July 2019

SULFUR DIOXIDE BASED CHEMICALS REACH CONSORTIUM

SDIOConsortium.com

Dear SIEF-member,

You are surely aware that the REACh regulation (EC 1907/2006) requires every SIEF to share the costs of registrations on a fair, transparent and non-discriminatory basis. The past years have shown that this apparently simple request is quite challenging to transfer in practice, especially to satisfy different parties with different opinions on the quite complex issue of REACh registrations. However, all SIEF members participating or not participating in the initial preparation and submission of dossiers for the REACH registration are required to pay an equal share of the costs that have arisen to register their substances.

REACH is an evolving system. With the initial Reach regulation, there were hardly any definitive instructions on how to share cost. Every lead registrant or consortium therefore more or less developed their own model of cost sharing. The situation changed with the EU Commissions implementing regulation (EU 2016/9), and fortunately now rather precise requirements on cost sharing need to be met.

The SDIOConsortium had revised the cost calculation scheme for its Letter of Access (LOA) in January 2018 according to the EU Commissions implementing regulation (EU 2016/9). The amendment of the cost sharing model includes a cost itemisation of all accrued cost based on the information requirement per tonnage band (REACH annexes VII, VIII, XI, and X), the allocation of cost items to the categories “data cost” and “administrative cost”, and the calculation of an individual cost share on a per substance basis that will apply for each registrant.

In addition to the costs listed in Annex II, members of the SDIOConsortium also bore expenses for participation in meetings incl. travel costs, working time for conference calls and email communications on important decisions concerning the compilation of dossiers. These company individual expenses and efforts are NOT included in the calculation of the LOA price. As a consequence, this time and effort has not been allocated to that any SIEF member purchasing an LOA over the past years, also applying to the future.

The first **Reimbursement Mechanism Exercise** was finalised in June 2019. The cost price of the LOA for your company as regards to each substance was assessed. The Reimbursement Mechanism Exercise takes into account the number of registrants for a substance in a particular tonnage band and the initial payment made by each LOA purchaser and SDIOC member respectively.

Based on the reimbursement calculation we will assess the actual LOA price for your individual request. The LOA Payment made by your company will be taken into account and will be offset against the actual cost for your individual registration in the next reimbursement exercise. Depending on whether the LOA cost price exceeds or comes within your LOA Payment each SIEF member will receive a credit note or an invoice for additional payment.

Each SIEF member shall continue to benefit from the rights of access to data needed to register the substance/s under REACH as long as relevant invoice(s) are fully paid by relevant deadlines.

Cost calculation scheme:

A cost itemisation was performed to comply with the requirements of the EU commissions implementing regulation (2016/9). All cost items from founding of the consortium in January 2009 until 31.05.2019 were itemised and then categorised into **data costs** and **administrative costs** based on ECHA guidance[1] (see Annex II). Income from terminated membership was deducted from the overall cost so that the complete

[1] ECHA guidance on data sharing Version 3.1, January 2017, Annex 3

SIEF benefits from the cost share already borne by former members. The reimbursement exercise included a budget for ongoing and upcoming scientific effort in 2019/20.

Cost item	**EUR**	**Future cost included**
Total cost	3,348.764.62	
Thereof administrative cost	884,702.21	111,000.00
Thereof data cost (read across)	1,217,738,50	417,000.00
Thereof data cost (substance specific)	1,089,221.48	

Administrative costs are allocated to all substances and then shared equally per registration. The result corresponds to amount (a).

Data costs are divided by the number of substances that require this information. These substance-specific costs are allocated per tonnage band and then divided by the number of registrants in that tonnage band. The result relate to amount (b).

Since SDIOC makes use of an extensive read-across concept and weight of evidence approach (see Annex I), we need to apply a system that gives credit to the different information requirements in each tonnage band. Data cost of information that is used in all dossiers is allocated to all substances and a factor system comparable to ECHA guidance[2] is applied. The percentage share per tonnage band reflects the data requirements of the sulfite substances that are comparably higher in the lower tonnage bands.

