

AR201-13406A

**HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM**

TEST PLAN

For

ETHYL MONOCHLOROACETATE

Prepared by:

The Dow Chemical Company

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EXECUTIVE SUMMARY

The Dow Chemical Company hereby submits for review and public comment the test plan for ethyl monochloroacetate (EMCA) (CAS No. 105-39-5), which we have classified as a closed-system intermediate, under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of The Dow Chemical Company to primarily use existing data and scientific judgment and analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this chemical. Additional data will be collected under the HPV Challenge Program as defined in this test plan.

Please note that we are aware that there is another importer of EMCA into the United States. We have tried to reach this company to determine if they were interested in joining with Dow in our commitment to the HPV Chemical Challenge Program. Further, we asked them to assess whether or not their import, handling, and use of EMCA would fulfill the criteria outlined by EPA for a closed-system intermediate. Unfortunately, the company declined to respond to our invitation and did not provide any information on their handling or use of EMCA.

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TEST PLAN FOR ETHYL MONOCHLOROACETATE

I. INTRODUCTION

The Dow Chemical Company has voluntarily committed to develop and/or summarize screening level human health effects, environmental effects and fate, and physicochemical test data for ethyl monochloroacetate under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program.

This plan identifies the chemical and its CAS number, identifies existing data of adequate quality for the chemical, provides justification for why additional toxicity data is not needed to characterize human health effects, and describes additional testing to be conducted for the chemical under the Program

II. DESCRIPTION OF ETHYL MONOCHLOROACETATE

A. The Chemical

Ethyl monochloroacetate (CAS No. 105-39-5) is a member of a group of chemicals referred to as esters of monocarboxylic halogenated acids. The halogenated acetates are used primarily as intermediates in organic synthesis processes. As is typical in this group, ethyl monochloroacetate is a colorless liquid with a relatively high density, good solubility in water, and good stability to hydrolytic processes. Halogenated acetates tend to have similar toxicity profiles, with a primary effect being pulmonary edema, as well as lacrimatory and irritant properties.

Table 1. Chemical/physical properties Ethyl *Monochloroacetate*

| | |
|--|---|
| <i>Chemical Abstract Number</i> | <i>105-39-5</i> |
| <i>Molecular formula</i> | <i>C₄H₇ClO₂</i> |
| <i>Molecular weight</i> | <i>122.56</i> |
| <i>Physical State</i> | <i>Clear, Colorless liquid</i> |
| <i>Melting Point</i> | <i>-26°C</i> |
| <i>Boiling point</i> | <i>144 °F @ 760 mmHg</i> |
| <i>Vapor pressure</i> | <i>4.5 hPa @20°C</i> |
| <i>Water Solubility</i> | <i>20 g/l @ 19.8°C</i> |
| <i>Specific Gravity</i> | <i>1.1585g/cm³ @ 20°C</i> |
| <i>Flash Point</i> | <i>53° C</i> |

The health hazards to humans can be summarized as follows:

Eyes: Liquid EMCA and its vapors can cause severe irritation and corneal injury sufficient to result in permanent impairment.

Skin: Prolonged or repeated exposure may produce severe irritation with burns, if confined, and may be absorbed through the skin in acutely toxic amounts to the extent that systemic injury may be sufficient to cause death.

Ingestion: There is little likelihood that ingestion will occur in routine industrial applications. Nevertheless, small amounts ingested incidentally to industrial handling are not likely to cause injury. Ingestion of large amounts would likely be injurious to the mouth, throat, and gastrointestinal tract.

Inhalation: Exposure to vapors may result in severe consequences and intolerable irritation to the respiratory passage.

III. TEST PLAN RATIONALE

A. Classification of the Chemical as a Closed-System Intermediate

1. Requirements

Classification of ethyl monochloroacetate as a closed-system intermediate under the EPA HPV program is dependent upon a number of criteria outlined by EPA. The Dow Chemical Company asserts that ethyl monochloroacetate should be regarded as a closed-system intermediate, based on satisfaction of these criteria. In the following paragraphs, we have provided information on the extremely limited potential for exposure during manufacturing, transport and processing.

