sittig 1981
(5) CCINFO 1991

TABLE 2-1: PHYSICAL AND CHEMICAL PROPERTIES OF BIS(CHLOROMETHYL) ETHER

CAS NUMBER	542-88-1	(1)
MOLECULAR FORMULA	$C_2H_4Cl_2O$	(2)
MOLECULAR WEIGHT	114.96	(3)
PHYSICAL STATE	Colourless Liquid Suffocating Odour	(1) (4)
HENRY'S LAW CONSTANT ($Atmos\,m^3\,mol^{-1}$)	$2.1x10^{-4}$	(5)
MELTING POINT (°C)	-41.5	(5)
BOILING POINT (°C)	104 105 104-106	(5) (2) (1)
FLASH POINT (°C)	<19	(2)
VAPOUR PRESSURE (mm Hg)	30 @ 22°C	(5)
VAPOUR DENSITY (Air = 1)	3.97 4.0	(3) (2)
SOLUBILITY IN WATER ($mg\,L^{-1}$)	22 000 @ 25°C	(5)
SPECIFIC GRAVITY	1.315 @ 20°C/4°C 1.328 @ 15°C/4°C	(3) (6)
LOG OCTANOL/WATER PARTITION COEFFICIENT (Log K_{ow})	2.4	(5)
LOG SEDIMENT/WATER PARTITION COEFFICIENT (Log K_{oc})	1.2	(3)
HYDROLYSIS RATE CONSTANT	0.16 - 0.53 min^{-1} (Gaseous) 0.0025 sec^{-1} @ 0°C (Water) 0.018 sec^{-1} @ 20°C (Water) 0.10 sec^{-1} @ 40°C	(13) (8) (8) (8)

TABLE 2-1 (CONT'D): PHYSICAL AND CHEMICAL PROPERTIES OF BIS(CHLOROMETHYL) ETHER

HYDROLYSIS RATE CONSTANT		(Water) 0.050 sec^{-1}	(12)
		(Aqueous HCl/formaldehyde) >3.5x10^{-1} min^{-1} @ 0°C	(7)
		(3:1 water:dimethylformamide) 0.00047 min^{-1} @ 25°C	(11)
		(Gaseous, RH = 81%) 1.70x10^{-1} sec^{-1} @ 45°C	(9)
		(3:1 water:dimethylformamide)	
PHOTOLYSIS RATE CONSTANT		3 to <360 $mol^{-1}h^{-1}$	(5)
		(Water)	
HALF-LIFE ($t_{1/2}$)			
	WATER	<2 min @ 0°C	(7)
		(Hydrol; 3:1 water:dimethylformamide) 14 sec	(12)
		(Hydrol; aqueous HCl/formaldehyde) 10 - 20 sec	(11)
		(Hydrol) 280 sec @ 0°C	(14)
		38 sec @ 20°C	(14)
		7 sec @ 40°C	(14)
		(Hydrol)	
	WATER	1.5 to 9.5 min @ 0°C	(9)
		(Hydrol) 4.1 sec @ 45°C	(9)
		(Hydrol; 3:1 water:dimethylformamide)	
	AIR	1.36 h (Ind Photol)	(10)
		>25 h @ 25°C	(11)
		(Hydrol; RH = 81%)	

RH = Relative Humidity
Hydrol = Hydrolysis
Ind Photol = Indirect Photolysis

TABLE 2-1 (CONT'D): PHYSICAL AND CHEMICAL PROPERTIES OF BIS(CHLOROMETHYL) ETHER

References:

(1) CCINFO 1991
(2) Sax 1984
(3) Verschueren 1983
(4) Sittig 1981
(5) Mabey *et al.* 1982
(6) Weast 1984
(7) Van Duuren *et al.* 1972
(8) Tou *et al.* 1974
(9) Nichols and Merritt 1973
(10) Clement Associates 1989
(11) Tou and Kallos 1974a
(12) Tou and Kallos 1974b
(13) Tou and Kallos 1976
(14) U.S. EPA 1980a

TABLE 2-2: PHYSICAL AND CHEMICAL PROPERTIES OF CHLOROMETHYL METHYL ETHER

CAS NUMBER	107-30-2 (1)
MOLECULAR FORMULA	C_2H_5ClO (2)
MOLECULAR WEIGHT	80.52 (3)
PHYSICAL STATE	Colourless Liquid (3) Irritating Odour (1)
MELTING POINT (°C)	-103.5 (3) -104 (1)
BOILING POINT (°C)	59 (4) 55 - 57 (1) 60 (7) 59.15 (1) 59.5 (6) 61 (5)
FLASH POINT (°C)	-17.78 (1) <23 (2) 15 (1) -8 (1) <-18 (1) -18 (1)
VAPOUR PRESSURE (mm Hg)	122 @ 20°C (1)
VAPOUR DENSITY (Air = 1)	2.8 (1)
SOLUBILITY IN WATER ($mg \cdot L^{-1}$)	Decomposes (3)
SPECIFIC GRAVITY	1.0625 @ 10°C/4°C (3) 1.0605 @ 20°C/4°C (6) 1.070 @ 20°C/4°C (1)
LOG OCTANOL/WATER PARTITION COEFFICIENT (Log K_{ow})	-0.21 (Calculated) (8)
REFRACTIVE INDEX	1.3974 @ 20°C (6)
DIPOLE MOMENT ($ux10^{18}$)	2.03 (5)

TABLE 2-2 (CONT'D): PHYSICAL AND CHEMICAL PROPERTIES OF CHLOROMETHYL METHYL ETHER

HYDROLYSIS RATE CONSTANT		>3.5x10^{-1} min^{-1} @ 0°C	(9)
		(3:1 water:dimethylformamide)	
		0.0018 min^{-1} @ 29°C	(11)
		(Gaseous, RH = 39%)	
		>90 sec^{-1} @ 25°C (Water)	(8)
PHOTOLYSIS RATE CONSTANT		1.0x10^{-10} mol^{-1}·sec^{-1} (Gaseous)	(8)
HALF-LIFE ($t_{1/2}$)			
	WATER	<2 min @ 0°C (Hyrol; 3:1 water:dimethyl-formamide)	(9)
		<0.007 sec @ 25°C	(8)
		(Hydrol)	
		<1 sec (Hydrol)	(11)
	AIR	3.5 to 6 min @ 25°C (Hydrol; RH = 70%)	(10)
		>6.5 h @ 29°C	(11)
		(Hydrol; RH = 39%)	
		230 h	(8)
		(Ind Photol)	

RH = Relative Humidity
Hydrol = Hydrolysis
Ind Photol = Indirect Photolysis

References:

(1) CCINFO 1991
(2) Sax 1984
(3) Verschueren 1983
(4) Sittig 1981
(5) Durkin *et al.* 1975
(6) Weast 1984
(7) Hawley 1981
(8) Radding *et al.* 1977
(9) Van Duuren *et al.* 1972
(10) Nichols and Merritt 1973
(11) Tou and Kallos 1974a

Table 7-1. Acute Toxicity.

