ANALYSIS OF ALTERNATIVES

Non-confidential report

Legal name of applicant(s): DEZA, a.s.

Submitted by: DEZA, a.s.

Substance: Dibutyl phthalate

Use title: Use as an absorption solvent in a closed system in the manufacture of maleic anhydride (MA)

Use number: 1
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1 SUMMARY

1.1 Background to this Analysis of Alternatives

The substance of concern is dibutyl phthalate (hereafter referred to as DBP), EC No 201-557-4, CAS No 84-74-2, and its use for which Authorisation is sought is as a solvent in the manufacture of maleic anhydride (MA) in a closed system.

This Analysis of Alternatives (AoA) constitutes part of the Application for Authorisation submitted by DEZA, a.s. (hereafter referred to as “the applicant” or “DEZA”), the Czech-based manufacturer of the substance. By way of context, Huntsman Petrochemical LLC (hereafter referred to as Huntsman) is the licensor of a MA manufacturing technology that requires the use of DBP. Sasol-Huntsman is a joint venture between Huntsman and Sasol Solvents Germany GmbH (hereafter referred to as Sasol Solvents). The collection of information and scientific analysis for the preparation of this AoA was conducted by an independent third party to ensure appropriate handling of confidential business information in accordance with EU Competition Law.

DBP is used as an absorption solvent in the manufacture of MA by Sasol-Huntsman for the absorption of MA from the off-gas generated by the reaction of n-butane and air, under a licence to use the Huntsman technology (see a more detailed description in Section 2.1.2). Manufacture of MA takes place at Moers in Germany on a plant situated within a large site operated by Sasol Solvents. DBP does not itself participate in the reactions that lead to the formation of MA; it only acts as a processing agent within a closed system.

MA is a versatile and widely used industrial intermediate chemical. Major applications for MA include the manufacture of unsaturated polyester resins (UPR), which in turn are used in the production of lighter, stronger, fibreglass composites for boats, cars, construction, wind turbine blades and many other products. MA is a key ingredient in the manufacture of co-polymers that enable the use of more sustainable raw materials, for example, to bind wood fibres into plastic, to inhibit corrosion, create protective coatings for wire and to repel water in sunscreens. Through conversion to fumaric and malic acids, MA is a vital component of gelling agents, flavour enhancers and food preservatives. It is also essential to the production of elastane (Spandex) fibres, artificial sweeteners, paper-sizing, water treatments, hardeners for epoxy curing, hairsprays, pharmaceuticals, agricultural chemicals and motor oil additives. More detail on the downstream applications of MA is given in the SEA (Section 1.1.4.4). MA is used to produce many consumer products, but there are no consumer products containing MA. MA will not long remain as free MA outside industrial use as the anhydride is readily hydrolysed to maleic acid, due to humidity in the air. Thus, it is by nature that free MA cannot exist in consumer products.

Huntsman’s technology for MA manufacture has safety, economic, and environmental advantages over competing technologies (see detailed descriptions in Sections 4.1.2.2 and 4.2.2.2):

- as a direct result of the fact that the consumption of steam within the Huntsman MA manufacturing process is lower than within competing technologies, the process is a net energy producer. This allows the export of energy generated from MA manufacture to neighbouring plants;
- it produces lower amounts of carbon emissions than competing technologies;
- it consumes a lower amount of water and produces lower amounts of wastewater compared to competing technologies;
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- it affords improved control of fouling of the process equipment, through better control of the formation of by-products and polymeric tars compared to competing technologies, thus affording greater operating reliability and reduced maintenance requirements; and

- it is currently the state-of-the-art technology for the manufacture of MA, with ca. 50% of global MA manufactured coming from plants holding a Huntsman technology licence, as of early 2013 (see Table 4.4). World-leading chemical producers have consistently selected Huntsman’s MA technology since the 1990s and no world-scale MA plant has been constructed anywhere between the mid-1990s and the time of writing this AoA (beginning of 2013) using any technology other than Huntsman’s (see Section 4.1.2.2 under the heading Market success as a measure of technical suitability). Energy efficiency and raw material utilisation efficiency are consistently noted as key decision criteria by licensing companies in selecting Huntsman’s MA manufacturing technology.

In this context, DBP is a critical element in the commercially successful and environmentally attractive implementation of the Huntsman technology. The Authorisation is applied for so that Huntsman’s technology will continue to be used in the EU and is based on the demonstration of adequate control of risks to workers from exposure to DBP at the Moers plant.

1.2 Identification of suitable alternatives

For the assessment of alternative substances, nine technical comparison criteria have been identified (see Section 2.2.2); meeting these would allow the successful replacement of DBP within the Huntsman MA manufacturing process. On the other hand, for alternative techniques, four criteria have been identified (see Section 2.2.3); meeting these would allow the commercially viable replacement of the Huntsman MA manufacturing process with an alternative one.

Extensive research on the identification of suitable absorption solvents for MA has been undertaken by researchers over recent decades (see Section 3.2.1.1). Huntsman has screened more than 13,000 substances for technical and economic feasibility without identifying any suitable alternative to DBP (see Section 3.2.1.2). When the potential substitutes were assessed against the technical comparison criteria, they all demonstrated inferior technical performance in one or more attributes. On-going research and development (R&D) has confirmed that the choice of DBP as the absorption solvent in Huntsman’s technology is the most beneficial from a technical perspective. Moreover, the assessment of the economic feasibility of a selection of potential alternatives confirms that the price of potential alternatives is considerably higher than the price of DBP. As a result, none of the alternative substances that are known to Huntsman (and by inference to the applicant) can replace DBP within the existing Huntsman technology (see Section 3.2.1.4 for a discussion on potential alternatives that have not found commercial applications).

In light of the technical shortcomings and poor economics of unproven alternative substances, the focus of this AoA has been on alternatives known to be in commercial practice.

Two commercially proven alternatives have been identified in the preparation of this AoA:

(a) a solvent-based technology for the recovery of MA: the so-called ALMA technology uses as an absorption solvent the substance diisobutyl hexahydrophthalate (also known as DIBE, EC Number: 275-069-5, CAS Number: 70969-58-3) (see description of the technology in Section 4.1.2.2 and the identity of DIBE in Section 4.1.1), and

(b) a water-based technology for the recovery of MA: the recovery of MA using a combination of water and xylene (see description in Section 4.2.1.1).
A third alternative has also been considered in this Analysis, the non-use and non-replacement of DBP (see Section 4.3). This is a purely theoretical alternative, as this would result in the closure of the Moers MA plant since the manufacture of MA necessitates the absorption of the product from the off-gas of the reaction of n-butane and air. This theoretical alternative has been considered primarily as a ‘benchmark’ of the economic feasibility and commercial realism of the only other demonstrated alternatives (of which there are two).

1.3 Suitability of commercially proven alternatives

1.3.1 Reduction of overall risks

The CSR accompanying this Application for Authorisation demonstrates that exposure of workers to DBP at the Sasol-Huntsman plant is kept well below the effect threshold. Therefore, the risks associated with the endpoint of concern (reproductive toxicity) are adequately controlled. Consequently, the use of any alternative (whether commercially proven or not) would not result in a discernible benefit to workers’ health. In any case, the alternatives raise concerns of their own: for DIBE there are grounds for concern with regard to its developmental and/or endocrine profile (including with respect to its ability to interact with the androgen receptor), and for its environmental toxicity. Based on publicly available information and to the applicant’s knowledge, DIBE has been investigated to a far lesser extent than DBP (see Section 4.1.3.2).

For the water-based recovery technology, a considerable additional release of greenhouse gases (CO$_2$) would be expected due to the increased energy demand of the alternative MA manufacturing process and the generation of increased amounts of wastewater, which would need to be incinerated (see Section 4.2.3.2 which estimates that more than 42.2 ktonnes of additional CO$_2$ would be released each year if the Moers plant converted from Huntsman’s technology to the water-based recovery technology).

For both alternatives, an additional release of 170 ktonnes of CO$_2$ would occur during the conversion of the plant due to the stoppage of steam generation at the MA plant and the consequent increase of natural gas consumption at the Sasol Solvents power plant over the two years of the conversion work.

1.3.2 Technical feasibility of alternatives

DEZA cannot manufacture or supply either of the two commercially proven alternatives. DEZA does not currently have access to commercially viable hydrogenation technology which would allow it to manufacture a hydrophthalates such as DIBE. Hydrogenation methods are either patented by third parties or pose technical challenges that are difficult to overcome. On the other hand, the water-based extraction of MA is licensed by companies other than DEZA. As a result, these two alternatives cannot be considered to be technically feasible for the applicant.

From the perspective of Sasol-Huntsman, the assessment of technical feasibility of the identified potential alternatives clearly demonstrates that a switch to either of the two commercially proven alternatives would present significant technical challenges.

Implementation of the ALMA technology that uses DIBE as the absorption solvent would require a costly conversion of the Moers plant. This is estimated to require more than 2 years for completion,
during which the plant would have to shut down (see Section 4.1.4.2). The economic consequences of a shutdown of more than 2 years would lead to the permanent closure of the Moers plant. It is important to note that the capacity of the Moers plant was only recently (2011) expanded, from 60 ktonnes MA per year to 105 ktonnes per year, on the basis of its current licence to use the Huntsman technology. It is now the largest MA manufacturing plant in the EU. A major conversion of the plant into a new technology cannot be justified, either on strategic or commercial/economic grounds. Moreover, the physicochemical properties of DIBE would adversely affect the performance of the MA manufacturing process (see Section 4.1.2.2):

(a) the poorer solubility of fumaric acid in DIBE would result in higher solvent consumption and increased solids deposition with consequent equipment fouling;

(b) the very small difference between the density of DIBE and the density of water would increase losses of DIBE thus increasing cost. It would also generate an additional waste stream and increasing the probability of an industrial accident due to contamination of DIBE with caustic (which is used for washes in the ALMA technology) – MA reacts violently with caustic; and

(c) the lower flash point of DIBE, compared to DBP, would increase the likelihood of fire within the absorber column.

Finally, to the applicant’s knowledge, the ALMA technology has not been selected for use in a new plant since the mid-1990s.

Similarly, implementation of a water-based technology at Moers would require an even more costly conversion of the Moers plant over a period of time similar to that described for the conversion to ALMA/DIBE (see Section 4.2.4.2). As above, the economic consequences of a shutdown of more than 2 years would lead to the permanent closure of the Moers plant. Even if plant conversion could be undertaken, the new technology would suffer from lower MA recovery efficiency, higher energy consumption, the generation of wastewater that would need to be incinerated, increased fouling and potentially poorer MA product quality, due to the presence of xylene impurities in the MA product (see Section 4.2.2.2). In should be noted that the water/xylene-based technology (which was considered state-of-the art in the 1970s) was abandoned by Condea Chemie GmbH (hereafter referred to as Condea) the predecessor to Sasol Solvents in favour of the more technically and economically advantageous Huntsman technology. In the last 20 years, many European MA producers have shut down MA plants utilising the water/xylene technology, notably with benzene as the feedstock (see SEA, Section 2.2.1.8), and the idea of Sasol-Huntsman returning to such a technology would be inconceivable and impossible to justify, either on strategic or commercial/economic grounds.

1.3.3 Economic feasibility of alternatives

DEZA cannot currently manufacture or supply either of the two commercially proven alternatives. Moreover, the lack of technical and economic feasibility of these alternatives for the Downstream User reinforces the conclusion that neither of these two alternatives can be considered to economically feasible for the applicant.

From the perspective of Sasol-Huntsman, the assessment of the economic feasibility of the two commercially proven alternatives has further confirmed their shortcomings in comparison to DBP.

1 If there were a realistic prospect for commercially viable operation after the conversion of the plant, up to a further 18 preceding (operational) months would be required for obtaining agreement of the company owners/shareholders, drawing up of engineering plans, undertaking cost estimation and raising capital.
The key cost element in both cases would be the very high cost of plant modifications: for DIBE, the cost of plant modification has been estimated to exceed €150 million (see Section 4.1.4.2 and Part 3 of the Confidential Annex to AoA) while for water-based recovery, it would exceed €170 million (see Section 4.2.4.2 and Part 5 of the Confidential Annex to AoA). When additional cost elements are considered (see same Sections for DIBE and for water-based recovery for a comprehensive analysis of the various cost elements), the Net Present Value of the cost of conversion to either DIBE-based absorption or water-based recovery would exceed €403 million and €539 million respectively (these values have been based on lost turnover estimates and are calculated over 20 years at a 4% discount rate). These figures include a cost component allocated to Sasol-Huntsman and a smaller one allocated to Sasol Solvents (the latter associated with an increase in energy costs for the on-site power plant). These costs are so substantially high that it can only be assumed to result in bankruptcy and the closure of the Sasol-Huntsman plant, thus making it completely unrealistic to consider converting to either of the alternatives.

If, for the sake of discussion, it were to be assumed that conversion to either alternative would be implemented, the Sasol-Huntsman plant would face further challenges:

- inactivity of the largest EU manufacturer of MA for more than two years would not only seriously upset the EU market, but would also drive customers (users of MA) to the hands of competitors, out of business, or out of the EU. The theoretical conversion to a higher cost solvent (DIBE, see Section 4.1.4.2) or a less efficient production technology (water/xylene-based recovery, see Sections 4.2.2.2 and 4.2.4.2), would result in Sasol-Huntsman’s MA production costs increasing upon restarting operations at the Moers plant. This would further undermine Sasol-Huntsman’s competitiveness and would hinder the return of past customers back to Sasol-Huntsman’s MA product. Realistically, removing 35% of the capacity currently supplying the European MA market (which is regional in nature) would have a significant effect on users both in terms of the price of the product, as well as their ability to source sufficient supply of the product to meet their requirements (also see SEA, Section 2.2.1.3). This is because there is insufficient idle MA capacity in the EU to fill the gap created by Sasol-Huntsman’s loss; and

- Sasol-Huntsman is currently servicing loans associated with a recent capacity expansion (details regarding outstanding loans are given Section 4.1.4.2 under the heading Cost element 3: Cost of plant conversion). The need for another round of investment and conversion at the Moers plant would require another large loan. Beyond the certain reluctance of banks to finance such a fundamental change to the operational parameters of the plant, the need to repay the new loan would add further upward pressure to the price of Sasol-Huntsman’s MA product, thus further impacting on the company’s competitiveness.

The combination of loan repayments, selling at a less competitive price and the need to re-build their customer base would lead to such difficulties in the short term as to render any thought of converting the plant, and hoping for commercial success completely unrealistic. Overall, even if the conversion of the Sasol-Huntsman MA plant could be financed and technically achievable, there would be no justification from a commercial perspective for undergoing such a fundamental change without a minimum guarantee of commercial success – even more so when considering that risks to workers’ health from exposure to DBP are already adequately controlled.

1.4 Availability of commercially proven alternatives

In terms of availability, DIBE’s market availability is highly uncertain. It is not available in the portfolio of the manufacturer of DBP and the company does not currently have, and cannot foresee, acquiring access to the relevant hydrogenation technology that would allow its manufacture (see
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Section 4.1.5). Furthermore, DEZA does not have access to the water-based technology as it is completely alien to its operations.

From the perspective of Sasol-Huntsman, DIBE is known to be manufactured by only one company, which is a direct competitor to both Huntsman (in terms of licensing technology) and Sasol-Huntsman (in terms of the manufacture of MA). Preliminary calculations made in this AoA (see Sections 4.1.5.1 and 4.1.5.2) suggest that, due to the lack of the REACH registration for DIBE at the time of writing this AoA (June 2013), and having due regard to the need of its manufacturer to both use the substance internally and supply it to his licensees, the amount of DIBE available on the market would be unlikely to cover the (theoretical) future demands of Sasol-Huntsman.

With regard to the alternative technology based on water/xylene recovery of MA, this is available on the market for Sasol-Huntsman if it wished to switch to it. The technology is licensed by competitors to Huntsman and its uptake by Sasol-Huntsman would require the payment of a licence fee.

As indicated above, due to technical and economic feasibility considerations, the availability of commercially unproven alternatives has not been examined in detail, but is expected to vary by substance (see Section 3.2.1.4 under the heading Availability).

1.5 Actions required for making the alternatives suitable and available

It is fundamentally impossible for either the DIBE-based technology or the water/xylene technology to offer technical performance that could match that of Huntsman’s technology, as is detailed in Sections 4.1.2.2 and 4.2.2.2. Improvement of their technical and economic disadvantages cannot be envisaged, as they are intrinsic to the physico-chemical properties of the substances involved in the recovery of the MA product. It would be unjustifiable to invest time, effort and capital into converting the Moers MA plant to inferior technologies, particularly given that risks to workers’ health from exposure to DBP are already adequately controlled.

It is more realistic and commercially prudent to focus instead on the development of a suitable new alternative substance, which, even if not finding commercial applications at present, can be properly researched and adapted to the Huntsman technology so that it meets the needs of Sasol-Huntsman without the prerequisite of a prohibitively costly and technically unjustified conversion. Such research is currently underway by Huntsman with the aim of identifying and developing a technically suitable and economically feasible alternative that can be obtained from the market in sufficient quantities (details of the R&D programme are given in Section 5.3 and in Part 6 of the Confidential Annex to the AoA). Huntsman is committed to continuing this R&D even in the event of the applicant being granted an Authorisation under this present Application.
2 ANALYSIS OF SUBSTANCE FUNCTION

2.1 Background to the use of DBP in the manufacture of MA

2.1.1 Overview

DBP is used as an absorption solvent in the manufacture of MA by Sasol-Huntsman at the Moers plant in Germany using Huntsman technology. At present, the industrial preparation of MA is predominantly carried out by partial oxidation of n-butane by air or oxygen in the gas phase in the presence of a catalyst. The MA produced in the reactor is recovered from the off-gas. In the case of the Sasol-Huntsman plant, the MA product is absorbed in an organic solvent, DBP. The MA-enriched solvent stream is then sent to the purification section to recover pure MA and DBP is recovered and reused within the MA manufacturing process. It is important to note that whilst DBP plays a critical role in the production of MA, it does not itself participate in the reactions that lead to the formation of MA and is not incorporated into the MA product.

The Huntsman technology is a state-of-the-art process for the preparation and recovery of MA in which the concentration of contaminants in the circulating absorbing solvent (DBP) is maintained at a low level; the technology prevents the build-up of polymeric tars in the circulating solvent and subsequent fouling of heat transfer surfaces (Brown & Alumbaugh, 2004).

The Huntsman technology for MA manufacture is licensed by Huntsman to several licensee plants around the globe. Sasol-Huntsman is one of the licensees, with the company being a 50/50 joint venture between Huntsman and Sasol Solvents. Sasol-Huntsman produces MA in Germany and markets MA, in both molten and solid forms, in Central and Western Europe, Scandinavia, Eastern Europe, the Iberian Peninsula, Turkey and Northern Africa. It also exports limited quantities of MA, in solid form, to the Americas (Huntsman, 2009).

MA is a vital chemical intermediate, used only by industrial producers of downstream products; it is not itself a consumer product. As shown in Figure 2.1. The versatility of this molecule is linked to its reactivity as a result of (Burdick & Leffler, 2010):

- the anhydride group;
- the double bond; and
- the carboxylic acid grouping that (re-)forms when MA is mixed with water.

2 Huntsman is also a major supplier of the catalyst used to manufacture MA from butane feedstock.

3 The company was founded in 1997 by Huntsman Corporation and RWE-DEA Aktiengesellschaft für Mineraloel und Chemie (Condea Chemie GmbH). Sasol Solvents took over the shares of Condea during the acquisition of the Condea Chemie business in 2001.
ANALYSIS OF ALTERNATIVES

Figure 2.1: Structure of the MA molecule

Unlike other common uses of DBP\(^4\), in particular plasticiser applications, MA produced by Sasol-Huntsman contains only extremely low traces of DBP (at the ppb level) and is thus a negligible source of exposure to DBP for either downstream industrial workers or, even more so, users of downstream products based on MA. All waste streams emanating from the MA process are destroyed by incineration, thus also excluding the possibility of releases of DBP to the environment.

2.1.2 Description of the use of DBP

The Huntsman technology can be briefly described as follows: air containing 2.05% or less n-butane is sent to a reactor from which the off-gas contains MA, n-butane, \(\text{H}_2\text{O}\) and \(\text{CO}_2\). This mixture is cooled to recover energy and contacted with DBP inside an absorber. The bottom of the absorber gives a mixture of DBP with MA (called Rich Oil), which is sent to a stripper. The recovered DBP is treated to remove by-products using proprietary technology (this separates water, phthalic acid and any water-soluble components) and is returned to the absorber. Crude MA is batch-refined to give the final pure product. The process is schematically presented in Figure 2.2.

\(^4\) It is worth noting that this use of DBP was not present in the Annex XV dossier that identified the substance as a Substance of Very High Concern and indeed departs significantly from the commonly known uses of the substance. The Annex XV dossier only referred to uses of the substance as a plasticiser in (among others) PVC consumer products, inks, adhesives, sealants, paints, lubricants, etc. Consequently, the Annex XV discussion of alternatives is not relevant to this use (the Annex XV dossier is available at: [http://echa.europa.eu/documents/10162/13640/svhc_axvrep_austria_cmr_dbp_20083006_en.pdf](http://echa.europa.eu/documents/10162/13640/svhc_axvrep_austria_cmr_dbp_20083006_en.pdf), accessed on 22 February 2013).
Figure 2.2: Simplified description of the Huntsman process for MA manufacture (Huntsman, pers. comm.)

The major chemical reactions that take place are:

\[
\text{C}_4\text{H}_{10} + 3.5 \text{O}_2 \rightarrow \text{C}_4\text{H}_2\text{O}_3 + 4 \text{H}_2\text{O} \\
\text{Butane} + \text{Oxygen} \rightarrow \text{MA} + \text{Water}
\]

\[
\text{C}_4\text{H}_{10} + 4.5 \text{O}_2 \rightarrow 4 \text{CO} + 5 \text{H}_2\text{O} \\
\text{Butane} + \text{Oxygen} \rightarrow \text{Carbon monoxide} + \text{Water}
\]

\[
\text{C}_4\text{H}_{10} + 6.5 \text{O}_2 \rightarrow 4 \text{CO}_2 + 5 \text{H}_2\text{O} \\
\text{Butane} + \text{Oxygen} \rightarrow \text{Carbon dioxide} + \text{Water}
\]

It is important for the discussion presented later in this document to note that tars build-up in the solvent system; these may cause blockages at high concentrations. The tars include both those formed from the decomposition of the DBP solvent, as well as those introduced in the minor reactor off-gas by-products. The two primary by-product impurities are phthalic anhydride (PA), formed by decomposition of the solvent, and fumaric acid (FAc), formed from the isomerisation of hydrolysed MA. The relevant reactions that form these by-products are as follows:

\[
\text{Ph(COOC}_4\text{H}_9)_2 + \text{H}_2\text{O} \rightarrow \text{Ph(C}_2\text{O}_3) + 2 \text{C}_4\text{H}_9\text{OH} \\
\text{DBP} + \text{Water} \rightarrow \text{Phthalic anhydride} + \text{Butanol}
\]

\[
\text{C}_4\text{H}_2\text{O}_3 + \text{H}_2\text{O} \rightarrow \text{C}_4\text{H}_4\text{O}_4 \\
\text{MA} + \text{Water} \rightarrow \text{Maleic acid}
\]

\[
\text{C}_4\text{H}_4\text{O}_4 \rightarrow \text{C}_4\text{H}_4\text{O}_4 \\
\text{Maleic acid} \rightarrow \text{Fumaric acid (structural isomerisation)}
\]

2.2 Conditions of DBP use

2.2.1 Overview

The following Table summarises the role of DBP in the manufacture of MA and provides an overview of how the substance has to be used under the Huntsman technology.
## Table 2.1: Parameters for DBP use in the manufacture of MA

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Task(s) performed by the substance</td>
<td>Absorption solvent for removal of MA from the reaction product gases</td>
</tr>
<tr>
<td>Physical form of product</td>
<td>Liquid</td>
</tr>
<tr>
<td>Concentration of substance in product</td>
<td>DBP is used as a processing aid and is not detectable in the MA product by routine manufacturing quality control methods</td>
</tr>
<tr>
<td>Critical properties and quality criteria it must fulfil</td>
<td>Key properties of DBP include: 1. Boiling point 2. Solubility of MA 3. Solubility of FAc 4. Low solubility in water 5. Difference from water density 6. Decomposition products easily separable from MA 7. Vapour pressure at the temperatures used 8. Thermal stability These, plus its flash point, are discussed in more detail below – see Table 2.2</td>
</tr>
<tr>
<td>Function conditions (frequency of use and quantity used)</td>
<td>Continuous use; the Exposure Scenario in the CSR covers daily exposures up to 8 hours per shift; operation 365 days/y (the plant operates 24 h/day) Consumption of DBP is variable, depending on the MA output of the plant. Design conditions allow for a typical actual consumption of 7-9.5 kg of solvent per tonne of MA produced</td>
</tr>
<tr>
<td>Process and performance constraints</td>
<td>Temperature at which the lean solvent is introduced into the absorption step is below 75°C, ideally 30-40°C, to minimise overhead losses</td>
</tr>
<tr>
<td>Conditions under which the use of the substance could be eliminated</td>
<td>Use of DBP could only be eliminated if a suitable substitute could be used or if the Moers plant converted to an alternative MA manufacturing technology. The functionality of DBP cannot be eliminated – MA needs to be recovered from the reaction off-gas. Currently available alternatives, substances and technologies, are considered inferior in physico-chemical, safety, technical, commercial, economic and environmental impact terms</td>
</tr>
<tr>
<td>Customer requirements associated with the use of the substance</td>
<td><strong>DBP user:</strong> for the user of DBP, the critical properties referred to above apply. <strong>MA users:</strong> DBP is not incorporated into MA and is not detectable according to routine manufacturing quality control testing. Thus, the use of DBP in the manufacture of MA is of no consequence to downstream users. On the other hand, certain users of MA demand to receive MA product that has low xylene impurities. This can be achieved with the use of the Huntsman technology which utilises DBP as the absorption solvent, rather than water/xylene absorption which leads to xylene impurities</td>
</tr>
<tr>
<td>Industry sector and legal requirements for technical acceptability that must be met and the function must deliver</td>
<td>There are no legal requirements of relevance to the use of DBP in the manufacture of MA or the use of the MA product by the immediate customers of Sasol-Huntsman</td>
</tr>
</tbody>
</table>

*Source: (Brown & Alumbaugh, 2004); CSR; applicant’s own information*

### 2.2.2 Technical criteria for alternative substances

A patent awarded to Brown & Alumbaugh in 2004 provides a useful description of the Huntsman technology. According to this, an absorbing solvent that may be used to remove MA from the reaction off-gases must have the desired solubility for MA, a relatively low vapour pressure at the temperatures used in the process, sufficient thermal stability to avoid excessive decomposition, and be substantially immiscible with water. DBP obviously meets these criteria; any other substance that might be considered as a potential alternative to DBP for the Huntsman technology must also meet the same criteria.
A more recent patent (dated 2012) and attributed to Huntsman researchers describes in a more quantified fashion the requirements that an absorption solvent needs to meet. Smith & Chernyak (2012) suggest the following technical criteria for absorption solvents:

- a normal boiling point between ca. 250°C and ca. 350°C;
- solubility of FAc at least about 0.06% by weight at 60°C;
- solubility of MA at least about 20% by weight at 100°C;
- solubility in water not higher than ca. 100 mg/L;
- density different from the density of water by at least ca. 0.020 g/mL; and
- water-soluble hydrolysis products with a molecular weight no higher than the molecular weight of pentanol (just over 88)\(^5\).

Based on the aforementioned patents, but also on the expertise of Huntsman and the practical experience of Sasol-Huntsman, the key technical characteristics that have been identified as relevant to the use of DBP in the manufacture of MA are described in Table 2.2.

