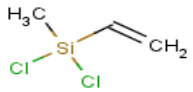
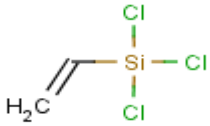
SIDS INITIAL ASSESSMENT PROFILE

Category Name	Vinyl Chlorosilanes
CAS No(s).	124-70-9 75-94-5
Chemical Name(s)	Dichloromethyl(vinyl)silane (**VDCS**) Trichlorovinylsilane (**VTCS**)
Structural Formula(s)	 **VDCS**  **VTCS**

SUMMARY CONCLUSIONS OF THE SIAR

Analogue/Category Rationale

Chlorosilanes react rapidly when exposed to moisture or polar reagents, producing hydrogen chloride (HCl; CAS No. 7647-01-0) and the corresponding silanols (in general, siloxane oligomers and polymers). For the two vinyl chlorosilanes in the category, the half-lives are expected to be <1 minute based on data from two analogous substances, dimethyldichlorosilane (DMDCS; CAS No. 75-78-5) and methyltrichlorosilane (MTCS; CAS No. 75-79-6).

The silanols expected to be produced following vinyl chlorosilane hydrolysis are vinylmethylsilanediol, CAS No 3959-12-4 (from **VDCS**) and vinylsilanetriol, CAS No 143-48-6 (from **VTCS**). The silanols can condense spontaneously to form highly cross-linked polymeric gels in uncontrolled environments. Because of these properties, they cannot be readily isolated without spontaneously forming highly cross-linked polymeric gels in uncontrolled environments and as such cannot be tested.

VDCS hydrolyzes to form two moles of HCl and one mole of vinylmethylsilanediol, whereas **VTCS** forms three moles of HCl and one mole of vinylsilanetriol. The category is supported by (1) similar structures of category members, (2) the common hydrolysis product HCl and (3) similarities in physical-chemical properties of the silanol products (high water solubility and low log K_{ow}).

Hydrolysis Analogues. It is appropriate to use other chlorosilane data to estimate hydrolysis of the sponsored substances. As noted above, analogues used for hydrolysis are DMDCS and MTCS.

Human Health and Aquatic Toxicity Analogues. Trimethoxyvinylsilane (VTMS; CAS No. 2768-02-7) hydrolyzes at pH 4, 7 and 9 with $t_{1/2} \leq$10 minutes, < 2.4 hours and <10 minutes, respectively. The final products of hydrolysis are expected to be methanol and vinylsilanetriol; toxicity due to hydrolysis to methanol is expected to be negligible.

In aqueous environments, exposures to VTMS are likely to be transient and observed toxicity is likely due primarily to the hydrolysis products methanol, vinylsilanetriol, and condensed silanetriol materials (high molecular weight polymers). Because one of the sponsored substances (**VTCS**) has the same expected product (vinylsilanetriol) as VTMS and due to similarities between this product and vinylmethylsilanediol, the analogue VTMS can be used as a supporting substance for the vinyl chlorosilanes. Due to rapid hydrolysis of the vinyl chlorosilanes and expected corrosive effects of one of the products (HCl), the data for HCl are also presented for a complete consideration of the toxicity of hydrolysis products for both human health and aquatic toxicity endpoints. No test data are available for short-term toxicity of **VDCS** to aquatic organisms. Reliable data are available for the read-across substance, dimethylsilanediol (DMSD, CAS 1066-42-8). DMSD is a close structural analogue of vinylmethylsilanediol. Read-across from DMSD to vinylmethylsilanediol is appropriate because both are small molecule alkylsilanols whose properties are dominated by presence of the silanediol group.

HCl, VTMS, DMDCS, and MTCS have been previously presented and agreed in the OECD programme; DMSD has been previously used as an analogue, most recently for chloroalkylchlorosilanes at CoCAM 3. These data can be found at http://www.oecd.org/env/hazard/data.