Species/strain/sex/ No.[a]	Chemical/Route/Duration	Parameter	Dose	Reference
BCME				
Rat/Sprague-Dawley/male/number not specified	BCME Inhalation (7 h)	LC_{50}	7 ppm (33 mg/m^3)	Drew et al. 1975
Rat/strain, sex not specified/6 per group	BCME Inhalation (time not specified)	LC_{50}	10.3 ppm (8.3-13.4 ppm) (48 mg/m^3)	Union Carbide 1968
Mice/A/Heston/male/number not specified	BCME Inhalation (6 h)	LC_{50}	5.3 ppm (25 mg/m^3)	Leong et al. 1971
Hamster/Golden Syrian/male/number not specified	BCME Inhalation (7 h)	LC_{50}	7 ppm (33 mg/m^3)	Drew et al. 1975
Rat/Wistar/male/5 per group	BCME (undiluted) Peroral	LD_{50}	0.21 ml/kg b.w. (278 mg/kg b.w.)	Union Carbide 1968
Rabbit/New Zealand albino/male/4 per group	BCME (undiluted) Dermal (24 h)	LD_{50}	0.28 ml/kg b.w. (370 mg/kg b.w.)	Union Carbide 1968
CMME[b]				
Rat/strain, sex and number not specified	CMME Inhalation (7 h)	LC_{50}	55 ppm (182 mg/m^3)	Drew et al. 1975
Hamster/strain, sex and number not specified	CMME Inhalation (7 h)	LC_{50}	65 ppm (215 mg/m^3)	Drew et al. 1975
Rat/strain, sex and number not specified	CMME Oral (method not specified)	LD_{50}	817 mg/kg b.w.	NIOSH (1974) cited in EPA 1980a

[a] M = male, F = female, No. = total number of animals per exposure group.
[b] CMME containing BCME.
BCME Conversion Factor: 1 ppm = 4.7 mg/m^3 (ATSDR 1989).
CMME Conversion Factor: 1 ppm = 3.3 mg/m^3 (Leong et al. 1971).

Table 7-2. Short-Term Repeated Dose Toxicity.

Study Protocol	Results
BCME[a]	
Groups of 50 male Sprague-Dawley rats and Golden Syrian hamsters were exposed (by inhalation) to 0 and 1 ppm (0, 4.7 mg/m^3) BCME for 1, 3, 10, or 30 multiple 6-hour exposures (duration between exposures not specified). The animals were observed for their entire lifespan and the trachea and bronchia examined histopathologically.	Rats: After 0, 1, 3, 10 and 30 (6-hour) exposures to BCME, 50% mortality was observed after 66, 66, 20, 4 and 4 weeks, respectively. The incidence of tracheal hyperplasia, with and without atypias, increased from 27% after 1 exposure to 89% after 30 exposures to BCME. The incidence of tracheal squamous metaplasia increased after 3 to 30 exposures. The incidence of bronchial hyperplasia and squamous metaplasia increased with greater exposure to BCME. Bronchoalveolar squamous metaplasia and cuboidal transformations of alveolar epithelium were also observed in rats receiving multiple exposures to BCME. Hamsters: After 0, 1, 3, 10 to 30 (6-hour) exposures to BCME, 50% mortality was observed after 95, 95, 70, 22 and 8 weeks, respectively. The incidence of tracheal hyperplasia, with and without atypias, increased with more frequent exposure to BCME. The incidence of tracheal squamous metaplasia increased after 10 and 30 exposures to BCME, with atypias observed in approximately 50% of the animals after 3 or more exposures. Exposure to BCME also produced bronchoalveolar metaplasia, squamous metaplasia with atypia and atypical alveolar epithelium.
CMME[b]	
Groups of 25 male Sprague-Dawley rats were exposed (by inhalation) to 0, 1, and 10 ppm (0, 3.3, 33 mg/m^3) CMME for 30 days (duration and frequency of exposure not specified).	Exposure to 10 ppm (33 mg/m^3) CMME increased mortality to 88% within 30 days (data for controls not presented); marked (not quantified) weight decrease was observed with some recovery towards the end of exposure. Significant (not quantified) increases in lung/body weight ratios were observed in rats which died after exposure to CMME; regenerative hyperplasia of bronchial epithelium was also observed. Exposure to 1 ppm (3.3 mg/m^3) CMME increased mortality to 8% within 30 days. Exposure had no significant effect upon body weight. Regenerative hyperplasia and squamous metaplasia were observed in rats sacrificed 2 weeks after the last exposure.

Source: Drew et al. 1975.

[a] BCME Conversion Factor: 1 ppm = 4.7 mg/m^3 (ATSDR 1989).

[b] CMME containing BCME.
CMME Conversion Factor: 1 ppm = 3.3 mg/m^3 (Leong et al. 1971).

Table 7-3. Chronic Toxicity/Carcinogenicity

Protocol	Results	Reference
BCME		
Fifty A/Heston male mice were exposed (by inhalation) to 0 or 5 mg/m^3 BCME (industrial grade) for 6 hours/day, 5 days/week for 82 days, after which time exposure was terminated and survivors observed for a further 10 weeks. The animals were necropsied and lungs examined pathologically.	Exposure to BCME produced loss of body weight, respiratory distress and death. Survival of control and BCME-exposed mice was 90% and 28%, respectively. The incidence of pulmonary adenomas was 20/49 and 26/47 in control and BCME-exposed mice respectively (statistical significance not specified). The average number of pulmonary adenomas/animal among tumour-bearing mice was 2.2 for controls and 5.2 for the BCME-exposed group.	Leong et al. 1971
Groups comprising 144 to 157 male Ha/ICR mice were exposed (by inhalation) to 0, 1, 10 or 100, ppb (0, 0.0047, 0.047, 0.47 mg/m^3) BCME for 6 hours/day, 5 days/week for 6 months, after which time exposure was terminated, mice observed for a further 18 months, necropsied and examined histopathologically.	Six-month survival of mice exposed to 0, 1, 10 or 100 ppb (0, 0.0047, 0.047 or 0.47 mg/m^3) BCME was 55%, 35%, 25% and 18%, respectively. After 6 months the incidence of pulmonary adenomas in surviving mice exposed to 0, 1, 10 or 100 ppb (0, 0.0047, 0.047 or 0.47 mg/m^3) BCME was 9/86, 5/45, 3/37, and 8/27, respectively; increased tumour incidence in the group exposed to 100 ppb (0.47 mg/m^3) was statistically ($p < 0.05$) significant. After 24 months, the incidence of pulmonary adenomas in animals exposed to 0, 1, 10 or 100 ppb (0, 0.0047, 0.047 or 0.47 mg/m^3) BCME was 10/157, 7/138, 3/143 and 10/144, respectively. Exposure to BCME had no adverse effect on body weight and produced no nasal or eye irritation.	Leong et al., 1981