**Table 2.2: Key properties and technical characteristics of DBP**

<table>
<thead>
<tr>
<th>Technical comparison criterion</th>
<th>Threshold value or ideal range</th>
<th>Reasoning and linkages to the functions, tasks and conditions under which DBP is used in the manufacture of MA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal boiling point</td>
<td>250-350°C</td>
<td>MA has a normal boiling point of 202°C; therefore, a solvent with normal boiling point of at least about 250°C is typically used with an upper threshold of 350°C. Lower boiling point solvents would experience relatively higher rates of loss from the absorber and distillation column overheads. The theoretical use of a more volatile solvent than DBP could result in the need to use refrigeration to mitigate its losses and this would make the production process very costly and energy intensive. High losses of the solvent would also increase the volumes sent to the incinerator, which has been designed for a certain fuel volume.</td>
</tr>
<tr>
<td>Dissolution of MA</td>
<td>&gt;20% wt at 100°C</td>
<td>Solubility of MA needs to be sufficient at the temperature of the off-gases, so that the solvent effectively and efficiently absorbs MA.</td>
</tr>
<tr>
<td>Dissolution of fumaric acid</td>
<td>&gt;0.06% wt at 60°C</td>
<td>A solvent usable for MA absorption generally has at least some ability to dissolve by-products of the MA reaction. The by-products are generally removed in the stripping and the solvent purification processes. Solubility of FAc needs to be sufficiently high; otherwise, it would result in a combination of higher solvent use and increased solids deposition with consequent equipment fouling. Increased maintenance frequency may also result in increased likelihood of worker exposure and environmental releases.</td>
</tr>
<tr>
<td>Solubility in water</td>
<td>&lt;100 mg/L</td>
<td>DBP’s water solubility is very low at 11.2 mg/L. Solvents with higher water solubility would be lost to wastewater at a higher rate than DBP, increasing operating costs and wastewater production. Additionally, there could be material consequences with respect to the capacity limitations of the incinerator in which wastewater is disposed of and the possibility that the quantity of wastewater might exceed the capacity of the existing equipment to evaporate it before being fed to the incinerator.</td>
</tr>
<tr>
<td>Difference from water density</td>
<td>&gt;0.020 g/mL</td>
<td>Density should not be too close to that of water, as separation of solvent from water relies on density differences. If the difference became smaller, additional separation equipment would have to be added to the process to accomplish adequate recovery and re-use of the solvent. Even after such modifications, solvent recovery would likely be less efficient than with DBP.</td>
</tr>
</tbody>
</table>

\(^5\) Decomposition products of higher molecular weight do not have an escape from the process.
2.2.3 Technical criteria for alternative MA recovery technologies

This AoA also discusses the availability and suitability of alternative technologies. It will be explained that alternative technologies essentially involve the use of water-based recovery of MA from the reaction off-gas.

Information submitted by Huntsman and a review of the available literature confirm that the technical criteria that need to be considered for the comparison of the DBP-based technology to the use of water/xylene recovery systems include the following.

Table 2.3: Key properties and technical characteristics of DBP-based recovery technology

<table>
<thead>
<tr>
<th>Technical comparison criterion</th>
<th>Threshold value</th>
<th>Reasoning and linkages to the functions, tasks and conditions under which DBP is used in the manufacture of MA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decomposition products easily separable from MA</td>
<td>Not applicable</td>
<td>When esters and diesters are used as solvents to absorb MA at elevated temperatures and in the presence of water and acids, a portion of the solvent may decompose into its corresponding carboxylic acid and alcohol components. It is preferred that these components of the solvent be readily separable from MA, in the absorption solvent, to facilitate the purification of MA. Decomposition of DBP gives PA and butanol, which are readily separated</td>
</tr>
<tr>
<td>Vapour pressure at the temperatures used</td>
<td>No specific threshold available</td>
<td>Vapour pressure needs to be low (the vapour pressure of DBP is 9.7 mPa at 20°C). The amount of solvent that is not condensed (and is thus lost) is proportional to its vapour pressure. Most alternative substances with boiling points below that of DBP would have a vapour pressure above DBP. This would lead to proportionally higher overhead losses, even after major changes to the tower overhead condensers</td>
</tr>
<tr>
<td>Thermal stability</td>
<td>Not applicable</td>
<td>Thermal stability at process conditions must be sufficient to avoid excessive solvent decomposition during the MA production process. If losses to decomposition were to increase, there could be severe operational consequences and waste stream effects</td>
</tr>
<tr>
<td>Flash point</td>
<td>≥191°C (OC*)</td>
<td>Flash point is a safety criterion; a substance with a lower flash point than DBP would be inherently more likely to ignite than DBP (i.e. its use might lead to a fire in the absorber column)</td>
</tr>
</tbody>
</table>

Sources: (Smith & Chernyak, 2012); applicant’s own information

* Open Cup
<table>
<thead>
<tr>
<th>Technical comparison criterion</th>
<th>Threshold value</th>
<th>Reasoning and linkages to the functions, tasks and conditions under which DBP is used in the manufacture of MA</th>
</tr>
</thead>
</table>
| Incidence and consequences of fouling | Not applicable | The Hunstman technology has been developed with the aim of alleviating fouling problems inherent to the manufacture of MA:  
  • by-products of the partial oxidation reaction such as acrylic acid tend to accumulate in the circulating absorbing solvent, along with other contaminants such as maleic, fumaric and phthalic acids, phthalic anhydride and polymeric tars formed in the absorption and stripping loop. The accumulated contaminants, especially the tars, cause plugging and fouling of the process equipment (e.g., heat transfer surfaces), and may have an adverse impact on MA quality; and  
  • tar generation reactions tend to be autocatalytic, so that accumulation of the tars may also have an adverse effect on yields.  
Past efforts to filter the absorbing solvent (after it has been stripped of MA) to remove FAc, and distillation of solvent to remove soluble tars have added to equipment costs, increased thermal degradation of the absorbing solvent and complicated the recovery of MA. Fouling incidence and maintenance requirements and costs under any alternative technology should match if not improve upon those of the DBP-based technology. |
| Quality of MA product | ≤100 ppm xylene impurity in the MA product | Some users of MA may refuse to buy MA from producers using xylene in their recovery processes, especially where MA is intended for use in the manufacture of environmentally friendly (biologically degradable) or ‘green’ products, where such xylene presence would be unacceptable. |

*Source: (Brown & Alumbaugh, 2004); applicant’s own information*
3 IDENTIFICATION OF POSSIBLE ALTERNATIVES

3.1 Introduction and list of potential alternatives

The focus of this AoA will be:

1. the only identified alternative substance known to have found commercial application, **diisobutyl hexahydrophthalate** (also known as DIBE – EC Number: 275-069-5, CAS Number: 70969-58-3) (see Section 4.1); and

2. the commercially proven alternative technology of a **water-based recovery system**, which is based on the use of water and xylene for the recovery of MA (see Section 4.2).

A third alternative to be considered will be the non-use and non-replacement of DBP, i.e. the cessation of the function of DBP without its replacement by any alternative substance or technology. This is discussed for completeness only (see Section 4.3).

Potential alternatives that are still at the R&D stage and have not come close to a commercialisation stage are also considered in some detail (Section 3.2.1.4) with the aim of demonstrating their shortcomings and the challenges faced by Huntsman and Sasol-Huntsman in using them as replacements for DBP. These substances have not been included in the detailed analysis in Section 4 of the AoA.

3.2 Description of efforts made to identify possible alternatives

3.2.1 Research and development

3.2.1.1 Past research

Consultation and online sources have been used to identify relevant patents that describe the use of DBP and to identify potential alternatives as absorption solvents for MA. The sources used include those shown in Table 3.1.

**Table 3.1: Key information sources used in patent searches**

<table>
<thead>
<tr>
<th>Source</th>
<th>Details</th>
</tr>
</thead>
</table>

It has been established that there have been efforts towards the development of MA separation technologies over the last 60-70 years. US patent 2,574,644 (Landau, 1951) has been referred to as...
the first application mentioning the use of DBP as a selective absorbent for MA (Simola, Cassarino, & Iosco, 2012). MA has great solubility in DBP, even at low temperatures. The patent explains that, thanks to this fact, MA can be recovered in a column using DBP as an absorption medium, even at moderate conditions of temperature and pressure. Subsequently, the MA is removed from the solvent by stripping under vacuum conditions and elevated temperature.

Similarly, GB patent 727,828 (Landau, 1955) and US patent 2,942,005 (Brown & White Colton, 1960) refer to the use of DBP for simultaneous absorption of MA and PA from a mixture gas, followed by vacuum stripping and separation of the products by fractionation (Landau, 1955) or by crystallisation (Brown & White Colton, 1960). GB patent 763,339 (Landau, 1956) and GB patent 768,551 (Landau, 1957) represented improvements of the organic solvent recovery system, where the rich solvent is subject to two subsequent stripping operations at controlled conditions of pressure and temperature.

However, alternative absorption solvents have also been looked at over the years:

- US patent 3,818,680 (Marquis, 1974) discloses the use of an alkenyl or alkyl substituted succinic anhydride as absorption liquid in a column having a number of theoretical trays – from 5 to 15 – and operating at a temperature between 65 and 125°C;
- US patent No. 3,891,680 (Katsumoto & Lind, 1975) describes how MA can be effectively recovered from a gaseous mixture by contacting the mixture with a dialkyl phthalate having from 4 to 8 carbon atoms in each alkyl group and a total of from 10 to 14 carbon atoms in the two alkyl groups. These dialkyl phthalate esters have lower vapour pressures than DBP and were described as being capable of preventing carryover loss of solvent out of the gas-scrubbing column and out of the vacuum stripper. The preferred solvents were in the group of dihexyl orthophthalates (Simola, Cassarino, & Iosco, 2012);
- US patent 4,118,403 (White, 1978) discloses the use of DBP as an absorption solvent but also mentions a series of other solvents that were considered at the time, all of them phthalates (a total of 18 phthalates in addition to DBP);
- US patent 4,071,540 (Marquis, 1978) discloses the absorption of MA by counter-current contacting in a column, by using a liquid solvent comprising polymethyl benzophenones;
- US patent 4,314,946 (Neri & Sanchioni, 1982) refers to a process for recovering MA from reaction gases, by using dialkyl esters of hexahydrophthalic acid, tetrahydrophthalic acid, methyl tetrahydrophthalic acid or methyl hexahydrophthalic acid;
- Chinese patent CN 1062344 (Zunqing, Shiyi, & Fangtian, 1992) refers to the use of different types of organic solvents, like phthalic dioctyl ester or dewaxed oil from refinery, to recover MA from the catalytic oxidation of hydrocarbons;
- Japanese patent JP5025154 discloses the use of an organic solvent consisting of tetrahydrothiophene 1,1-dioxide (Simola, Cassarino, & Iosco, 2012);
- European patent EP 0 815 098 B1 (Brown & Alumbaugh, 2004), already discussed above, discusses dialkyl phthalate compounds that have two to eight carbon atoms in each alkyl chain. Suitable dialkyl phthalate compounds include ordinary phthalates and hydrophthalates (DBP was described as the preferred MA-absorbing solvent); and
- patent WO 2012/154479 A1 (Smith & Chernyak, 2012) describes that an appropriate MA absorption solvent may be non-cyclic, non-aromatic, linear, and/or branched, and may have the
general structure $R_1\text{COOR}_2\text{COOR}_3$, where $R_1$ and $R_3$ are each linear or branched C$_3$ to C$_5$ groups, and $R_2$ is a linear or branched C$_3$ to C$_8$ group.

Much of the research presented in the above patents has been undertaken by the creators and licensors of the Huntsman technology, which has been developed and continuously improved over many years. Huntsman acquired the MA business from Monsanto that had licensed its fixed-bed MA production technology for the first time in 1988.

In the 1970s, Monsanto undertook extensive R&D in the development of the technology and for selecting a suitable absorption solvent. Monsanto’s original work utilised literature research and both laboratory and pilot plant testing. Acceptance criteria for the absorption solvent were established for a wide range of parameters, both physicochemical and also those of toxicity, commercial availability and cost. The selection of DBP as the solvent of choice was based on its stability, the process operation parameters and its cost.

3.2.1.2 Current research by Huntsman

Huntsman continues its research into the identification of suitable absorption solvents. Certainly, the placing of DBP into Annex XIV of the REACH Regulations has provided further incentive for the development of a technically and economically feasible alternative with an acceptable risk profile.

In recent years, Huntsman has made extensive use of modern electronic physical property databases and process simulation. More than 13,000 chemicals have been examined for close matches of key physical properties. These 13,000 substances have been screened against technical and other selection criteria under a rigorous approach. Information on the key physical properties of substances was obtained from the physiochemical databases DIPPR (maintained by the American Institute of Chemical Engineers), DECHEMA (the database of the German Society for Chemical Engineering and Biotechnology) and Huntsman’s own proprietary database. The subsequently selected materials were then subjected to laboratory testing of unpublished parameters such as MA and FAc solubility. ‘Surviving’ candidates were then incorporated into an Aspen model of Huntsman’s MA process.

3.2.1.3 Long list of theoretical alternative solvents based on past and current research

Taking into consideration the potential alternative substances referred to in recent patents (Brown & Alumbaugh, 2004) (Smith & Chernyak, 2012) (Simola, Cassarino, & Iosco, 2012) and the work that Huntsman’s laboratories have undertaken, we have developed a list of potential alternatives, shown in Table 3.2. The Table also indicates whether any of the identified substances had been registered under REACH by May 2012 and whether information is available on the likely registration timing.

The Table presents alternative substances that are commonly referred to in the patent literature; however, it should be noted that the alternative substances presented in the Table are only a few out of the thousands of potential alternatives investigated by Huntsman (and previously by its predecessor). Although this cannot be considered to be a shortlist of the ‘best’ or ‘most suitable’ potential alternatives, it provides a useful overview of the families of substances that might be considered as possible pools for the selection of suitable alternatives, i.e. phthalates, hydrophthalates, benzophenones, adipates, maleates and succinic anhydrides. All offer performance inferior to DBP, as will be discussed below.
### Table 3.2: Indicative list of potential alternative solvents

<table>
<thead>
<tr>
<th>Substance (solvent)</th>
<th>EC No.</th>
<th>CAS No.</th>
<th>Registration intention</th>
<th>Envisaged registration deadline (from pre-registration)</th>
<th>REACH Registered?</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Phthalates</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimethyl phthalate</td>
<td>205-011-6</td>
<td>131-11-3</td>
<td>N/A</td>
<td>-</td>
<td>Yes</td>
</tr>
<tr>
<td>Diethyl phthalate</td>
<td>201-550-6</td>
<td>84-66-2</td>
<td>N/A</td>
<td>-</td>
<td>Yes</td>
</tr>
<tr>
<td>Dipropyl phthalate</td>
<td>205-015-8</td>
<td>131-16-8</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td>Diisopropyl phthalate</td>
<td>210-086-3</td>
<td>605-45-8</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td>Diisobutyl phthalate</td>
<td>201-553-2</td>
<td>84-69-5</td>
<td>N/A</td>
<td>-</td>
<td>Yes</td>
</tr>
<tr>
<td>Di-n-octyl phthalate</td>
<td>204-214-7</td>
<td>117-84-0</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td><strong>Hydrophthalates</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimethyl dihydrophthalate</td>
<td>N/A</td>
<td>14309-54-7</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Diethyl dihydrophthalate</td>
<td>N/A</td>
<td>6268-45-7</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Dipropyl dihydrophthalate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Diisopropyl dihydrophthalate</td>
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<tr>
<td>Dibutyl dihydrophthalate</td>
<td>-</td>
<td>-</td>
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<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Diisobutyl dihydrophthalate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Diethyl dihydrophthalate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Dimethyl tetrahydrophthalate</td>
<td>N/A</td>
<td>4336-19-0</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Diethyl tetrahydrophthalate</td>
<td>N/A</td>
<td>5048-50-0</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Dipropyl tetrahydrophthalate</td>
<td>N/A</td>
<td>92687-40-6</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Diisopropyl tetrahydrophthalate</td>
<td>N/A</td>
<td>7497-50-9</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Dibutyl tetrahydrophthalate</td>
<td>N/A</td>
<td>62950-20-3</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Diisobutyl tetrahydrophthalate</td>
<td>N/A</td>
<td>81667-22-3</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Dimethyl hexahydrophthalate</td>
<td>605-528-0</td>
<td>1687-29-2</td>
<td>-</td>
<td>2018</td>
<td>No</td>
</tr>
<tr>
<td>Diethyl hexahydrophthalate</td>
<td>N/A</td>
<td>10138-59-7</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Dipropyl hexahydrophthalate</td>
<td>N/A</td>
<td>65646-25-5</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Diisopropyl hexahydrophthalate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Dibutyl hexahydrophthalate</td>
<td>N/A</td>
<td>62950-20-3</td>
<td>-</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>Diisobutyl hexahydrophthalate</td>
<td>275-069-5</td>
<td>70969-58-3</td>
<td>2013</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td><strong>Dimethyl benzophenones</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2,4-Dimethylbenzophenone</td>
<td>214-523-9</td>
<td>1140-14-3</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td>2,5-Dimethylbenzophenone</td>
<td>223-740-8</td>
<td>4044-60-4</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td>4,4’-Dimethylbenzophenone</td>
<td>210-287-6</td>
<td>611-97-2</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td><strong>Adipates</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diethyl adipate</td>
<td>205-477-0</td>
<td>141-28-6</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td>Di-n-butyl adipate</td>
<td>203-350-4</td>
<td>105-99-7</td>
<td>-</td>
<td>2010</td>
<td>No</td>
</tr>
<tr>
<td>Di-isobutyl adipate</td>
<td>205-450-3</td>
<td>141-04-8</td>
<td>N/A</td>
<td>-</td>
<td>Yes</td>
</tr>
<tr>
<td><strong>Maleates</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dibutyl maleate</td>
<td>203-328-4</td>
<td>105-76-0</td>
<td>N/A</td>
<td>-</td>
<td>Yes</td>
</tr>
</tbody>
</table>
### 3.2.1.4 Suitability of potential alternatives still being researched

**Overview**

The following paragraphs demonstrate the difficulties in identifying a suitable alternative from within a large pool of potentially feasible solvents. It presents the technical challenges but also the economic hurdles in replacing DBP with some of the alternatives that are still commercially unproven and are currently at the R&D stage.

Obviously, it is not feasible to present here the entire list of 13,000 substances screened by Huntsman. Nevertheless, for demonstrating the selection process that Huntsman follows in its quest to identify a suitable replacement for DBP, a range of potential alternative solvents have been selected for comparison to DBP. This comparison is shown in Table 3.3. The substances have been selected to represent a variety of different substance groups (phthalates, adipates, benzophenones, terephthalates, maleates) likely to include the ‘most promising’ alternative substances. However, no guarantee can be made that Huntsman has been able to identify all possible theoretical alternatives to DBP.

**Technical feasibility**

It should be clear that it only takes failing a single critical parameter to abandon any particular candidate substance in favour of other more feasible alternatives. Failure to meet any parameter
means that the substance cannot meet the requirements of the established Huntsman technology. The substances presented in Table 3.2 generally fail one or more of the technical criteria discussed in Section 2.2.2; therefore, they do not constitute realistic and technically feasible alternatives.

For each of the selected potential alternatives listed in Table 3.3, boiling point, water solubility, density and flash point values are presented. On the other hand, for solubility in MA and FAc solubility, a relative value in comparison to DBP is generally given. The data in the Table have largely been provided by Huntsman, but additional research has been undertaken in the open literature to obtain some missing values for the key physico-chemical and technical parameters of these substances.

The following points must be noted:

- some information is proprietary to Huntsman and cannot be disclosed, however, a clear indication is given (where possible) of whether each substance performs better, similarly or worse than DBP;
- values given in the colour red indicate that the selected potential alternative substance does not meet the relevant technical performance criterion;
- for vapour pressure, for which a specific threshold has not been set, only values that are well above the vapour pressure of DBP are marked in the colour red; and
- the Table also contains (on the right hand side) commentary on specific shortcomings of the selected substances.

**Economic feasibility**

In order to obtain up-to-date information on prices of DBP and the potential alternative substances, information was collected from ‘Alibaba.com’ (self-described as “the world's largest online business-to-business marketplace”) – a site which has been used to gather similar information in a number of professional studies. Annex 2, at the end of this AoA document, explains the relevance of the Alibaba.com price of DBP and the actual price at which the applicant sells the substance, as of July 2013. The actual price is not given here due to the need to respect confidentiality.

Information specifically concerning European traders was given priority; however, where this information was unavailable or lacking (we considered this to be when information was available from fewer than three individual European-based suppliers), data was instead obtained from Chinese traders, as they typically account for the dominant market share/supply source of each substance.

In addition to the price of the substances, information was collected on company names and locations, the purity of the substances as well as the supply ability, minimum order quantity and type of shipping included in the price. If no information was available from ‘Alibaba.com’ on a certain chemical, several separate business-to-business, wholesale marketplaces were searched – these included TradeKey (http://www.tradekey.com/), EC21 (http://www.ec21.com/), ECPlaza (http://www.ecplaza.net), TradeEasy (http://www.tradeeasy.com/), and Made in China (http://www.made-in-china.com/). Where a conversion in currency was required, the average conversion rate for US dollars into Euros was undertaken (US$1 = €0.76, for 20 June 2013)².

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6 Available at: http://www.alibaba.com/

7 We used the exchange rates provided here: http://www.xe.com.
Table 3.3: Comparison of selected potential alternative substances currently at the R&D stage against key technical comparison criteria

<table>
<thead>
<tr>
<th>Solvent name</th>
<th>CAS No</th>
<th>EC No</th>
<th>NBP (°C)*</th>
<th>Density at 25°C (g/cm³)</th>
<th>Vapour pressure (kPa) at 20°C</th>
<th>Flash Pt OC, (°C)**</th>
<th>MA Solubility</th>
<th>FAc Solubility</th>
<th>Water solubility (mg/L)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyl phthalate</td>
<td>84-74-2</td>
<td>201-557-4</td>
<td>340</td>
<td>1.043</td>
<td>9.7 x 10⁻⁵</td>
<td>191</td>
<td>&gt;20 wt%</td>
<td>0.066%</td>
<td>11.40 ± 0.71</td>
<td>Optimum combination of properties</td>
</tr>
<tr>
<td>Diethyl phthalate</td>
<td>84-66-2</td>
<td>201-550-6</td>
<td>295</td>
<td>1.12</td>
<td>&lt;2.8</td>
<td>140</td>
<td>No data</td>
<td>No data</td>
<td>1.080</td>
<td>Losses via solvent purification system would be very high. Higher vapour pressure than DBP would lead to higher losses in absorber off-gas</td>
</tr>
<tr>
<td>4,4’-Dimethyl benzophenone</td>
<td>611-97-2</td>
<td>210-287-6</td>
<td>200</td>
<td>1.05</td>
<td>4.57 x 10⁻⁶</td>
<td>200</td>
<td>No data</td>
<td>No data</td>
<td>9.238 - 14.067</td>
<td>Decomposition products adversely affect MA colour stability. Colour stability is important for the main application of MA, in the manufacture of UPR</td>
</tr>
<tr>
<td>Diethyl adipate</td>
<td>141-28-6</td>
<td>205-477-0</td>
<td>251</td>
<td>1.009</td>
<td>0.0036</td>
<td>127</td>
<td>~DBP</td>
<td>&gt;&gt;DBP</td>
<td>403.8 - 694.95</td>
<td>Higher vapour pressure than DBP would lead to higher losses in absorber off-gas. Density difference from water too small. Water solubility too high</td>
</tr>
<tr>
<td>Dibutyl adipate</td>
<td>105-99-7</td>
<td>203-350-4</td>
<td>305</td>
<td>0.962</td>
<td>2.1 x 10⁻³</td>
<td>155</td>
<td>~DBP</td>
<td>0.15%</td>
<td>35 at 25°C</td>
<td>Somewhat higher water solubility than DBP. Lower flash point, higher vapour pressure</td>
</tr>
<tr>
<td>Dibutyl terephthalate</td>
<td>1962-75-0</td>
<td>217-803-9</td>
<td>337-341</td>
<td>1.045</td>
<td>3.8 x 10⁻³</td>
<td>196</td>
<td>~DBP</td>
<td>&lt;DBP</td>
<td>0.00451</td>
<td>Decomposition product not water soluble, thus no outlet from process</td>
</tr>
<tr>
<td>Tetraethylene glycol dimethyl ether</td>
<td>143-24-8</td>
<td>205-594-7</td>
<td>276</td>
<td>1.009</td>
<td>&lt;0.001</td>
<td>141 (CC)</td>
<td>No data</td>
<td>No data</td>
<td>&gt;&gt;DBP</td>
<td>Very highly water soluble, so losses in solvent purification system would be high. Density too close to water</td>
</tr>
<tr>
<td>Dibutyl maleate</td>
<td>105-76-0</td>
<td>203-328-4</td>
<td>280</td>
<td>0.99</td>
<td>0.00027</td>
<td>121 (CC)</td>
<td>No data</td>
<td>&lt;DBP</td>
<td>170 mg/L</td>
<td>Does not dissolve FAc. May co-boil with MA making solvent-product separation difficult</td>
</tr>
</tbody>
</table>

* NBP - Normal Boiling Point
** Flash Pt - Flash Point
FAc - Formic Acid
MA - Maleic Acid

Use number: 1
Legal name of applicant: DEZA, a.s.
## ANALYSIS OF ALTERNATIVES

<table>
<thead>
<tr>
<th>Solvent name</th>
<th>CAS No</th>
<th>EC No</th>
<th>NBP (°C)*</th>
<th>Density at 25°C (g/cm³)</th>
<th>Vapour pressure (kPa)</th>
<th>Flash Pt OC, (°C)**</th>
<th>MA Solubility</th>
<th>FAc Solubility</th>
<th>Water solubility (mg/L)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diphenyl ether</td>
<td>101-84-8</td>
<td>202-981-2</td>
<td>259</td>
<td>1.073</td>
<td>0.0027 at 25°C</td>
<td>115</td>
<td>No data</td>
<td>&lt;DBP</td>
<td>18-21</td>
<td>Does not dissolve FAc. Butyric acid decomposition product may cause an odour problem</td>
</tr>
<tr>
<td>Glyceryl tributyrate</td>
<td>60-01-5</td>
<td>200-451-5</td>
<td>287</td>
<td>1.032</td>
<td>5.1x10⁻⁵ at 25°C</td>
<td>174 (CC)</td>
<td>No data</td>
<td>&lt;DBP</td>
<td>17.74 - 46.614</td>
<td>No data</td>
</tr>
</tbody>
</table>

* “NBR” indicates Normal Boiling Point  
** “CC” indicates values generated by the closed cup method  

Sources:  
- Smith & Chernyak, 2012; CSR; applicant’s own information  
- Dibutyl terephthalate: ECHA Dissemination Portal: [http://apps.echa.europa.eu/registered/data/dossiers/DISS-9eac3c49-4e66-1d4e-e044-00144f67d031/AGGR-1b02ebb2-d81b-40a6-a1fb-8d77b4c69fc_DISS-9eac3c49-4e66-1d4e-e044-00144f67d031.html#AGGR-1b02ebb2-d81b-40a6-a1fb-8d77b4c69fc](http://apps.echa.europa.eu/registered/data/dossiers/DISS-9eac3c49-4e66-1d4e-e044-00144f67d031/AGGR-1b02ebb2-d81b-40a6-a1fb-8d77b4c69fc_DISS-9eac3c49-4e66-1d4e-e044-00144f67d031.html#AGGR-1b02ebb2-d81b-40a6-a1fb-8d77b4c69fc)  

Table generated in May 2012
Using this approach, a series of Tables with prices for DBP and for the potential alternatives were created. These are available in Annex 2 to this AoA and a summary given in Table 3.4. This Table shows that all of the selected alternatives are likely to be more costly than DBP, with all of them, bar diethyl phthalate, potentially being at least +50% more costly than DBP. Some alternatives (dibutyl adipate and tetraethylene glycol dimethyl ether) are considerably more expensive, making them particularly unattractive as DBP replacements.

### Table 3.4: Cost comparison of DBP to selected commercially unproven potential alternatives

<table>
<thead>
<tr>
<th>Solvent name</th>
<th>Average cost (€/t)</th>
<th>Median cost (€/t)</th>
<th>Cost range (€/t)</th>
<th>Difference compared to DBP (average cost)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibutyl phthalate</td>
<td>1,489</td>
<td>1,520</td>
<td>760 - 2,280</td>
<td>N/A</td>
</tr>
<tr>
<td>Diethyl phthalate</td>
<td>1,705</td>
<td>1,456</td>
<td>1,210 - 3,025</td>
<td>+15%</td>
</tr>
<tr>
<td>Diethyl adipate</td>
<td>2,269</td>
<td>N/A</td>
<td>756 - 3,781</td>
<td>+52%</td>
</tr>
<tr>
<td>Dibutyl adipate</td>
<td>5,886</td>
<td>5,886</td>
<td>756 - 11,349</td>
<td>+295%</td>
</tr>
<tr>
<td>Tetraethylene glycol dimethyl ether</td>
<td>17,693</td>
<td>17,100</td>
<td>760 - 76,000</td>
<td>+1,090%</td>
</tr>
<tr>
<td>Dibutyl maleate</td>
<td>2,270</td>
<td>N/A</td>
<td>756 - 3,783</td>
<td>+52%</td>
</tr>
<tr>
<td>Diphenyl ether</td>
<td>2,447</td>
<td>2,752</td>
<td>75 - 3,783</td>
<td>+64%</td>
</tr>
<tr>
<td>Glyceryl tributyrate</td>
<td>2,268</td>
<td>N/A</td>
<td>756 - 3,780</td>
<td>+52%</td>
</tr>
</tbody>
</table>

It should be noted that the discussion in Section 4.1 will demonstrate that the replacement of DBP by an alternative absorption solvent such as DIBE would likely result in significant modifications to the MA manufacturing plant that would be accompanied by very high costs. It is reasonable to assume that if one of the potential unproven alternatives were to be adopted as a DBP replacement, analogous significant costs would arise in addition to the increased cost of the absorption solvent.