Each registrant is allocated a certain number of points per tonnage band. The cost item in questions is then divided by the total number of points of all registrations. Each registrant pays a proportionate share of the cost based on the following factors:

- REACH Annex VII: all registrants factor 0.75 (12 %)
- REACH Annex VIII: all w tpy 10-100 factor 1.25 (20 %)
- REACH Annex IX: all w tpy 100-1000 factor 2.00 (32 %)
- REACH Annex X: all w tpy > 1000 factor 2.25 (36 %)

The result is represented by amount (c). The sum of amounts (a), (b), and (c) is the actual cost share for each registration.

Please note that in earlier calculations, SDIOC provided an LOA that was valid for all Substances from the substance portfolio. Since this approach is not in accordance with the implementing regulation EU 2016/9, SDIOC had to adapt the model to share the cost on a per substance basis. Some substances have a larger SIEF than others, meaning more registrants share the cost of one substance while in other cases only few registrants share the cost of another substance. This leads to different cost shares for each substance.

IMPORTANT: Please note that our REACh dossiers make reference to some studies for which SDIOC does not hold ownership. SDIOC itself is therefore not authorised to pass on the right to refer to these studies for REACH registrations. If you purchase a Letter of Access, either for a full dossier or for an intermediate registration, you have to acquire the right to refer to those “Third party studies” that you may need for your REACH registration from the respective data owner. SDIOC is not liable for a reimbursement of cost out of these studies. SDIOC members also purchased the right to use these studies and the cost item is not part of the cost itemisation for non-consortium members.

Despite the latest REACH registration deadline having expired, the responsibility for the dossiers continues to exist (see Annex III) and will also continue in the future. SDIOConsortium and its lead registrants are continuously working on the dossiers and the SIEF is still growing as further requests for LOA purchases are coming in. The LOA cost share will be re-calculated regularly based on the actual costs and the actual number of SIEF-members i. E. future LOA-purchases will be considered accordingly. The reimbursement

[2] Compare to example 9 in ECHA guidance

exercise will be repeated annually from now onward. The next reimbursement exercise will occur in 2020 and the SIEF will be informed accordingly. Please make sure to keep SDIOConsortium up to date on your contact information.

Further steps:

In case your company wishes to purchase a Letter of Access, please proceed as follows:

- Please refer to our homepage and download the required Letter of access document. You will find the documents here: http://www.sdioconsortium.com/loa.html
- Read the document thoroughly.
- Consider possible information requirements out of Annex 1 of the LoA agreement (if so contact the data owner and negotiate access)
- Fill in the relevant information in the LoA agreement; company information and substance identification (for the latter please refer to the substance list below);
- In case you act as an ONLY REPRESENTATIVE, you may use the same template, but please fill in the respective space in the head of the LOA
- Print two copies of the duly completed Letter of access.
- Sign both copies by a person duly authorised to represent the company.
- Send both copies via courier to the following address:

SDIOC EWIV, Raffaelstraße 4, 30177 Hannover, Germany

You will receive:

1. The invoice for the LOA incl. your individual SDIOC-reference number.
2. The countersigned copy of the Letter of Access incl. your individual SDIOC-reference number.
3. After full payment has been received, SDIOC will send the joint submission information and a pdf file of the Dossier incl. CSR via E-Mail to the buyer's E-Mail-address as stated in the LoA as soon as possible but within two weeks at the latest.

Safety data sheet and guidance on safe use have to be submitted by each SIEF member individually and are not part of the LOA.

In case you have any further queries concerning the Letter of Access, please contact the SDIOC headquarters:

SDIOC EWIV
REACH Management
Raffaelstr. 4, 30177 Hannover, Germany
Phone: +49 (511) 898389-0
Web: www.sdioconsortium.com
Email:sief@sdioconsortium.com

Annex I: Read-across between sulfur dioxide based chemicals

In order to minimise the overall experimental costs for studies and due to animal welfare, SDIOC has developed a comprehensive read-across concept which is encouraged by the REACH legislation and thus highly preferred.

Common assessment elements for category approaches

The common assessment elements (AE) are introduced below following the principles laid down in the ECHA Read-Across Assessment Framework.

HH / ENV - Substance characterisation / Characterisation of source and target substances

The structural similarity is based on the fact that the common (eco)toxicological moiety of concern is the sulfite/hydrogensulfite anion which is either present in the substance as such or is formed as degradation product of unstable substance analogues (e.g. thiosulfates, dithionites) under environmental or physiological conditions.