Four groups of 120 male Sprague-Dawley rats were exposed (by inhalation) to 0, 1, 10 or 100 ppb (0, 0.0047, 0.047, 0.47 mg/m^3) BCME 6 hours/day, 5 days/week for 6 months, after which time, exposure was terminated and the rats observed for a further 22 months. Eight rats from each group were sacrificed after 6 months for hematological, cytological, cytogenetic and histopathological analyses.	Six-month survival was greater than 97% for control and BCME-exposed rats. Nineteen-month survival for animals exposed to 0, 1 or 10 ppb (0, 0.0047 or 0.047 mg/m^3) BCME was approximately 45%, while no animals exposed to 100 ppb (0.47 mg/m^3) BCME survived. After 6 months there was no significant difference in the weights of the total body, liver, kidneys, brain, heart and testes; exposure to BCME produced no adverse haematological or cytogenetic effects. The incidence of "respiratory tract" tumors in animals exposed to 0, 1, 10 or 100 ppb (0, 0.0047, 0.047 or 0.47 mg/m^3) BCME was 0/112, 0/113, 0/111 and 102/111, respectively; in the highest-concentration group, there were 96 esthesioneuroepitheliomas (significantly different [$p < 0.05$] than controls), four pulmonary adenomas, one carcinoma of the nasal passage and an esthesio-neuroepithelioma metastasis in the lung.	Leong et al. 1981
Six groups of 20 to 50 male Sprague-Dawley rats were exposed (by inhalation) to 0 or 0.1 ppm (0, 0.47 mg/m^3) BCME 6 hours/day, 5 days/week for 2, 4, 8, 12, 16 and 20 weeks (10, 20, 40, 60, 80 or 100 exposures), after which time the rats were necropsied and examined histopathologically.	Sixty exposures to BCME had no effect upon mortality, although the time at which 50% mortality was reached was reduced approximately 24% in animals receiving 80 or 100 exposures to BCME. Animals surviving 30 weeks had "respiratory tract" cancers (26 in the nasal cavity and 13 in the lung). The incidence of "respiratory tract cancer" in animals surviving for more than 210 days and receiving 10, 20, 40, 60, 80 or 100 exposures of BCME was, 1/41 (2.4%), 3/46 (6.5%), 4/18 (22.2%), 4/18 (22.2%), 15/34 (44.1%) and 12/20 (60.0%), respectively (statistical significance not specified). No lung tumors were observed following up to 40 exposures to BCME. The incidence of squamous cell carcinomas of the lung was 2/20, 3/50 and 8/30, after 60, 80 and 100 exposures, respectively.	Kuschner et al. 1975

CMME

Fifty A/Heston male mice were exposed (by inhalation) to 0 or 2 ppm (0, 6.6 mg/m^3) (industrial grade) CMME for 6 hours/day, 5 days/week for 101 days, after which time exposure was terminated and survivors observed for a further 7 weeks. The animals were necropsied and lungs examined histopathologically.	The incidence of pulmonary tumors in CMME-exposed mice (25/50) was not significantly ($p < 0.05$) different than in the unexposed controls (20/49). The average number of pulmonary tumors/animal among tumour-bearing mice was 2.2 and 3.1 for the control and CMME-exposed group, respectively.	Leong et al. 1971
Seventy-four male Sprague-Dawley rats were exposed (by inhalation) to 0 or 1 ppm (0 or 3.3 mg/m^3) (industrial grade) CMME for 6 hours/day, 5 days/week for their entire lifespan (up to 852 days). The rats were necropsied and tissues examined histopathologically.	Exposure to CMME had no effect upon mortality or body weight gain. The incidence of tracheal squamous metaplasia and bronchial hyperplasia was 3% and 10%, and 35% and 59%, in the control and BCME-exposed animals respectively (statistical significance not stated). Two respiratory tract cancers (lung squamous cell carcinoma and an esthesioneuroepithelioma of olfactory epithelium) were found in animals exposed to CMME (but presumably not in unexposed controls).	Laskin et al. 1975
Ninety male Golden Syrian hamsters were exposed (by inhalation) to 1 ppm (3.3 mg/m^3) (industrial grade) CMME for 6 hours/day, 5 days/week for their entire lifespan (up to 852 days). The hamsters were necropsied and tissues examined histopathologically. Eighty-eight animals unexposed animals served as controls.	Exposure to CMME had no effect upon mortality or body weight gain. The incidence of tracheal squamous metaplasia was 0% and 2%, and incidence of bronchial hyperplasia was 5% and 8%, in the control and BCME-exposed animals respectively (statistical significance not stated). One lung adenocarcinoma and a tracheal squamous papilloma were observed in two animals exposed to CMME.	Laskin et al. 1975

Table 7-4. Carcinogenicity in Skin Tumour Bio-Assay

Animals	Primary Treatment	Secondary Treatment	No. mice with squamous cell carcinomas of the skin (papillomas)	Reference
Twenty female ICR/Ha Swiss mice per treatment group.[1]	None	None	0(0)	van Duuren et al. 1969
	None	Acetone	0(0)	
	None	Benzene	0(0)	
	None	2 mg BCME	12(13)	
	1 mg BCME	Acetone	0(0)	
	1 mg BCME	25 µg TPA	2(5)	
	0.15 mg B[a]P	Acetone	0(1)	
	0.15 mg B[a]P	25 µg TPA	7(20)	
	0.15 mg B[a]P	2 mg BCME	12(13)	
	None	2 mg CMME	0(0)	
	1 mg CMME	Acetone	0(0)	
	1 mg CMME	25 µg TPA	1(5)	
	0.1 mg CMME	25 µg TPA	4(7)	
	0.15 mg B[a]P	2 mg CMME	0(1)	

Twenty-eight male XVIInc/Z mice in each treatment group[2]	None	2 µg TPA	0(4)	Zajdela et al. 1980
	1 mg BCME	2 µg TPA	3(12)	

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[1] BCME, CMME and benzo[a]pyrene (B[a]P) were dissolved in benzene; TPA was dissolved in acetone. In the primary treatment, the indicated substances (dissolved in 0.1 ml of the appropriate solvent) were applied to the dorsal skin. The secondary treatment commencing 14 days later involved the thrice weekly application of the indicated substances (dissolved in 0.1 ml of the appropriate solvent) to the dorsal skin of the animals for their entire lifespan (up to 540 days), except for with animals receiving BCME and CMME where treatment was terminated after 325 days.