**Availability**

No research has been undertaken on the commercial availability of unproven alternative substances. It is expected that availability will vary; among the nine substances presented in Table 3.3, three do not appear to have been registered\(^8\).

DEZA was asked to detail its ability to manufacture and supply any of the theoretical alternative substances that have been identified in the open literature. The information submitted by DEZA is presented in tabular format in Part 1 of the Confidential Annex. Generally, DEZA manufactures some phthalates and adipates but has no knowledge or expertise in the manufacture of the potential alternatives that belong to other chemical families.


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\(^8\) Searches on the ECHA Dissemination Portal were undertaken on 10 July 2013.
Actions required for improving availability of unproven potential alternatives

From DEZA’s perspective, only the acquisition of knowledge and, hence, ability to produce the selected potential alternative at an industrial scale would potentially improve the availability of the potential alternatives. At present, it cannot be foreseen that this knowledge would be acquired by DEZA in the near future.

3.2.1.5 Conclusion

The aforementioned substances have not found commercial applications as absorption solvents. Their technical suitability has not been proven and the examination of their key physico-chemical properties suggests that they could not be feasibly used as replacements for DBP in Huntsman’s MA technology, at least with current knowledge and expertise.

When the cost of these potential alternatives is further considered, it is clear that the majority of the selected alternatives are considerably more costly than DBP on a per tonne basis. Moreover, based on the discussion that follows for DIBE (in Section 4.1), it is likely that the use of these potential alternatives could be accompanied by significant cost due to the need to modify the plant in which MA is manufactured. In light of the adequate control of risks to workers’ health from exposure to DBP, the adoption of any of these unproven, costly solvents as a replacement for DBP would be commercially and technically unjustified. In conclusion, the focus of the detailed analysis of the suitability and availability of alternatives is only based on realistic, commercially proven solutions.

3.2.2 Data searches

A literature review was undertaken by the authors of this AoA for potential alternatives. The open literature has been searched for information on both potential alternative substances and alternative methods of manufacture of MA using keywords such as “maleic anhydride”, “manufacture of maleic anhydride” and others. Once some information had been collected (for example, names of providers or licensors of manufacturing methods), the data searches were expanded to include additional relevant key words.

Information was sought on:

- the identities of potential alternative substances and alternative technologies;
- information on the technical parameters of alternative technologies, in particular information from those licensing or using the available technologies; and
- information on the technical feasibility, economic feasibility and human health and environmental impacts profile of alternative substances and technologies.

Table 3.5 provides the main sources of information used, although as new leads were being found, a much larger number of individual Internet sites were consulted. In addition, important sources of information on the MA market are the reports by the market research company Tecnon Orbichem9.

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9 See [http://www.tecnon.co.uk/_iNeedInfo.aspx](http://www.tecnon.co.uk/_iNeedInfo.aspx).
Table 3.5: Key information sources used in the identification of potential alternatives

<table>
<thead>
<tr>
<th>Source</th>
<th>Details</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Google</td>
<td><a href="http://www.google.com">http://www.google.com</a></td>
<td>Search engine</td>
</tr>
<tr>
<td>Google Scholar</td>
<td><a href="http://scholar.google.co.uk">http://scholar.google.co.uk</a></td>
<td>Scientific articles</td>
</tr>
<tr>
<td>Google Books</td>
<td><a href="http://books.google.co.uk/bkshp?hl=en&amp;tab=wp">http://books.google.co.uk/bkshp?hl=en&amp;tab=wp</a></td>
<td>Books</td>
</tr>
</tbody>
</table>

With regard to the characteristics and properties of potential alternative substances, a range of specialist websites have been systematically consulted. The following Table gives an overview of some of the most important information sources that were used in the preparation of this AoA.

Table 3.6: Key information sources used in the collection of information on the properties of potential alternatives

<table>
<thead>
<tr>
<th>Source</th>
<th>Details</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Google</td>
<td><a href="http://www.google.com">http://www.google.com</a></td>
<td>Search engine</td>
</tr>
<tr>
<td>Scirus</td>
<td><a href="http://www.scirus.com/">http://www.scirus.com/</a></td>
<td>Scientific search engine</td>
</tr>
<tr>
<td>ESIS</td>
<td><a href="http://esis.jrc.ec.europa.eu/home.php">http://esis.jrc.ec.europa.eu/home.php</a></td>
<td>Substance inventory</td>
</tr>
<tr>
<td>KEMI PRIO Database</td>
<td><a href="http://www2.kemi.se/templates/PRIOEngframes_4144.aspx">http://www2.kemi.se/templates/PRIOEngframes_4144.aspx</a></td>
<td>Substance inventory</td>
</tr>
<tr>
<td>SIN List</td>
<td><a href="http://w3.chemsec.org/">http://w3.chemsec.org/</a></td>
<td>Inventory of substances of concern</td>
</tr>
<tr>
<td>US EPA Substance Registry Services</td>
<td><a href="http://iaspub.epa.gov/sor_internet/registry/substreg/searchandretrieve/substsearch/search.do">http://iaspub.epa.gov/sor_internet/registry/substreg/searchandretrieve/substsearch/search.do</a></td>
<td>Substance inventory</td>
</tr>
<tr>
<td>New Zealand Inventory of Chemicals</td>
<td><a href="http://www.epa.govt.nz/search-databases/Pages/nzioc-search.aspx">http://www.epa.govt.nz/search-databases/Pages/nzioc-search.aspx</a></td>
<td>Substance inventory</td>
</tr>
<tr>
<td>OECD Screening Information Datasets</td>
<td><a href="http://www.oecd.org/chemicalsafety/assessments/chemicals/theoecdqsartoolbox.htm#Download_qsar_application">http://www.oecd.org/chemicalsafety/assessments/chemicals/theoecdqsartoolbox.htm#Download_qsar_application</a>_</td>
<td>Risk assessment information</td>
</tr>
<tr>
<td>OECD QSAR Toolbox</td>
<td></td>
<td>Human health and environmental data</td>
</tr>
<tr>
<td>GESTIS Database</td>
<td><a href="http://gestis-en.itrust.de/nxt/gateway.dll/gestis_en/000000.xml?f=templates$5fn=default.htm$3.0">http://gestis-en.itrust.de/nxt/gateway.dll/gestis_en/000000.xml?f=templates$5fn=default.htm$3.0</a></td>
<td>Chemical hazards database</td>
</tr>
<tr>
<td>CAMEO Chemicals</td>
<td><a href="http://cameochemicals.noaa.gov/">http://cameochemicals.noaa.gov/</a></td>
<td>Chemical hazards database</td>
</tr>
<tr>
<td>WHO IARC Monographs</td>
<td><a href="http://monographs.iarc.fr/ENG/Classification/index.php">http://monographs.iarc.fr/ENG/Classification/index.php</a></td>
<td>Carcinogenicity effects information</td>
</tr>
<tr>
<td>ECETOC Joint Assessment of Commodity Chemicals</td>
<td><a href="http://www.ecetoc.org/jacc-reports">http://www.ecetoc.org/jacc-reports</a></td>
<td>Risk assessment information</td>
</tr>
<tr>
<td>TOXNET</td>
<td><a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search">http://toxnet.nlm.nih.gov/cgi-bin/sis/search</a></td>
<td>Human health and environmental data</td>
</tr>
<tr>
<td>NLM Gateway</td>
<td><a href="http://gateway.nlm.nih.gov/">http://gateway.nlm.nih.gov/</a></td>
<td>Scientific articles</td>
</tr>
<tr>
<td>Google Scholar</td>
<td><a href="http://scholar.google.co.uk">http://scholar.google.co.uk</a></td>
<td>Scientific articles</td>
</tr>
</tbody>
</table>
The core of the literature search was undertaken in the period January 2012 – March 2013.

3.2.3 Consultations

3.2.3.1 Identities of key consultees

The authors of this AoA undertook consultation with DEZA, Sasol-Huntsman and Huntsman. As noted earlier, the use of DBP is essentially not of relevance to the users of MA. As a result, consultation with customers downstream of Sasol-Huntsman on the issue of alternative substances and technologies has not been undertaken.

The core of the consultation regarding the suitability and availability of alternatives was undertaken in the period September 2011 – December 2012.

3.2.3.2 Consultation tools utilised

Consultation with DEZA

By means of two written questionnaires (sent in May 2012 and June 2013) and subsequent numerous email exchanges and telephone communications, DEZA was asked to provide information on:

- whether it manufactures any of the potential alternative substances that have been identified;
- whether specific plans exist to start the manufacture of any potential alternative substance, including what tonnage could potentially be placed on the market;
- potential problems with the manufacture of any of the identified potential alternative substances;
- the possibilities for manufacture and supply DIBE by DEZA, with specific regard to:
  - the availability and accessibility of precursors to DIBE; and
  - the foreseeable economic feasibility of DIBE’s production.

Several meetings were held with DEZA in preparation of this AoA in Germany and the UK. The information collected has been used in the preparation of this AoA and the Confidential Annex to the AoA.

Consultation with Sasol-Huntsman and Huntsman

Consultation took several forms:

- written questionnaires: a questionnaire was originally used for the collection of information. This was submitted to Sasol-Huntsman and Huntsman in October 2011. The aim of the questionnaire was to collect information on:
• the use of DBP in the manufacture of MA and the downstream applications of MA;
• the technical criteria that DBP meets in this use;
• the importance of DBP in this use;
• the technical suitability, economic feasibility and market availability of alternative substances and technologies; and
• information on past, current and planned future R&D on the replacement of DBP.

Responses started being submitted in October 2011 and several additional questions were subsequently added as the questionnaire evolved into a living document that facilitated the exchange of information between RPA and the two companies;

• exchange of draft documents: preliminary outputs were shared with Huntsman and Sasol-Huntsman. These were accompanied by a series of questions aimed at filling gaps, addressing queries and exploring new issues that arose as information was being collected and processed; and

• face-to-face meetings and telephone conversations: several meetings were held with Huntsman and Sasol-Huntsman (and DEZA) in preparation of this AoA. When necessary, telephone interviews and conference calls were held.

Huntsman was consulted alongside Sasol-Huntsman, as indicated above. Huntsman’s knowledge of the global MA market is unparalleled and Huntsman’s staff, based in the USA, have very extensive experience in the MA manufacture field. They have been able to provide significant insights to the advantages and disadvantages of different alternative technologies.

3.2.4 Identified commercially proven alternatives

3.2.4.1 Commercially proven alternative absorption solvents

The starting point for the identification of realistic alternative substances was the identification of where MA is manufactured across the globe and how manufacture is undertaken. However, readily (or less readily) accessible sources may not necessarily provide conclusive answers. For instance, publications by the market research company Tecnon Orbichem explain whether a fixed- or fluidised-bed technology is employed and what the feedstock is (n-butane or another hydrocarbon), but they do not shed light on the identities of absorption solvents used at each plant.

This information is generally not widely available, as companies do not wish to disclose to competitors the details of the technologies they license or use. Therefore, publicly available information on absorption solvents currently in use is very sparse and no particular alternative substance has been confirmed in the open literature as being currently in use in the manufacture MA anywhere in the world. As a result, we have to rely on market intelligence available to Huntsman and Sasol-Huntsman. Huntsman has confirmed that when solvent-based recovery is used, only two solvents are known to be commercially used globally: DBP and DIBE. DIBE is thought to be used by one EU plant, located in Italy, as shown in Table 3.7 which summarises the MA manufacturers in the EU (including a plant in Bosnia & Herzegovina) and indicates the feedstock and absorption solvent each plant is believed to use. The SEA (Section 2.2.1.8) provides more detail on the state of the EU MA market. Apart from the Belgian plant, which closed in 2010, other plants ceased
production in the 2000s, such as the Polioli plant in Italy (shut down in 2003) and a Cray Valley plant in France (shut down in 2007).10

Table 3.7: MA manufacture in the EU (plus Bosnia & Herzegovina) and solvents used

<table>
<thead>
<tr>
<th>Producer</th>
<th>Country</th>
<th>Capacity (kt/y)</th>
<th>Feedstock</th>
<th>Absorption solvent</th>
<th>Operation status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sasol-Huntsman</td>
<td>Germany</td>
<td>105</td>
<td>n-butane</td>
<td>DBP</td>
<td>Operating</td>
</tr>
<tr>
<td>Polynet</td>
<td>Italy</td>
<td>65</td>
<td>n-butane</td>
<td>DIBE</td>
<td>Operating</td>
</tr>
<tr>
<td>Polynet</td>
<td>Italy</td>
<td>36</td>
<td>Benzene</td>
<td>Water/xylene</td>
<td>Intermittently operating</td>
</tr>
<tr>
<td>DSM</td>
<td>Austria</td>
<td>36</td>
<td>n-butane</td>
<td>Water/xylene</td>
<td>Operating</td>
</tr>
<tr>
<td>MOL</td>
<td>Hungary</td>
<td>17</td>
<td>n-butane</td>
<td>Water/xylene</td>
<td>Operating</td>
</tr>
<tr>
<td>Cepsa</td>
<td>Spain</td>
<td>10</td>
<td>n-butane</td>
<td>Water/xylene</td>
<td>Operating</td>
</tr>
<tr>
<td>ZAK</td>
<td>Poland</td>
<td>7</td>
<td>Benzene</td>
<td>Water/xylene</td>
<td>Idle</td>
</tr>
<tr>
<td>BASF (former Sisas)</td>
<td>Belgium</td>
<td>115</td>
<td>n-butane</td>
<td>DBP</td>
<td>Closed in 2010</td>
</tr>
<tr>
<td>GIKIL</td>
<td>Bosnia</td>
<td>10</td>
<td>n-butane</td>
<td>Water/xylene</td>
<td>Operating</td>
</tr>
</tbody>
</table>

3.2.4.2 Commercially proven alternative recovery technologies

It has been relatively easier to collect details on the aqueous methods of MA recovery that are used in several plants across the globe through literature review and through Huntsman’s contribution.

Table 3.8 provides an overview of the different technologies for the manufacture of MA that have been marketed and licensed around the world. The Table does not specify the MA recovery methods used by each licensed technology, but it should be understood that all plants using the Huntsman technology currently employ DBP as an absorption solvent. In addition, the Conser/Sisas plant operated by Lanxess in Baytown, Texas, USA is also believed to use DBP as the absorption solvent. The plants which are not believed to use DBP are marked in the Table in a grey background colour.

Table 3.8: MA manufacture technologies around the globe

<table>
<thead>
<tr>
<th>Technology name</th>
<th>Developer</th>
<th>Type of catalyst</th>
<th>Feed</th>
<th>Owner / Licensor</th>
<th>User plants operating or under construction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Huntsman</td>
<td>Monsanto</td>
<td>Fixed-bed</td>
<td>n-butane</td>
<td>Huntsman</td>
<td>Pensacola, FL, USA Geismar, LA, USA Moers, Germany, AJ Jubail, Saudi Arabia Kuantan, Malaysia Ulsan, South Korea Kaohsiung, Taiwan Chang Hwa, Taiwan Lanzhou, China Yizheng, China Nanjing, China</td>
</tr>
<tr>
<td>Conser/Sisas</td>
<td>Sisas</td>
<td>Fixed-bed</td>
<td>n-butane</td>
<td></td>
<td>Baytown, TX, USA</td>
</tr>
<tr>
<td>ALMA</td>
<td>ABB Lummus Global &amp; Lonza (joint)</td>
<td>Fluid-bed</td>
<td>n-butane</td>
<td>Lonza &amp; ABB Lummus Global (joint)</td>
<td>Linz, Austria Ravenna, Italy Kawasaki, Japan Ulsan, Korea Dongying City, China</td>
</tr>
</tbody>
</table>

10 Both these were using benzene as their feedstock. The information in the Table supports the view that benzene-based plants do not face favourable operating conditions due to a high feedstock cost.
### Analysis of Alternatives

<table>
<thead>
<tr>
<th>Technology name</th>
<th>Developer</th>
<th>Type of catalyst</th>
<th>Feed</th>
<th>Owner / Licensor</th>
<th>User plants operating or under construction</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP</td>
<td>BP</td>
<td>Fluid-bed</td>
<td>n-butane</td>
<td>Ineos</td>
<td>Lima OH, USA</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Algeciras, Spain</td>
</tr>
<tr>
<td>BP-5</td>
<td>BP</td>
<td>Fixed-bed</td>
<td>n-butane</td>
<td>Ineos</td>
<td>Joliet IL, USA</td>
</tr>
<tr>
<td>Lonza / ALMA</td>
<td>Lonza</td>
<td>Fixed-bed</td>
<td>Benzene</td>
<td>Lonza</td>
<td>Ranipet, India</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cakung, Indonesia</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Bergamo, Italy</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Kashima, Japan</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Danyang City, China</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Suzhou, China</td>
</tr>
<tr>
<td>Mitsubishi / PETROX</td>
<td>Mitsubishi / BOC</td>
<td>Fluid-bed</td>
<td>n-butane</td>
<td>Mitsubishi / BOC</td>
<td>Mizushima, Japan</td>
</tr>
<tr>
<td>Scientific Design</td>
<td>Scientific Design</td>
<td>Fixed-bed</td>
<td>Benzene</td>
<td>SABIC / Sud-Chemie JV</td>
<td>Durban, South Africa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Tarapur (Mumbai), India</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Ulsan, Korea</td>
</tr>
<tr>
<td>Scientific Design</td>
<td>Scientific Design</td>
<td>Fixed-bed</td>
<td>n-butane</td>
<td>SABIC / Sud-Chemie JV</td>
<td>Ensenada, Argentina</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Durban, South Africa</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Oita, Japan</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Ulsan, South Korea</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Panjin, China</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Szazhalombatta, Hungary</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Kemaman, Malaysia</td>
</tr>
<tr>
<td>Not reported</td>
<td>Not reported</td>
<td>Fixed-bed</td>
<td>Benzene</td>
<td>Not reported</td>
<td>Kędzierzyn-Koźle, Poland</td>
</tr>
<tr>
<td>Not reported</td>
<td>Not reported</td>
<td>Fixed-bed</td>
<td>n-butane</td>
<td>Not reported</td>
<td>Lukavac, Bosnia-Herzegovina</td>
</tr>
</tbody>
</table>

Source: Based on Tecnon Orbichem (2011) with additional information from consultation

Two key points arise from the Table when considered alongside Huntsman’s knowledge of the global MA market:

- **Availability of alternative recovery technologies**: the key alternative technology, both within and outside the EU, is based on an aqueous absorption of MA. Water-based methods typically involve scrubbing the reaction off-gases with water to produce a solution of maleic acid. This is subsequently concentrated by azeotropic distillation or evaporation. The most common solvents for water-based recovery of MA are mixed xylenes, ortho-xylene and ortho-dichlorobenzene in a dual-purpose dehydrator/refiner in which the acid solution is converted to crude MA (Felthouse, Burnett, Horrel, Mummey, & Kuo, 2001). In a somewhat different method (the so-called BP MAH (formerly UCB) process), the water in the maleic acid solution is evaporated to concentrate the acid solution. The concentrated acid solution and condensed crude MA is converted to MA by a thermal process in a specially designed reactor (Felthouse, Burnett, Horrel, Mummey, & Kuo, 2001); and

- **Availability of alternative feedstocks**: as shown in Table 3.8, MA may also be manufactured from an alternative feedstock, for example benzene rather than n-butane. In the present AoA, the focus will be on the alternative MA recovery systems rather than the alternative feedstocks. The reason for this is that the choice of feedstock does not necessarily influence the choice of MA recovery technology. In other words, the use of benzene as feedstock would not really require, or lead to, the replacement/elimination of the use of DBP.

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11 Another far less common feedstock is phthalic anhydride waste.
3.3 Relevance of alternatives to MA

In the context of this AoA, alternative materials might include materials that could replace MA in its applications. Detailed consideration of the potential replacement of MA derivatives would greatly and unnecessarily expand the scope of this analysis. The alternatives would have no relevance to the operations of DEZA or Sasol-Huntsman, since the latter’s plant does not actually use MA in any further reaction or manufacturing process (it is a merchant plant simply selling the MA product downstream). Therefore, this Application for Authorisation only focuses on alternative solvents and alternative MA recovery technologies. In any case, due to its very widespread use in some very important applications, it would be impossible for MA to be replaced with a different molecule, thus eliminating the need for the use of DBP (also see SEA, Section 1.1.4.4 and Section 2.2.1.3).
4 SUITABILITY AND AVAILABILITY OF POSSIBLE ALTERNATIVES

4.1 Alternative 1: Use of the alternative substance DIBE

4.1.1 Substance ID and properties of DIBE

4.1.1.1 Name and other identifiers for the substance

The identity of DIBE is shown in the following Table.

**Table 4.1: Identity of DIBE**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>EC number</td>
<td>275-069-5</td>
<td>1</td>
</tr>
<tr>
<td>EC name</td>
<td>Diisobutyl hexahydrophthalate</td>
<td>2</td>
</tr>
<tr>
<td>CAS number</td>
<td>70969-58-3</td>
<td>1</td>
</tr>
<tr>
<td>CAS name</td>
<td>Diisobutyl 1,2-cyclohexanedicarboxylate</td>
<td>2</td>
</tr>
<tr>
<td>IUPAC name</td>
<td>Bis(2-methylpropyl) cyclohexane-1,2-dicarboxylate</td>
<td>4</td>
</tr>
<tr>
<td>Other names</td>
<td>1,2 – Cyclohexanedicarboxylic acid, bis(2-methylpropyl)ester</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Diisobutyl 1,2-cyclohexanedicarboxylate</td>
<td>2</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C₁₆H₂₈O₄</td>
<td>1</td>
</tr>
<tr>
<td>SMILES notation</td>
<td>O=C(OCC(C)C1C(C(=O)OCC(C)C)CCCC1</td>
<td>2</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>284.39</td>
<td>3</td>
</tr>
</tbody>
</table>

**Sources:**
1: (Polynt, 2007)
3: Chemical Book Internet site: [http://www.chemicalbook.com/ProductChemicalPropertiesCB8930051_EN.htm](http://www.chemicalbook.com/ProductChemicalPropertiesCB8930051_EN.htm)

4.1.1.2 Composition of the substance

No information is available on constituents or impurities of the commercially available substance. A technical data sheet for the product suggests the presence of moisture to a concentration of max. 0.1% (Polynt, 2007).

4.1.1.3 Physicochemical properties

The following Table summarises the available information on the physico-chemical properties of DIBE. The information has been collected from a variety of literature sources, which often disagree on the value of specific properties.
### Table 4.2: Physico-chemical properties of DIBE

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Remarks (models used, etc.)</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state at 20°C and 101.3 kPa</td>
<td>Clear liquid</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-4.68°C</td>
<td>MPBPWIN v1.42</td>
<td>2</td>
</tr>
<tr>
<td>Boiling point</td>
<td>296°C</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Density</td>
<td>0.995 mg/L at 20°C</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>1.01 mg/L</td>
<td>ACD/PhysChem Suite</td>
<td>2</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>6.19 x 10^-6 kPa at 25°C</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>1.7 x 10^-4 kPa at 25°C</td>
<td>EPI Suite (Modified Grain method)</td>
<td>2</td>
</tr>
<tr>
<td>Surface tension</td>
<td>34.93 dyne/cm</td>
<td>ACD/PhysChem Suite</td>
<td>2</td>
</tr>
<tr>
<td>Water solubility</td>
<td>0.9702 mg/L at 25°C</td>
<td>Estimate from Log Kow (WSKOW v1.41)</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>11.431 mg/L</td>
<td>Estimate from Fragments</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>0.477 - 11.4 mg/L</td>
<td>WS (Multicase) and EPI Suite (range of predictions based on undefined domain)</td>
<td>4</td>
</tr>
<tr>
<td>Partition coefficient n-octanol/water</td>
<td>4.44</td>
<td>Low quality, out of domain prediction from EPI Suite</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>4.5 - 4.91</td>
<td>Multicase and EPI Suite (Range of predictions based on undefined domain)</td>
<td>4</td>
</tr>
<tr>
<td>Flash point</td>
<td>172°C</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>162.566 °C</td>
<td>ACD/PhysChem Suite</td>
<td>2</td>
</tr>
<tr>
<td>Flammability</td>
<td>No data</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Self-ignition temperature</td>
<td>No data</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>No data</td>
<td>Unlikely to be of relevance</td>
<td></td>
</tr>
<tr>
<td>Granulometry</td>
<td>Not relevant</td>
<td>Not in solid form</td>
<td></td>
</tr>
</tbody>
</table>

**Sources:**
1. (Polynt, 2007)
4. OECD QSAR Toolbox: [Link](#)

#### 4.1.1.4 Classification and labelling

Online searches have been performed using the substance name, CAS number and EC number, but no information has been identified. The ECHA C&L Inventory was checked using the EC number for the substance. The Inventory includes an entry for the substance with an indication that it has not been classified by two notifiers. Based on this information, a more benign hazard profile for DIBE compared to DBP is assumed, although this must be considered uncertain given the lack of a Registration dossier and the fact that no new toxicity testing is required for the purposes of classification under the CLP Regulation.

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4.1.2 Technical feasibility of DIBE

4.1.2.1 Technical feasibility for DEZA

DEZA does not currently manufacture DIBE and does not currently have the knowledge to hydrogenate the ester that would be produced from the reaction of the relevant anhydride and alcohol. Information on the technical feasibility of DIBE for DEZA is given in the Confidential Annex to this AoA, Part 2.

Most importantly, the discussion below will demonstrate that DIBE is not a technically suitable alternative which Sasol-Huntsman could use. Therefore, DEZA would have virtually no incentive to develop technology that would allow it to manufacture the substance because it would be unable to sell it for use in this particular application.

4.1.2.2 Technical feasibility for Sasol-Huntsman

Scope of the analysis

DIBE is used in a commercial MA manufacturing technology which utilises a fluidised bed reactor and solvent recovery that is known as the ALMA (Alusuisse Italia Lummus Crest) technology. The ALMA technology produces MA from n-butane (as the Huntsman technology does) and was jointly developed and licensed by Lummus Technology and Polynt SpA (Lummus, 2009).

The use of DIBE as an absorption solvent in the place of DBP would mean that the Sasol-Huntsman MA plant would require the modification of the MA manufacturing technology currently used in the Moers plant to meet the requirements of the ALMA technology. Therefore, for the assessment of the technical suitability of this potential alternative substance, we will be looking both at the comparison between the two absorption solvents and at the practical implications of the conversion of the Moers plant.

Description of the use of the substance

The ALMA joint development programme began in 1981 and a semi-commercial unit started up in 1984. The first full-scale commercial plant in Yokkaichi, Japan started up in 1989. Five additional plants (in South Korea, Taiwan, Japan, Italy, and China) which use the ALMA reactor came on-stream in the 1990s (Lummus, 2009) but, importantly, no new plant has started using this technology since 1995-1996. In the EU, the method is currently used by Polynt SpA in Ravenna, Italy. Additionally, at least one of the foregoing Asian plants is believed to have now discontinued the use of the ALMA process.

The process is shown schematically in Figure 4.1 overleaf. n-butane and air are fed separately into the fluidised bed catalytic reactor to produce MA. In a fluidised bed process, reaction gases flow upward through a bed of catalyst particles (Kababji, 2009). The exothermic heat of the reaction is removed by generating high-pressure steam (as in the Huntsman technology). After cyclone separation of the elutriated solids, the reactor effluent is cooled, filtered and fed to the absorber. In

13 A further sixth plant is believed to use the front-end of the ALMA technology but this is not relevant to the discussion on the conversion of the Moers plant.
the absorber, a solvent, typically DIBE, is used to selectively remove MA from the cooled reactor effluent. The tail gas is exhausted to an incinerator for recovery of its heating value. The bottoms are fed to the stripper where crude MA is separated as distillate from recirculated solvent. A small slipstream of the circulating solvent is purified to remove solvent degradation products in order to prevent the build-up of impurities in the solvent recycle loop (Lummus, 2009).