Read Across Strategy

	Environmental fate		**Mammalian toxicity**			**Environmental effects**
Substance	**Hydrolysis**	**Biodegradation**	**Skin, Eye, Resp. tract (RT) irritation**	**Repeated dose toxicity, Reproductive toxicity**	**Genetic toxicity (chromosome aberration)**	**Aquatic toxicity to Fish, Daphnid and Algae**
VDCS	DMDCS	X	**VTCS** (RT)	VTMS, HCl	X, HCl, VTMS	VTMS, DMSD, HCl
VTCS	MTCS	**VDCS**; VTMS	HCl (skin, eye, RT)		X, HCl, VTMS	VTMS, HCl

X= data available

Physical-chemical Properties

The sponsored substances are liquids with a measured melting point of -95 °C, measured boiling points of 91.4 °C (**VTCS**) to 93.8 °C (**VDCS**), and vapour pressures of 58.75 hPa (**VDCS**, extrapolated) to 87.99 hPa (**VTCS**, extrapolated). The calculated octanol-water partition coefficients (log K_{ow}) are 2.4 (**VTCS**) and 2.6 (**VDCS**), and the calculated water solubilities are 802.3 (**VDCS**) and 1338 (**VTCS**) mg/L at 25 °C. The calculated water solubility and log Kow values may not be relevant because the substances are hydrolytically unstable.

Human Health

No data are available on the toxicokinetics, metabolism and distribution of the vinyl chlorosilanes. However,

these substances are expected to rapidly hydrolyze on contact with moisture. Although the silanol hydrolysis products are not expected to be absorbed across the skin or respiratory epithelium,damage to membranes caused by HCl's corrosivity might enhance the uptake of the sponsored substances or the silanol hydrolysis products. The hydrophilic nature of the silanol hydrolysis products is expected to limit diffusion across membranes and accumulation in fatty tissues. Hydrogen and chloride ions will enter the body's natural homeostatic processes. HCl will rapidly dissociate and its effects are thought to be a result of pH change (local deposition of H^+). The low molecular weight and water solubility of the silanols suggest elimination via the kidneys in urine.

The acute inhalation toxicity of the vinyl chlorosilanes is well characterized, and is expected to result from HCl exposure. The 1-hour nominal acute inhalation LC_{50} for **VDCS** in rats was > 8.61 mg/L and $\leq$ 9.61 mg/L. For **VTCS**, the 4-hour value in rats is < 0.73 mg/L, and the 1-hour values in rats were 10.63 and 13.13 mg/L (both nominal values). Clinical signs and necropsy findings for animals that died during the study reflected the corrosive nature of the test substance. Inhalation LC_{50} values for HCl were determined to be 4.2-4.7 mg/L for 1 hour for rats. The dermal LD_{50} of **VTCS** in rabbits was ca. 864 mg/kg bw; dermal toxicity data were not located for **VDCS**. The oral LD_{50}s in rats were between 200 and 2000 mg/kg (**VDCS**) and 1280 mg/kg (**VTCS**); corrosive effects were observed in the gastrointestinal tract (site of contact). The acute oral LD_{50} values of HCl were determined to be 238-277 mg/kg bw for female rats.

Based on results from HCl the sponsored substances are considered corrosive to the skin and eyes. Vinyl chlorosilanes are considered respiratory tract irritants based on data from acute inhalation toxicity studies with HCl and the sponsored substances

No data are available to evaluate the sensitisation of vinyl chlorosilanes.

Data from the supporting substance VTMS and the hydrolysis product HCl are used to fill the repeated-dose toxicity endpoint for the vinyl chlorosilanes. Systemic effects following repeated inhalation of VTMS (exposure likely as a mixture with silanol hydrolysis products) and HCl have been observed. In a repeated-dose toxicity study [TG unknown], rats (20/sex/concentration) were exposed for six hours per day, five days per week, for 14 weeks to vapor of VTMS at concentrations of 0, 0.06, 0.6 or 2.4 mg/L, respectively, resulting in effects primarily on the urinary bladder and kidney. The LOAEC was determined to be 0.6 mg/L and the NOAEC was 0.06 mg/L. During 90-day repeated dose inhalation toxicity studies, local effects of HCl irritation were observed in groups exposed to 0.015 mg/L and above. The NOAEC for systemic toxicity for HCl, excluding the local effects of irritation, has been determined to be 0.030 mg/L for rats and mice. Based on these data, the vinyl chlorosilanes may result in repeated dose inhalation toxicity, with an NOAEC of 0.60 mg/L (HCl) for both category members.