Within this category, because of the structural similarity, the specified toxicological and ecotoxicological properties are similar.

The similarity rules specified in Annex XI, Section 1.5 of the REACH Regulation in the REACH Guidance on IR & CSA, Chapter R.6 of apply and the category ”sulfites/thiosulfates/ dithionite” is formed on the following basis:

The basis for the read-across concept for this project is the equilibrium between sulfites, hydrogensulfites, and metabisulfites in aqueous solutions depending on pH value which is clearly described in published literature and summarised in the following equations:[3,4]

$SO_2 + H_2O$ <->`H_2SO_3´ H_2SO_3<->$H^+ + HSO_3^-$ <-> $2H^+ + SO_3^{2-}$ $2HSO_3^-$ <->$H_2O + S_2O_5^{2-}$

As the nature of the cation should make no significant difference in this case concerning toxicity and solubility (all compounds are very soluble in water), only the chemical and biological properties of the anion are considered relevant. Based on the described equilibrium correlations, we propose unrestricted read-across between the groups of sulfites, hydrogensulfites and metabisulfites. Additionally, it is known that sodium dithionite disproportionates in water to form sodium hydrogen sulfite and sodium thiosulfate (equation II) so that this substance can also be added to the read-across concept.[3,4]

It is expected for this case that the substance is not stable enough under physiological conditions to fulfil the requirements of study guidelines and so the products of decomposition have to be considered.

$2\ S_2O_4^{2-} + H_2O \rightarrow 2HSO_3^- + S_2O_3^{2-}$

Not completely included in this read-across concept is the substance class of thiosulfates. Although thiosulfates may also disproportionate in aqueous solution to form polythionic acids and SO2(HSO3-), the required conditions are somewhat different (more acidic) and are therefore not strictly comparable with physiological conditions, except for the case of oral application where read-across should be considered unrestricted due to the strongly acidic conditions in the stomach:

$HS_2O_3^- + H_2S_2O_3 \rightarrow HS_3O_3^- + SO_2 + H_2O$

[3] Hollemann Wiberg, Lehrbuch der Anorganischen Chemie, 101.Auflage

[4] Handbook of Chemistry and Physics, Ed. Lide, DR, 88thedition, CRC Press

Nevertheless, read-across for all other routes (dermal, inhalation) should also be considered. The proposed read-across concept only applies to toxicological and ecotoxicological/environmental fate endpoints.

Chemical similarity and environmental fate

Sulfur-containing oxyacids such as sulfurous, dithionous and thiosulfric acid and their respective salts dissociate upon contact with water releasing their respective cations and anions. The majority of the sulfur-containing oxyacids are bibasic and have a similar stoichiometric composition $H_2S_nO_m$.

Sulfites/ hydrogensulfites/ metabisulfites:

Sulfurous acid is an acid of weak to medium strength. Sulfite (SO_3^{2-}), the respective anion and relevant species under most environmental conditions, is in solution in equilibrium with hydrogensulfite (HSO_3^{2-}) and metabisulfite ($S_2O_5^{2-}$), the latter being a hybrid of dithionite ($S_2O_4^{2-}$) and dithionate ($S_2O_6^{2-}$). All sulfite, hydrogensulfite and metabisulfite substances are highly soluble in water. The substances readily dissociate and form an equilibrium that depends on solution pH (Holleman & Wiberg, 1995). The following transformation reactions may be anticipated:

$SO_2 + H_2O \rightleftharpoons H_2SO_3$

$H_2SO_3 + H_2O \rightleftharpoons HSO_3^- + H_3O^+$ pka_1: 1.85

$HSO_3^- + H_2O \rightleftharpoons SO_3^2 + H_3O^+$ pka_2: 7.20

$2\ HSO_3^- \rightleftharpoons H_2O + S_2O_5^{2-}$

In acidic solutions, sulfites and hydrogen sulfites may release SO_2 but this is not likely to occur under e.g. normal natural environmental conditions.

$SO_3^{2-} + 2\ H_3O^+ \rightleftharpoons SO_2 + 3\ H_2O$

Under oxidising conditions, e.g., in surface waters, sulfite is rapidly oxidized to sulfate catalytically by (air) oxygen or by microbial action. A half-life of 77 hour was measured in deionized water, already suggesting substantial abiotic degradation.

