

concaawe

ENVIRONMENTAL SCIENCE FOR THE EUROPEAN REFINING INDUSTRY

# review

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Environmental science for the European refining industry

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# Foreword



*Robin Nelson  
Science Director  
Concawe*

Three of the five articles in this edition of the *Review* once again illustrate the prescience of the founders of an Association working on the ‘**C**onservation of **C**lean **A**ir and **W**ater in **E**urope’ back in 1963. The articles on the real driving emissions of the latest diesel vehicles should be seen in the context of a long chapter on improving air quality, from removing lead in gasoline fuel, to low-sulphur diesel fuel and at last, exhaust treatment technology that will meet NO<sub>x</sub> emissions regulations under real driving conditions. In the article on marine sulphur emissions our industry is increasing its focus on the changes needed to meet the 0.5% sulphur limit imposed by the IMO for 2020. The third article, on the water survey, is designed to improve our ability to monitor and analyse data on effluents to water, needed to meet the requirements of several pieces of EU legislation.

The remaining two articles touch on another priority topic for our industry—improving the health and safety performance of our industry, not just in our refinery operations but also in the marketing and distribution of our products. Thus one article summarises the 2016 HSSE performance and highlights the need for continuous improvement and the importance of behavioural safety, while the final article focuses on the health effects of low-dose exposure to benzene.

My thanks to the contributors to Concawe in 2017, either as a member company contributing to a Concawe special task force or management group, or as a partner, collaborator to the management groups.

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Real driving emissions (RDE) from passenger cars has come under close scrutiny in recent times due to a perceived divergence between stated certification and measured on-road performance. This has been most pointed in the case of NO<sub>x</sub> emissions from diesel cars. To build understanding of the emissions performance of the latest available diesel passenger cars, Concawe asked Ricardo consulting engineers to conduct a study on the 'Expectations for actual Euro 6 vehicle emissions' and to carry out Concawe work involving a study of the chassis dynamometer (CD) and RDE performance of three Euro 6b+ vehicles. As well as having diesel particulate filters (DPFs), two of the vehicles featured high- and low-pressure exhaust gas recirculation (EGR) and aqueous urea-dosed selective catalytic reduction (SCR) aftertreatment systems, while the third used high pressure EGR and was fitted with a lean NO<sub>x</sub> trap (LNT). For each vehicle, tests were conducted over RDE, WLTC, NEDC and US06 cycles. Both studies provide insight into the on-road emissions performance of the latest diesel passenger cars, and into how this compares with regulated emissions limits and results from CD tests run under comparable conditions.

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## Concawe Safety Management Group: strategy review **Improving safety performance in the European downstream oil industry** 10

Improvement in European downstream oil refining industry safety performance is evident over the years since the first Concawe safety report in 1993. However, the Safety Management Group (SMG) recognised in the 2016 strategy review that further improvement is necessary, and will need to be addressed with a focus on the role of human behaviour in incidents and the sharing of best practice in learning from incidents. In 2017, the SMG initiated work in these areas while continuing to deliver its annual safety statistics report.

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## New Concawe web-based water use/effluent quality survey **A new survey aims to address EU initiatives on the sustainable use of water resources** 13

In recent years the development and implementation of EU legislation, including the Water Framework Directive, the Industrial Emissions Directive, the European Pollutant Release and Transfer Register Regulation and REACH, has led to a growing need for data on refining sector water use and effluent quality. In particular, additional data on water use and consumption is needed to address legislative initiatives under the 2012 Blueprint to Safeguard Europe's Water Resources and the EU initiative on the circular economy. To address these challenges, the Concawe refinery effluent special task force has developed a new web-based data collection system to streamline data capture, provide sites with an immediate overview of their water use, and expedite the process of data analysis and reporting. This article explains the design concept behind the new web-based survey and provides an introduction to some of its key features.

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 **The EU refining industry and the challenge of the IMO global sulphur limit for bunker fuels** **17**

The bunker residual fuel oil market is now facing significant changes due to regulations adopted by the IMO a year ago to reduce emissions of sulphur oxides (SO<sub>x</sub>) from the combustion of bunker fuels. The refining industry will be strongly impacted as the demand for heavy fuels will change drastically. These changes will affect the entire industry, with impacts on producers, blenders and suppliers, all of which will need to adapt in an uncertain and moving environment. According to linear programming simulations, meeting demand will be a considerable challenge for EU refiners as many technical constraints have been identified. New fuel formulations will be introduced to the market, and their stability and compatibility could potentially be problematic if the challenges are not taken seriously by each individual actor.

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 **The low-dose benzene debate needs a sharp blade**  
**Concawe sheds new light on the recently reported low-dose benzene phenomenon** **22**

The health effects of benzene have been a major concern for regulators and health experts for many years. This has led to significantly lower regulatory threshold limits (such as occupational exposure limits, OELs) and the implementation of corresponding risk management measures to reduce benzene concentrations and human exposure to benzene in the production, transport and use of petroleum products such as gasolines. Over the past decade, a series of research papers has been published by a group of researchers at the University of California, Berkeley, who postulated effects of benzene at very low dose exposures—levels which are relevant to current operations in the oil and gas industry and are currently (well) below the occupational exposure limits in most jurisdictions. A strong public scientific debate followed the publication of these papers, and in response to this, Concawe concluded a research project this year with two independent consultants who reanalysed the dataset to shed new light on this ongoing debate.