![Figure 4.1: Flow sheet of the ALMA process (Lummus, 2009)](image)

There are evident similarities between the Huntsman and ALMA technologies. Moreover, Sasol-Huntsman is in a well-informed position to assess the technical implications of replacing DBP with DIBE and moving closer to the ALMA technology. In the mid-1990s, Condea (the predecessor to Sasol Solvents) was considering a plant expansion and examined all commercially proven methods. After careful consideration of detailed technical proposals by technology licensors (including those promoting the ALMA technology) and evaluation of the advantages and disadvantages of the different technologies, Condea opted for the Huntsman technology to which it converted in 1999. Documentation that was submitted to Condea provides very useful and quantitative insights into how the ALMA technology would work.

**Important Note**

It should be noted that, in 1990s, the Moers plant had a much smaller capacity than it has currently and the engineering plans made available to Condea are now almost 20 years old. Although these plans are considered reliable (given that since the mid-1990s the ALMA technology has not been introduced into a new plant), it cannot be precluded that some elements of the ALMA technology may have been modified in the intervening period. Therefore, although presumptions made in this document are based on the best available information, material changes may have been made to this alternative technology, which may affect the accuracy of estimates presented here.

**Comparison of DIBE to DBP against technical comparison criteria**

Table 4.3 summarises the comparison between DBP and DIBE across the selected technical criteria (originally presented in Table 2.2). The criteria that DIBE fails to meet are marked with a grey
ANALYSIS OF ALTERNATIVES

Vapour pressure is not included in the Table as it is adequately addressed under the normal boiling point row (the two parameters are clearly interlinked).

### Table 4.3: Comparison of DIBE to DBP against key technical performance criteria

<table>
<thead>
<tr>
<th>Technical comparison criteria</th>
<th>Values for DBP</th>
<th>Values for DIBE</th>
<th>Threshold value / Desired range</th>
<th>Comparison result and comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal boiling point</td>
<td>340°C</td>
<td>296°C</td>
<td>250-350°C</td>
<td><strong>Criterion met</strong> (based on Table 4.2) but boiling point considerably lower than DBP thus increasing overhead losses and solvent costs</td>
</tr>
<tr>
<td>Dissolution of MA</td>
<td>&gt;20% wt</td>
<td>&gt;20% wt</td>
<td>&gt;20% wt</td>
<td><strong>Criterion met</strong></td>
</tr>
<tr>
<td>Dissolution of fumaric acid</td>
<td>0.066% wt</td>
<td>&lt;0.05 wt% at 60°C</td>
<td>&gt;0.06% wt at 60°C</td>
<td><strong>Criterion not met</strong>. This would result in higher solvent consumption and increased solids deposition with consequent equipment fouling</td>
</tr>
<tr>
<td>Solubility in water</td>
<td>11.40 ± 0.71 mg/L at 25°C</td>
<td>0.48-11.4 mg/L at 25°C</td>
<td>&lt;100 mg/L</td>
<td><strong>Criterion met</strong> (based on Table 4.2)</td>
</tr>
<tr>
<td>Difference from water density</td>
<td>+0.046 g/mL</td>
<td>-0.005 to +0.01 g/mL</td>
<td>&gt;0.020 g/mL</td>
<td>Losses of solvent to water would thus be higher than when using DBP. Loses to water would mean (a) increased costs, (b) generation of an additional waste stream, and (c) increased probability of contamination of DIBE with caustic (used for washes in the ALMA technology). The conveyance of caustic into the MA process by DIBE could initiate an explosive decomposition of MA</td>
</tr>
<tr>
<td>Decomposition products easily separable from MA</td>
<td>Decomposition of DBP gives phthalic anhydride</td>
<td>No data</td>
<td>Not relevant</td>
<td>No judgement can be made due to the lack of sufficient information</td>
</tr>
<tr>
<td>Thermal stability</td>
<td>Stable at process temperature</td>
<td>No data</td>
<td>Not relevant</td>
<td>No judgement can be made due to the lack of sufficient information</td>
</tr>
<tr>
<td>Flash point (OC)</td>
<td>191°C</td>
<td>172°C</td>
<td>≥191°C</td>
<td><strong>Criterion not met</strong> (based on Table 4.2). The lower flash point of DIBE would suggest an increased safety hazard compared to DBP</td>
</tr>
</tbody>
</table>

Source: CSR; applicant’s own information

The Table demonstrates the technical shortcomings of DIBE, more specifically, its poorer boiling point, its inferior dissolution of FAc and the small difference between its density and that of water, which have profound technical performance, equipment suitability, maintenance and economic implications. DIBE’s flash point is also lower than that of DBP thus resulting in a higher probability that a fire may occur in the absorber column.

**Required changes to MA manufacture equipment**

The ALMA technology appears to have similarities to the Huntsman technology, as shown in Figure 4.1. Given the similarities, if DIBE were to be used by Sasol-Huntsman, one would expect the equipment downstream from the absorber to be of a similar size. On the other hand, a key difference is that the Huntsman technology uses a fixed bed reactor, while the ALMA method uses a fluidised bed reactor. This difference, though important, it is not critical to the comparison of solvent recovery technology. It is assumed that if the Sasol-Huntsman plant had to switch from DBP to DIBE, a reactor change would not be required.
However, certain changes would be required before the plant could adapt to the ALMA technology:

- the absorber column would likely have to be entirely replaced. The MA concentration in the off-gas of an ALMA technology plant is different to the concentration in the off-gas in a Huntsman technology plant. The reason for this is the difference in reactor types explained above. The fluidised bed requires a much higher consumption of butane gas but also a reduced consumption of air. With the ALMA technology, the reaction off-gas would have MA concentrations higher than those generated by the Huntsman technology. Therefore, the absorber column would have to be re-designed in order to accommodate the reactor off-gas of a Huntsman-designed reactor; and

- the Moers plant would likely have to convert to the ALMA mixer/settler/decanter technology. Information available to Huntsman indicates that the ALMA technology delivers the separation of MA by using caustic washing of the solvent and multiple mixing and decanting steps. Crude MA is separated by a stripper, similar to the Huntsman process. The density difference between water and DIBE would be too small to allow for efficient separation of the two using the current Huntsman technology, so a new mixer/settler/decanter would be needed.

These key differences, between the reactor types, do pose a problem for estimating the plant modification requirements that would arise from a switch from DBP to DIBE. The approach taken in this AoA is to assume that a change in the absorption solvent would not require a concomitant switch to a fluidised bed reactor; instead, only a change to the MA recovery system downstream from the reactor would be required while still using the Huntsman technology reactor. The assumption that the reactor type does not matter is untested and unproven; if conversion were ever to be actually implemented, this assumption might well prove to be wrong. The ALMA technology has never been commercially practiced at the scale successfully demonstrated by Huntsman (>100 ktonnes MA per year) and whether conversion would actually work is uncertain.

Market success as a measure of technical suitability

The consistent selection of Huntsman technology over ALMA technology by world-leading producers of MA, has demonstrated that the market believes that the ALMA technology is inferior to Huntsman’s technology. DBP-based recovery is widely considered the current state-of-the-art and continues to be the focus of on-going process development R&D within the worldwide MA industry. For example, a 2012 patent by Italian inventors (WO 2012/081043 Al) on MA absorber design features the use of DBP. A Japanese licensor has also patented and recently begun to offer DBP-based MA recovery technology. Although other technologies are sometimes selected for small projects or in developing countries, every large-scale butane-to-MA project in the world has chosen Huntsman’s technology since the mid-1990s, including projects by leading global MA manufacturers such as BASF and Sinopec.

Table 4.4 shows the locations and capacities of all large-scale plants using Huntsman’s DBP-based technology. The Moers plant is the only plant based in the EU and is the fourth largest on the list in terms of MA production capacity. It should be noted, however, that the Sinopec Yizheng plant in China and the BASF-Petronas plant in Malaysia produce MA only as feedstock for 1,4-butanediol, while Sasol-Huntsman sells its entire product to downstream users. Overall, Sasol-Huntsman is the second largest merchant MA plant in the world.

With the commissioning of two new Huntsman-licensed plants in 2013, it is expected that Huntsman technology will become the basis for more than half of global MA production capacity (estimated at 1.6 million tonnes). Again, this is a clear indication that the market has a preference for Huntsman’s technology. On the other hand, the licensing of the fluidised bed technology has had limited market success so far. Literature suggests that no more than six plants currently use the
ALMA fluidised bed technology (Tecnon OrbiChem, 2011) and it is understood that not all of these plants use DIBE-based recovery technology. As indicated above, since the mid-1990s, there has been no plant that was set up or converted to the ALMA technology.

Table 4.4: Global MA production plants based on the Huntsman DBP-based technology

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Licensed</th>
<th>Start-Up</th>
<th>Capacity (t/y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sinopec Yizheng Fibers Co.</td>
<td>Yizheng, China</td>
<td>2010</td>
<td>2013</td>
<td>117,000</td>
</tr>
<tr>
<td>BASF-Petronas</td>
<td>Malaysia</td>
<td>1999</td>
<td>2003</td>
<td>113,000</td>
</tr>
<tr>
<td>Huntsman (Pensacola)</td>
<td>Florida, USA</td>
<td>Owned</td>
<td>1983</td>
<td>110,000</td>
</tr>
<tr>
<td>SASOL-Huntsman</td>
<td>Germany</td>
<td>1996/2008</td>
<td>1999/2011</td>
<td>105,000</td>
</tr>
<tr>
<td>International Diol Corp</td>
<td>Saudi Arabia</td>
<td>2002</td>
<td>2005</td>
<td>85,000</td>
</tr>
<tr>
<td>Zhejiang Jiangshan Chemical</td>
<td>Ningbo, China</td>
<td>2011</td>
<td>2013</td>
<td>82,000</td>
</tr>
<tr>
<td>Huntsman (Geismar)</td>
<td>Louisiana, USA</td>
<td>Owned</td>
<td>2009</td>
<td>45,000</td>
</tr>
<tr>
<td>TCC Chemical Corp</td>
<td>Taiwan</td>
<td>1997</td>
<td>2000</td>
<td>40,000</td>
</tr>
<tr>
<td>TPCC</td>
<td>Taiwan</td>
<td>2006</td>
<td>2009</td>
<td>40,000</td>
</tr>
<tr>
<td>GUCC</td>
<td>Taiwan</td>
<td>1988</td>
<td>1990</td>
<td>27,000</td>
</tr>
<tr>
<td>Yongsan Chemical Inc.</td>
<td>Korea</td>
<td>1996</td>
<td>1998</td>
<td>20,000</td>
</tr>
<tr>
<td>Lanlian</td>
<td>China</td>
<td>2005</td>
<td>2006</td>
<td>20,000</td>
</tr>
<tr>
<td><strong>Total Owned / Licensed Capacity</strong></td>
<td></td>
<td></td>
<td></td>
<td><strong>804,000</strong></td>
</tr>
</tbody>
</table>

Source: applicant’s own information

4.1.3 Reduction of overall risk due to transition to DIBE

4.1.3.1 Introduction and important note

The information below is given for completeness and to inform decision-makers. The key point of this Application for Authorisation is that the risks from worker exposure to DBP during the manufacture of MA are adequately controlled and the replacement of DBP by an alternative substance would not result in any discernible benefit to workers’ health.

4.1.3.2 Human health hazard profile of DIBE

Research has been undertaken to identify and collect information on the hazard profile of DIBE. It has not been possible to identify sources of specific relevant information on the substance.

In the absence of any published information on the toxicity profile of DIBE to mammalian species, the OECD QSAR toolbox\textsuperscript{14} was employed to derive predictions for hazard endpoints for which models are currently available. The US Food and Drug Administration Endocrine Disruptor Knowledge Base (FDA EDKB) androgen receptor binding dataset\textsuperscript{15} was also utilised to explore the potential androgenicity/anti-androgenicity of this substance. The results are given in Table 4.5.

\textsuperscript{14} Available at: http://www.oecd.org/chemicalsafety/assessmentofchemicals/theoecdqsartoolbox.htm#Download_qsar_application_toolbox (accessed on 27 November 2012).

\textsuperscript{15} Available here: http://www.fda.gov/ScienceResearch/BioinformaticsTools/EndocrineDisruptorKnowledgebase/default.htm (accessed on 27 November 2012).
**Acute and chronic toxicity:** while a high rate of intestinal absorption is predicted via the oral (gastrointestinal) route, the chemical structure was noted to possibly not fit well within the domain limitations of the OECD models; hence, such a prediction should be regarded with caution.

Although there is no suitable QSAR model within the OECD toolbox that informs on acute toxicity, the behaviour of similar substances does not suggest immediate concerns for high toxicity under acute exposure conditions. No information was available from the QSAR toolbox to inform on DIBE’s repeat dose toxic potential.

**Irritancy and sensitisation:** predictions generated on irritancy and sensitisation potential show a somewhat variable picture with no strong, consistent indication of high concern being predicted for irritancy. A read-across approach identified a possible concern for sensitization, but this should be weighed against QSAR-based modelling from the Danish Environmental Protection Agency (Danish EPA) database, which suggests a negative response. Overall, therefore, although no definitive conclusions are possible, there does not appear to be significant grounds for concern for these endpoints at present.

**Genotoxicity and carcinogenicity:** with regard to DIBE’s genotoxic potential, most predictions on in vitro prokaryotic and eukaryotic mutagenicity are negative with only isolated exceptions. Those related to in vivo activity also do not raise any particular concerns. Similarly, there appears to be little basis for concern with regard to carcinogenic potential.

**Reproductive toxicity and endocrine disruption potential:** a QSAR prediction of teratogenicity (from the FDA Teratogen Information System (TERIS))\(^\text{16}\), reported in the Danish EPA Database, does warrant attention given that the substance was reported to fall within the model’s domain. Alongside this suggestion of potential developmental toxicity, it should be noted that an entry in the RiscTox database of the Spanish Instituto Sindical de Trabajo, Ambiente y Salud (ISTAS)\(^\text{17}\) reports that DIBE is included in a blacklist because of endocrine disruption effects.

According to the ISTAS website, the blacklist includes substances which damage health and the environment for which their use or presence in the workplace and their discharge to the environment should be avoided. These substances, whose elimination is a priority, include carcinogens, mutagens, substances toxic to reproduction, endocrine disruptors, sensitisers, neurotoxic substances, PBT/vPvB substances or those that may cause long-term adverse effects in the aquatic environment.

However, it is unclear if this is because of generic concerns regarding endocrine effects relevant to humans or non-human species and, indeed, no experimental evidence to substantiate the inclusion is given. Hence, it cannot be discounted that an ‘endocrine disrupter’ label might have been applied solely because of generic concerns regarding any substance embodying a ‘phthalate’ structure or a derivative thereof.

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\(^{16}\) For further information, please see here: [http://depts.washington.edu/terisweb/teris/](http://depts.washington.edu/terisweb/teris/).

### Table 4.5: Human health and environmental hazard profile for DIBE – QSAR results

<table>
<thead>
<tr>
<th>Hazard endpoint</th>
<th>Finding</th>
<th>Data source</th>
<th>Study design</th>
<th>Assessed robustness/Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicokinetics</td>
<td>Extent of absorption = 93%</td>
<td>OECD QSAR</td>
<td>QSAR prediction of human intestinal absorption by Multicase expert system</td>
<td>Result reported to be undefined with regard to domain applicability, hence considered of doubtful reliability</td>
</tr>
<tr>
<td>Acute toxicity</td>
<td>No suitable QSAR model available</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Irritation/Corrosion</td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for ‘severe’ skin irritation</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Undefined</td>
<td>OECD QSAR</td>
<td>QSAR prediction for BfR skin irritation/corrosion assay</td>
<td>Result reported to be undefined with regard to domain applicability, hence considered of doubtful reliability</td>
</tr>
<tr>
<td>Sensitisation</td>
<td>Positive</td>
<td>OECD QSAR</td>
<td>Read-across from Givaudan (based on following criteria: Strong sensitiser: EC3 &lt; 10%; Weak sensitiser: EC3 ≥10% &lt; 50%; Non-sensitiser: EC3 ≥50%)</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR</td>
<td>QSAR prediction for skin sensitisation, from Danish EPA Database</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>Respiratory</td>
<td>No information available</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Repeat dose toxicity</td>
<td>Oral</td>
<td>No suitable data available to inform read-across according to the OECD QSAR toolbox</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Genetic toxicity</td>
<td>Positive</td>
<td>OECD QSAR (citing Romualdo Benigni)</td>
<td>Read-across on Ames Test with S9 activation</td>
<td>Reported to be outside of QSAR domain; hence considered of doubtful reliability</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Romualdo Benigni)</td>
<td>Read-across on Ames Test without S9 activation</td>
<td>Reported to be outside of QSAR domain; hence considered of doubtful reliability</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for Ames test (Salmonella typhimurium) with no S9 activation</td>
<td>Reported to be outside of QSAR domain; hence considered of doubtful reliability</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for Ames test (Salmonella)</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for Ames test (Salmonella) for which is no S9 information</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for Ames test (Salmonella) with S9 activation</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
</tbody>
</table>
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<table>
<thead>
<tr>
<th>Hazard endpoint</th>
<th>Finding</th>
<th>Data source</th>
<th>Study design</th>
<th>Assessed robustness/Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for Ames test (Salmonella) without S9 activation</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR</td>
<td>Prediction for mammalian cell unscheduled DNA-synthesis assay without definition of metabolic activity status</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR</td>
<td>DNA-reactivity (based on Ashby Fragments)</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>In vitro – Chromosomal effect</td>
<td>Negative</td>
<td>OECD QSAR</td>
<td>Prediction for mammalian cell chromosome aberration assay</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR</td>
<td>Prediction for sister chromatid exchange assay for mouse bone marrow without definition of metabolic activity status</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>Prediction for SCE stands for sister chromatid exchange assay for mouse bone marrow without definition of metabolic activity status</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Positive</td>
<td>OECD QSAR</td>
<td>Sister chromatid exchange in Syrian Hamster Embryo (SHE) assay, without definition of metabolic activity status</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>In vivo - Mutation</td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>Prediction for sex-linked recessive lethal assay in Drosophila melanogaster</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>In vivo - Chromosomal effect</td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>Prediction for rodent dominant lethal assay</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>Prediction for mouse micronucleus assay</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>Carcinogenicity</td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction based on FDA Cancer Female Mouse</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td></td>
<td>Carcinogenic potency value (TD50) = 1.00E+03 mg/kg</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction from Mouse Carcinogenic Potency Database (CPDB)</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>Hazard endpoint</td>
<td>Finding</td>
<td>Data source</td>
<td>Study design</td>
<td>Assessed robustness/Comment</td>
</tr>
<tr>
<td>-----------------</td>
<td>---------</td>
<td>-------------</td>
<td>--------------</td>
<td>-----------------------------</td>
</tr>
<tr>
<td>Toxicity to reproduction</td>
<td>Reproductive</td>
<td>No information available</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Developmental/teratogenicity</td>
<td>Positive</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for teratogenicity (FDA TERIS)</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>Protein binding potential</td>
<td>No alert found</td>
<td>OECD QSAR</td>
<td>QSAR prediction</td>
<td>No indication identified that model was operating outside of its operational limits</td>
</tr>
<tr>
<td>Oestrogen Receptor Binding Activity</td>
<td>Probability of estrogenic activity = 10%</td>
<td>OECD QSAR</td>
<td>QSAR prediction for oestrogen receptor binding by RBA (Multicase) expert system</td>
<td>Reported to be outside of QSAR domain; hence considered of doubtful reliability</td>
</tr>
<tr>
<td></td>
<td>Negative</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for oestrogen receptor binding</td>
<td>Reported to be within QSAR domain, hence considered acceptable</td>
</tr>
<tr>
<td>Other toxic endpoints</td>
<td>Negative</td>
<td>FDA EKDB model</td>
<td>Model reports ‘inactive’ prediction with regard to ER binding and ER gene activation</td>
<td>N/A</td>
</tr>
<tr>
<td>Androgen Receptor Binding Activity</td>
<td>Active</td>
<td>FDA EKDB model</td>
<td>Model reports ‘active’ prediction for AR binding</td>
<td>N/A</td>
</tr>
<tr>
<td>Aquatic toxicity</td>
<td>Invertebrate</td>
<td>EC50 = 5.26 mg/L</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for lethality in <em>Daphnia magna</em></td>
</tr>
<tr>
<td></td>
<td>Protozoan</td>
<td>IGC50 = 45.6 mg/L</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for immobilisation potential in <em>Tetrahymena pyriformis</em></td>
</tr>
<tr>
<td></td>
<td>Algal</td>
<td>EC50 = 27.6 mg/L</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for lethality in <em>Pseudokirchneriella subcapitata</em></td>
</tr>
<tr>
<td></td>
<td>Fish</td>
<td>LC50 = 3.83 mg/L</td>
<td>OECD QSAR (citing Danish EPA Database)</td>
<td>QSAR prediction for lethality in Fathead minnow</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.78 (0.333-68.7)</td>
<td>OECD QSAR</td>
<td>QSAR prediction for lethality in Fathead minnow from by M1 - LC50 model</td>
</tr>
</tbody>
</table>

Sources:
OECD QSAR data obtained using OECD QSAR Toolbox at Internet site: [Link](#)
FDA EKDB data obtained using FDA EKDB Database at Internet site: [Link](#)
The output of the OECD toolbox modelling did not identify any concern as to either protein binding or oestrogen receptor binding potential. The FDA EKDB model did, however, suggest potential activity with regard to the substance’s ability to interact with the androgen receptor, although it does not inform as to whether this might result in androgenic and/or anti-androgenic properties, depending on conditions; the robustness of this prediction is uncertain.

Safety concerns

As explained earlier, if Sasol-Huntsman were to opt for the use of DIBE, this would involve a conversion of the Moers plant to (a variant of) the ALMA technology and the concomitant conversion to the ALMA mixer/settler/decanter technology which uses caustic washing. The use of caustic is strictly prohibited in the Huntsman technology since caustic and MA are known to react violently\(^\text{18}\). A process upset within ALMA’s technology, that might allow caustic to come into contact with MA, could have severe safety consequences. Thus, the ALMA technology is exposed to an intrinsic safety hazard that is fundamentally absent from Huntsman’s technology.

Environmental fate and behaviour and ecotoxicology of DIBE

The OECD toolbox predictions of bioaccumulation potential give a value of only 4.3 at 25°C.

As discussed above, the RiscTox database of ISTAS suggests that the substance may show endocrine effects and it is suggested by a Danish EPA list of advisory CLP-classifications to warrant a Chronic 1 environmental toxin classification\(^\text{19}\). However, available data based purely on QSAR predictions (see Table 4.5) seem to be suggestive of a somewhat lower chronic aquatic toxicity classification: the acute EC\(_{50}/LC\(_{50}\) values predicted across three trophic levels and the range of predicted octanol/water partition coefficients noted for DIBE (see Table 4.2) would appear to only warrant consideration as a tentative Aquatic Chronic Category 2.

REACH Registration and classification and labelling of DIBE

The substance was pre-registered\(^\text{20}\), with an originally envisaged REACH Registration deadline of 30/11/2010\(^\text{21}\). However, no such registration has yet taken place\(^\text{22}\) although ECHA’s website had suggested that the substance was intended for registration by 2013\(^\text{23}\). The lack of an early REACH Registration may be taken as indicative that the substance may not possess significant hazardous

\(^{18}\) Literature confirms that contamination with sodium salts can drastically decrease the stability of MA at elevated temperatures. Serious accidents on an industrial scale have resulted from sodium salt contamination, and the scientific literature refers to additives designed to mitigate the effects of sodium ion contamination of MA (Vogler, Cecil, & Koerner, 1983).

\(^{19}\) Available at http://www.mst.dk/English/Chemicals/assessment_of_chemicals/The_advisory_list_for_selfclassification/CLPclassification.htm (accessed on 18 December 2012)

\(^{20}\) The only known manufacturer of the substance, Polyni SpA, based in Italy, announced in 2008 that it pre-registered the substance under reference number: 05-2114132000-78-0000 (see http://eng.polynt.it/user/download.aspx?FILE=OBJ00353.PDF&TIPO=FLE&NOME=Announcement).


properties, such as CMR or PBT potential; though, as noted above, the situation with regard to
developmental toxicity and endocrine activity remains somewhat unclear.

Additionally, the anticipated Registration date is also indicative of the limited scale of current
manufacture or use of this substance in the EU.

4.1.3.3 Conclusion on the risks from the potential use of DIBE

The limited available data does not allow firm conclusions to be reached on the hazards of DIBE. However, there is reason to believe that DIBE may have a more benign mammalian hazard profile than DBP, given the lack of a REACH Registration dossier (so far) and some aspects of the OECD QSAR outputs. In particular, it appears that it is unlikely that the substance would meet the requirements for classification as a CMR 1A/1B.

There exist, however, grounds for concern with regard to its developmental and/or endocrine profile (including with respect to its ability to interact with the androgen receptor), and for its environmental toxicity.

Table 4.6 below summarises the limited insights available on the hazard profile of DIBE in comparison with that established for DBP. Better characterisation of the extent to which such concerns are justified would, however, require additional research, potentially involving use of vertebrate animals.

Table 4.6: Hazard comparison of DBP with DIBE

<table>
<thead>
<tr>
<th></th>
<th>DBP</th>
<th>DIBE</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Human health</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acute toxicity</td>
<td>Very low</td>
<td>No data</td>
</tr>
<tr>
<td>Irritancy</td>
<td>Uncertain</td>
<td></td>
</tr>
<tr>
<td>Sensitisation</td>
<td>Uncertain</td>
<td></td>
</tr>
<tr>
<td>Repeat dose toxicity</td>
<td>Toxic</td>
<td>No data</td>
</tr>
<tr>
<td>STOT</td>
<td>Liver; kidney; testes</td>
<td></td>
</tr>
<tr>
<td>Reproductive toxicity</td>
<td>1B (male fertility)</td>
<td>No data</td>
</tr>
<tr>
<td>Developmental toxicity</td>
<td>1B (males)</td>
<td>Uncertain</td>
</tr>
<tr>
<td>Carcinogenicity</td>
<td>Data are insufficient to determine the carcinogenic potential. No evidence of carcinogenicity is available. The CSR assumes that the substance is not carcinogen</td>
<td></td>
</tr>
<tr>
<td><strong>Environment</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Aquatic</td>
<td>Very toxic</td>
<td>Uncertain</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other concerns</td>
<td>Potential endocrine disruptor</td>
<td>Uncertain endocrine disruptor</td>
</tr>
</tbody>
</table>

Based on the limited information available and if viewed simplistically, it would appear that – if it were assumed that the extent and mode of use of DIBE would be similar to that of DBP – its adoption might represent some, although an uncertain, lessening of hazard. However, the lack of dose-response information for the endpoints of concern precludes the assessment of the relative potency of this substance compared to that shown by DBP. Finally, the use of caustic washing within the ALMA technology could raise safety concerns in respect to the possible violent reaction.
of caustic with MA which is currently absent from the Huntsman technology. The risk of fire within the absorber column would appear to be materially greater than under the Huntsman technology.

4.1.3.4 Other environmental impacts

Additional release of greenhouse gases

As will be explained in Section 4.1.4.2, the conversion of the Sasol-Huntsman plant to the ALMA technology to allow the replacement of DBP by DIBE would mean that, for over two years (25 months), the MA plant would not be able to generate steam which is required by the Sasol Solvents power plant for serving the needs of Sasol Solvents and for exporting electricity to the grid. It will be explained that for two years, the Sasol Solvents power plant would be deprived of 650 GWh of steam currently exported from the MA plant. To obtain this from fuel gas, an additional 459 GWh would have to be obtained each year from natural gas purchased from the open market, as shown in the Confidential Annex to this AoA.

Additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf, Part 5.

This additional consumption of natural gas (equivalent to a total of 918 GWh over two years) would mean an additional release of CO₂ to the atmosphere that would normally not occur under the “Applied for use” Scenario. Using greenhouse gas emission factors available from the UK Department for Environment, Food and Rural Affairs\(^{24}\), it can be calculated that the consumption of natural gas equivalent to 918 GWh would result in the release of an additional 918,000,000 kWh x 0.18404 = ca. 170 ktonnes CO₂ (eq) per year on a gross calorific value basis.