$2\ SO_3^{2-} + O_2 \rightarrow 2\ SO_4^{2-}$ (in presence of oxygen)

The reaction is accompanied with consumption of dissolved oxygen. Thus, observed toxic effects to aquatic organisms may be indirect effects, i.e. caused by lack of oxygen.

Dithionite:

Dithionous acid and salts are unstable in solution, rapidly hydrolyse and are ultimately slowly converted to sulfate (SO_4^{2-}) and SO_2 depending on solution pH. The respective anion ($S_2O_4^{2-}$) acts as strong reducing agent[5]. The following principal reactions occur in aqueous media (Münchow, 1992) depending on the solution pH:

$H_2S_2O_4 + H_2O \rightleftharpoons HS_2O_4^- + H_3O^+$ pka_1: 0.35

$HS_2O_4^- + H_2O \rightleftharpoons S_2O_4^{2-} + H_3O^+$ pka_2: 2.45

An aqueous solution of dithionite is acidic and dithionite disproportionates rapidly to form to thiosulfate and bisulfite due to the weak S-S binding. The reaction rate increases with increasing acidity and temperature.

$2\ S_2O_4^{2-} + H_2O \rightleftharpoons S_2O_3^{2-} + 2\ HSO_3^-$

[5] Housecroft, C. and Sharpe, A.G. (2005): Inorganic Chemistry, Second Edition.

Under aerobic conditions, dithionite decomposes to bisulfate and bisulfite, i.e. oxidises with a significant oxygen depletion to finally form sulfate as final oxidation/decomposition product. This environmental behaviour is also observed in soils, where these anions are unstable and do not persist (Lindsay, 1979).

$S_2O_4^{2-} + O_2 + H_2O \rightleftharpoons HSO_4^- + HSO_3^-$

$S_2O_4^{2-} + O_2 + 2\ OH^- \rightleftharpoons SO_3^{2-} + SO_4^{2-} + H_2O$ (in the presence of oxygen)

Bisulfate and bisulfite in turn decrease the solution pH and therewith accelerate the reaction. Sulfur dioxide is only formed under strongly acidic conditions.

$2\ H_2S_2O_4 \rightleftharpoons 3\ SO_2 + S + 2\ H_2O$

$3\ H_2S_2O_4 \rightleftharpoons 5\ SO_2 + H_2S + 2\ H_2O$

In a basic solution (pH 9–11), dithionites are more stable and decompose slowly (about 1% in an hour). Dithionites have strong reducing properties and decompose to sulfurous acid and sulfide.

$3\ S_2O_4^{2-} + 6\ OH^- \rightleftharpoons 5\ SO_3^{2-} + S^{2-} + 3H_2O$

Thiosulfate:

The structure of the thiosulfate ion ($S_2O_3^{2-}$) is comparable to the sulfate ion with one oxygen atom replaced by a sulfur atom. It is considered to be metastable and has only moderate reducing properties (Cotton et al., 1999). Thus, thiosulfate is an oxyanion of sulfur, is the respective anion of the strong thiosulfuric acid and the only species relevant upon dissolution in an aqueous medium under environmental conditions:

$H_2S_2O_3 + H_2O \rightleftharpoons HS_2O_3^- + H_3O^+$ pka_1: 0.6

$HS_2O_3^- + H_2O \rightleftharpoons S_2O_3^{2-} + H_3O^+$ pka_2: 1.74

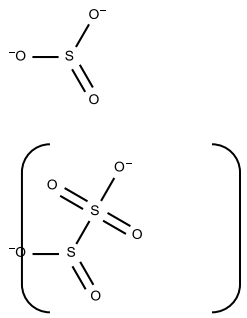
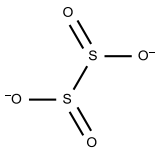
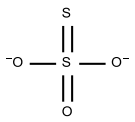
Thiosulfates occur naturally and are produced by certain biochemical processes. Thiosulfates are stable only in neutral or alkaline solutions, but not in acidic (physiological) solutions, due to decomposition to sulfite and sulfur, the sulfite being dehydrated to SO_2:

$S_2O_3^{2-}(aq) \rightleftharpoons SO_3^{2-}(aq) + S(s)$

$S_2O_3^{2-}(aq) + 2\ H_3O^+(aq) \rightleftharpoons SO_2(g) + S(s) + H_2O$

Thus, in contrast to sulfite and dithionite, the disproportion of thiosulfates occurs only under acid but not under alkaline conditions. Under normal environmental conditions, a break down to sulfite and a subsequent oxidation to sulfate may be anticipated.