In a combined repeated-dose/reproductive/developmental toxicity screening test [OECD TG 422], male and female rats were administered VTMS via gavage at 62.5, 250 and 1000 mg/kg bw/day for up to 43 days, resulting in effects primarily on the urinary bladder, intestine, kidney, and thymus in both sexes at all doses. The NOAEL was not established in this study. The LOAEL was 62.5 mg/kg bw/day (decreased urine osmolality and sodium, potassium and chloride concentrations (males) and slight decrease in body weight and body weight gain (females)). Similar effects are expected for the vinyl chlorosilane category members. Based on these data, the vinyl chlorosilanes may result in repeated dose oral toxicity, with a LOAEL of 62.5 mg/kg bw (VTMS) for both category members.

VTCS did not induce gene mutations in two bacterial mutagenicity assays (OECD TG 471). **VDCS** is considered mutagenic in *Salmonella* strain TA 1535 in the presence of hamster microsomal enzyme with metabolic activation (reducing conditions) (OECD TG 471) and was negative in the presence and absence of rat liver S9 metabolic activation (OECD TG 471), negative in the mouse lymphoma assay (OECD TG 476) and negative for the induction of chromosome aberrations in mammalian cells (OECD 473). The hydrolysis product, HCl, did not induce gene mutations in bacteria. Positive results in the *in vitro* chromosome aberration test with HCl were considered to be the effect of low pH. **VTMS** was negative in a reliable and valid *in vivo* micronucleus assay (OECD TG 474).

The weight of evidence suggests that the Vinyl Chlorosilanes may not be genotoxic. However, the positive finding in one bacterial strain under reducing conditions leaves a residual uncertainity for gene mutation potential.

No data are available for the carcinogenicity of the vinyl chlorosilanes.

No data are available on the reproductive toxicity of the vinyl chlorosilanes; data are available for the supporting substance, VTMS and the hydrolysis product, HCl. In the combined repeated-dose/reproductive/developmental toxicity screening test [OECD TG 422], there were no effects on reproductive performance of parental rats when VTMS was administered by oral gavage. The NOAEL was 1000 mg/kg bw/day for males, and 250 mg/kg bw/day for females (based on a reduced number of estrous cases). There were no effects on developmental parameters; the NOAEL for developmental effects was 1000 mg/kg bw.

Exposure of pregnant rats to VTMS by inhalation including 14 days pre-mating through lactation day 4 resulted in a NOAEC of 0.15 mg/L for maternal toxicity. There was evidence of slightly delayed skeletal ossification in fetuses from the 1.8 mg/L group; the NOAEC for developmental effects was 0.60 mg/L. No reliable studies have been reported regarding toxicity to reproduction and development in animals after oral, dermal or inhalation exposure to hydrogen chloride/hydrochloric acid. Because the proton (H^+) and chloride (Cl^-) ions are the normal constituents in the body fluid of animal species, lower concentration of hydrogen chloride gas/mist or solution does not seem to cause adverse effects to animals. In fact, the cells of gastric glands secrete hydrochloric acid into the cavity of stomach and orally administered sulfuric acid, which result in pH change as well, did not cause developmental toxicity to laboratory animals. These facts indicate that hydrogen chloride/hydrochloric acid is not expected to have developmental toxicity. In addition, no effects on the gonads were observed in a 90-day inhalation repeated-dose study with HCl up to concentrations of 0.073 mg/L. Based on these data, the vinyl chlorosilanes may result in developmental toxicity at high concentrations in inhalation studies, with a NOAEC of 0.60 mg/L (VTMS) for both category members.

The vinyl chlorosilanes possess properties indicating a hazard for human health (lethality from acute studies (inhalation, oral, and dermal); corrosivity and severe irritation to the skin, eyes, respiratory tract, and GI tract; repeated dose toxicity, potential *in vitro* gene mutation; developmental toxicity (only at high concentrations via inhalation at maternally toxic concentrations). Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD Cooperative Chemicals Assessment Programme.