Monetisation of externalities

Monetisation of greenhouse gas emissions is based on the estimate of marginal abatement costs in a recent publication by the European Environment Agency\(^{25}\). The valuation adopted for CO₂ emissions is £33.6 per tonne, based on a methodology developed by the UK government for carbon

\(^{24}\) Available at: http://www.ukconversionfactorscarbonsmart.co.uk (accessed on 23 June 2013).

\(^{25}\) There are two reasons for using a control cost approach for greenhouse gas (GHG) emissions (EEA, 2011):

a. There are concerns over the very high uncertainty in estimates of climate costs. This uncertainty is unavoidable as damage is dependent on the future development of society, particularly with respect to population and economic growth, neither of which can be forecast with great confidence, and the extent to which value is attached to future events.

b. Where national emission ceilings effectively exist for GHGs (as under the Kyoto Protocol), the marginal effect of a change in emissions is not to alter the amount of damage that is done to health, infrastructure and the environment, but to change the cost of reaching the national ceiling. To assume otherwise assumes that countries are very willing to exceed the agreed emission reduction targets (abating emissions more than they are legally required to do). The difficulty in gaining international consensus on effective GHG controls suggests that this is unlikely at present.

There are issues with this approach in that the marginal costs of abatement for GHGs are subject to their own significant uncertainties, and that they are specific to a certain level of emission control. However, the use of an approach involving use of marginal abatement costs can be considered a pragmatic response to the problems faced in this part of the analysis. Notably, damage cost methods applied by other studies estimate a range between £5 and £120 per tonne of CO₂, so the cost value given in the main text is within this range and rather conservative.
valuation in public policy appraisal. The latest update of this methodology provides a central short-term traded price of carbon of £29 per tonne CO$_2$-equivalent in 2020. The present day exchange rate was used to convert the value in £ to €$^{26}$.

Therefore, one-off external (damage) costs due to the emission of an estimated additional 170 ktonnes of CO$_2$ are calculated at ca. **€5.7 million**. It is clear that the stoppage of steam generation from the MA production plant during its conversion would have a detrimental effect on the environment.

### 4.1.4 Economic feasibility of DIBE

#### 4.1.4.1 Economic feasibility for DEZA

Without access to a technology that allows the manufacture of hydrophthalates, DEZA would not be able to manufacture DIBE. Acquisition of the required technology would be very costly, as described in the Confidential Annex to this AoA, Part 2.

Importantly, based on the discussion on the technical shortcomings of DIBE (see Section 4.1.2) and the analysis of the economic infeasibility of DIBE and the ALMA technology for Sasol Huntsman (to be discussed in Section 4.1.4.2), DIBE is not a suitable alternative. Thus, even if DEZA were to become capable of manufacturing DIBE, it is unlikely that Sasol-Huntsman would be purchasing this solvent. Therefore, DEZA would lose the sales of DBP and would not be able to replace these by sales of DIBE. The turnover of DBP that would be lost is presented in the SEA (Section 2.2.11).

Importantly, the SEA points out that the loss of sales of DBP to Sasol-Huntsman would cause the collapse of the entire sales of DBP by DEZA and would lead to the cessation of the production of the substance, even if Authorisation were to be granted for other uses of the substance. For these reasons, DIBE cannot be considered to be an economically feasible alternative for DEZA.

#### 4.1.4.2 Economic feasibility for Sasol-Huntsman

**Overview**

For the assessment of the economic feasibility of DIBE (and the concomitant conversion to the ALMA technology) for Sasol-Huntsman, the following cost elements will be considered:

1. costs arising from the increased price of the absorption solvent;
2. costs arising from increased absorption solvent consumption (due to the poorer physico-chemical characteristics of DIBE in comparison to DBP);

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$^{26}$ A value for the year 2020 was selected rather than, for example, the current spot trading price for carbon, to remove one element of uncertainty with respect to short-term price fluctuations affecting the value of the marginal abatement cost. The year 2020 is also the end of the phase III period of the EU Emissions Trading System. While it is stressed that this figure reflects the views of the United Kingdom government rather than a consensus-based estimate widely recognised across Europe, it is considered reasonably representative and consistent with other figures that have been discussed, either in relation to damage costs or abatement costs. For illustrative purposes, the UK methodology further recommends an increased value of carbon by 2030, with a central price of £74 per tonne CO$_2$-equivalent (EEA, 2011).
3. costs arising from the modifications to the plant in order to convert from the Huntsman technology to the ALMA technology;

4. costs arising from increased fouling of the production line and associated maintenance requirements associated with the reduced solubility of FAc in DIBE; and

5. the cost of a new licence to operate under the ALMA technology.

Some additional cost elements are considered insignificant and have not been investigated in detail. For example, it is estimated that the caustic wash process utilised by the ALMA technology consumes 3.8 kg of caustic per tonne of MA produced and consequently produces a waste stream, which is unsuitable for incineration and thus imposes a waste treatment burden not required under the Huntsman technology. The cost associated with a (maximum) consumption of 400 tonnes of caustic soda (corresponding to a maximum MA production of 105 ktonnes per year) and the associated disposal of wastewater has not been taken into account in the discussion below.

It is also important to note that during the plant conversion phase, the Sasol Solvents power plant would be deprived of steam currently exported from the MA plant. Therefore, the theoretical use of DIBE under the ALMA process would be accompanied by a cost to Sasol Solvents associated with the purchase of energy to compensate for the loss of the steam imports.

The discussion here aims to demonstrate that the cost of switching to DIBE and the ALMA technology, particularly the cost and duration of the modification of the Moers plant, would ultimately result in the closure of the Sasol-Huntsman plant.

Cost element 1: Price of DIBE

**Current price information:** there is only one known supplier of DIBE, the Italian company Polynt that is a direct competitor to both Huntsman (as it acts as the licensor of the ALMA technology) and Sasol-Huntsman (as it manufactures MA in two plants in Italy). It has not been possible to directly obtain specific information on the price of DIBE.

Publicly available sources have been researched for price data for DIBE, but information has not been identified. Therefore, assumptions had to be made regarding the price ‘premium’ of DIBE over DBP. A higher price than DBP is assumed due to the additional production stage (hydrogenation) required for the manufacture of DIBE, which attracts an additional cost for the manufacturer.

DEZA’s experience suggests that the additional cost of the hydrogenation reaction might add a further €300 per tonne of DIBE in comparison to the price of DBP. This is only an informed assumption, as there is no actual experience with the manufacture of this substance. Details on the source of this estimate are given in the Confidential Annex, Part 2.

An additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf, Part 2.

Such a price premium would mean a price increase of ca. 20% compared to the price of DBP shown in Table 3.4.

**Future price projections:** judging from the absence of a REACH Registration dossier for DIBE, the tonnage of DIBE manufactured and placed on the market in the EU (presumably only by Polynt) would appear to be below 1,000 t/y. Moreover, assuming that Polynt manufactures DIBE, which needs to be used both by Polynt internally at its Ravenna plant and probably externally by licensees...
of the ALMA technology, the amount of DIBE that could, theoretically, become available to Sasol-Huntsman is uncertain. Below we calculate Sasol-Huntsman’s estimated demand of DIBE if DBP were to be replaced. The estimated figure is high enough to raise concerns as regards the market availability of DIBE. Poor market availability and a theoretical future increased demand (from Sasol-Huntsman) could put upward pressure on the market price of DIBE, unless Polynt were able to increase its production of the substance in time for serving the needs of all potential customers. In light of all this, the future price of DIBE cannot be quantitatively estimated.

**Conclusion**: since the potential future price of DIBE cannot be estimated with reasonable certainty, the assumption is made here that DIBE’s price will remain at a level €300 higher than DBP’s price per tonne.

**Cost element 2: Increased solvent consumption**

**Approach**: the replacement of DBP by DIBE would not occur on a 1:1 basis due to the different physico-chemical characteristics of DIBE that affect its losses during the manufacture of MA.

The information originally proposed to Condea in the mid-1990s showed a required airflow of 61,648 Nm³/hr for a 40 kt MA/y plant. In comparison, Huntsman’s fixed bed technology requires 121,000 Nm³/hr. Therefore, the air consumption under the ALMA technology is calculated to be 1.96 times lower than under the Huntsman technology. The same factor of 1.96 would apply to the volume of the produced off-gas when the two production technologies are considered.

Furthermore, the information proposed to Condea described a 45.1 kg/hr DIBE loss for a 40 kt/y plant. Of this, the losses from the off-gas (due to the substance’s higher vapour pressure) were 33.1 kg/hr; the remaining 12 kg/hr of DIBE losses were due to its dissolution into process water leading to the formation of decomposition products. It is assumed that this latter proportion of losses would remain the same if the Sasol-Huntsman plant converted to the ALMA technology.

Using the calculated off-gas factor of 1.96, the overhead losses with DIBE would be higher by a factor of 1.96, i.e. 33.1 x 1.96 = 64.9 kg/hr. Overall, the losses of DIBE per tonne of MA would be: 12 kg/hr + 64.9 kg/hr = ca. 77 kg/hr. For a plant with a MA production capacity of 40,000 t/y and an operation of 8,000 hr/y, the amount of MA produced per hour is 5 t/hr, meaning that the consumption of DIBE would be 77/5 = ca. 15.4 kg per tonne of MA.

This is higher than the consumption rate of DBP per tonne of MA that Sasol-Huntsman can currently achieve. As shown in Table 2.1, the Huntsman technology allows the operation of the MA production line with a consumption rate of DBP of 7-9.5 kg/t MA.

It can, therefore, be assumed that the replacement ratio of DBP by DIBE could be between 15.4:9.5 and 15.4:7 or between 1.6:1 and 2.2:1.

**Overall cost calculation**: due to the inherent uncertainties in our analysis, for the calculation of the cost of using DIBE as an absorption solvent, we make the following assumptions:

- the consumption rate for DBP is conservatively assumed to be at the high end of the aforementioned range, i.e. 9.5 kg per tonne of MA manufactured;
- the consumption rate for DIBE is 15.4 kg per tonne of MA manufactured;

---

27 For this comparison it is assumed that although the concentrations of MA are different (see airflow rates above), the size of the absorber column will be the same because of the same total MA flow rate.
• the tonnage of DBP consumed is assumed to be a maximum 1,000 t/y. This figure is based on the MA production capacity of the Moers plant (105 kt/y) and the consumption rate of DBP of 9.5 kg/t MA. For the purposes of this calculation, the capacity of the Moers plant is assumed to remain at current levels for the next 20 years;

• the price increase per tonne of solvent consumed is €300 and the prices of the two substances are, for simplicity, assumed to remain stable during the assessment period. The cost of DBP is presented in Annex 2 of this AoA and is assumed to be €1,520 per tonne. This is considered a good approximation of the actual market price (excluding transport costs) as of July 2013. The actual price is not provided here for reasons of confidentiality (but is disclosed in the SEA);

• the present value of the cost of the solvent is calculated over a time horizon of 20 years. This length of time is based on the time required for an adequate return on investment following a plant conversion, rather than the commercialised lifetime of the plant/equipment (which could be much longer). As will be discussed below, these 20 years would be preceded by downtime for the plant conversion of an estimated 2 years (25 months); and

• a discount rate of 4% has been used, as per ECHA’s Guidance on the Application for Authorisation.

The following Table presents our calculations. The annual cost of the solvent would increase by €1.4 million, corresponding to a present value cost of €18 million over 20 years. The use of the actual market price for DBP would make little difference, particularly in comparison to the plant conversion costs that are quantified below.

Table 4.7: Increased cost of absorption solvent (DIBE) use

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>DBP consumption rate</td>
<td>9.5</td>
<td>kg/t MA</td>
</tr>
<tr>
<td>DIBE consumption rate</td>
<td>15.4</td>
<td>kg/t MA</td>
</tr>
<tr>
<td>DBP annual consumption</td>
<td>1,000</td>
<td>t/y</td>
</tr>
<tr>
<td>DIBE annual consumption</td>
<td>1,617</td>
<td>t/y</td>
</tr>
<tr>
<td>Additional solvent consumption</td>
<td>617</td>
<td>t/y</td>
</tr>
<tr>
<td>Additional solvent cost (price of DBP: €1,520/t, price of DIBE: €1,820/t)</td>
<td>1.4 million</td>
<td>€/y (rounded)</td>
</tr>
<tr>
<td>Present value over 20 years (following plant conversion) at 4% discount rate</td>
<td>18 million</td>
<td>€ (rounded)</td>
</tr>
</tbody>
</table>

Cost element 3: Cost of plant conversion

Overview: replacing the DBP-based absorption process at the Moers site with the DIBE-based process of the ALMA technology would require the following plant changes:

• it is assumed that the existing air compression and the reactor section, as well as the incineration units, could still be used with only minor modifications. Because the ALMA technology uses less air for the reaction, it has been assumed that MA absorption must be as large as in the fixed bed method\(^\text{28}\); and

• it is assumed that if the available fixed bed reactors would continue to be used, the recovery unit would have to allow for the higher off-gas flow (see Section 4.1.2.2). The absorber section of

\(^{28}\) It is assumed that the design of the absorber first order is ruled by the rate of MA that has to be absorbed and not by the flow rate of the off-gas.
the ALMA recovery system has to be designed for the 1.96-fold increased off-gas flow and, in addition, the stripper column would have to accommodate the higher rich oil flow. Neither of these have been commercially demonstrated; and

- it is assumed that the Moers plant would need to replace its heat exchangers and pumps.

Sasol-Huntsman is capable of estimating the duration, cost and manpower demand of the switch to the ALMA technology on the basis of information from two key sources:

- the information submitted to Condea in the mid-1990s; and

- the experience of the recent expansion of the capacity of the Moers plant that was completed in 2011 and which increased the capacity of the plant from 60kt MA per year to 105 kt/y.

A detailed estimate of the duration, cost and manpower demand of the theoretical conversion to the ALMA technology is provided in the Confidential Annex (Part 2).

Additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf, Part 3.

**Summary of cost estimates:** The following points outline the costs that would arise for Sasol-Huntsman:

- **Timeline of cost estimates:** It is estimated that the decision making on whether or not to grant an Authorisation might take 18-24 months and the European Commission’s decision to grant (or not) an Authorisation will be around the Sunset Date for DBP. Therefore, cost estimates apply from the Sunset Date onwards. It is fair to assume that conversion could not start immediately after publication of the Commission’s decision. It can be estimated that an additional eighteen (operational) months would be required for obtaining agreement of the company owners/shareholders for the conversion, drawing up of engineering plans, cost estimation and raising capital. Ideally, this delay should be considered in the calculation of costs. Similarly, cost estimates should ideally be discounted to allow for the delay. However, the cost of conversion and the scale of modifications are of such magnitude that any attempt to over-analyse, or aim for high accuracy, would be of little real benefit to this discussion. We have, therefore, ignored this theoretical 18-month (operational) preparatory period.

- **Cost of plant conversion:** As described in the Confidential Annex, the total cost of switching from the DBP-based method to the ALMA technology could be **over €150 million**. The most important costs would be associated with:
  - the rebuild of the absorption, stripping and afterflasher section;
  - the rebuild of the distillation section;
  - the rebuild of the solvent cleaning system; and
  - the installation of a gas cooling system.

As noted earlier, it is assumed that existing reactors, compressors/turbines and incineration units can be reused with no, or very little, modification.
ANALYSIS OF ALTERNATIVES

- **Cost of inactivity/downtime**: an important characteristic of the Sasol-Huntsman plant is that it comprises two trains, which are highly integrated. To execute the conversion described above, it would be necessary to shut down both trains of the existing plant for demolition over seven months and a total shutdown of the plant with no production of MA for a total of twenty-five months. This estimate takes into account the experiences of the recently installed MA 2nd train (reactor) when Sasol-Huntsman needed two years’ construction time. It would not be possible to shorten this time because of both the high integration of both trains and the spatially tight layout of the Moers site, with Sasol Solvents’ plants operating at close proximity to the Sasol-Huntsman MA plant.

100% of Sasol-Huntsman’s turnover is associated with the production of MA. Sasol-Huntsman’s turnover stands at €100-120 million per year (or €8.3-10 million per month) and varies each year. We assume that this turnover range would also apply to the year 2015. Consequently, downtime lasting for 25 months would be associated with a lost turnover of ca. €208-250 million.

This cost of inactivity would be extremely detrimental to Sasol-Huntsman and could only lead to the closure of the MA plant. Even if it could be contemplated that conversion to the ALMA technology would create a viable business model, the 25-month loss of production would result in significant upset in the EU MA market, cause MA prices to increase significantly (owing to the shortage of MA in the EU) and lead customers to finding alternative MA suppliers, possibly outside the EU. Furthermore, some downstream users of MA finding high MA prices and short supply in the EU may close down their business or relocate outside the EU. By definition, due to Sasol-Huntsman having to move to a higher cost solvent, the cost of production would increase when the plant would come back on line. This would lead to an increase in the price of MA placed on the market by the company. Furthermore, Sasol-Huntsman would also need to increase prices in order to ensure that they could repay both the existing and any new loan. The combination of selling at a less competitive price and the need to re-build their customer base would lead to severe difficulties in the short-term. Therefore, even if the conversion of the Moers plant could be financed and successfully engineered, there would be no justification, from a commercial perspective, for going through this conversion process, especially in light of the fact that risks to workers’ health from exposure to DBP are already adequately controlled.

- **Cost of raising capital**: Sasol-Huntsman has indicated that, in order to obtain the €150+ million required for the conversion of the plant, a bank loan would have to be obtained. There would be obvious difficulties in obtaining such a large amount in the current economic climate, especially given that the Moers plant only recently completed a major expansion of its capacity, which required significant investment on the Huntsman technology and is subject to an outstanding loan. Therefore, it is very unlikely that a new large loan would be easily obtainable.

- **Cost of lost investment**: Sasol-Huntsman has invested significantly in its operations. The company has made a capital investment of ca. €150 million in the last 12 years for two rounds of capacity expansion in 1999 and 2011, which is equivalent to ca. €200 million when finance costs are taken into account. As a result, the company is still committed to banks, customers, suppliers and shareholders, while the plant and equipment acquired through these investments have not run through their intended lifecycle – a switch to the ALMA technology would mean

29 A “train” is a series of process equipment which are connected to each other and through which the process flows from front to back. The Moers plant has two MA trains, one with 60 kt/y capacity and the other (new) with 45 kt/y MA production capacity.
that certain equipment would have to be replaced before the end of its useful lifetime. The SEA (Section 2.2.1.2) discusses the amount of outstanding loan that would have to be repaid in 2015, if the Moers plant were not able to continue producing MA. Additionally, Sasol-Huntsman also invested, in 2005 and 2012, a further amount (discussed in more detail in the SEA, see Section 2.2.1.2) into a state-of-the-art MA pastillation unit in order to support small businesses in the EU and Europe with sales of solid MA. Closure of the company would also mean the loss of this investment.

Overall cost calculation: the following Table summarises the above cost estimates.

Table 4.8: Cost element 3 summary: Conversion of the MA plant to the ALMA technology

<table>
<thead>
<tr>
<th>Cost element</th>
<th>Type of cost</th>
<th>Present value cost</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quantifiable costs</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cost of plant modification</td>
<td>One-off (investment)</td>
<td>€150 million</td>
</tr>
<tr>
<td>Cost of inactivity/downtime</td>
<td>One-off (expenditure)</td>
<td>€208-250 million</td>
</tr>
<tr>
<td><strong>Non-quantifiable costs</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cost of raising capital</td>
<td>One-off (expenditure)</td>
<td>Not quantified</td>
</tr>
<tr>
<td>Cost of lost investment</td>
<td>One-off (sunk costs)</td>
<td>Not quantified – see SEA</td>
</tr>
<tr>
<td><strong>Total (rounded)</strong></td>
<td></td>
<td>&gt;€358 million</td>
</tr>
</tbody>
</table>

The overall cost is estimated at over €358 million. These high costs could not be passed on to customers and confirm again the view that the ultimate result of converting to the ALMA technology would be the closure of the Sasol-Huntsman MA plant.

Cost element 4: Cost of increased fouling and maintenance

Based on the information available, it has not been possible to quantify the costs that would arise from an increased incidence of fouling and the associated increase in maintenance activities due to DIBE’s poorer FAc solubility. It is considered that in the context of Cost element 3 (conversion cost), this cost element would be of limited significance.

Cost element 5: Cost of a new licence

Sasol-Huntsman has already paid a licence fee to Huntsman in order to operate under the Huntsman technology. Should the company decide to move to a new technology, the ALMA technology in this case, a new licence would have to be purchased. Quantitative information is available in the Confidential Annex (Part 3).


Cost element 6: Cost of changes in steam generation and consumption

For the first two years of the 20-year assessment period, the Sasol Solvents power plant would be deprived of 650 GWh of steam currently exported from the MA plant. To obtain this from fuel gas, an additional 459 GWh would have to be obtained each year from natural gas purchased from the open market, as shown in the Confidential Annex to this AoA. The cost of acquiring this amount of energy over 2 years of MA plant shutdown can be calculated as follows:

\[ 2 \times 459,000 \text{ MWh/y} \times \varepsilon 29/\text{MWh} = \varepsilon 26.6 \text{ million}. \]
Additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf, Part 5.

Summary of costs

The following Table summarises the costs that would arise for the downstream user of DBP (Sasol-Huntsman). The Table and the calculations of present value costs show that conversion of the plant to the ALMA technology would result in the closure of the Moers plant.

It is considered appropriate that the summary of costs not only presents the losses in turnover, but also the losses in profit that is associated with the lost turnover, or, in other words, the value added lost. Sasol-Huntsman does not wish to disclose in a document intended for publication the profit margin of its operations. In order to provide an indication of the value added lost, we will hereby assume a profit margin of 10%. It must be understood that this figure has no bearing on the real profit margin of Sasol-Huntsman; it has merely been selected as a typical margin for companies in the EU chemicals industry.

Table 4.9: Summary of costs of the replacement of DBP-based absorption with DIBE-based absorption

<table>
<thead>
<tr>
<th>Cost element</th>
<th>Actor incurring cost</th>
<th>Type of cost</th>
<th>Cost impact on…</th>
<th>Annual cost (where available)</th>
<th>Present value cost (20 years, 4% discount)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Annual cost</td>
<td>Present value cost</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(based on turnover)</td>
<td>(Based on profit (10% margin))</td>
</tr>
<tr>
<td>1-2 Cost of new solvent</td>
<td>Sasol-Huntsman</td>
<td>Recurrent</td>
<td>Profit</td>
<td>€1.4 million</td>
<td>€18 million</td>
</tr>
<tr>
<td>3 Cost of plant conversion</td>
<td>Sasol-Huntsman</td>
<td>One-off</td>
<td>Profit</td>
<td>€150 million</td>
<td>€150 million</td>
</tr>
<tr>
<td>4 Cost of fouling</td>
<td>Sasol-Huntsman</td>
<td>Recurrent</td>
<td>Profit</td>
<td>Not quantified</td>
<td>Not quantified</td>
</tr>
<tr>
<td>5 Cost of licence fee</td>
<td>Sasol-Huntsman</td>
<td>One-off</td>
<td>Profit</td>
<td>See Confidential Annex</td>
<td>See Confidential Annex</td>
</tr>
<tr>
<td>6 Cost of lost steam</td>
<td>Sasol Solvents</td>
<td>One-off</td>
<td>Profit</td>
<td>€27 million</td>
<td>€27 million</td>
</tr>
<tr>
<td>Total (rounded)</td>
<td></td>
<td></td>
<td></td>
<td>&gt;€403 million</td>
<td>&gt;€216 million</td>
</tr>
</tbody>
</table>

The present value of the overall cost would be:

- for Sasol-Huntsman, **over €376 million, based on lost turnover, or over €189 million based on lost profit for a theoretical 10% profit margin.** This is clearly an unacceptable cost that could not be passed on to the customers or absorbed by Sasol-Huntsman; and
- for Sasol Solvents, **€27 million,** as a result of the loss of steam that would otherwise be generated by the MA reaction and would be passed onto the on-site power plant.

Overall, the use of DIBE within the ALMA technology is not an economically feasible alternative for the user of DBP.
4.1.5 Availability of DIBE

4.1.5.1 Current and projected availability for DEZA

Market availability

As discussed earlier, DEZA cannot currently manufacture hydrophthalates, such as DIBE, since it does not have access to the relevant technology. DIBE is not considered available to DEZA.

Actions required for improving availability

Due to the technical and economic feasibility issues explained above, DIBE is not a suitable alternative for DBP from the perspective of the downstream user; therefore, there is no realistic incentive for DEZA (or for any other interested third party) to engage in research and develop technologies and means for the manufacture of DIBE for the specific purpose of selling to Sasol-Huntsman for use in the manufacture of MA.

4.1.5.2 Current and projected availability for Sasol-Huntsman

Market availability

As discussed under Section 4.1.4.2 (under the sub-heading Cost element 1: Price of DIBE), the market availability of DIBE appears to be limited and the lack of a REACH Registration dossier would support this assertion. The conservative calculations made on the potential future demand of DIBE by Sasol-Huntsman (see Table 4.7), indicate that the amount of DIBE needed for the operation of the Moers plant might exceed 1,000 t/y, when operating at capacity. Given that only one manufacturer of DIBE is known, there is justified concern over Sasol-Huntsman’s future ability to source the substance.

Actions required for improving availability

Due to the technical and economic feasibility issues explained above, DIBE is not a suitable alternative for DBP; therefore, there is no realistic incentive for any interested party (DEZA or others) to improve the market availability of DIBE for the specific purpose of it being used by Sasol-Huntsman in the manufacture of MA.

4.1.6 Conclusion on suitability and availability for DIBE

4.1.6.1 Summary of findings

Technical feasibility

In assessing the suitability of DIBE (and of the ALMA technology that uses this substance) it must be remembered that this Application for Authorisation, in its CSR, demonstrates that risks to workers’ health from exposure to DBP during the manufacture of MA are very low and are adequately controlled. Therefore, the use of DIBE (or other alternative substance) would not confer any discernible benefit to the health of workers employed by Sasol-Huntsman.
Nevertheless, the detailed analysis of the suitability of DIBE above has identified the following fundamental issues:

- a lower FAc solubility of DIBE leads to increased deposits and maintenance requirements;
- a boiling point lower than that of DBP would lead to higher vapour losses from the absorber overhead, meaning that additional quantities of solvent would be required;
- the relatively small difference between the density of DIBE and that of water would impact upon the recovery of the used solvent, further increasing solvent losses. DIBE cannot be used as a drop-in replacement for DBP within Huntsman’s technology and its use would preclude the reuse of some existing expensive equipment;
- modifications that could be implemented to the MA manufacturing plant would be lengthy, very disruptive to the operation of the Moers plant, would be accompanied by significant cost and ultimately jeopardise the existence of the MA manufacturing plant at Moers; and
- DIBE’s worse flash point compared to DBP would increase the risk of a process upset causing a fire.

DIBE is currently used in the ALMA technology and relies on a fluidised bed reactor. Market research suggests that, in the last 15 years, MA manufacturers have consistently opted for Huntsman’s technology. The ALMA technology does not appear to have the confidence of the global MA markets, especially when compared to the success that Huntsman has had in licensing its fixed bed DBP-based technology.

Economic feasibility

Although the assumption is made that existing key (expensive) equipment such as reactors, compressors/turbines and incineration units could still be used with DIBE with no or very little modification, the cost that would arise from the conversion of the plant and the associated downtime (estimated at twenty-five months after completion of detailed engineering and procurement of capital financing) would exceed €358 million, based on turnover losses. Other less significant costs elements include the increased cost of solvent (due to a higher per tonne cost and a worse consumption rate in comparison to DBP), the increased maintenance cost (due to increased fouling) and the one-off cost of a new licence for the ALMA technology. The overall cost of switching to DIBE would exceed €403 million, based on lost turnover, or €216 million based on lost profit for a theoretical 10% profit margin.

Availability

DIBE is not available in the portfolio of the manufacturer of DBP and its availability crucially depends on access to technology that allows its manufacture – certain companies have patented such technology but this is currently unavailable to DEZA. From the perspective of the downstream user, there are concerns about the tonnage of the substance available on the market as a result of the existence of only one known manufacturer, the lack of REACH Registration (as of March 2013) and the presence of a number of licensees of the ALMA technology which may require access to a considerable tonnage of DIBE. Therefore, there are reasons to question the market availability of this alternative substance.