2. Satisfaction of Requirements

a. Review of Manufacture / Transport / Consumption:

Ethyl Monochloroacetate (EMCA) is produced in a single facility within The Dow Chemical Company's Michigan Operations Site located in Midland, Michigan. EMCA is manufactured from chloroacetyl chloride in a completely closed system. The sole use of EMCA is as an on-site intermediate in the production of another chlorinated derivative, manufactured within the same manufacturing site where EMCA is produced. After the EMCA is manufactured, it is placed in a storage tank, which is vented to a caustic scrubber, located in a diked area. EMCA is transferred to the downstream facility via pipeline. There is no offsite transfer of this material.

b. Environmental Fate

The potential for environmental exposure to EMCA is negligible. There are minimal releases to the air, which occur through both point source and fugitive releases, but these represent a fraction of the EMCA produced. There are no releases to water or land unless a major plant upset occurred. In case of a plant upset or storage tank leak, EMCA would be contained in the dike that surrounds the manufacturing and storage area

Since the EMCA is consumed entirely as an intermediate, the downstream processing will result in yet a smaller fraction of air emissions than during manufacturing. As the residual

level of EMCA in its downstream product is non-detectable (L.O.D. - 1 ppm level), there is essentially no potential for environmental exposure through its use.

c. Human Exposure

The potential for human exposure is also extremely low. The total number of workers within our production and processing facility is less than 20. Due to the inherent irritant nature of EMCA, personal protective equipment is worn during production, maintenance, distribution and processing to ensure no personal contact. During normal operation, this would include goggles and hard hats. During an operation, such as a line opening, where there is a potential for EMCA to be present, the protective equipment would include goggles, face shield, hard hat, protective full rubber suit, boots and a full-face respirator. Suitable positive-pressure self-contained breathing apparatus would be used for longer-term exposure in emergency situations such as a spill clean up.

Available monitoring data from the production of EMCA, which is conducted periodically, indicates that the exposures are well below the industrial hygiene guideline established for EMCA. The 8-hour Time-Weighted Average exposure limit for EMCA is 0.1ppm, Skin.

A summary of the actual monitoring data, from the activities, which are expected to have the greatest potential for worker exposures, is included in the following table. During these activities, personal protective equipment is worn.

WORKER EXPOSURE DATA FOR EMCA

| ACTIVITY | MONITORING DATA | SAMPLE DURATION | COMMENT |
|-------------------------------------|-----------------|-----------------|-----------------|
| Collected Process Sample | ND (0.02 ppm) | 6 min. | Personal Sample |
| Collected Process Sample | 0.08 ppm | 6 min. | Personal Sample |
| Outdoors near Sample Collection Box | 0.07 ppm | 5 min. | Area Sample |

As the residual level of EMCA in the downstream product is non-detectable (L.O.D. – 1ppm), there is essentially no potential for worker or public exposure during processing. There is no potential for public exposure unless there would be a significant manufacturing plant upset or catastrophic event. We have a program in place to conduct extensive root cause investigations if any such incidents were to occur and to develop a corrective action plan to prevent reoccurrence.

3. Conclusion

The Dow Chemical Company believes that the information above fully satisfies the EPA's criteria for closed-system intermediates. Further, the above information suggests that there appears to be little additional action that could be taken to prevent any further exposure, as the potential exposure opportunity is extremely limited.

B. Human Health Effects

There are six mammalian toxicity endpoints in the HPV Program (Results summarized in the table on Page 7):

- Acute Toxicity
- Repeated Dose Toxicity
- Genetic Toxicity *In Vitro*
- Genetic Toxicity *In Vivo*
- Reproductive Toxicity
- Developmental Toxicity

Published and unpublished data, as detailed in the attached Robust Summaries, satisfy the requirements of Acute, Repeated Dose, and *In Vitro* Genetic Toxicity endpoints. Since *in vitro* genetic toxicity endpoints are negative, *in vivo* testing has not been addressed.

As EMCA satisfies the EPA's criteria as a closed-system intermediate, the only data gap that exists is for a Developmental Toxicity study. Based on our demonstration above that the potential for any human and environmental exposure is highly unlikely and that repeated human and environmental exposure are even less likely, we do not believe that a development toxicity test is justified. Further, the corrosive nature of the compound will limit the dose that can be tolerated by the animals, which limits the potential to show any adverse effect if such a study were conducted.

The attached Robust Summaries provide adequate data to characterize the human health effects endpoints under the Program.

C. Ecotoxicity

There are three aquatic toxicity endpoints in the HPV Program:
(Results summarized in the table on Page 7)

- Acute Toxicity to Fish
- Acute Toxicity to Aquatic Invertebrates
- Toxicity to Algae (Growth Inhibition)

Published and unpublished data, as detailed in the attached Robust Summaries, satisfies requirements for Acute Toxicity to Fish and Aquatic Invertebrates. To satisfy the remaining requirement, a test for acute toxicity to algae is planned, in compliance with OECD Guideline

201. The recommended testing, in conjunction with existing data, will provide adequate data to characterize ecotoxicity endpoints under the Program.