[2] The primary treatment involved the application of BCME (dissolved in 80 µl benzene) to the dorsal skin. The secondary treatment commencing 14 days later involved the thrice weekly application of TPA (dissolved in acetone) to the dorsal skin of these animals for 42 weeks.

Monenco

$$CH_3OH + HCl + HCHO \rightleftharpoons CH_3OCH_2Cl + H_2O$$

(CMME)

Source: Fishbein (1979); Durkin et al. (1975)

FIGURE 3-1
THE FORMATION OF CHLOROMETHYL METHYL ETHER (CMME) FROM METHANOL, HYDROGEN CHLORIDE, AND FORMALDEHYDE

R420T07

Monenco

$$2\ CH_3OCH_3 + Cl_2 \rightleftharpoons 2\ CH_3OCH_2Cl$$

(CMME)

Source: Durkin et al. (1975)

FIGURE 3-2
THE FORMATION OF CHLOROMETHYL METHYL ETHER (CMME) VIA THE DIRECT CHLORINATION OF DIMETHYL ETHER

R42DT08

Monenco

$$CH_3OCH_2Cl + H_2O \rightleftharpoons CH_3OH + HCl + HCHO$$

(CMME)

$$2\,HCHO + 2\,HCl \rightleftharpoons ClCH_2OCH_2Cl + H_2O$$

(BCME)

Source: Travenius (1982)

FIGURE 3-3
THE FORMATION OF BIS(CHLOROMETHYL) ETHER (BCME) FROM THE DECOMPOSITION PRODUCTS OF CHLOROMETHYL METHYL ETHER (CMME)

R420T05

APPENDIX 1. COMPUTERIZED DATA BASES USED FOR LITERATURE SEARCHES

AQUIRE	1976 TO PRESENT
AQUALINE	1967 TO PRESENT
AQUAREF	1980 TO PRESENT
BIOSIS	1980 TO PRESENT
CAS ONLINE	1987 TO PRESENT
CAB	1980 TO PRESENT
CCINFO	1990
CESARS	1960 TO PRESENT
CODOC	1640 TO PRESENT
ELIAS	1976 TO PRESENT
ENVIROLINE	1971 TO PRESENT
FEDERAL REGISTRY	1980 TO PRESENT
MICROLOG	1979 TO PRESENT
POLLUTION ABSTRACTS	1970 TO PRESENT
TOXLINE	1960 TO PRESENT
TRI (TOXNET)	1990

Appendix II : BCME

LEVEL 3 FUGACITY MODEL

Predicted fate of bcme in Southern Ontario

compound properties

molecular weight	114.96 g/mol				
aqueous solubility	2.2000E+04 g/m3	or	1.9137E+02 mol/m3		
vapour pressure	3.9996E+03 pa	or	3.9473E-02 atm	or	(2.9999E+01 mm Hg)
henry's constant	2.0900E+01 pa m3/mol				
octanol-water part coeff (log)	2.40				

temperature 25.0 deg C or 298.2 K

bulk compartment	volume m3	height/ depth (m)	area m2	Z mol/m3.Pa	density kg/m3
1 bulk air	4.000E+14	2.000E+03	2.000E+11	4.034E-04	1.19
2 bulk water	4.000E+12	5.000E+01	8.000E+10	4.786E-02	1000.01
3 bulk soil	1.200E+10	1.000E-01	1.200E+11	1.330E-01	1500.24
4 bulk sediment	8.000E+08	1.000E-02	8.000E+10	1.758E-01	1420.00

total area (m2) 2.000E+11

subcompartment	volume m3	Z mol/m3.Pa	density kg/m3	mass fraction organic content	volume fraction
1., 1 air	4.000E+14	4.034E-04	1.19		1.00E+00
1., 3 air particles	8.000E+03	6.052E-01	2400.00		2.00E-11
2., 2 water	4.000E+12	4.785E-02	1000.00		1.00E+00
2., 3 water particles	2.000E+07	2.371E+00	2400.00	0.20	5.00E-06
2., 4 biota	4.000E+06	5.769E-01	1000.00		1.00E-06
3., 1 soil air	2.400E+09	4.034E-04	1.19		2.00E-01
3., 2 soil water	3.600E+09	4.785E-02	1000.00		3.00E-01
3., 3 soil solids	6.000E+09	2.371E-01	2400.00	0.02	5.00E-01
4., 2 pore water	5.600E+08	4.785E-02	1000.00		7.00E-01
4., 3 sed. solids	2.400E+08	4.742E-01	2400.00	0.04	3.00E-01

Reaction Parameters

bulk compartments	rate constant h-1	half-life h	D value mol/pa.h
1 bulk air	3.5200E+00	1.9688E-01	5.6801E+11
2 bulk water	6.5000E+01	1.0662E-02	1.2444E+13
3 bulk soil	6.5000E+01	1.0662E-02	1.0373E+11
4 bulk sediment	6.5000E+01	1.0662E-02	9.1394E+09
Subcompartments			
1., 1 air	0.0000E+00	0.0000E+00	0.0000E+00
1., 3 air particles	0.0000E+00	0.0000E+00	0.0000E+00
2., 2 water	0.0000E+00	0.0000E+00	0.0000E+00
2., 3 water particles	0.0000E+00	0.0000E+00	0.0000E+00
2., 4 biota	0.0000E+00	0.0000E+00	0.0000E+00
3., 1 soil air	0.0000E+00	0.0000E+00	0.0000E+00
3., 2 soil water	0.0000E+00	0.0000E+00	0.0000E+00
3., 3 soil solids	0.0000E+00	0.0000E+00	0.0000E+00
4., 2 pore water	0.0000E+00	0.0000E+00	0.0000E+00
4., 3 sed. solids	0.0000E+00	0.0000E+00	0.0000E+00

Advective Parameters

compartment	flow m3/h	inflow concn mol/m3	rate constant h-1	D value mol/pa.h	residence time h
1 bulk air	3.30E+12	0.00E+00	8.25E-03	1.33E+09	1.21E+02
2 bulk water	3.30E+08	0.00E+00	8.25E-05	1.58E+07	1.21E+04
3 bulk soil	0.00E+00	0.00E+00	0.00E+00	0.00E+00	infinity
4 bulk sediment	0.00E+00	0.00E+00	0.00E+00	0.00E+00	infinity