Environment

Not all programs within EPI Suite have been validated for chemicals that contain the element Si, but recent upgrades to the Kow module, found in the current version of EPI Suite (v4.10), may improve estimates for silanes and siloxanes for this endpoint. However, there is still uncertainty associated with the calculated values and they should be used with caution whenever they are reported.

The chlorine group is the most active functional group of these molecules and determines many aspects of the behaviour of the category members. The vinyl chlorosilanes are expected to undergo rapid hydrolysis in the presence of water to form two or three moles of HCl and one mole of silanediol or silanetriol, depending on the parent substance. Hydrolysis is the primary reaction in aqueous systems. Hydrolysis studies were not conducted on the vinyl chlorosilanes. The vinyl chlorosilanes hydrolyze rapidly; the half-lives are expected to be <1 minute based on data from two analogous substances, DMDCS and MTCS. Observed rates of hydrolysis were so rapid that it was not possible to distinguish among the different pH conditions.

The overall rate constants for reaction with OH radicals in the atmosphere for the vinyl chlorosilanes and resulting half-lives due to indirect photolysis are ca. 26 x 10^{12} cm^3/molecule-sec and 5 hours for the category members. Any potential for photodegradation might be superseded by hydrolysis of the parent compound depending on the concentration of water vapor in the air. The sponsored substance, **VDCS**, was not readily biodegradable in an OECD TG 301A test and the supporting substance VTMS was not readily biodegradable in an OECD TG 301F test. Based on this information, the sponsored substance, **VTCS**, is not expected to be readily biodegradable. Due to rapid hydrolysis of the sponsored and supporting substances, any potential for biodegradation is likely to be of the hydrolysis products. Consequently, the only biodegradable materials in the test system will be silanols, and condensed silanol materials (high molecular weight polymers). At high concentrations, the silanols will condense to form highly cross-linked, high molecular weight polymers that are water insoluble and effectively nonbiodegradable.

A level III fugacity model calculation with equal and continuous distributions to air, water and soil

compartments suggests that the vinyl chlorosilanes will distribute mainly to the air (ca. 48 %) and soil (ca. 47%) compartments, with minor distribution to water (ca. 5%) and negligible distribution to sediments (<0.1). Since the parent materials are not expected to be released to soil or water based on their uses and handling, a scenario of 100% emission to air is more realistic. When the vinyl chlorosilanes are released to air exclusively, the fugacity model predicts that 99.8% is reacted. The unreacted 0.2% remains in air (100%). The modeling results show that the environmental fate of the vinyl chlorosilanes is controlled by their high reactivity with water in all compartments. Level III fugacity modeling using equal loading rates of 1000 kg/h each for air, soil and water predicts that the hydrolysis products will distribute mainly to soil (c. 70-80 %), with a smaller fraction to water (ca. 20-27 %) and negligible amounts to sediment and air. Based on the more realistic scenario of 100% release to air, the model predicts that vinylmethylsilanediol and vinylsilanetriol will be distributed mainly in soil (ca. 93%) and water (ca. 7%). Fugacity modeling of HCl is not applicable. The calculated Henry's law constants for both vinyl chlorosilanes are not applicable due to their rapid hydrolysis.

The bioaccumulation potential of the vinyl chlorosilanes was not measured due to rapid hydrolysis. The estimated BCFs using the BCFBAF Program (v3.01) are 16.8 L/kg wet-wt for **VTCS** and 24.1 L/kg wet-wt for **VDCS**, indicating the vinyl chlorosilanes are not expected to bioaccumulate. For both the hydrolysis products, the estimated BCF is 3.2 L/kg wet-wt.

Acute aquatic toxicity data are not available for vinyl chlorosilanes. The vinyl chlorosilanes undergo rapid hydrolysis, which would occur during testing; therefore, exposure to parent chlorosilane is likely to be transient and observed toxicity would likely be due to its hydrolysis products, HCl and the respective silanol hydrolysis products. Data are available for the supporting substance, VTMS and the silanol, DMSD.