For completeness, a comparison of the hazard profiles of DIBE and DBP has been attempted. Almost no information has been identified on DIBE’s hazards in publicly available sources, apart from an entry in the blacklist of the Spanish Institute ISTAS, which identifies the substance as a potential endocrine disruptor, and an aquatic toxicity classification suggested by the Danish EPA.
The ECHA C&L Inventory suggests that two notifiers have made a non-classification entry for the substance; the lack of a REACH Registration would also point in the direction of lack of grounds for classification. Having used QSARs for a preliminary assessment, only limited cause for concern has been identified with regard to DIBE’s possible environmental toxicity potential, its possible mammalian developmental toxicity, and its potential influence on androgen receptors. To better characterise the extent to which such concerns are justified would, however, require additional research (potentially involving use of vertebrate animals).

Based on the limited information available and if viewed simplistically, it would appear that the adoption of DIBE might represent some, uncertain, reduction in hazard potential. Nevertheless, risks to workers’ health from exposure to DBP are already adequately controlled.

On the other hand, the use of caustic under the ALMA technology might result in higher safety concerns for workers due to the need for caustic washing.

**Conclusion:**

DIBE cannot be considered a suitable alternative to DBP for use as an absorption solvent in the manufacture of MA, especially since the risks to workers’ health from exposure to DBP are adequately controlled.

### 4.1.6.2 Actions to make the alternative suitable and available

We can distinguish the following areas:

- **the inherent shortcomings of the alternative substance:** DIBE has inferior physicochemical properties relative to DBP. Therefore, DIBE cannot realistically be used within the Huntsman technology. The properties of the substance cannot improve;

- **the shortcomings of the alternative technology that uses DIBE:** the above discussion has explained the challenges that Sasol-Huntsman would face in the conversion of the Moers plant to the ALMA technology. It is impossible to make a switch from DBP to DIBE at Moers while maintaining commercially viable operations, particularly considering the investment and expansion work that has recently been completed and which has centred on the use of DBP as the absorption solvent. The lack of new licensees of the ALMA technology in the last 15 years raises legitimate doubts that any major breakthrough to the engineering and economic parameters of the ALMA technology have materialised in this period.

With regard to the availability of DIBE, given the above technical and economic shortcomings of DIBE and the ALMA technology, issues of availability and how this may improve in the future are not considered to be of importance.

### 4.2 Alternative 2: Use of the water-based alternative MA recovery technology

#### 4.2.1 Description of water-based recovery of MA

#### 4.2.1.1 Background

There are generally two methods for the water-based recovery of MA from the reactor off-gas. One relies on a combination of water and o-xylene and the other only uses absorption in water and distillation under vacuum (Luciani, 2009). The former is the main water-based competitor to the
ANALYSIS OF ALTERNATIVES

Huntsman technology and the AoA will focus on this. Historically, water-based recovery technology was originally developed in concert with the production of MA from benzene and was adapted to the recovery of MA produced from n-butane when n-butane oxidation technology was introduced in the 1970s. It is worth noting that water-based recovery was used at the Moers plant in the past when, between 1990 and 1999, Condea operated the Moers plant under a Scientific Design licence (some detail on Scientific Design was given in Table 3.8). The Moers plant switched to the Huntsman technology with DBP as the solvent in 1999, converting the plant from an energy consuming to an energy producing unit.

4.2.1.2 MA recovery through a combination of water and xylene

The key licensor of this technology is Scientific Design. Although others have developed variations of water-based recovery technology, they fundamentally rely on the same principles. Under the Scientific Design variant, the recovery of MA is performed through two mechanisms:

- **recovery of MA through condensation**: the effluent stream from the reactor contains gaseous MA, carbon monoxide, carbon dioxide, water, oxygen, nitrogen, and unreacted butane. It is cooled to about 120°C in a chain of heat exchangers, raising low-pressure steam and preheating boiler feedwater.

  As the off-gas is cooled below the dew point of MA, liquid droplets of MA are formed and are separated from the off-gas by a separator. The condensed crude MA is pumped to a tank for storage (Felthouse, Burnett, Horrel, Mummey, & Kuo, 2001).

  The final cooling stage is in a condenser using tempered cooling water (around 50-55°C) to avoid freezing. Great care must be taken to condense as much MA as possible without condensing any water, since it would react with MA to give fumaric and maleic acids. FAc is insoluble and would block the condenser. The MA will also absorb moisture from the gas stream, so residence time in this condenser must be minimised; and

- **recovery of MA through scrubbing and distillation**: the MA remaining in the gas stream after partial condensation is removed in a water scrubber by conversion to maleic acid, which accumulates in the acid storage section at the bottom of the scrubber. The concentration of the maleic acid solution may be undertaken by azeotropic distillation or evaporation. The common solvents for extractive distillation are mixed xylenes, ortho-xylene and ortho-dichlorobenzene in a dual-purpose dehydrator/refiner and water from the dehydration step is recycled to the scrubber. When the conversion of the acid solution to crude MA is complete, condensed crude MA is added to the still pot and a batch distillation refining step is conducted (Felthouse, Burnett, Horrel, Mummey, & Kuo, 2001).

4.2.1.3 MA recovery through a combination of water absorption and distillation

The owner of this technology is BP Chemicals. The technology was formerly known as UCB collection and refining technology and is now marketed as BP MAH technology. This also depends on partial condensation of MA and scrubbing with water to recover the MA present in the reaction off-gas. The BP MAH technology departs from the Scientific Design technology where the maleic acid is dehydrated to MA. In the BP MAH technology, the water in the maleic acid solution is evaporated to concentrate the acid solution. The concentrated acid solution and condensed crude MA is converted to MA by a thermal process in a specially designed reactor. The resulting crude MA is then purified by distillation (Felthouse, Burnett, Horrel, Mummey, & Kuo, 2001). As shown in Table 3.8, this technology only finds use in the USA and combines either a fixed bed or a fluidised bed with n-butane feedstock.
There have been suggestions in the literature (Shelley, Fouhy, & Moore, 1993) that the BP MAH technology does not use xylene. However, xylene may be used as an entrainer for water in a two-phase distillation process that eventually separates the xylene from water. In theory, benzene might be used instead of xylene, but this would make the separation process more complicated because of its hazardous characteristics. The use of xylene is suggested in the open literature (Weissermel & Arpe, 2008) (Forgac, 1999). Knowledge of the xylene-free version of water-based absorption is more limited than the xylene/water technology. Nevertheless, absorption in water is undertaken in any case; it is the re-work of maleic acid that can be done with or without xylene. The technology without xylene still suffers the same intrinsic disadvantages due to the fact that hydrolysis to acid and re-conversion to anhydride is more energy intensive.

4.2.2 Technical feasibility of water-based recovery

4.2.2.1 Technical feasibility for DEZA

This alternative technology is not relevant for DEZA as it is outside its portfolio and areas of expertise. Thus, it cannot be considered technically feasible for DEZA.

4.2.2.2 Technical feasibility for Sasol-Huntsman

Overview

The following paragraphs discuss key technical aspects and characteristics of the water-based recovery technology and how it compares to the solvent-based Huntsman technology. The key advantages of the Huntsman technology that have been considered in this analysis relate to:

- the recovery efficiency for the manufactured MA;
- the energy consumption of the MA technology;
- the generation of wastewater;
- the incidence and implications of fouling; and
- the quality of the final MA product.

Recovery efficiency for the manufactured MA

Argument: the Huntsman technology has superior recovery efficiency than water-based recovery technology.

Information from literature: a 1993 article in the Chemical Engineering magazine confirms that one of the upsides of a solvent-based recovery system is a yield advantage. The reaction of MA in the off-gas with water to form maleic acid (which isomerises to FAc) means that recovery rates of 92-95% are typical in a water-based process. In contrast, 97-98% of the MA produced in the reactor can be recovered using a solvent-based system (Shelley, Fouhy, & Moore, 1993). Nevertheless, in the early 1990s, the BP technology claimed a demonstrated efficiency of 96-98%\(^{30}\).

Information from the applicants’ own information: presently, Huntsman’s solvent-based recovery and refining technology achieves 99% recovery of all MA produced in the reactor.

\(^{30}\) Only a few plants are currently using MA technology developed by BP, as shown in Table 3.8.
Huntsman’s experience with water-based recovery plants\textsuperscript{31} indicates that water-based recovery and refining typically achieves no more than 95% recovery. Indeed, Huntsman is familiar with cases where values as low as 90% are observed. Thus, water-based recovery suffers an intrinsic disadvantage in that a significant percentage of the MA product is unavoidably and irreversibly converted to FAc.

**Conclusion:** the recovery efficiency of water-based recovery is lower than that achieved with solvent (DBP)-based absorption of MA, thus reducing the raw material utilisation efficiency of the MA manufacturing process and adversely affecting its economics and stewardship of fossil resources. Our calculations later in this document will be consistent with a recovery efficiency of 99% for the Huntsman technology and 95% recovery efficiency for the water-based recovery of MA, giving an **efficiency difference of 4%**.

**Energy consumption**

**Argument:** water-based recovery of MA consumes a larger amount of steam than the Huntsman method; therefore, it significantly reduces the steam (i.e. energy) that can be exported from the manufacture of MA for onward use.

**Steam production and export with DBP- and water-based recovery:** to estimate the differences between both production routes, Sasol-Huntsman has used information from a comparison of MA production technologies that was undertaken in 1996 when the company (then Condea) was considering options for plant conversion. All data that Sasol-Huntsman has used for the calculations presented herein are based on licensors’ information supplied for the then proposed 40,000 t/y capacity expansion, which at the time included a recovery unit designed for a production capacity of 56,000 kt/y\textsuperscript{32}.

**Similarities between the two technologies:** the Huntsman technology and the water-based recovery technology have nearly equivalent steam production characteristics. More specifically, the off-gas from the reactors has similar heating values under both technologies and the thermal incineration process produces amounts of steam of the same order of magnitude in both cases. Energy recovery from hot reactor off-gases is the same for either case and can vary depending upon plant configuration.

**Differences between the two technologies:** the key difference between the two technologies relates to the operation of the recovery unit. While the Huntsman technology requires ca. 2.5 tonnes of steam per tonne of MA, the water-based technology needs more than 5 tonnes of steam per tonne of MA. Based on this information, the following Table that compares steam production, consumption and export under the Huntsman and the water-based technologies can be created.

The Table above shows the steam production figures for both technologies based on compressors driven by electrical motors. In the case of a steam turbine drive, the internal consumption would increase by ca. 4 tonnes of steam per 1,000 tonnes of MA\textsuperscript{33}. This would turn the water-based

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\textsuperscript{31} These observations of recovery inefficiencies in water-based plants are based on Huntsman’s experience as a supplier of catalyst to both solvent-based and water-based plants.

\textsuperscript{32} There was an existing 16 kt/y plant with aqueous recovery, to which a 40 kt/y plant was added in 1999 and the old aqueous recovery was demolished and replaced with a single solvent-based recovery system for the combined 56 kt/y plant. The 56 kt/y plant was debottlenecked to 60 kt/y and then expanded in 2011 to 105 kt/y via the addition of a new 45 kt/y plant.

\textsuperscript{33} Steam turbines use steam directly to turn the air compressor in lieu of using an electrical motor to accomplish the same result. Steam turbines are used in plants which either do not have sufficient demand at the site for steam export or
technology into a net importer of high-pressure steam (steam consumption would then increase to ca. 9.5 tonnes of steam compared to an overall production of 8.5 tonnes). Based on these results, it is clear that the water-based technology shows significantly higher internal steam consumption than the solvent-based technology (more than 100% higher than under the Huntsman technology). Overall, the above calculations show that the solvent (DBP)-based technology is the most energy efficient one.

Table 4.10: Approximate steam production, consumption and export under the DBP-based and water-based technologies, per 1,000 tonnes of MA product

<table>
<thead>
<tr>
<th>Steam production, consumption and exports</th>
<th>Water-based technology</th>
<th>DBP-based technology</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam export</td>
<td>3 tonnes</td>
<td>8.3 tonnes</td>
<td>Figures based on technology comparison by Condea in 1996 and experience of current steam production at Moers</td>
</tr>
<tr>
<td>Steam internal consumption</td>
<td>5.5 tonnes</td>
<td>2.6 tonnes</td>
<td>Based on 5.2 tonnes of steam per tonne of MA vs. 2.5 tonnes of steam per tonne of MA</td>
</tr>
<tr>
<td>Overall steam production</td>
<td>8.5 tonnes</td>
<td>10.9 tonnes</td>
<td>Aggregate of figures in two previous rows</td>
</tr>
</tbody>
</table>

Source: applicant’s own information

It must be noted that at the Moers site, all steam produced by the MA plant which is not used by the recovery unit is sent to the adjacent Sasol Solvents power plant. The power plant uses the steam from the MA plant plus natural gas fuel to produce 100% electricity (this requires 120-140 t/hr high pressure steam). The majority of the generated electricity is used to operate the Sasol Solvents plants and the remainder is exported as electricity to the grid. The steam from the MA plant currently accounts for 60% of the energy inputs into the power plant, as shown in Part 4 of the Confidential Annex.

Technically, if steam supply from the MA plant would be lower following the conversion to the water-based technology, the deficit in the steam supply to the power plant would have to be covered by additional fuel gas supplied from the open market. From a cost perspective, this is less attractive. In addition, the CO$_2$ balance of the site would become less favourable if the ‘green’ chemical energy which would otherwise be generated from the steam produced by the strongly exothermic reaction of MA were to be replaced by energy generated from the burning of fuel oil. Sasol Solvents would be forced to purchase CO$_2$ certificates for the burning of additional fuel.

Additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf, Part 5.

Conclusion: similar to the Huntsman technology, water-based recovery produces steam, as the energy contained in the reactor off-gases is of the same order of magnitude. However, water-based recovery uses more energy and is thus less advantageous at best and a net energy consumer at worst.

The use of a water-based method to extract MA from the reaction gases would be accompanied by a reduced export of energy to the Sasol Solvents power plant, which serves adjoining plants which are located at the Moers site. This would be accompanied by an increased cost of fuel gas consumption and a concomitant increased release of CO$_2$ (note that a calculation of the additional CO$_2$ emissions where the relative values (due to local circumstances) of steam and electrical energy favour the use of steam (Huntsman, pers. comm.).

Use number: I  Legal name of applicant: DEZA, a.s.  59
is provided in Section 4.2.3.2). From an economic and sustainability perspective, the use of water-based recovery is clearly unfavourable.

Wastewater generation

**Argument:** the use of water-based recovery of MA results in increased wastewater generation; the wastewater needs to be disposed of by incineration leading to increased costs and additional CO$_2$ emissions.

**Operational conditions associated with wastewater production:** the Huntsman technology is a water-free absorption process, as the MA from the reactor off-gas is absorbed in the organic solvent. Losses of MA through hydrolysis to FAc are very small (see Section 2.1.2). Conversely, under the water-based technology, MA reacts very quickly with water (the recovery medium) leading to the formation of maleic acid. This maleic acid, which accounts for a significant part of the MA produced at the synthesis stage, must be reworked and dehydrated in an additional refining step.

The dehydration water is sent back to the absorption column, but a part must be purged in order to prevent accumulation of impurities. Washing steps are more frequent, which ultimately results in a higher tonnage of washing water being generated.

**Comparison of wastewater production:** to estimate the differences in wastewater production between the DBP-based technology and the water-based technology, Sasol-Huntsman has used information from the comparison of MA manufacturing technologies that was performed by Condea in 1996. All data used are based on licensors’ information provided for the then 40,000 t/y capacity MA plant.

**Table 4.11: Wastewater production under the solvent-based and water-based processes**

<table>
<thead>
<tr>
<th>Wastewater production</th>
<th>Water-based technology</th>
<th>DBP-based technology</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wastewater production (40 kt/y capacity)</td>
<td>25 kt/y</td>
<td>24 kt/y</td>
<td>Based on 1996 comparison of technologies in the Basic Engineering Package provided to Condea</td>
</tr>
<tr>
<td>Wastewater production (105 kt/y capacity)</td>
<td>65 kt/y</td>
<td>48 kt/y</td>
<td>Figure for the water-based technology is extrapolated from row above. Figure for DBP-based technology is based on actual operation data from the Sasol-Huntsman plant</td>
</tr>
<tr>
<td>Biological Oxygen Demand</td>
<td>30,000 mg/L</td>
<td>12,800 mg/L</td>
<td></td>
</tr>
<tr>
<td>Chemical Oxygen Demand</td>
<td>85,400 mg/L</td>
<td>23,200 mg/L</td>
<td></td>
</tr>
</tbody>
</table>

Source: applicant's own information.
Note: figures are rounded; BOD and COD values are experimental figures

The Table confirms that the water-based technology would be accompanied by the generation of a higher wastewater flow volume (65 - 48 = 17 kt/y). This wastewater must be decomposed in a biological water treatment plant or be incinerated. Biological treatment of the wastewater is not possible at the Moers site as the existing treatment plant is a comparatively small one and could not handle such additional wastewater loads. Therefore, this waste stream would have to be incinerated.
Conclusion: in relation to wastewater generation, the consequences of a theoretical move to water-based recovery would be:

1. The rebuild of the existing treatment facilities; or, alternatively,

2. The combustion of the additional 17 kt/y of wastewater generated. The combustion of this waste stream would require an estimated consumption of ca. 1,000,000 m$^3$/y natural gas$^{34}$. Using greenhouse gas emission factors available from UK Department for Environment, Food and Rural Affairs$^{35}$, it can be calculated that the consumption of this amount of natural gas would result in the release of an additional ca. 2,020 tonnes CO$_2$ (eq) per year.

Importantly, the difference in wastewater flow was one of the reasons why Condea decided not to continue with the water-based technology at Moers in the 1990s and switched to Huntsman’s solvent-based technology in 1999. Wastewater minimisation is also known to be a contributing factor to the decision of other MA producers to select the Huntsman technology.

Incidence and implications of fouling

Argument: the use of water for the recovery of MA increases the generation of by-products and polymeric tars, which require increased maintenance, wastewater generation and MA production rate and consequently increase operating costs.

Fouling issues: Section 2.2.3 explains that one of the strong technical points of the Huntsman technology is that it allows for an improved control of fouling of the process equipment through better control of the formation of by-products and polymeric tars, compared to other technologies used in the MA industry. Indeed, experience confirms that the length of time a water-based plant is on-stream is typically lower compared to the Huntsman technology owing to the frequent fouling of process equipment by FAc deposits.

Increased fouling incidence could be important in three aspects:

- it may require additional personnel/man-hours for equipment cleaning and maintenance, which also increases the potential for worker exposure;
- it results in the generation of increased amounts of waste that needs to be disposed of; and
- increases operating costs through blockages that cause the plant to operate at reduced rates, increased maintenance costs and increased waste disposal costs.

Sasol-Huntsman has considered the likely cleaning and maintenance requirements that might arise under the water-based technology. Although the cleaning frequency and the duration of cleaning sessions under the water-based technology would certainly be less attractive from a cost perspective, it has been concluded that the differences to the current situation would be of limited importance in the context of other major changes to the plant and its operating costs. More frequent cleaning procedures would be possible to take place while the plant would be on-line and cleaning would be undertaken by the operation staff, as is now. Consequently, this aspect of fouling is considered of limited criticality and will not be considered further in our estimates of economic feasibility.

34 This estimated volume has been based on the evaporation rate of wastewater and is only a rough estimate. A more rigorous calculation would suggest that to evaporate 17,100 tonnes of wastewater per year 1,100,000 m$^3$/y gas would be required.

35 Available at: http://www.ukconversionfactorscarbonsmart.co.uk (accessed on 23 June 2013).
On the other hand, as regards waste disposal, the 1996 technology comparison showed the following waste arisings (such as filter waste) that have to be combusted.

### Table 4.12: Organic waste arisings under the water-based and DBP-based technologies

<table>
<thead>
<tr>
<th>Organic waste arisings</th>
<th>Water-based technology</th>
<th>DBP-based technology</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 kt/y capacity</td>
<td>240 t/y</td>
<td>0 t/y</td>
<td>Based on 1996 comparison of MA technologies by Condea</td>
</tr>
<tr>
<td>105 kt/y capacity</td>
<td>603 t/y</td>
<td>2 t/y</td>
<td>Figure for water-based technology is extrapolated from figure in row above (linear extrapolation). For the Huntsman technology, the experience of running the Moers plant on the Huntsman technology between 1999 and 2012 suggests that ca. 2 t/y of solid organic waste have to be removed from wastewater cleaning services and filter changes</td>
</tr>
</tbody>
</table>

Source: applicant’s own information

**Conclusion**: a switch to the water-based recovery technology would result in the generation of an additional ca. 600 t/y of organic waste with the associated disposal requirements.

**Quality of MA product**

**Argument**: the use of xylene within the water-based recovery technology adversely affects the quality of the MA product to the extent that some customers of Sasol-Huntsman might be reluctant to continue purchasing MA from the company should a conversion be effected.

**Presence of xylene impurities and market acceptability of MA**: the use of xylene in the water-based recovery of MA results in the presence of traces of xylene in the final MA product. Therefore, the quality of MA from water-based plants is inherently inferior compared to the DBP-based technology. Detectable xylene traces in the MA product may render it unacceptable to companies manufacturing products considered environmentally friendly (biologically degradable) or ‘green’. Relevant affected products would include polyacrylic acids used in water additives, laundry and dishwashing detergents.

**Role of recovery method in the market acceptability of MA**: although the specific xylene content in competitors’ MA product is not known, Huntsman notes that, prior to the formation of Sasol-Huntsman and adoption of the Huntsman technology at Moers, Condea would only guarantee a 100 ppm max. concentration of xylene in MA produced from its water-based process. Some customers required a limit much lower than 100 ppm and thus would not buy from Condea. Sasol-Huntsman cannot be certain whether such requirements are placed upon the MA product of plants currently using water-based recovery systems. However, it can be confirmed that some of Sasol-Huntsman’s customers continue to be sensitive to xylene and actively request that they are supplied MA with low xylene impurities.

**Conclusion**: the use of the water-xylene MA recovery technology could result in the presence of xylene impurities in the final MA product. This would cause problems with the sale of the product to specific customers of Sasol-Huntsman. Due to this degradation in the quality of its product, Sasol-Huntsman might potentially lose a part of its turnover that is associated with sales of MA for such xylene-sensitive applications.

Sasol-Huntsman estimates that its sales of MA to customers for xylene-sensitive applications may account for a small but considerable percentage of total turnover. As it cannot be certain that turnover losses might arise from the potential inability of Sasol-Huntsman to meet certain customers’ requirements on xylene impurities, no attempt will be made in this document to quantify...
these impacts. In any case, this cost element would likely be quite modest compared to the cost of converting the Moers plant back to the water-based technology.

4.2.3 Reduction of overall risk from a potential transition to water-based recovery

4.2.3.1 Human health issues associated with the use of o-xylene

Introduction and important note

The information below is given for completeness and to inform decision-makers. The key point of this Application for Authorisation is that the risks to workers’ health from exposure to DBP during the manufacture of MA are adequately controlled, as shown in the accompanying CSR, and the replacement of DBP-based recovery by an alternative recovery technology would not confer any discernible benefit to workers’ health.

Name and other identifiers for the substance

The one chemical input in a water-based recovery system that requires some attention is o-xylene. The Table below presents the identity of the substance. It should be clear that o-xylene should not be considered an alternative substance to DBP as its role departs radically from what DBP delivers within the Huntsman technology but its hazard profile is given consideration as the water-based recovery technology involves its use.

Table 4.13: Identity of o-xylene

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>EC number</td>
<td>202-422-2</td>
<td>1</td>
</tr>
<tr>
<td>EC name</td>
<td>o-xylene</td>
<td>1</td>
</tr>
<tr>
<td>CAS number</td>
<td>95-47-6</td>
<td>1</td>
</tr>
<tr>
<td>CAS name</td>
<td>o-xylene</td>
<td>1</td>
</tr>
<tr>
<td>IUPAC name</td>
<td>o-xylene</td>
<td>1</td>
</tr>
<tr>
<td>Other names</td>
<td>benzene, 1,2-dimethyl-1,2-dimethylbenzol</td>
<td>2</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C₈H₁₀</td>
<td>1</td>
</tr>
<tr>
<td>SMILES notation</td>
<td>Cc1ccc1c</td>
<td>2</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>106.17</td>
<td>3</td>
</tr>
<tr>
<td>Molecular structure</td>
<td><img src="image" alt="Structure" /></td>
<td>4</td>
</tr>
</tbody>
</table>

Sources:
1: ECHA Dissemination Portal: [Link](#)
2: ChemSpider Internet site: [Link](#)
3: GESTIS Substance Database: [Link](#)
4: ESIS Database: [Link](#)
Competition of o-xylene

The ECHA Dissemination Portal provides information on a variety of commercial o-xylene products, some of which contain certain impurities, such as:

- benzene (EC Number 200-753-7, CAS Number 71-43-2), a Carc Cat 1A substance;
- ethyl benzene (EC Number 202-849-4, CAS Number 100-41-4);
- p-xylene (EC Number 203-396-5, CAS Number 106-42-3), a skin irritant; and
- m-xylene (EC Number 203-576-3, CAS Number 108-38-3), a skin irritant.

Physicochemical properties of o-xylene

The following Table summarises the available information on the physicochemical properties of o-xylene. The information has been collected from several literature sources.

**Table 4.14: Physicochemical properties of ortho-xylene**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Remarks (models used, etc.)</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state at 20°C and 101.3 kPa</td>
<td>Colourless liquid</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-25.2°C</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Boiling point</td>
<td>144.5 °C</td>
<td>148.29°C (adapted Stein and Brown method)</td>
<td>1, 2</td>
</tr>
<tr>
<td>Density</td>
<td>0.8755 g/cm³ at 25°C</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>0.8801 g/cm³ at 20°C/4°C</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>8.82 hPa at 25°C</td>
<td>Experimental</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>9.08 hPa at 25°C</td>
<td>Vapour Pressure, Mean of Antoine &amp; Grain methods</td>
<td>2</td>
</tr>
<tr>
<td>Surface tension</td>
<td>29.76 dyne/cm at 25°C</td>
<td></td>
<td>1, 2</td>
</tr>
<tr>
<td>Water solubility</td>
<td>170.5 mg/L at 25°C</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>162 -242 mg/L at 25°C</td>
<td>WSKOW v.1.41, WATERNT v.1.01 (US EPA, EPI Suite v 4.00)</td>
<td>2</td>
</tr>
<tr>
<td>Partition coefficient n-octanol/water</td>
<td>3.12</td>
<td></td>
<td>1, 2</td>
</tr>
<tr>
<td>Flash point</td>
<td>32°C Closed cup</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>23°C Closed cup</td>
<td></td>
<td>4</td>
</tr>
<tr>
<td>Flammability</td>
<td>Classified as Flam. Liq. 3</td>
<td></td>
<td>See next Table</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>Lower explosion limit: 0.97 vol. %, 43 g/m³</td>
<td>Maximum explosion pressure: 8.7 bar</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>Upper explosion limit: 7.6 vol. %, 335 g/m³</td>
<td></td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>0.9 -9.0 vol. %</td>
<td></td>
<td>1, 2</td>
</tr>
<tr>
<td>Self-ignition temperature</td>
<td>463 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>No data</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Granulometry</td>
<td>Not relevant</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Sources:**
1: ECHA Dissemination Portal: [Link](#)
2: ECHA Dissemination Portal: [Link](#)
3: GESTIS Substance Database: [Link](#)
4: (Huntsman, pers. comm.)
Classification and labelling of o-xylene

Xylene is flammable, irritating to the skin and harmful if exposed to via inhalation or skin. The main intake pathway for o-xylene is via the respiratory tract. Uptake through the skin should also be taken into account whenever there is contact with the liquid. The main acute toxic effects are irritation to the eyes, airways and skin, and disturbance to the central nervous system (narcotic effects at high concentrations). The main chronic effects are chronic local effects to the skin and mucous membranes and disturbances to the central-nervous system.

The harmonised classification and labelling of o-xylene under the CLP Regulation is given below.