Transfer to higher altitude,sediment burial and leaching from soil to groundwater

process	velocity m/y	velocity m/h	flow m3/h	rate constant h-1	D value mol/pa.h	residence times h	y
transfer to higher alt	9.00E+01	1.03E-02	2.05E+09	5.14E-06	8.29E+05	1.95E+05	2.22E+01
leaching from soil	3.40E-01	3.88E-05	4.66E+06		2.23E+05		
sediment burial	3.00E-04	3.42E-08	2.74E+03	1.14E-05	1.30E+03	8.76E+04	1.00E+01

Transfer parameters between compartments

Total D Values and Fluxes

compartment	D (mol/h*pa)	flux mol/h)	tau(i,j) h
from 1 to 2	5.290E+07	1.293E-07	1.151E+03
from 2 to 1	5.253E+07	-1.293E-07	1.151E+03
from 1 to 3	1.307E+06	3.196E-09	1.449E+03
from 3 to 1	7.502E+05	-3.196E-09	1.449E+03
from 2 to 4	1.824E+06	1.895E-14	7.269E+04
from 4 to 2	1.816E+06	-1.895E-14	5.363E+01
from 3 to 2	2.235E+05	6.886E-15	4.948E+03

Individual D Values, Flows and Velocities

compartments	by	D (mol/h*pa)	flow (m3/h)	flow (m3/y)	velocity (m/h)	velocity (m/y)
from 1 to 2	diffusion	5.253E+07				
	rain	3.714E+05	7.763E+06	6.800E+10	9.703E-05	8.500E-01
	wet deposition	1.879E+01	3.105E+01	2.720E+05	3.881E-10	3.400E-06
	dry deposition	1.046E+01	1.728E+01	1.514E+05	1.080E+01	3.000E-03 (m/s)
from 2 to 1	diffusion	5.253E+07				
from 1 to 3	diffusion	7.502E+05				
	rain	5.571E+05	1.164E+07	1.020E+11	9.703E-05	8.500E-01
	wet deposition	2.819E+01	4.658E+01	4.080E+05	3.881E-10	3.400E-06
	dry deposition	1.569E+01	2.592E+01	2.271E+05	1.080E+01	3.000E-03 (m/s)
from 3 to 1	diffusion	7.502E+05				
from 2 to 4	diffusion	1.815E+06				
	deposition	8.661E+03	3.653E+03	3.200E+07	4.566E-08	4.000E-04
from 4 to 2	diffusion	1.815E+06				
	resuspension	4.331E+02	9.132E+02	8.000E+06	1.142E-08	1.000E-04
from 3 to 2	water flow	2.229E+05	4.658E+06	4.080E+10	3.881E-05	3.400E-01
	soil flow	6.496E+02	2.740E+03	2.400E+07	2.283E-08	2.000E-04

Input Transport Parameters

Mass Transfer Coefficients (MTC) (m/h)

Air-Water	air-side MTC	3.00E+00
	water-side MTC	3.00E-02
	overall water-side MTC	1.37E-02
Air-Soil		
	air-side MTC	1.000E+00
Water-Sediment		
	water-side MTC	1.000E-02

Diffusivities

air molecular diffusivity	0.40E-01	m2/h	air effective diffusivity	0.75E-03	m2/h	mean path length	0.0500	m
water molecular diffusivity	0.40E-05	m2/h						
soil			water effective diffusivity	0.29E-06	m2/h	mean path length	0.0500	m
sediment			water effective diffusivity	0.25E-05	m2/h	mean path length	0.0050	m

D Values for Diffusive Flow in Soil Air and Water

Soil	air diffusion	7.286E+05
	water diffusion	3.334E+04

D Value for Diffusive Flow in Sediment Pore Water

Sediment	water diffusion	1.906E+06

Bulk Compartments

compartment	amount mol	percent	concentrations mol/m3	concentrations microg/g	concentrations microg/m3	fugacity Pa
1 bulk air	3.945E-04	99.999	9.862E-19	9.564E-14	1.134E-10	2.445E-15
2 bulk water	1.990E-09	0.001	4.974E-22	5.718E-20	5.718E-14	1.039E-20
3 bulk soil	4.917E-11	0.000	4.097E-21	3.140E-19	4.710E-13	3.081E-20
4 bulk sediment	2.916E-16	0.000	3.645E-25	2.951E-23	4.190E-17	2.074E-24
Total	3.945E-04	100.000				

Subcompartments

compartment	amount mol	percent	concentrations mol/m3	concentrations microg/g	concentrations microg/m3	fugacity Pa
1., 1 air	3.945E-04	99.999	9.862E-19	9.564E-14	1.134E-10	2.445E-15
1., 3 air particles	1.184E-11	0.000	1.479E-15	7.087E-14	1.701E-07	2.445E-15
2., 2 water	1.989E-09	0.001	4.973E-22	5.717E-20	5.717E-14	1.039E-20
2., 3 water particles	4.929E-13	0.000	2.464E-20	1.180E-18	2.833E-12	1.039E-20
2., 4 biota	2.398E-14	0.000	5.996E-21	6.893E-19	6.893E-13	1.039E-20
3., 1 soil air	2.983E-14	0.000	1.243E-23	1.205E-18	1.429E-15	3.081E-20
3., 2 soil water	5.307E-12	0.000	1.474E-21	1.695E-19	1.695E-13	3.081E-20
3., 3 soil solids	4.383E-11	0.000	7.305E-21	3.499E-19	8.398E-13	3.081E-20
4., 2 pore water	5.556E-17	0.000	9.922E-26	1.141E-23	1.141E-17	2.074E-24
4., 3 sed. solids	2.360E-16	0.000	9.833E-25	4.710E-23	1.130E-16	2.074E-24

summary of 4 bulk compartment mass balances (mol/h)

	emissions	inflow	reaction	outflow	net flux out to other compts
bulk air	1.392E-03	0.000E+00	1.389E-03	3.255E-06	1.325E-07
bulk water	0.000E+00	0.000E+00	1.293E-07	1.641E-13	-1.293E-07
bulk soil	0.000E+00	0.000E+00	3.196E-09	0.000E+00	-3.196E-09
bulk sediment	0.000E+00	0.000E+00	1.895E-14	0.000E+00	-1.895E-14
Total	1.392E-03	0.000E+00	1.389E-03	3.255E-06	

total input (emissions and inflow) 1.392E-03 mol/h
total output (reactions and outflow) 1.392E-03 mol/h

