## Section A7.3.1-01 Phototransformation in air (estimation method)

**Annex Point IIIA VII.5**

| | | | Official use only |
|---|---|---|---|
| | | **1 REFERENCE** | |
| **1.1** | **Reference** | Mamouni A. (2006): 2-n-octyl-4-isothiazolin-3-one (OIT): Estimation of Degradation by Photo-oxidation in Air – Model calculation according to Atkinson. [redacted] | |
| **1.2** | **Data protection** | Yes | |
| 1.2.1 | Data owner | Thor GmbH | |
| 1.2.2 | Companies with letter of access | None | |
| 1.2.3 | Criteria for data protection | Data submitted on existing a.s. for the purpose of its entry into Annex I. | |
| | | **2 GUIDELINES AND QUALITY ASSURANCE** | |
| **2.1** | **Guideline study** | Not applicable.<br>The calculation of the substance decay rate in air was performed using [redacted] | |
| **2.2** | **GLP** | Not applicable.<br>The estimation was conducted using a widely accepted calculation method [redacted] | |
| **2.3** | **Deviations** | No | |
| | | **3 MATERIALS AND METHODS** | |
| **3.1** | **Test material** | No test material used, computer simulation | |
| 3.1.1 | Lot/Batch number | Not applicable. | |
| 3.1.2 | Specification | Not applicable. | |
| 3.1.3 | Purity | Not applicable. | |
| 3.1.4 | Further relevant properties | Not applicable. | |
| **3.2** | **Reference substance** | Not applicable. | |
| 3.2.1 | Initial concentration of reference substance | Not applicable. | |
| **3.3** | **Relevant information on the test substance modelled** | Name: 2-n-octyl-4-isothiazolin-3-one (OIT)<br>CAS number: 26530-20-1<br>physical appearance: white to yellowish powder<br>empirical formula: $C_{11}H_{19}NOS$<br>Molecular weight: 213.34 g/mol | |
| **3.4** | **Testing procedure** | | |
| 3.4.1 | Calculation of half-lives | The estimation methods used by the [redacted] are based on the [redacted] developed by [redacted]. The program estimates the rate constant for the atmospheric gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. It also estimates the rate constant for the gas-phase | |

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reaction between ozone and olefinic/acetylenic compounds. The atmospheric decay of OIT by hydroxyl radicals is determined by the addition of hydroxyl radicals to the olefinic bond, by reactions with N, S and O and by hydrogen abstraction.

The rate constants provided by the modelling were used to calculate the atmospheric half-lives of OIT based upon assumed average concentrations of hydroxyl radicals and ozone in air.

For the calculation, OIT was entered into the program by its CAS number.

### 4 RESULTS

**4.1 Degradation of test substance**

The half-life and rate constant for the photochemical oxidative degradation of OIT in air via the hydroxyl reaction was estimated to be 3.26 hours and 39.372 x $10^{-12}$ $cm^3$ $molecule^{-1}$ $s^{-1}$, respectively, based on 1.5 x $10^6$ OH radicals per $cm^3$, which is considered to be a representative value for daylight hours (12-hour day). The OIT half-life of 3.26 hours is equivalent to 0.272 daylight periods (12-h day). During night-time OH radical concentrations will be much lower and hence the decay rate will decrease correspondingly.

Similarly, the half life and rate constant for the photochemical oxidative degradation of OIT in air via the ozone reaction was estimated to be 157 hours and 0.175 x $10^{-17}$$cm^3$ $molecule^{-1}$ $s^{-1}$, respectively, based on 7 x $10^{11}$ mol ozone/$cm^3$ (=55 µg ozone/$m^3$), which is considered to be a representative value for ozone over a 24 hours period. The OIT half-life of 157 hours is equivalent to 6.549 days (24-h day).

### 5 APPLICANT'S SUMMARY AND CONCLUSION

**5.1 Materials and methods**

The photochemical oxidative degradation half-life of OIT in air was estimated using the [redacted], which is based on the [redacted] methods developed by [redacted]. Photodegradation of the compound by hydroxyl radicals and by ozone was considered during the simulations.

**5.2 Results and discussion**

The reaction with hydroxyl radicals dominates the decay of OIT during daylight, resulting in a half-life of 3.26 hours, i.e. 0.272 days (12-h day), while at night the much slower decay due to ozone may dominate with a half-life of 157 hours, i.e. 6.549 days (24-h day). X

The half-life of OIT for the reaction with OH-radicals taking into account a concentration of OH-radicals in atmosphere of 5 x $10^5$ molecules · $cm^{-3}$ as recommended in the TGD (2203) is equivalent to 9.78 hours or 0.815 days (12-h day).

**5.3 Conclusion**

The model substance 2-n-octyl-4-isothiazolin-3-one (OIT) is predicted to be efficiently removed from air by OH radical reactions during daylight situations, whereas at night the decay will predominantly be determined by reactions with ozone, however, at a much lower rate.

5.3.1 Reliability: 1

5.3.2 Deficiencies: None

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## Evaluation by Competent Authorities

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| | **EVALUATION BY RAPPORTEUR MEMBER STATE** |
| **Date** | 11 Nov 2009 |
| **Materials and Methods** | Applicant's version is considered acceptable. |
| **Results and discussion** | Applicant's version is considered acceptable. |
| **Conclusion** | Applicant's version is considered acceptable, noting the following:<br>**5.2:** Comment regarding half-life of OIT when taking into account a concentration of OH-radicals in atmosphere of 5 x $10^5$ molecules · $cm^{-3}$ is not mentioned in the study report. |
| **Reliability** | 2<br>The study has been conducted in accordance with generally accepted scientific principles, rather than agreed protocols |
| **Acceptability** | Acceptable |
| **Remarks** | None |
| | **COMMENTS FROM ...** |
| **Date** | |
| **Materials and Methods** | |
| **Results and discussion** | |
| **Conclusion** | |
| **Reliability** | |
| **Acceptability** | |
| **Remarks** | |