Table 4.15: Harmonised classification and labelling for o-xylene (EC No: 202-422-2, CAS No: 95-47-6)

<table>
<thead>
<tr>
<th>Classification</th>
<th>Hazard Statement Code(s)</th>
<th>Pictogram Code(s)</th>
<th>Hazard Statement Code(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flam. Liq. 3</td>
<td>H226</td>
<td></td>
<td>H226</td>
</tr>
<tr>
<td>Acute Tox. 4 *</td>
<td>H332</td>
<td></td>
<td>H332</td>
</tr>
<tr>
<td>Acute Tox. 4 *</td>
<td>H312</td>
<td></td>
<td>H312</td>
</tr>
<tr>
<td>Skin Irrit. 2</td>
<td>H315</td>
<td></td>
<td>H315</td>
</tr>
</tbody>
</table>

Source: ECHA C&L Inventory: Link (accessed on 23 February 2013)

ECHA C&L Inventory suggests that classifications notified by individual companies may vary. Classifications that appear in the Inventory in addition to those shown in the CLP Regulation might relate to impurities contained in some o-xylene products placed on the market.

Due to inadequate data, the International Agency for Research on Cancer (IARC) determined that it is not known whether xylene causes cancer and thus considered it as not being classifiable (HPA, 2010).

Furthermore, xylene is a flammable liquid with a flash point of 23-32°C and an explosion limit of 0.9-9.0% by volume. In the areas where xylene is used, it is necessary to have a higher standard (explosion-proof) of installed instruments and process equipment. Vapours of xylene are heavier than air and have to be kept away from systems below ground like sewers, sumps and cable channels.

Potential for worker exposure to o-xylene

The Moers plant has a history of use of the water/xylene recovery technology; therefore, there is experience with the use of such an alternative to DBP. The handling of xylene shows significant downsides as worker exposure to xylenes and waste streams containing xylenes may occur during the manufacture of MA. In addition, worker exposure associated with the higher frequency of process equipment wash-outs should also be taken into consideration.

Comparison of hazards and risks for DBP and o-xylene

A comparison of the hazards of DBP to those of o-xylene is not provided as the use of xylene is only a minor component in the water-based recovery technology and o-xylene cannot be considered

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to constitute a direct replacement for DBP. Thus, a direct comparison would not be appropriate or informative.

Similarly, no attempt has been made to investigate the potential exposure of workers to o-xylene at the Moers plant given that the two substances are employed in a completely different fashion; still, the downsides of using xylene mentioned above need to be considered. Finally, the above information, as well as information from the REACH Registration of this xylene isomer would indicate that the substance has an overall more benign hazard profile than DBP.

4.2.3.2 Environmental issues associated with the use of o-xylene and greenhouse gas emissions

Hazards from the use of o-xylene

Only a very short review of the environmental hazards from xylene is given here for completeness.

Xylene is readily volatile and flammable and as a VOC (Volatile Organic Compound) contributes to the formation of ozone in the lower atmosphere (in the air, xylenes are broken down by sunlight). Xylene isomers are harmful to aquatic organisms but overall risk to the aquatic environment is low, except near localised industrial discharges or spillages. Only very small amounts are taken up by plants, fish and birds. In soil and water, o-xylene is readily biodegraded under a wide range of aerobic and anaerobic conditions (Environment Agency for England and Wales, 2011).

There is currently legislation on the reduction of releases of VOCs across the EU. Xylene releases are regulated under EC Directive 76/464/EEC (plus daughter directives) and was also regulated under (EC) Regulation 793/93. As a VOC, the main international legislation is the UN/ECE Convention on Long-Range Transboundary Air Pollution and Basel Conventions. Directive 99/13/EC on solvents (VOC emissions) will also apply (Environment Agency for England and Wales, 2011).

Some information on releases of xylene from the manufacture of MA is given in the literature. Information from the Austrian Environment Agency (Umweltbundesamt, 2001) and the US Environmental Protection Agency (US EPA, 1994) indicates that in the past (1990s) the use of the substance in MA recovery processes was accompanied by releases, for example from the dehydration columns, the xylene columns, the distillation equipment, the pure MA columns and the condensers. However, it is understood that emission controls have since improved and the emissions of xylene referred to in these literature sources are no longer representative of a typical water-based MA manufacturing plant.

It has not been possible to identify more recent information from current users of this recovery technology in the open literature. We have looked into the xylenes emission data available for 2009 on the European Pollutant Release and Transfer Register37 and releases of xylene were not reported for any relevant plant in Italy, Austria, Hungary, Poland or Spain where EU-based MA manufacturers are known to be located.

It must be noted that whilst DBP bears classification for aquatic toxicity (Aquatic Acute 1), o-xylene does not have a classification for environmental hazards.

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37 Available at: [http://prtr.ec.europa.eu/PollutantReleases.aspx](http://prtr.ec.europa.eu/PollutantReleases.aspx)
Other environmental impacts

As explained in Section 4.2.2.2, water-based recovery uses more energy and is thus less advantageous than the Huntsman technology at best, and a net energy consumer at worst. To compensate for the loss of energy exports from the MA plant, additional energy has to be purchased and used with a consequent additional release of CO\(_2\). Furthermore, the use of the water-based recovery process results in increased wastewater production, increased cleaning requirements and increased generation of organic waste. The incineration of this waste will release an additional amount of CO\(_2\), the most significant greenhouse gas influencing climate change (EEA, 2011).

**CO\(_2\) emissions from one-off impacts on the energy balance during plant conversion:** as will be explained in Section 4.2.4.2, the conversion of the Sasol-Huntsman plant to the water-based technology would mean that for over two years (25 months) the MA plant would not be able to generate steam, which is required by the Sasol Solvents power plant for serving the needs of Sasol Solvents and for exporting electricity to the grid. It will be explained in Section 4.2.4.2 that, for two years, the Sasol Solvents power plant would be deprived of 650 GWh of steam currently exported from the MA plant. To obtain this from fuel gas, an additional 459 GWh would have to be obtained each year from natural gas purchased from the open market, as described in the Confidential Annex to this AoA.

**CO\(_2\) emissions from on-going impacts on the energy balance and incineration of wastewater:** with regard to the higher consumption of energy by the water-based technology, Table 4.17 will show that the energy demand for the water-based technology is almost double that for the DBP-based technology. The energy deficit is calculated at 197 GWh/y, which would have to be covered by natural gas purchased from the open market.

Using greenhouse gas emission factors available from UK Department for Environment, Food and Rural Affairs\(^{38}\), it can be calculated that the consumption of natural gas equivalent to 459 x 2 = 918 GWh would result in the release of an additional ca. 170 ktonnes CO\(_2\) (eq) on a gross calorific value basis.

**CO\(_2\) emissions from on-going impacts on the energy balance and incineration of wastewater:** with regard to the higher consumption of energy by the water-based technology, Table 4.17 will show that the energy demand for the water-based technology is almost double that for the DBP-based technology. The energy deficit is calculated at 197 GWh/y, which would have to be covered by natural gas purchased from the open market.

Using greenhouse gas emission factors available from UK Department for Environment, Food and Rural Affairs, it can be calculated that the consumption of natural gas capable of producing 197 GWh/y would result in the release of an additional 197,000,000 x 0.20421 = ca. 40,230 tonnes CO\(_2\) (eq) per year on a net calorific value basis.

Additionally, the incineration of the additional wastewater would add a further ca. 2,020 tonnes of CO\(_2\) releases to the atmosphere per year (see calculation earlier in Section 4.2.2.2 under the heading Wastewater generation).

Therefore, the total additional release of CO\(_2\)-equivalent would be **42,250 tonnes per year**.

**Monetisation of externalities:** monetisation is based on the approach taken in Section 4.1.3.4. Therefore,

- one-off external (damage) costs due to the emission of an estimated additional 170 ktonnes of CO\(_2\) per year are calculated at ca. **€5.7 million**; and

\(^{38}\) Available at: [http://www.ukconversionfatorscarbonsmart.co.uk](http://www.ukconversionfatorscarbonsmart.co.uk) (accessed on 23 June 2013).
ANALYSIS OF ALTERNATIVES

- on-going external (damage) costs due to the emission of an estimated additional 42,250 tonnes of CO₂ per year are calculated at just over €1.4 million per year. Over an 18-year horizon and with a discount rate of 4% (assuming that the valuation for CO₂ emissions remains at €33.6 per tonne), the present value of these environmental externalities would be ca. €19 million.

The overall calculated externalities would therefore be ca. €25 million. It is clear that the replacement of DBP by the water-based method would have a detrimental effect on the environment.

Conclusion

Whilst the use of o-xylene for the recovery of MA from the reaction gases may not lead to significant environmental releases, water-based recovery is environmentally more burdensome than the Huntsman technology in terms of energy consumption and wastewater generation which result in increased CO₂ emissions. The environmental externalities of these emissions are estimated at ca. €23 million over the assumed 20-year assessment period.

4.2.4 Economic feasibility of water-based recovery

4.2.4.1 Economic feasibility DEZA

DEZA does not market the alternative technique. Therefore, if water-based recovery were to replace the DBP-based process, DEZA would lose the sales of DBP without being able to replace them. The turnover of DBP that would be lost is presented in the SEA (Section 2.2.2.1). Overall, water-based recovery technology cannot be considered to be economically feasible for DEZA.

4.2.4.2 Economic feasibility for Sasol-Huntsman

Overview

For the assessment of the economic feasibility of water-based recovery for Sasol-Huntsman, the following cost elements will be considered:

1. costs arising from converting the Moers MA plant from the Huntsman technology back to water-based recovery of MA;
2. costs arising from impacts on the process efficiency of the MA recovery;
3. costs arising from changes in steam consumption and export to the Sasol Solvents power plant;
4. costs arising from the expected increase in wastewater generation;
5. costs arising from increased fouling of the production line and associated maintenance requirements; and
6. costs associated with the loss of turnover due to adverse effects on the quality of the MA product (xylene impurities).

Other cost elements, for example the cost of o-xylene, would be of relatively low significance and have not been investigated.
The discussion here demonstrates that the cost of switching to the water-based recovery technology, particularly the cost and duration of the modification of the Moers plant, would result in the closure of the Sasol-Huntsman plant.

Cost element 1: Cost of plant conversion

**Approach:** the replacement of the solvent-based recovery technology by the water-based recovery technology would be accompanied by significant modifications to existing installations and equipment for both the MA plant but also for the neighbouring Sasol Solvents site that relies on the steam generated from the MA reaction.

In the MA plant, the entire liquid side\(^{39}\) would have to be modified for both trains, requiring demolition of these parts and installation of the water-based recovery system. Because of the high integration of both MA trains, this cannot be done in one step. Based on the experiences of the recently installed MA 2\(^{nd}\) train (reactor), where Sasol-Huntsman needed two years’ construction time, it is expected that at least two years downtime would be required for the conversion of the whole plant including demolition.

For estimating the cost and duration of conversion, two key assumptions are made:

- parts of the existing plant would still be suitable for use with water-based recovery: the air compression and reactor section, as well as the incineration units could be used with only minor modifications because they are similar in both technologies; and

- using the existing condensing steam turbines compressors would mean that the water-based process would be a net steam importer because of the higher internal usage of the produced steam (see earlier discussion in Section 4.2.2.2 under the heading *Energy consumption*).

Sasol-Huntsman has undertaken an estimate of the duration, cost and man-power demand of the theoretical switch to the water-based process, as shown in the Confidential Annex. A summary of the findings is presented below.

**Summary of cost estimates:** the following is the summary of estimated costs:

- **Cost of plant conversion:** as described in the Confidential Annex, the total cost of switching from the solvent-based technology to the water-based technology could be **ca. €170 million**. The key cost elements include:
  - the rebuild of the absorption, stripping and afterflasher section;
  - the rebuild of the distillation section;
  - the rebuild of the solvent cleaning system; and
  - the installation of a gas cooling system.

- **Cost of inactivity/downtime:** the discussion presented in Section 4.1.4.2 would apply here. The calculation of conversion costs assumes a total shutdown of the Moers plant with no production

\(^{39}\) Liquid side is the recovery section (downstream of the reactors).
of MA for a total of 25 months. As for the conversion to the ALMA technology, it is estimated that such downtime would be associated with a lost turnover of ca. **€208-250 million**. Again, this estimate is based on the simplifying assumption that the current turnover figures will generally remain valid in the future.

**This cost of inactivity would be extremely detrimental to Sasol-Huntsman and could only lead to the closure of the MA plant.** Even if it could be contemplated that conversion back to the water-based technology would create a viable business model, the 25-month loss of production would result in significant upset in the EU MA market, cause MA prices to increase significantly owing to the shortage of MA in the EU and lead customers to finding alternative MA suppliers, possibly outside the EU. Furthermore, some downstream users of MA, finding high MA prices and short supply in the EU, may close down their business or relocate outside the EU. By definition, due to Sasol-Huntsman having to move to a much less efficient production technology, the cost of production would increase when the plant would come back on line. This would lead to an increase in the price of MA placed on the market by Sasol-Huntsman. Furthermore, Sasol-Huntsman would also need to increase prices in order to ensure that they could repay both the existing and any new loan. The combination of selling at a less competitive price and the need to re-build their customer base would lead to difficulties in the short term. Therefore, even if the conversion of the Moers plant could be financed and successfully engineered, there would be no justification from a commercial perspective for going through this process, especially in light of the fact that risks to workers’ health from exposure to DBP are already adequately controlled.

- **Cost of raising capital**: the discussion presented in Section 4.1.4.2 would apply here.
- **Cost of lost investment**: the discussion presented in Section 4.1.4.2 would apply here.

As stated earlier, the cost estimates presented in this document assume a 20-year lifetime of a new production plant. This is based on the time required for return on investment rather than the commercial lifetime of the plant/equipment, which might be much longer. In addition, a discount rate of 4% is used, as per ECHA’s Guidance on Applications for Authorisation.

**Summary**: the following Table summarises the above cost elements. The overall cost of plant conversion is estimated at over **€378 million** (figure is rounded). This high cost could not be passed on to customers and confirms again the view that the ultimate result of converting back to the water-based technology would be the closure of the Sasol-Huntsman MA plant.

**Table 4.16: Cost element 1 summary: Modifications to MA plant to introduce the water-based technology**

<table>
<thead>
<tr>
<th>Cost element</th>
<th>Type of cost</th>
<th>Present value cost</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quantifiable costs</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cost of plant alternation activities</td>
<td>One-off (investment)</td>
<td>€170 million</td>
</tr>
<tr>
<td>Cost of inactivity/downtime</td>
<td>One-off (expenditure)</td>
<td>€208-250 million</td>
</tr>
<tr>
<td><strong>Non-quantifiable costs</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cost of raising capital</td>
<td>One-off (expenditure)</td>
<td>Not quantified</td>
</tr>
<tr>
<td>Cost of lost investment</td>
<td>One-off (sunk costs)</td>
<td>Not quantified</td>
</tr>
<tr>
<td><strong>Total (rounded)</strong></td>
<td></td>
<td>&gt;€378 million</td>
</tr>
</tbody>
</table>
Cost element 2: Cost of impacts on recovery efficiency

A reduction of MA recovery efficiency by 4% would impact upon the tonnage of MA produced and could erode up to 4% of the turnover of Sasol-Huntsman.

To estimate this cost, we assume that for the first two years during the switch from solvent-based to water-based recovery, the Moers plant would be shut down for the conversion to be implemented. Thereafter, over the assumed 20-year assessment period, Sasol-Huntsman would lose 4% of its turnover, due to the poorer MA recovery efficiency of the water-based technology.

With a turnover of €100-120 million per year, it can be estimated that €4-4.8 million per year would be lost at current prices. The present value of this loss over 20 years at a 4% discount rate would be ca. €52-63 million (rounded), assuming the Moers plant would continue to operate at current levels of capacity utilisation.

Cost element 3: Cost of changes in steam generation and consumption

Huntsman and Sasol-Huntsman have no information about their competitors’ actual cost of MA manufacture. How steam is valued can vary significantly according to host chemical park requirements and the value of alternative steam sources. Therefore, the following analysis is based on a series of assumptions.

The Moers MA plant is highly integrated into the Sasol Solvents site. Particularly, the steam balance matches the demand and production of other Sasol Solvents plants at the Moers site. Switching to water-based technology would significantly reduce steam production by the MA plant. Consequently, the utility consumptions will negatively change for steam consumption, cooling water (a new cooling tower would be required) and fuel gas consumption for the incineration units.

As described earlier, Sasol-Huntsman has relied on information on the steam generation and consumption characteristics of the water-based recovery that was made available to Condea in the mid-1990s to estimate the difference in steam consumption under the two recovery technologies. The estimates are shown in the following Table and suggest an annual difference in energy consumption of 197 GWh/y.

**Table 4.17: Steam consumption for DBP-based and water-based recovery of MA**

<table>
<thead>
<tr>
<th>Energy consumption parameters</th>
<th>Water-based technology</th>
<th>DBP-based technology</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal steam consumption</td>
<td>550.1 TJ/y</td>
<td>279.4 TJ/y</td>
<td>Figures based on technology comparison in 1996</td>
</tr>
<tr>
<td>(based on a 40 kt MA/y capacity)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Internal steam consumption</td>
<td>1,444.0 TJ/y</td>
<td>733.4 TJ/y</td>
<td>Figures extrapolated from figures in above row</td>
</tr>
<tr>
<td>(based on a105 kt MA/y capacity)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Energy demand</td>
<td>400 GWh/y</td>
<td>203 GWh/y</td>
<td>Rounded figures. Conversion from TJ to GWh was undertaken using an online calculator: [Link](accessed on 23 February 2013)</td>
</tr>
</tbody>
</table>

Source: applicant’s own information

The annual cost of purchasing this additional energy by Sasol-Huntsman has been calculated on the basis of the cost of purchased fuel gas of €29 per MWh\(^40\). The cost to Sasol-Huntsman of obtaining

\(^{40}\) Price valid in January 2013.
the missing 197GWh/y would be €5.7 million per year. The present value of this cost over 20 years with a discount rate of 4% can be calculated at ca. €75 million (rounded).

It is worth noting that for the first two years of the 20-year assessment period, the Sasol Solvents power plant would be deprived of 650 GWh of steam currently exported from the MA plant. To obtain this from fuel gas, an additional 459 GWh would have to be obtained each year from natural gas purchased from the open market, as shown in the Confidential Annex to this AoA. The cost of acquiring this amount of energy over 2 years of MA plant shutdown can be calculated as follows:

\[2 \times 459,000 \text{ MWh/y} \times €29/\text{MWh} = €26.6 \text{ million.}\]

Additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf, Part 5.

Cost element 4: Cost of increased wastewater generation

It was described above that the use of water-based recovery would generate an additional 17 ktonnes of wastewater each year. Two options have been identified by Sasol-Huntsman as possibilities for the treatment of this additional wastewater stream:

- the rebuild of the existing wastewater treatment facilities at the Moers plant; or
- the incineration of this additional stream of waste.

The biological wastewater treatment plant currently operating at Moers can handle 60 m³/hr and a certain freight of organics for the whole of the Moers site. To be able to cope with a conversion to the water-based technology, doubling the capacity of the wastewater treatment plant would be required as a minimum.

If it were decided to modify the existing wastewater treatment plant, there would be a considerable one-off investment and an increased operating cost due to the increased throughput of wastewater. This option would be particularly costly in comparison to the incineration of the additional stream of waste and therefore it is considered that the most realistic option would be to simply incinerate the additional wastewater volume.

Thus, if incineration of the waste was selected, it is estimated that the combustion of the additional 17 ktonnes of wastewater would require the consumption of ca. 1,000,000 m³/y fuel gas. It is assumed that 1m³ of natural gas provides equivalent energy of 11 kWh. Therefore, 1,000,000 m³/y of gas is equivalent to 11,000 MWh/y. Using the same price of fuel gas per MWh as above, the annual cost of incineration would be ca. €0.32 million per year. The present value of this cost over 20 years and a discount rate of 4% can be calculated at ca. €4.2 million.

Cost element 5: Cost of increased fouling incidence

As indicated in Section 4.2.2.2, the use of the water-based recovery technology would generate an additional ca. 600 t/y of organic waste. Sasol-Huntsman estimates that the cost of incinerating 1 tonne of organic waste is €317 (price valid for 2012). Therefore, the annual cost of disposing of ca. 600 t/y will be ca. €0.19 million. The present value of this cost over 20 years at a 4% discount rate is ca. €2.5 million.

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41 Figure taken from http://www.thegreenblue.org.uk/pdf/z%201088.%20Energy%20and%20carbon%20conversions.pdf (accessed on 21 September 2011).
**ANALYSIS OF ALTERNATIVES**

Cost element 6: Cost of revenue loss due to xylene impurities in the MA product

As explained earlier, this cost element would likely be quite modest compared to the cost elements quantified above and no attempt to quantify this has been made.

**Summary of costs**

Table 4.18 summarises the costs that would arise for the downstream user of DBP (Sasol-Huntsman).

In accordance with the approach followed for the assessment of the economic feasibility of DIBE/ALMA, the summary of costs not only presents the losses in turnover but also the losses in profit that is associated with the lost turnover, or in other words, the value added lost. A theoretical profit margin of 10% is again assumed.

**Table 4.18: Summary of costs of the replacement of DBP-based absorption with water-based recovery**

<table>
<thead>
<tr>
<th>Cost element</th>
<th>Actor incurring cost</th>
<th>Type of cost</th>
<th>Cost impact on...</th>
<th>Annual cost (where available)</th>
<th>Present value cost (20 years, 4% discount)</th>
<th>Based on turnover</th>
<th>Based on profit (10% margin)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Cost of plant conversion</td>
<td>Sasol-Huntsman</td>
<td>One-off</td>
<td>Profit</td>
<td>–</td>
<td>€170 million</td>
<td>€170 million</td>
<td>&gt;€208 million</td>
</tr>
<tr>
<td>2 Cost of impacts on recovery</td>
<td>Sasol-Huntsman</td>
<td>Recurring</td>
<td>Turnover</td>
<td>&gt;€4 million</td>
<td>&gt;€52 million</td>
<td>&gt;5.2 million</td>
<td>&gt;5.2 million</td>
</tr>
<tr>
<td>3 Cost of changes in steam ending</td>
<td>Sasol Solvents</td>
<td>One-off</td>
<td>Profit</td>
<td>€5.7 million</td>
<td>€75 million</td>
<td>€75 million</td>
<td>&gt;€75 million</td>
</tr>
<tr>
<td>4 Cost of increased wastewater</td>
<td>Sasol-Huntsman</td>
<td>Recurring</td>
<td>Profit</td>
<td>€0.32 million</td>
<td>€4.2 million</td>
<td>€4.2 million</td>
<td>&gt;€4.2 million</td>
</tr>
<tr>
<td>5 Cost of increased fouling</td>
<td>Sasol-Huntsman</td>
<td>Recurring</td>
<td>Profit</td>
<td>€0.19 million</td>
<td>€2.5 million</td>
<td>€2.5 million</td>
<td>&gt;€2.5 million</td>
</tr>
<tr>
<td>6 Cost of xylene impurities</td>
<td>Sasol-Huntsman</td>
<td>Recurring</td>
<td>Turnover</td>
<td>Not quantified</td>
<td>Not quantified</td>
<td>Not quantified</td>
<td>&gt;€305 million</td>
</tr>
</tbody>
</table>

The present value of the overall cost would be:

- for Sasol-Huntsman over €437 million, based on lost turnover, or over €203 million, based on lost profit for a theoretical 10% profit margin. This is clearly an unacceptable cost that could not be passed on to the customers or absorbed by Sasol-Huntsman; and
- for Sasol Solvents €102 million, as a result of the loss of steam that would otherwise be generated by the MA reaction and would be passed onto the on-site power plant.
Overall, the conversion to the water-based technology is not an economically feasible alternative for Sasol-Huntsman and would also severely impact upon Sasol Solvents.

4.2.5 Availability of water-based recovery technology

4.2.5.1 Current and projected availability DEZA

Market availability

From DEZA’s perspective, water-based recovery technologies are globally marketed by completely different companies. This alternative is not available to DEZA.

Actions required for improving availability

Availability is unlikely to change for DEZA in the foreseeable future.

4.2.5.2 Current and projected availability for Sasol-Huntsman

Market availability

Water-based methods of MA recovery have a long history of application. Water-based recovery is neither the most modern nor an efficient technology for the recovery of MA from the reaction off-gas but it is employed by several plants across the globe; in that sense, water-based recovery is available for use. The Moers plant also used this method in the past, before the switch to solvent-based recovery. Moreover, there are no legal barriers to conversion that would arise from the existing licensing agreement between Sasol-Huntsman and Huntsman.

Nevertheless, the time and cost implications of the conversion make such conversion impractical and unrealistic, as explained earlier.

Actions required for improving availability

Not relevant, as the technique is already available on the market.

4.2.6 Conclusion on suitability and availability for water-based recovery

4.2.6.1 Summary of findings

Technical feasibility

In assessing the suitability of water-based recovery of MA, it must be remembered that this Application for Authorisation in its accompanying CSR demonstrates that risks to workers’ health from exposure to DBP during the manufacture of MA are very low and are already adequately controlled. Therefore, the use of an alternative technology which does not use DBP would not confer any material benefit to the health of workers employed by the downstream user.

In any case, the detailed analysis presented above has demonstrated the following clear drawbacks of the water-based recovery of MA:

- **efficiency of recovery**: literature and practical experience agree that water-based absorption offers a worse recovery rate than solvent-based absorption. The difference in efficiency is estimated at ca. 4%, adversely affecting the economics of the MA manufacturing process;
• **energy consumption**: the water-based recovery of MA has greater energy requirements than the solvent-based process: it consumes 5.2 tonnes of steam per tonne of MA while the solvent-based process requires only 2.5 tonnes of steam per tonne of MA. Currently the MA plant in Moers is a net exporter of steam to the adjacent Sasol Solvents power plant. Conversion of the plant to water-based recovery would turn the MA plant from a net exporter into a net importer of steam. The changes in steam consumption would result in an energy shortage at the Sasol Solvents power plant of 197 GWh per year;

• **wastewater production**: the use of water-based recovery would create a new wastewater stream, which would add an estimated 17 ktonnes of wastewater outputs each year. The Moers plant is not currently able to biologically treat this additional wastewater. Its incineration would require an additional consumption of an estimated 1 million m$^3$ of fuel gas each year;

• **fouling**: the Huntsman technology allows for an improved control of fouling of the process equipment through better control of the formation of by-products and polymeric tars. Whilst cleaning and maintenance activities would probably not impose an insurmountable burden, an additional organic waste stream would be generated (equivalent to ca. 600 t/y) which would require disposal by incineration; and

• **xylene impurities**: some downstream users of MA demand that the MA product composition does not exceed a certain low level of xylene impurities. Sasol-Huntsman’s experience confirms that guaranteeing xylene impurity content below 100 ppm when employing water-based recovery technology would be difficult. Therefore, a switch to water/xylene-based recovery could result in revenue losses as certain customers might refuse to purchase MA from Sasol-Huntsman.

**Economic feasibility**

It is demonstrated that the replacement of DBP-based absorption by water-based recovery of MA would require plant modifications at a significant cost. Although the assumption is made that some of the existing equipment could be reused, the cost that would arise from rebuilding the liquid side for both trains and the associated downtime (estimated at 25 months) would exceed €378 million (present value based on lost turnover). Additional costs would arise from the partial loss of steam exports, the increased incidence of fouling, the reduction of recovery efficiency, the increased generation of wastewater and the presence of xylene impurities in the final MA product. The overall cost of switching to water-based recovery would exceed a present value of €539 million over 20 years based on lost turnover or €305 million based on lost profit for a theoretical 10% profit margin.

In light of the magnitude of these costs, and considering that worker risks from exposure to DBP are already adequately controlled, this alternative technology can only be seen as commercially unrealistic, thus cannot be considered to be economically feasible for the user of DBP.

**Availability**

With regard to the market availability of water-based recovery technology, this is well known and available, although this is not the case for DEZA as far as licensing the downstream user is concerned. From a legal perspective, Sasol-Huntsman is not prohibited from switching back to water-based recovery of MA. However, after spending a considerable amount of time and making significant investments to expand the capacity of the Moers plant to 105 kt MA/y, a change to water-based recovery would be completely unrealistic, particularly since Condea abandoned the water-based technology back in 1999. The less favourable economics and the increased
ANALYSIS OF ALTERNATIVES

The environmental impact of water-based absorption could not be justified on grounds of eliminating the currently very low and adequately controlled risks to workers’ health from exposure to DBP.

Reduction of risks

Irrespective of the reality of adequate control of risks at the Moers plant, under the water-based technology, a considerable additional release of greenhouse gases (CO$_2$), estimated at over 42 ktonnes per year, would be expected due to the increased energy demand and increased generation of wastewater that would need to be disposed of by incineration.