Table 1: Comparison of chemical similarity.

	Sulfite/Disulfite	**Dithionite**	**Thiosulfate**
Structure			
	$S_nO_m^{2-}$ (n=1 or 2; m=3 or 5)	$S_nO_m^{2-}$ (n=2; m=4)	$S_nO_m^{2-}$ (n=2; m=3)
Sulfur content [%]	40.1 (44.5)	50.1	57.2
Sulfite equivalent	1.0/2.0	1.2	1.4
Solubility	Very soluble (>10000 mg/L)	Very soluble (>10000 mg/L)	Very soluble (>10000 mg/L)

pKa	pKa_1: 1.85 pKa_2: 7.20	pKa_1: 0.35 pKa_2: 2.45	pKa_1: 0.6 pKa_2: 1.74
Bioaccumulation	Not expected	Not expected	Not expected

Conclusion: Thiosulfates, sulfites and dithionites are sulfur and oxygen containing compounds that may reasonably be considered chemically unstable under most environmental conditions, are transformed into other sulfur species and become ultimately part of the sulfur cycle.

Upon contact with water, salts of sulfur oxyacids dissociate into sulfur oxyacid anions and the respective counterions. The subsequent environmental transformation reactions, including oxidation and reduction, differ depending on the anionic species, but ultimately follow a similar fate as part of the sulfur cycle resulting in sulfites and sulfates - indistinguishable from natural sulfur reservoirs. The ubiquitous presence of cations such as iron, copper or manganese in the environment further accelerate these oxidation reductions. Thus, the environmental fate and ultimate transformation and its products depend predominantly on the environmental conditions that thiosulfates, sulfites and dithionites are released into.

Limitation: read-across is only appropriate for HH and ENV sections but not for substance-specific physico-chemical data.

Annex II: The payments towards the consortium are based on the following cost allocation scheme:

A) Cost allocation scheme for intermediates < 1000 tpy:

IM < 1000tpy:	**calculation includes**	**calculation does not include**
Data costs	Share of costs for data gap analysis, literature search, IUCLID file preparation and updates, PNEC/ DNEL derivation, questionnaire survey. Share of costs for relevant studies, i.e. phys-chem.	Costs for exposure assessments (consumer, occupational, indirect, environmental and regional environmental), risk characterisation and generation of CSA/ CSR. All other human health studies, long term toxicity to fish (fish early life stage); Studies purchased by third parties. SDIOC does not have the right to grant access to these studies. Negotiation required with data owner.
Administrative costs	Share of total costs for REACH management, technical support and generic cost.	

B) Cost allocation scheme for substances at 1-10 tpy or intermediates > 1000 tpy:

The effort for compilation of our dossiers for substances in the tonnage band 1-10 tpy and intermediates > 1000 tpy is very similar. Thus, we have calculated one price for the LOA of such registrations.

1-10 tpy or IM < 1000 tpy:	**calculation includes**	**calculation does not include**
Data costs	Share of costs for data gap analysis, literature search,	Costs for exposure assessments (consumer, occupational, indirect,

	IUCLID file preparation and updates, PNEC/ DNEL derivation, questionnaire survey. Share of costs for relevant studies, i.e. phys-chem, human health (skin sensitisation)	environmental and regional environmental), risk characterisation and generation of CSA/ CSR. all other human health studies, long term toxicity to fish (fish early life stage); Studies purchased by third parties. SDIOC does not have the right to grant access to these studies. Negotiation required with data owner.
Administrative costs	Share of total costs for REACH management, technical support and generic cost.	

C) Cost allocation scheme for substances at 10-100 tpy:

10-100 tpy:	**calculation includes**	**calculation does not include**
Data costs	Share of costs for data gap analysis, literature search, IUCLID file preparation and updates, PNEC/ DNEL derivation, questionnaire survey. Costs for exposure assessments (consumer, occupational, indirect, environmental and regional environmental), risk characterisation and generation of CSA/ CSR. Share of costs for relevant studies, i.e. phys-chem, all human health studies, partly environmental studies	Long term toxicity to fish (fish early life stage); Studies purchased by third parties. SDIOC does not have the right to grant access to these studies. Negotiation required with data owner.
Administrative costs	Share of total costs for REACH management, technical support and generic cost.	