D. Environmental Fate

(Results summarized in the table on Page 7)

Predictive models were used to develop meaningful data for chemicals that are gaseous at relevant environmental temperatures and pressures. The environmental fate data include:

- Photodegradation
- Stability in Water (Hydrolysis)
- Transport and Distribution (Fugacity)
- Biodegradation

1. Photodegradation

Photodegradation was estimated using models accepted by the EPA. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows)¹ is used by The Dow Chemical Company. This program calculates a chemical half-life based on an overall OH reaction rate constant, a 12-hr day, and a given OH concentration. This calculation was performed for ethyl monochloroacetate, as detailed in the attached Robust Summaries.

2. Stability in Water (Hydrolysis Testing and Modeling)

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters⁴. Stability in water can be measured³ (EPA identifies OECD test guideline 111 as a test method). Experimentally determined data for ethyl monochloroacetate, as referenced in Howard² and as detailed in the attached Robust Summaries is available.

3. Chemical Transport and Distribution In The Environment (Fugacity Modeling)

The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model⁵. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data*³, which was prepared as guidance for the HPV Program.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model has been used to calculate distribution values for ethyl monochloroacetate. A computer model, EPIWIN - version 3.02¹, has been used to calculate the properties needed to run the Level I EQC

model. The distribution values for ethyl monochloroacetate are detailed in the attached Robust Summaries.

4. Biodegradation Testing

Biodegradation values for ethyl monochloroacetate, as detailed in the attached Robust Summaries, were experimentally determined using OECD Guideline 302B.

E. Physicochemical Properties

(Results are summarized in the “Description of the Chemical” on page 1.)

The physicochemical properties include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Octanol/Water Partition Coefficient

Data for physicochemical properties will be summarized from various resources and detailed in the attached Robust Summaries.

IV. TEST PLAN SUMMARY

The following testing will be conducted for ethyl monochloroacetate:

- Conduct an algal toxicity study.

For reasons indicated in the above paragraphs, we do not believe additional data needs to be generated beyond this algal toxicity study. Due to the manner in which the chemical is manufactured, distributed, and processed; the product stewardship measures taken to prevent exposure; and existing human/environmental data, we believe that our workers, the public and the environment are well protected from exposure to EMCA. Most importantly, we do not believe that generation of any additional data, especially developmental toxicity testing, will impact our handling or product stewardship practices. Due to the acute hazards of this compound, our process and procedures are designed to prevent any exposure to our workers and the public.

Test Plan for Ethyl monochloroacetate

| Endpoint | Data Availability | Acceptable (Reliability) | Planned Testing |
|--|---|---------------------------------|-------------------------------|
| Acute Toxicity | Oral LD50: 50 – 200 mg/kg (rat) Oral LD50: 350 mg/kg (mouse) Dermal LD50: 161 mg/kg (rat) Dermal LD50: 230 - 335 mg/kg (rabbit) Dermal Irritation: Moderately Irritating (rabbit) Eye Irritation: Highly Irritating (rabbit) | Acceptable (1) | None |
| Repeated Dose Toxicity (Carcinogenicity: 580 days) | Negative (See Robust Summary for details) | Acceptable (2) | None |
| Genetic Toxicity <i>In Vitro</i> | Ames – negative Genetic mutation - negative | Acceptable (1) | None |
| Genetic Toxicity <i>In Vivo</i> | Not available | Not necessary | None |
| Reproductive Toxicity | Not available | Not required | None |
| Developmental Toxicity | Not available | Not necessary | None |
| Acute Toxicity to Fish | LC50 1.48 mg/L (OECD 203) | Acceptable (2) | None |
| Acute Toxicity to Aquatic Invertebrates | EC50 3.3 mg/L (DIN 38412) | Acceptable (2) | None |
| Toxicity to Algae (Growth Inhibition) | Not available | To Be Conducted | Algal growth inhibition study |
| Photodegradation | 50% after 15.7 days (calculated) | Acceptable (1) | None |
| Stability in Water (Hydrolysis) | Half life: pH 7 – 9.1 day @25°C pH 8 – 21.8 hrs @25° C (calculated) | Acceptable (2) | None |
| Transport and Distribution (Fugacity) | Level I: Air – 45.1 Water – 54.5 Soil – 0.42 (calculated) | Acceptable (1) | None |
| Biodegradation | 75% after 28 days (OECD 301 F) 93% after 13 days (OECD 302 B) | Acceptable (1) | None |

REFERENCES

1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.02. Syracuse Research Corporation, Syracuse, NY, USA.
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4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
5. Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15:1627-1637.