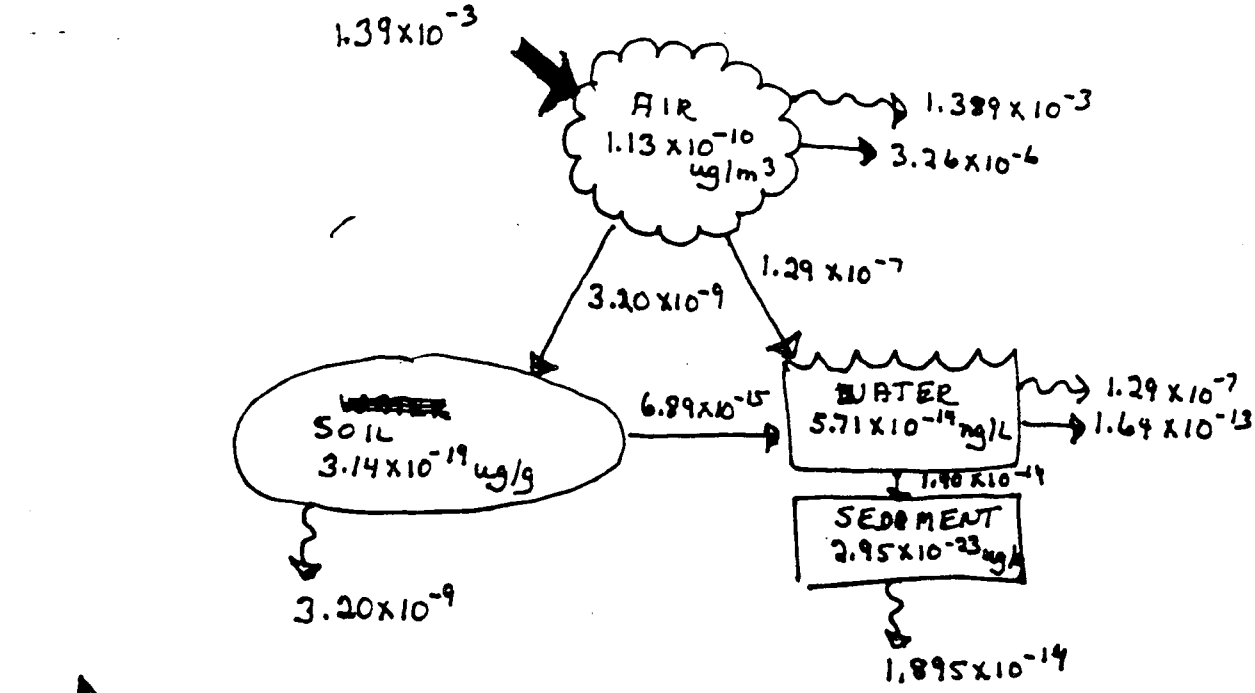
residence time (hours) .2834007 persistence .2840653
(days) 1.180836E-02 persistence 1.183605E-02

Transfer and Transformation rates (mol/h)

	Bulk air	Bulk water	Soil	Sediment	Total
emissions	1.392E-03	0.000E+00	0.000E+00	0.000E+00	1.392E-03
advective inflow	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
advective outflow	3.255E-06	1.641E-13	0.000E+00	0.000E+00	3.255E-06
reaction	1.389E-03	1.293E-07	3.196E-09	1.895E-14	1.389E-03
transfer to higher altitude	2.026E-09				2.026E-09
leaching from soil			6.866E-15		6.866E-15
sediment burial				2.694E-21	2.694E-21
transfer to air from	0.000E+00	-1.293E-07	-3.196E-09	0.000E+00	-1.325E-07
transfer to water from	1.293E-07	0.000E+00	6.886E-15	-1.895E-14	1.293E-07
by diffusion air-water	1.284E-07				
by diffusion water-air	-5.460E-13				
net diffusion	1.284E-07				
by rain	9.080E-10				
by wet deposition	4.594E-14				
by dry deposition	2.557E-14				
by water runoff			6.866E-15		
by soil runoff			2.001E-17		
transfer to soil from	3.196E-09	-6.886E-15	0.000E+00	0.000E+00	3.196E-09
by diffusion air-soil	1.834E-09				
by diffusion soil-air	-2.311E-14				
net diffusion	1.834E-09				
by rain	1.362E-09				
by wet deposition	6.891E-14				
by dry deposition	3.835E-14				
transfer to sediment from	0.000E+00	1.895E-14	0.000E+00	0.000E+00	1.895E-14
by diffusion water-sediment		1.887E-14			
by diffusion sediment-water		-3.764E-18			
net diffusion		1.886E-14			
by sediment deposition		9.002E-17			
by sediment resuspension		-8.980E-22			

Now we require advection rates (m3/h) and the corresponding inflow concentration
s (mol/m3)
Normally only air and water advection are included, and the background concentra
tions are zero. If no values are entered, zero will be assumed.

The same procedure is followed as for reaction rate constants except that the
requested numbers are: compartment no, advective flow rate (m3/h) and input conc
entration separated by commas. Advection may only be into bulk compartments (1 -
4)
a specimen input for Southern Ontario is 1,3.3e12,3e-12 indicating an inflow of
3.3e12 m3/h of air with a background concentration of 3e-12 mol/m3
do you want to enter an (or another) advective flow rate? y/n? y
? 1,3.3e12,0



BCME

FIGURE : MASS BALANCE DIAGRAM FOR BCME IN SOUTHERN ONTARIO.

Appendix II. CMME

LEVEL 3 FUGACITY MODEL

Predicted fate of cmme in Southern Ontario

compound properties

molecular weight	80.52 g/mol					
aqueous solubility	2.0000E+04	g/m3	or	2.4839E+02	mol/m3	
vapour pressure	1.6265E+04	pa	or	1.6052E-01	atm	or (1.2200E+02 mm Hg)
henry's constant	6.5483E+01 pa m3/mol					
octanol-water part coeff (log)	0.21					

temperature 25.0 deg C or 298.2 K

bulk compartment	volume m3	height/ depth (m)	area m2	Z mol/m3.Pa	density kg/m3
1. bulk air	4.000E+14	2.000E+03	2.000E+11	4.034E-04	1.19
2 bulk water	4.000E+12	5.000E+01	8.000E+10	1.527E-02	1000.01
3 bulk soil	1.200E+10	1.000E-01	1.200E+11	4.755E-03	1500.24
4 bulk sediment	8.000E+08	1.000E-02	8.000E+10	1.080E-02	1420.00

total area (m2) 2.000E+11

subcompartment	volume m3	Z mol/m3.Pa	density kg/m3	mass fraction organic content	volume fraction
1., 1 air	4.000E+14	4.034E-04	1.19		1.00E+00
1., 3 air particles	8.000E+03	1.488E-01	2400.00		2.00E-11
2., 2 water	4.000E+12	1.527E-02	1000.00		1.00E+00
2., 3 water particles	2.000E+07	1.858E-03	2400.00	0.20	5.00E-06
2., 4 biota	4.000E+06	4.520E-04	1000.00		1.00E-06
3., 1 soil air	2.400E+09	4.034E-04	1.19		2.00E-01
3., 2 soil water	3.600E+09	1.527E-02	1000.00		3.00E-01
3., 3 soil solids	6.000E+09	1.858E-04	2400.00	0.02	5.00E-01
4., 2 pore water	5.600E+08	1.527E-02	1000.00		7.00E-01
4., 3 sed. solids	2.400E+08	3.715E-04	2400.00	0.04	3.00E-01