D) Cost allocation scheme for substances at 100-1000 tpy or >1000 tpy:

The effort for compilation of our dossiers and study input for substances in the tonnage band 100-1000 tpy and >1000 tpy is highly similar. Thus, we calculated the same price for the LOA of such registrations.

100-1000 tpy and > 1000 tpy:	**calculation includes share of**	**calculation does not include**
Data costs	Costs for data gap analysis, literature search, IUCLID file preparation and updates, PNEC/ DNEL derivation, questionnaire survey, exposure assessments (consumer, occupational, indirect, environmental and regional environmental), risk characterisation and generation of CSA/ CSR. Costs for <u>all</u> studies incl. monitoring, i.e. phys-chem, all human health studies, and environmental studies	Studies purchased by third parties. SDIOC does not have the right to grant access to these studies. Negotiation required with data owner.
Administrative costs	Share of total costs for REACH management, technical support and generic cost.	

Annex III: Scientific budget:

The REACH regulation in Article 22 ("further duties of registrants") explicitly foresees the requirement to update registration dossiers under certain circumstances. The respective text passages of the regulation are as follows:

1. Following registration, a registrant shall be responsible on his own initiative for updating his registration without undue delay with relevant new information and submitting it to the Agency in the following cases:

(a) any change in his status, such as being a manufacturer, an importer or a producer of articles, or in his identity, such as his name or address;

(b) any change in the composition of the substance as given in Section 2 of Annex VI;

(c) changes in the annual or total quantities manufactured or imported by him or in the quantities of substances present in articles produced or imported by him if these result in a change of tonnage band, including cessation of manufacture or import;

(d) new identified uses and new uses advised against as in Section 3.7 of Annex VI for which the substance is manufactured or imported;

(e) new knowledge of the risks of the substance to human health and/or the environment of which he may reasonably be expected to have become aware which leads to changes in the safety data sheet or the chemical safety report;

(f) any change in the classification and labelling of the substance;

(g) any update or amendment of the chemical safety report or Section 5 of Annex VI;

(h) the registrant identifies the need to perform a test listed in Annex IX or Annex X, in which cases a testing proposal shall be developed;

(i) any change in the access granted to information in the registration.

The Agency shall communicate this information to the competent authority of the relevant Member State.

2. A registrant shall submit to the Agency an update of the registration containing the information required by the decision made in accordance with Articles 40, 41 or 46 or take into account a decision made in accordance with Articles 60 and 73, within the deadline specified in that decision. The Agency shall notify the competent authority of the relevant Member State that the information is available on its database.

3. The Agency shall undertake a completeness check according to Article 20(2) first and second subparagraphs of each updated registration. In cases where the update is in accordance with Article 12(2) and with paragraph 1(c) of this Article then the Agency shall check the completeness of the information supplied by the registrant and Article 20(2) shall apply adapted as necessary.

4. In cases covered by Articles 11 or 19, each registrant shall submit separately the information specified in paragraph 1(c) of this Article.

5. An update shall be accompanied by the relevant part of the fee required in accordance with Title IX.

This means that we continuously need to make sure that our dossiers are up-to-date. In this context, our budget for 2019 contains the item "dossier updates" which was not planned for in 2018. In 2019, we foresee the need for a complete update of the dossiers including the use- and exposure- sections. The work for those updates already started in 2018.

In this context, we also decided to closely monitor the current regulatory developments around sulfur dioxide which is the chemical basis for all our SDIOC substances. The potential additional classification for e.g. toxicity to reproduction which is proposed by the MS Germany will have (if agreed on) severe impacts on the substance SO_2 itself as well as potentially also on our sulfites. Hence, the intention is to proactively update the sulfite dossiers with information that is given in the CalEPA report for sulfur dioxide. Since this information will be used by the SO2 consortium as well, we propose to share the costs accordingly. The budget sum for this effort is may therefore be considered as preliminary and worst case.

In addition to the continuous work on the dossier updates we planned to install a hedge budget for additional ECHA requests (e.g. compliance checks).