<table>
<thead>
<tr>
<th>Conclusion:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water-based recovery technology cannot be considered a suitable alternative to DBP-based absorption during MA manufacture.</td>
</tr>
</tbody>
</table>

4.2.6.2 Actions to make the alternative suitable and available

Although water-based recovery is available on the market (but not through DEZA), it is not a suitable alternative for Sasol-Huntsman and there are no identifiable actions that would reverse this conclusion.

4.3 Alternative 3: Non-use and non-replacement of DBP

4.3.1 Description of the option

This option assumes that the use of DBP in the manufacture of MA ceases and that Sasol-Huntsman does not move to an alternative substance or technique. Given that Sasol-Huntsman only manufactures MA for sale to downstream users, this option would mean the outright closure of the Moers plant and the end of the Sasol-Huntsman business.

4.3.2 Technical feasibility of non-use/non-replacement of DBP

4.3.2.1 Technical feasibility for DEZA

The nature of this option is such that it cannot be considered beneficial or technically feasible to DEZA.

4.3.2.2 Technical feasibility for Sasol-Huntsman

This option would mean the closure of the Moers plant; Sasol-Huntsman only manufactures MA and engages in no other activity. An absorption system is necessary for the removal of gaseous MA from the reaction off-gases.

4.3.3 Reduction of overall risk from non-use/non-replacement of DBP

The removal of DBP from the manufacture of MA at Moers would certainly eliminate any risk to workers from DBP releases and exposure. However, the CSR demonstrates that risks are already adequately controlled; therefore, concerns over risks to workers’ health give no valid justification for the closure of the plant.
4.3.4 Economic feasibility of non-use/non-replacement of DBP

4.3.4.1 Economic feasibility for DEZA

The economic feasibility of this alternative would be similar to that for the other options: DEZA would lose its sales of DBP to Sasol-Huntsman. The turnover of DBP that would be lost is presented in the SEA (Section 2.2.2.1). An important point that the SEA makes is that the loss of sales of DBP to Sasol-Huntsman would cause the collapse of the sales of DBP by DEZA and would most likely lead to the cessation of the production of the substance, even if Authorisation were to be granted for other uses of the substance.

4.3.4.2 Economic feasibility for Sasol-Huntsman

Loss of turnover

Closure of the Moers plant would mean the complete loss of €100-120 million per year turnover currently associated with sales of MA, the only product manufactured and sold by the company.

Loss of investment

Sasol-Huntsman has invested significantly in its operations. The company has made a capital investment of ca. €150 million in the last 12 years for two rounds of capacity expansion (in 1999 and 2011), which is equivalent to ca. €200 million when finance costs are taken into account. As a result, the company is still committed to banks, customers, suppliers and shareholders, while the plant and equipment acquired through these investments have not run through their intended lifecycle. Additionally, Sasol-Huntsman also invested in 2005 and 2012 a further amount (discussed in more detail in the SEA, see Section 2.2.1.2.) into a state-of-the-art MA pastillation unit in order to support small businesses in the EU and Europe with sales of solid MA. Closure of the company would also mean the loss of this investment.

Cost of plant decommissioning

German law requires that in the event that the MA plant closes down, Sasol-Huntsman would be required to demolish the plant and return the MA site to a “grass-roots” condition suitable for re-use. This would be the case, even if the remainder of the neighbouring Sasol Solvents site remains in operation. Sasol-Huntsman is compelled to maintain adequate provision for demolition costs and these are calculated on an annual basis. An estimate of the decommissioning costs is provided in the SEA (Section 2.2.1.2).

It is unlikely that the company would realise any significant amount from the sale of any parts of the plant during demolition, as process equipment scrap is often passed on to the demolition company as part of their compensation for demolishing the site. Historical evidence supports the premise that it would be difficult to realise income from the sale of plant equipment in as much as Cray Valley, a past EU manufacturer of MA who has now shut down its MA business in France, tried unsuccessfully to sell its plant when it closed in 2007 and DSM, a current manufacturer of MA, has been trying unsuccessfully for several years to find a buyer for its plant.\footnote{According to Tecnon Orbichem, DSM announced in 2007 that it was planning a shift towards a life sciences and material sciences company by divesting or partnering some of its non-core businesses, including its MA and derivatives assets in Linz, Austria (Tecnon Orbichem, 2007). DSM’s Annual Report for 2010 also refers to “the expected disposal of the Maleic Anhydride and Derivatives business of DSM Pharmaceutical Products in Linz (Austria) in 2011” (DSM, 2011).}
Cost of paying existing loans

Sasol-Huntsman recently obtained a bank loan to fund the expansion of the Moers plant in 2008-2011 and loan repayments will be required until sometime in the future. In February 2015, a significant proportion of the total debt repayment, including fees and interest, is expected to be still outstanding. Since Sasol-Huntsman is a merchant seller of MA and it is the company’s only business, clearly, if it were unable to manufacture MA, then it would not have a source of revenue to make the loan payments due. Additional quantified detail is provided in the SEA, Section 2.2.1.2.

Commitments to customers and suppliers

Sasol-Huntsman holds a range of contracts with customers and suppliers. These do not only include multi-year contracts for the supply of MA downstream but also contracts for the provision of services by Sasol Solvents to Sasol-Huntsman. Sasol-Huntsman would not be able to deliver what is prescribed in these contracts if the closure of the Moers plant went ahead. Additional detail is given in the SEA, Sections 1.1.4.3 and 2.2.1.2.

Conclusion

It is clear that the closure of the Moers plant would have serious financial consequences for the management and shareholders of Sasol-Huntsman. The economic infeasibility of this alternative is undisputable.

4.3.5 Availability of non-use/non-replacement of DBP

This is not a relevant criterion for this alternative.

4.3.6 Conclusion on suitability and availability for non-use/non-replacement of DBP

It is clear that the non-use/non-replacement of DBP is not a realistic alternative.

Conclusion:

Non-use of DBP cannot be considered a suitable alternative for the applicant.

4.3.6.1 Actions to make the alternative suitable and alternative

This is not a relevant criterion for this alternative.
OVERALL CONCLUSIONS ON SUITABILITY AND AVAILABILITY OF POSSIBLE ALTERNATIVES FOR USE IN MALEIC ANHYDRIDE MANUFACTURE

5.1 Conclusions on the suitability and availability of commercially proven alternatives

5.1.1 Conclusion on the technical feasibility of commercially proven alternatives

The two commercially proven alternatives (the alternative substance DIBE and an alternative technology based on the water-based recovery of MA) are not available to DEZA; as such, they cannot be considered technically feasible.

In terms of technical feasibility for Sasol-Huntsman, DIBE does not meet all the technical criteria that were set out in Table 2.2; neither does water-based recovery perform as efficiently as DBP-based absorption against the criteria set out in Table 2.3. The technical shortcomings of these alternatives are summarised below.

<table>
<thead>
<tr>
<th>Technical shortcomings of Alternative 1: DIBE (within the ALMA technology)</th>
<th>Technical shortcomings of Alternative 2: water-based recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. A low solubility of FAc in DIBE resulting in increased solids deposition, thus increased maintenance frequency</td>
<td>1. A poorer MA recovery efficiency compared to DBP-based absorption</td>
</tr>
<tr>
<td>2. A lower boiling point than DBP which further increases solvent losses during use</td>
<td>2. A higher energy consumption, eliminating the energy surplus that can otherwise be exported to neighbouring facilities</td>
</tr>
<tr>
<td>3. The small difference between the density of DIBE and that of water makes recovery of the used solvent less efficient, further increasing its losses during MA manufacture</td>
<td>3. It creates a new wastewater stream that requires disposal</td>
</tr>
<tr>
<td>4. A lower flash point increases the risk of fire in the absorber column</td>
<td>4. Increased fouling leading to increased quantities of organic waste that require disposal</td>
</tr>
<tr>
<td>5. Use of DIBE requires modifications to the MA production plant which could only be accomplished at the cost of a 25-month stoppage of production operations</td>
<td>5. Xylene impurities in the MA product may render the product unsuitable for use in particularly sensitive or ‘green’ applications</td>
</tr>
<tr>
<td>6. DIBE is used within a technology that has not been successfully licensed since the mid-1990s</td>
<td>6. It requires modifications to the MA production plant which could only be accomplished at the cost of a 25-month stoppage of production operations</td>
</tr>
</tbody>
</table>

Technically, neither of the two alternatives can match the performance of DBP-based absorption of MA and the need for prolonged, complex and costly plant modifications renders these alternatives technically unfeasible and unrealistic, particularly given that the CSR demonstrates that risks to workers’ health are already adequately controlled.

5.1.2 Conclusion on the economic feasibility of commercially proven alternatives

For DEZA, the use of either alternative by Sasol-Huntsman would be accompanied by irreplaceable loss of turnover and thus cannot be considered economically feasible.

From the perspective of Sasol-Huntsman, the economic feasibility parameters for the two commercially proven alternatives are particularly disadvantageous and are summarised below.
### ANALYSIS OF ALTERNATIVES

<table>
<thead>
<tr>
<th>Economic feasibility of Alternative 1: DIBE</th>
<th>Economic feasibility of Alternative 2: water-based recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Implementation of DIBE would require plant modifications that would take 25 months and have a cost of over €150 million in turnover loss.</td>
<td>1. Implementation of the water-based technology would require plant modifications that would take 25 months and have a cost of over €170 million in turnover loss.</td>
</tr>
<tr>
<td>2. The cost of DIBE estimated to be up to 20% higher per tonne than DBP.</td>
<td>2. Additional costs would arise from the partial loss of steam exports, the increased incidence of fouling, the reduction of MA recovery efficiency, the increased generation of wastewater and the presence of xylene impurities in the final MA product.</td>
</tr>
<tr>
<td>3. The poorer physico-chemical properties of DIBE would result in higher losses of the solvent, thus requiring an increased consumption rate, by almost 2:1.</td>
<td>3. The overall cost of switching to water-based recovery would exceed €539 million present value over 20 years based on lost turnover or €305 million based on lost profit for a theoretical 10% profit margin, split between Sasol-Huntsman and Sasol Solvents.</td>
</tr>
<tr>
<td>4. The overall cost of switching to DIBE would exceed €403 million present value over 20 years based on lost turnover or €216 million based on lost profit for a theoretical 10% profit margin.</td>
<td></td>
</tr>
</tbody>
</table>

The estimated costs above would make Sasol-Huntsman’s operations unprofitable. Under either alternative, the cost of conversion is prohibitive, thus rendering these alternatives economically unfeasible and entirely unrealistic, particularly since exposure of workers to DBP is strictly controlled below the effects threshold.

#### 5.1.3 Conclusion on risk reduction potential of commercially proven alternatives

In terms of risk reduction, it is important to consider the key premise of this Application for Authorisation: exposure of workers at the Sasol-Huntsman plant is kept well below the effect threshold. Adequate control of risk is demonstrated in the CSR, thus, there is no unacceptable risk for the endpoint of concern (reproductive toxicity). Therefore, the replacement of DBP by an alternative substance or technology would not confer any discernible benefit to workers’ health.

Beyond the argument of adequate control, the information available on DIBE is limited; the lack of a REACH Registration for the substance would indicate that the substance is not a CMR 1A/1B, therefore its use in the place of DBP might result in a theoretical lessening of hazards. There exist, however, grounds for concern with regard to DIBE’s developmental and/or endocrine profile (including with respect to its ability to interact with the androgen receptor), and for its environmental toxicity. Moreover, the stoppage of steam generation at the MA plant for two years (during plant conversion) would result to an increased natural gas consumption with a concomitant release of 170 ktonnes of CO$_2$ with equivalent externalities of ca. €5.7 million.

On the other hand, the water-based recovery technology has a worse energy balance compared to solvent-based recovery. The shortfall would have to be made up by consuming increased amounts of fuel gas leading to a considerable additional release of greenhouse gases (CO$_2$). Additional CO$_2$ would also be released from the incineration of wastewater. The externalities of the release of an additional 170 ktonnes CO$_2$ during plant conversion and a further 42.2 ktonnes tonnes of CO$_2$-equivalent per year have been estimated ca. €25 million over 20 years.

#### 5.1.4 Conclusion on the availability of commercially proven alternatives

DEZA cannot supply either of the two commercially proven alternatives. DIBE is not available in DEZA’s portfolio of the manufacturer of DBP and its availability crucially depends on access to hydrogenation technology that DEZA does not currently have. The water-based technology is alien to DEZA’s areas of expertise.
From the perspective of Sasol-Huntsman, whilst water-based recovery is well known in the market, the availability of DIBE is much more obscure. The lack of REACH Registration and the pre-existing needs of licensees of the ALMA technology for DIBE create legitimate concern that the substance might not become available to Sasol-Huntsman at the required tonnage.

5.1.5 Overall conclusion

It is clear that Sasol-Huntsman, the sole user of DBP for the manufacture of MA in the EU, would have very little incentive to switch to either of the two commercially proven alternatives. These alternatives:

- would not confer any discernible benefit to workers’ health as the risks from exposure to DBP are already adequately controlled, as demonstrated in the CSR;
- would have a worse carbon footprint – water-based recovery would consume a considerable amount of steam and would generate additional wastewater and organic waste, while DIBE/ALMA technology might lead to increased fouling and consequent increased waste disposal requirements;
- could be detrimental to the quality of the MA product, with xylene impurities exceeding the limits set by customers, when water-based recovery is used;
- would require plant conversions involving a very long downtime of 25 months, which would consequently harm the EU industry that depends upon the supply of MA;
- would be accompanied by much poorer economics that would make the manufacture of MA unprofitable; and
- would require Sasol-Huntsman to obtain a new large loan in addition to an outstanding loan that financed the latest expansion of the Moers plant.

On the balance, if DBP could no longer be used, an outright closure of the plant would make better commercial and economic sense. Outright closure of the Moers plant in the event of a refused Authorisation for DBP is the only “Non-use” scenario that can be considered realistic and it is the only such scenario to be evaluated in the SEA.

5.1.6 Uncertainties

There is confidence in the conclusion that the commercially available alternatives are not technically and economically feasible. However, there is some uncertainty on certain elements of our analysis:

- information on the specifics of the ALMA technology, which utilises DIBE, is partly based on 20-year old data. This lack of more up-to-date information has been mitigated by the use of very recent actual data on plant modifications at Moers that were completed in 2011 but also by the knowledge that the ALMA technology has not been introduced into a new plant since the mid-1990s. The scale and complexity of the plant modifications that would be required for introducing an alternative substance or technology is such that despite the uncertainties in the cost estimates, the scale of the challenge that Sasol-Huntsman would face is clear and undisputable, particularly when considered in the light of the demonstrated adequate control of risks from exposure to DBP;
for the purpose of assessing the economic feasibility of the alternatives, the assumption has been made that the Sasol-Huntsman plant would undergo conversion over a period of 25 months before restarting operations. In this context, it would be uncertain how the market would react to the loss of 35% of the EU MA market which Sasol-Huntsman currently holds and to what extent Sasol-Huntsman would be able to regain old customers once MA production would recommence. However, such uncertainty does not critically impact upon the conclusions. Realistically, the scale of the cost of conversion is such that the use of these identified alternatives is purely theoretical. Instead, a refused Authorisation would simply lead to the Moers MA plant shutting down;

- some figures used in calculations may fluctuate, for example the price of fuel gas or the price used for the valuation of externalities of CO₂ emissions. However, the influence of this variability on the scale of the overall cost is limited; hence this uncertainty has immaterial impact on the conclusions; and

- the profit margin for the affected companies (primarily Sasol-Huntsman but also Sasol Solvents) cannot be disclosed. It has been assumed to be 10% which is a purely theoretical figure. A sensitivity analysis with different profit margin figures is not considered to be necessary. The main cost element is the cost of converting the Moers plant which is not affected by the profit margin figure selected.

5.2 Conclusions on the suitability and availability of commercially unproven alternatives

5.2.1 Conclusions on the suitability of commercially unproven alternatives

A selection of substances commonly mentioned in patent literature was presented in Table 3.3. The Table shows that each of the selected solvents fails one or more of the technical suitability criteria established for DBP alternatives and therefore cannot be considered technically feasible, and hence, realistic alternatives, at least at present.

With regard to the economic feasibility of commercially unproven alternatives, the discussion provided on the cost of conversion to the ALMA technology, certainly offers clear indications of the scale of cost and disruption that a change in the absorption solvent might cause. In addition, Table 3.4 has summarised the available information on the cost per tonne of the selected unproven alternatives. They appear to be much more costly than DBP (also see Annex 2).

5.2.2 Conclusions on the availability of commercially unproven alternatives

The availability of commercially unproven alternatives has not been examined in detail. It is expected that availability will vary amongst the substances.

5.3 Actions required for making the alternatives suitable and available

5.3.1 Overview

Making the commercially proven alternatives suitable is considered impossible with the current level of knowledge. Indeed, it is considered unwise to invest time, effort and funds in attempting to make the two alternatives (DIBE and water-based recovery technology) suitable for use at Moers. DIBE is used in a technology that has not been licensed since the 1990s and water-based recovery is no longer state-of-the-art in the global MA market. Any effort concentrated on them would be a
backward step towards inefficient processes with worse economics and greater environmental
impacts, which Sasol-Huntsman would not consider.

It is more realistic and practical to focus instead on the development of a suitable new alternative,
which, even if commercially unproven at present, can be properly researched and adapted to the
Huntsman technology so that it meets the needs of the downstream user without prohibitively costly
plant modifications.

5.3.2 Future research and development

From DEZA’s perspective, only the acquisition of knowledge, and hence ability to produce a
suitable alternative at an industrial scale, would improve the availability of any potential alternative
for the company. At present, it cannot be foreseen that this knowledge might be acquired in the
near future for DIBE. In any case, as the substance is not suitable for use by the downstream user,
DEZA would have no incentive to research its manufacture. In relation to researching
commercially unproved potential alternative substances, DEZA has not confirmed that any such
research is planned but this would change if the downstream user were to express an interest in a
specific alternative substance.

On the other hand, Huntsman is committed to continuing its R&D work with the aim of identifying
and developing technically suitable and economically feasible alternatives which can be obtained
from the market in sufficient quantities. Huntsman has provided details of its historical, ongoing
and planned R&D. These plans are highly proprietary and are presented in the Confidential Annex.

Additional confidential information is presented in: AoA Confidential Annex DBP MA DEZA.pdf,
Part 7
APPENDICES

Annex 1: List of data sources


ANALYSIS OF ALTERNATIVES


Annex 2: Information on the cost of DBP and potential alternative substances

The applicant does not wish to disclose the price per tonne of DBP for obvious reasons. For the purposes of the analysis presented in this AoA, the price of DBP has been obtained from Internet sources, more specifically from the Alibaba.com website. It is acknowledged that the actual price for DBP varies each year and is different to what is shown in Table 5.1. It can be noted that:

- the difference between the Alibaba-based median price (€1,520/t) and the actual price as of July 2013 is not large; and
- the use of price data for DBP and for the selected alternative substances from the same source (Alibaba) allows for consistency and comparability of the available data.

The following Table presents the information available from Alibaba.com on the cost of DBP per tonne.

Table 5.1: Cost information for DBP – From Alibaba.com (excludes transport cost)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (Free-on-Board price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>99.5</td>
<td>12,000</td>
<td>10</td>
<td>1,661 - 1,881</td>
</tr>
<tr>
<td>2</td>
<td>China</td>
<td>99.5</td>
<td>36,000</td>
<td>16</td>
<td>1,140 - 1,178</td>
</tr>
<tr>
<td>3</td>
<td>China</td>
<td>99.5</td>
<td>10,400</td>
<td>16</td>
<td>1,140 - 1,368</td>
</tr>
<tr>
<td>4</td>
<td>China</td>
<td>99.5</td>
<td>60,000</td>
<td>16</td>
<td>1,406 - 1,634</td>
</tr>
<tr>
<td>5</td>
<td>China</td>
<td>99.5</td>
<td>3,000</td>
<td>2.5</td>
<td>1,710 - 1,809</td>
</tr>
<tr>
<td>6</td>
<td>China</td>
<td>99.5</td>
<td>24,000</td>
<td>5</td>
<td>1,239 - 1,436</td>
</tr>
<tr>
<td>7</td>
<td>China</td>
<td>99.5</td>
<td>36,000</td>
<td>0.2</td>
<td>1,064 - 1,520</td>
</tr>
<tr>
<td>8</td>
<td>China</td>
<td>99-99.5</td>
<td>36,000</td>
<td>20</td>
<td>1,368 - 1,938</td>
</tr>
<tr>
<td>9</td>
<td>China</td>
<td>99.5</td>
<td>8,000</td>
<td>10</td>
<td>1,444 - 1,672</td>
</tr>
<tr>
<td>10</td>
<td>China</td>
<td>99.9</td>
<td>18,250</td>
<td>2</td>
<td>1,406 - 1,520</td>
</tr>
<tr>
<td>11</td>
<td>China</td>
<td>99.5</td>
<td>30,000</td>
<td>16</td>
<td>1,368 – 1,444</td>
</tr>
<tr>
<td>12</td>
<td>China</td>
<td>99.5</td>
<td>1,200</td>
<td>16</td>
<td>760 – 2,280</td>
</tr>
<tr>
<td>13</td>
<td>China</td>
<td>99-99.5</td>
<td>54,000</td>
<td>20</td>
<td>1,520 - 1,824</td>
</tr>
<tr>
<td>14</td>
<td>China</td>
<td>99.5</td>
<td>240</td>
<td>0.5</td>
<td>1,520 - 1,672</td>
</tr>
<tr>
<td>15</td>
<td>China</td>
<td>99</td>
<td>100,000</td>
<td>16</td>
<td>1,064 - 1,672</td>
</tr>
</tbody>
</table>

Average price: €1,489/t
Median price: €1,520/t
Range: €760 - €2,280/t

Sources: Link 1, Link 2, Link 3, Link 4, Link 5, Link 6, Link 7, Link 8, Link 9, Link 10, Link 11, Link 12, Link 13, Link 14, Link 15

Search date: 20 June 2012 – The above data were reviewed on 20 June 2013 and with the exception of certain links no longer being active (indicated in italics above), the average and median prices for the substance have remained almost identical

The sequence of Tables below summarises the information collected for DBP and for each of the substances shown in Table 3.3. These are followed by a summary table bringing the relevant information together and comparing this to information on the cost of DBP. For 4,4’-dimethyl benzophenone and dibutyl terephthalate, no price information was available.
### Table 5.2: Cost information for diethyl phthalate (CAS No. 84-66-2 / EC No. 201-550-6)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOB price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>99</td>
<td>3,360</td>
<td>3.086</td>
<td>1,210 - 1,361</td>
</tr>
<tr>
<td>2</td>
<td>China</td>
<td>99</td>
<td>1,440</td>
<td>1.2</td>
<td>1,512 - 3,025</td>
</tr>
<tr>
<td>3</td>
<td>China</td>
<td>99.5 min</td>
<td>24,000</td>
<td>20</td>
<td>1,399 - 1,512</td>
</tr>
<tr>
<td>4</td>
<td>China</td>
<td>99.5</td>
<td>24,000</td>
<td>20</td>
<td>1,361 - 1,512</td>
</tr>
<tr>
<td>6</td>
<td>China</td>
<td>99.9</td>
<td>120</td>
<td>1</td>
<td>1,891 - 2,269</td>
</tr>
</tbody>
</table>

Average price: €1,705/t  
Median price: €1,456/t  
Range: €1,210 - 3,025/t  
Sources: [Link 1](#), [Link 2](#), [Link 3](#), [Link 4](#), [Link 5](#), [Link 6](#)  
Search date: 20 June 2013

### Table 5.3: Cost information for diethyl adipate (CAS No. 141-28-6 / EC No. 205-477-0)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOB price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>98 min</td>
<td>N/A</td>
<td>1</td>
<td>756 - 3,781</td>
</tr>
</tbody>
</table>

Average price: €2,269/t  
Median price: N/A  
Range: €756 - 3,781/t  
Sources: [Link 1](#)  
Search date: 20 June 2013

### Table 5.4: Cost information for dibutyl adipate (CAS No. 105-99-7 / EC No. 203-350-4)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOB price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>High</td>
<td>1,200</td>
<td>0.001</td>
<td>756 - 7,566</td>
</tr>
<tr>
<td>2</td>
<td>China</td>
<td>99 min</td>
<td>5,200</td>
<td>1</td>
<td>3,873 - 11,349</td>
</tr>
</tbody>
</table>

Average price: €5,886/t  
Median price: €5,886/t  
Range: €756 - 11,349/t  
Sources: [Link 1](#), [Link 2](#)  
Search date: 20 June 2013
### Table 5.5: Cost information for tetraethylene glycol dimethyl ether (CAS No. 143-24-8 / EC No. 205-594-7)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOB price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>99</td>
<td>3,000</td>
<td>0.2</td>
<td>15,960 - 18,240</td>
</tr>
<tr>
<td>2</td>
<td>China</td>
<td>99</td>
<td>2,000</td>
<td>0.2</td>
<td>760 - 76,000</td>
</tr>
<tr>
<td>3</td>
<td>China</td>
<td>99.0 min</td>
<td>20,000</td>
<td>1</td>
<td>3,800 - 11,400</td>
</tr>
<tr>
<td><strong>Average price</strong></td>
<td><strong>€17,693/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Median price</strong></td>
<td><strong>€17,100/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Range</strong></td>
<td><strong>€760 - €76,000/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Sources:** Link 1, Link 2, Link 3

**Search date:** 15 May 2012 (fewer data were available on 20 June 2013 and the range of prices was too wide to be considered realistic; therefore, data from 2012 are presented here)

### Table 5.6: Cost information for dibutyl maleate (CAS No. 105-76-0 / EC No. 203-328-4)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOR price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>65-80</td>
<td>6,000</td>
<td>1 Litre or 0.001 tonne*</td>
<td>756 - 3,783</td>
</tr>
<tr>
<td><strong>Average price</strong></td>
<td><strong>€2,270/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Median price</strong></td>
<td><strong>N/A</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Range</strong></td>
<td><strong>€756 - 3,783/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Based on Table 3.2, the density of the substance is 0.99 g/cm³

**Sources:** Link 1

**Search date:** 20 June 2013

### Table 5.7: Cost information for diphenyl ether (CAS No. 101-84-8 / EC No. 202-981-2)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOB price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>No data</td>
<td>200</td>
<td>5 t</td>
<td>2,913 - 3,026</td>
</tr>
<tr>
<td>2</td>
<td>China</td>
<td>No data</td>
<td>12,000</td>
<td>1</td>
<td>75 - 756</td>
</tr>
<tr>
<td>3</td>
<td>China</td>
<td>99.9 min</td>
<td>1,000</td>
<td>1</td>
<td>2,837 - 2,875</td>
</tr>
<tr>
<td>4</td>
<td>China</td>
<td>99.9 min</td>
<td>4,800</td>
<td>23</td>
<td>2,497 - 2,799</td>
</tr>
<tr>
<td>5</td>
<td>China</td>
<td>No data</td>
<td>200</td>
<td>5</td>
<td>2,875 - 3,026</td>
</tr>
<tr>
<td>6</td>
<td>China</td>
<td>99.8 min</td>
<td>3,600</td>
<td>16</td>
<td>3,026 - 3,783</td>
</tr>
<tr>
<td>7</td>
<td>China</td>
<td>No data</td>
<td>2,400</td>
<td>1</td>
<td>2,042 - 2,270</td>
</tr>
<tr>
<td>8</td>
<td>China</td>
<td>No data</td>
<td>192</td>
<td>0.2</td>
<td>2,156 - 2,193</td>
</tr>
<tr>
<td><strong>Average price</strong></td>
<td><strong>€2,447/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Median price</strong></td>
<td><strong>€2,752/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Range</strong></td>
<td><strong>€75 - 3,783/t</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Sources:** Link 1, Link 2, Link 3, Link 4, Link 5, Link 6, Link 7, Link 8

**Search date:** 15 May 2012
### Table 5.8: Cost information for glyceryl tributyrate (CAS No. 60-01-5 / EC No. 200-451-5)

<table>
<thead>
<tr>
<th>Company</th>
<th>Location</th>
<th>Purity (%)</th>
<th>Supply Ability (t/y)</th>
<th>Minimum Order Quantity (t)</th>
<th>Price (€/t) (FOB price)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>China</td>
<td>No data</td>
<td>360</td>
<td>0.025</td>
<td>756 - 3,780</td>
</tr>
</tbody>
</table>

**Average price** €2,268/ t  
**Median price** N/A  
**Range** €756 - 3,780/ t  

_Sources: [Link 1]

_Search date: 20 June 2013_