Reaction Parameters

bulk compartments	rate constant h-1	half-life h	D value mol/pa.h
1 bulk air	3.1000E-02	2.2355E+01	5.0024E+09
2 bulk water	6.4000E+01	1.0828E-02	3.9094E+12
3 bulk soil	6.4000E+01	1.0828E-02	3.6518E+09
4 bulk sediment	6.4000E+01	1.0828E-02	5.5303E+08
Subcompartments			
1., 1 air	0.0000E+00	0.0000E+00	0.0000E+00
1., 3 air particles	0.0000E+00	0.0000E+00	0.0000E+00
2., 2 water	0.0000E+00	0.0000E+00	0.0000E+00
2., 3 water particles	0.0000E+00	0.0000E+00	0.0000E+00
2., 4 biota	0.0000E+00	0.0000E+00	0.0000E+00
3., 1 soil air	0.0000E+00	0.0000E+00	0.0000E+00
3., 2 soil water	0.0000E+00	0.0000E+00	0.0000E+00
3., 3 soil solids	0.0000E+00	0.0000E+00	0.0000E+00
4., 2 pore water	0.0000E+00	0.0000E+00	0.0000E+00
4., 3 sed. solids	0.0000E+00	0.0000E+00	0.0000E+00

Advective Parameters

compartment	flow m3/h	inflow concn mol/m3	rate constant h-1	D value mol/pa.h	residence time h
1 bulk air	3.30E+12	0.00E+00	8.25E-03	1.33E+09	1.21E+02
2 bulk water	3.30E+08	0.00E+00	8.25E-05	5.04E+06	1.21E+04
3 bulk soil	0.00E+00	0.00E+00	0.00E+00	0.00E+00	infinity
4 bulk sediment	0.00E+00	0.00E+00	0.00E+00	0.00E+00	infinity

Transfer to higher altitude,sediment burial and leaching from soil to groundwater

process	velocity m/y	velocity m/h	flow m3/h	rate constant h-1	D value mol/pa.h	residence times h	y
transfer to higher alt	9.00E+01	1.03E-02	2.05E+09	5.14E-06	8.29E+05	1.95E+05	2.22E+01
leaching from soil	3.40E-01	3.88E-05	4.66E+06		7.11E+04		
sediment burial	3.00E-04	3.42E-08	2.74E+03	1.14E-05	1.02E+00	8.76E+04	1.00E+01

Transfer parameters between compartments

Total D Values and Fluxes

compartment				D (mol/h*pa)	flux mol/h)	tau(i,j) h
from	1	to	2	2.671E+07	3.652E-04	1.154E+03
from	2	to	1	2.659E+07	-3.652E-04	1.154E+03
from	1	to	3	9.060E+05	1.239E-05	5.428E+01
from	3	to	1	7.282E+05	-1.239E-05	5.428E+01
from	2	to	4	5.793E+05	5.406E-11	7.219E+04
from	4	to	2	5.793E+05	-5.406E-11	1.033E+01
from	3	to	2	7.113E+04	2.413E-10	5.559E+02

Individual D Values, Flows and Velocities

compartments				by	D (mol/h*pa)	flow (m3/h)	flow (m3/y)	velocity (m/h)	velocity (m/y)
from	1	to	2	diffusion	2.659E+07				
				rain	1.185E+05	7.763E+06	6.800E+10	9.703E-05	8.500E-01
				wet deposition	4.621E+00	3.105E+01	2.720E+05	3.881E-10	3.400E-06
				dry deposition	2.572E+00	1.728E+01	1.514E+05	1.080E+01	3.000E-03 (m/s)
from	2	to	1	diffusion	2.659E+07				
from	1	to	3	diffusion	7.282E+05				
				rain	1.778E+05	1.164E+07	1.020E+11	9.703E-05	8.500E-01
				wet deposition	6.931E+00	4.658E+01	4.080E+05	3.881E-10	3.400E-06
				dry deposition	3.857E+00	2.592E+01	2.271E+05	1.080E+01	3.000E-03 (m/s)
from	3	to	1	diffusion	7.282E+05				
from	2	to	4	diffusion	5.793E+05				
				deposition	6.786E+00	3.653E+03	3.200E+07	4.566E-08	4.000E-04
from	4	to	2	diffusion	5.793E+05				
				resuspension	3.393E-01	9.132E+02	8.000E+06	1.142E-08	1.000E-04
from	3	to	2	water flow	7.113E+04	4.658E+06	4.080E+10	3.881E-05	3.400E-01
				soil flow	5.089E-01	2.740E+03	2.400E+07	2.283E-08	2.000E-04

Input Transport Parameters

Mass Transfer Coefficients (MTC) (m/h)

Air-Water	air-side MTC	3.00E+00
	water-side MTC	3.00E-02
	overall water-side MTC	2.18E-02
Air-Soil		
	air-side MTC	1.000E+00
Water-Sediment		
	water-side MTC	1.000E-02

Diffusivities

air molecular diffusivity 0.40E-01 m2/h air effective diffusivity 0.75E-03 m2/h mean path length 0.0500 m

water molecular diffusivity 0.40E-05 m2/h

soil	water effective diffusivity	0.29E-06	m2/h	mean path length 0.0500 m
sediment	water effective diffusivity	0.25E-05	m2/h	mean path length 0.0050 m

D Values for Diffusive Flow in Soil Air and Water

Soil	air diffusion	7.286E+05
	water diffusion	1.064E+04

D Value for Diffusive Flow in Sediment Pore Water

Sediment	water diffusion	6.082E+05

Bulk Compartments

compartment	amount mol	percent	concentrations mol/m3	concentrations microg/g	concentrations microg/m3	fugacity Pa
1 bulk air	2.207E+00	100.000	5.517E-15	3.747E-10	4.442E-07	1.367E-11
2 bulk water	5.706E-06	0.000	1.426E-18	1.149E-16	1.149E-10	9.341E-17
3 bulk soil	1.935E-07	0.000	1.613E-17	8.656E-16	1.299E-09	3.392E-15
4 bulk sediment	8.447E-13	0.000	1.056E-21	5.987E-20	8.502E-14	9.775E-20
Total	2.207E+00	100.000				