Fish

VTMS [*Brachydanio rerio*]	96 h LC50 >100 mg/L (nominal) [static]
DMSD [*Oncorhynchus mykiss*]	96 h LC50 >120 mg/L (measured) [static]
HCl [*Cyprinus carpio*]	96 h LC50 = 4.92 mg/L (pH 4.3) (measured; pH) [semi-static]

Invertebrate

VTMS [*Daphnia magna*]	48 h EC50 = 168.7 mg/L (nominal) [static]
DMSD [*Daphnia magna*]	48 h EC50 >117 mg/L (measured) [static]
HCl [*Daphnia magna*]	48 h EC50 = 0.492 mg/L (pH 5.3) (measured; pH) [semi-static]

Algae

VTMS [*Scenedesmus subspicatus*]	72 h ErC50; EbC50 >100 mg/L (nominal)
DMSD [*Pseudokirchneriella subcapitata*]	72 h ErC50, EbC50 > 118 mg/L (measured) [static]
HCl [Selenastrum capricornutum]	72 h ErC50 = 0.492 mg/L (pH 5.3) [static](measured; pH)

The hazard of hydrochloric acid for the environment is caused by the proton (pH) effect. For this reason the effect of hydrogen chloride on the organisms depends on the buffer capacity of the aquatic ecosystem. Also the variation in acute toxicity for aquatic organisms can be explained to a significant extent by the variation in buffer capacity of the test medium. For example, LC50 values of acute fish toxicity tests varied from 4.92 to 282 mg/L. The toxicity values to *Selenastrum capricornutum* 72h-EC50 is 0.780 mg/L at pH 5.1 for biomass, 0.492 mg/L at pH 5.3 for growth rate, and the 72h-NOEC is 0.097 mg/L at pH 6.0 for biomass and growth rate. The 48h-EC50 for *Daphnia magna* is 0.492 mg/L at pH 5.3 based on immobilization.

Based on the properties of the hydrolysis product, HCl, the vinyl chlorosilanes possess properties

indicating a hazard for the environment (acute toxicity to fish between 1 and 100 mg/L, acute toxicity to aquatic invertebrates and toxicity to algae < 1 mg/L). Toxic effects are expected primarily from the hydrolysis products (in particular hydrogen chloride, and depend on the buffering capacity of a particular aquatic environment. Therefore, the stated effect levels pertain to unbuffered systems and can be viewed as conservative). The vinyl chlorosilanes and their hydrolysis products are not expected to be readily biodegradable or to bioaccumulate. Adequate screening-level data are available to characterize the hazard for the environment for the purposes of the OECD Cooperative Chemicals Assessment Programme.

Exposure

The estimated annual production volumes for the category members are:

Substance	Estimated United States 2010 Production (metric tonnes)	Estimated European 2010 production (metric tonnes)	Estimated Japanese 2010 production (metric tonnes)
VDCS	454 – 4536	45 – 907	454 – 4536
VTCS	454 – 4536	0	0

100% of the vinyl chlorosilanes, by volume, are used as intermediates in the manufacture of commercial organosiloxanes. The vinyl chlorosilanes are reacted during use and lose their chemical identities.

The vinyl chlorosilanes are produced and processed in closed systems. There are no intentional releases to the environment from the manufacturing processes among the companies that are sponsoring this case. Many engineering controls are in place at all the companies sponsoring this case to prevent occupational exposure such as local and general ventilation, ventilation systems tied into scrubbers with nitrogen padding, ambient temperature, closed loop unloading and dry break connections. Employees involved in chlorosilane production and application are required to use personal protective equipment (PPE) such as a respirator with organic vapor cartridges, slicker suit, Viton (chemical resistant) gloves, and rubber boots. For any situation (e.g. equipment maintenance and repair) where potential exposure to chlorosilanes is expected, the use of acid resistant protective equipment, respiratory equipment and face shield is recommended because of their hazardous properties. Environmental exposure is not expected.

There are no consumer uses of the vinyl chlorosilanes.