Subcompartments

compartment	amount mol	percent	concentrations mol/m3	concentrations microg/g	concentrations microg/m3	fugacity Pa
1., 1 air	2.207E+00	100.000	5.517E-15	3.747E-10	4.442E-07	1.367E-11
1., 3 air particles	1.628E-08	0.000	2.035E-12	6.828E-11	1.639E-04	1.367E-11
2., 2 water	5.706E-06	0.000	1.426E-18	1.149E-16	1.149E-10	9.341E-17
2., 3 water particles	3.470E-12	0.000	1.735E-19	5.822E-18	1.397E-11	9.341E-17
2., 4 biota	1.689E-13	0.000	4.222E-20	3.399E-18	3.399E-12	9.341E-17
3., 1 soil air	3.284E-09	0.000	1.368E-18	9.294E-14	1.102E-10	3.392E-15
3., 2 soil water	1.865E-07	0.000	5.180E-17	4.171E-15	4.171E-09	3.392E-15
3., 3 soil solids	3.780E-09	0.000	6.301E-19	2.114E-17	5.073E-11	3.392E-15
4., 2 pore water	8.360E-13	0.000	1.493E-21	1.202E-19	1.202E-13	9.775E-20
4., 3 sed. solids	8.716E-15	0.000	3.632E-23	1.218E-21	2.924E-15	9.775E-20

summary of 4 bulk compartment mass balances (mol/h)

	emissions	inflow	reaction	outflow	net flux out to other compts
bulk air	8.700E-02	0.000E+00	6.841E-02	1.820E-02	3.776E-04
bulk water	0.000E+00	0.000E+00	3.652E-04	4.707E-10	-3.652E-04
bulk soil	0.000E+00	0.000E+00	1.239E-05	0.000E+00	-1.239E-05
bulk sediment	0.000E+00	0.000E+00	5.406E-11	0.000E+00	-5.406E-11
Total	8.700E-02	0.000E+00	6.878E-02	1.820E-02	

total input (emissions and inflow) 8.700E-02 mol/h
total output (reactions and outflow) 8.700E-02 mol/h

residence time (hours) 25.36389 persistence 32.08108
(days) 1.056829 persistence 1.336712

Transfer and Transformation rates (mol/h)

	Bulk air	Bulk water	Soil	Sediment	Total
emissions	8.700E-02	0.000E+00	0.000E+00	0.000E+00	8.700E-02
advective inflow	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
advective outflow	1.820E-02	4.707E-10	0.000E+00	0.000E+00	1.820E-02
reaction	6.841E-02	3.652E-04	1.239E-05	5.406E-11	6.878E-02
transfer to higher altitude	1.134E-05				1.134E-05
leaching from soil			2.412E-10		2.412E-10
sediment burial				9.950E-20	9.950E-20
transfer to air from	0.000E+00	-3.652E-04	-1.239E-05	0.000E+00	-3.776E-04
transfer to water from	3.652E-04	0.000E+00	2.413E-10	-5.406E-11	3.652E-04
by diffusion air-water	3.636E-04				
by diffusion water-air	-2.483E-09				
net diffusion	3.636E-04				
by rain	1.621E-06				
by wet deposition	6.319E-11				
by dry deposition	3.517E-11				
by water runoff			2.412E-10		
by soil runoff			1.726E-15		
transfer to soil from	1.239E-05	-2.413E-10	0.000E+00	0.000E+00	1.239E-05
by diffusion air-soil	9.957E-06				
by diffusion soil-air	-2.470E-09				
net diffusion	9.955E-06				
by rain	2.432E-06				
by wet deposition	9.478E-11				
by dry deposition	5.275E-11				
transfer to sediment from	0.000E+00	5.406E-11	0.000E+00	0.000E+00	5.406E-11
by diffusion water-sediment		5.412E-11			
by diffusion sediment-water		-5.663E-14			
net diffusion		5.406E-11			
by sediment deposition		6.339E-16			
by sediment resuspension		-3.317E-20			

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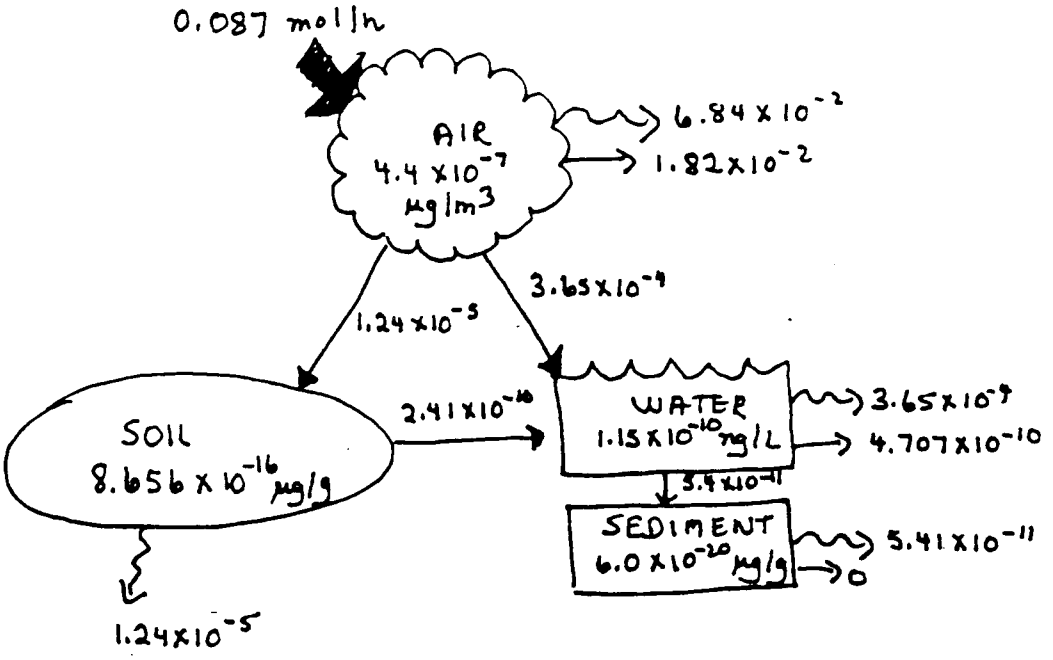

EMISSION

REACTION

ADVECTION AND/OR INTERMEDIA TRANSPORT

CMME

FIGURE: MASS BALANCE DIAGRAM FOR CMME IN SOUTHERN ONTARIO.