This Concawe *Review* article provides the reader with a short overview of the scientific argumentation in the ongoing discussions on this topic as an example of an educational scientific debate, and puts it into perspective based on the results of the Concawe project.

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# Recent studies on real driving emissions of diesel passenger cars

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**Two Concawe studies are commissioned to provide insight into the on-road emissions performance of the latest available diesel passenger cars.**  
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Emissions have been the focus of worldwide legislation for more than twenty-five years. European emissions legislation has set limits for particulate matter (PM) and oxides of nitrogen (NO<sub>x</sub>) emissions from diesel vehicles since the early 1990s, along with hydrocarbons (HC), which were initially included with NO<sub>x</sub> until 2000, and carbon monoxide (CO). For diesel passenger cars, PM limits were first introduced with the Euro 1 standards in 1992. Since then the limits have become progressively tighter, reaching 4.5 mg/km for the Euro 6 (2014) standards. More recently the focus has expanded to include particle number (PN), and a limit of 6x10<sup>11</sup> particles/km became effective for diesel vehicles from 2011 (new models) and 2013 (all models). NO<sub>x</sub> emissions limits have also reduced steadily and for diesel Euro 6 vehicles the limit has reached 80 mg/km. Similarly stringent standards have been introduced in other parts of the world. The introduction of these limits, along with clean fuels and advanced vehicle and after-treatment technologies, has resulted in a substantial reduction in automotive particulate mass (PM) emissions with a corresponding improvement in air quality. Figure 1 shows the breakdown of sources of emissions of particulate (in this case PM<sub>2.5</sub>) in urban areas in 2015.

Road transportation in 2015 only contributed 10% of total PM<sub>2.5</sub> emissions; only half of that value was due to exhaust particulate, with brake wear and tyre wear

making up the other half. Domestic heating was a much bigger contributor to particulate emissions than vehicles in urban areas.

NO<sub>x</sub> levels have not reduced as expected despite the limits mandated by the Euro standards.<sup>[1,2,3]</sup> As can be seen in Figure 2 on page 5, road transportation in 2015 accounted for more than 40% of NO<sub>x</sub> emissions contributing towards non-compliance with air quality standards. Figure 3a on page 5 shows attenuation of air quality standards for NO<sub>2</sub> in 2010; zones of compliance are shown in green, non-compliance shown in red and uncertain compliance shown in yellow. A Concawe study carried out with AERIS Europe<sup>[4]</sup> suggested that by 2030 these areas of non-compliance would be reduced down to smaller discrete islands (Figure 3b). This study made assumptions about the NO<sub>x</sub> levels that could be achieved, and these will be updated with new data based on the Ricardo study described below.

Part of the reason that real-world NO<sub>x</sub> levels have not come down in line with expectations is that emissions regulations for passenger vehicles have traditionally been based on the New European Driving Cycle (NEDC). Amid concerns that this test cycle does not represent closely enough real road driving in terms of CO<sub>2</sub> and other emissions levels including NO<sub>x</sub>, two new test procedures are under development—the Worldwide harmonized Light duty Test Procedure

**Figure 1 Sources of PM<sub>2.5</sub> emissions in urban areas in 2015**

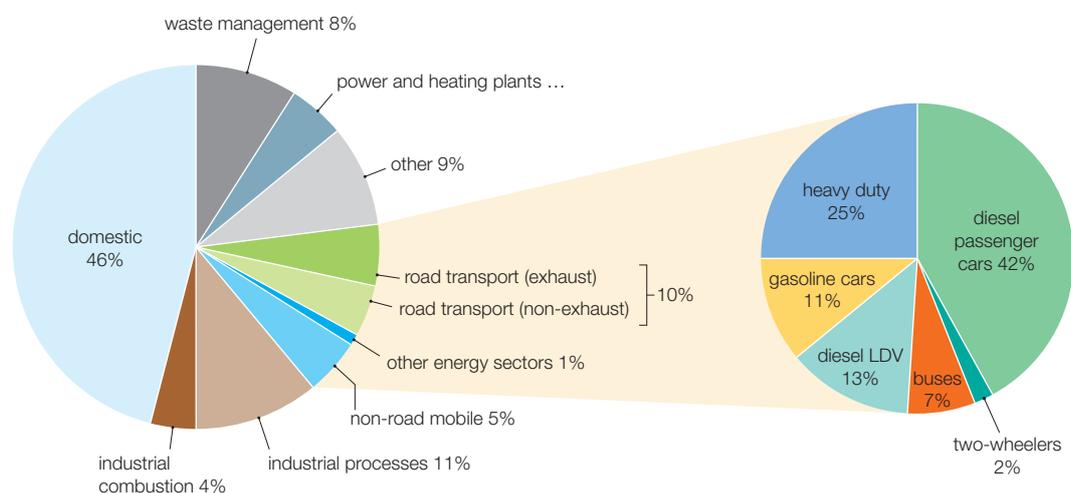
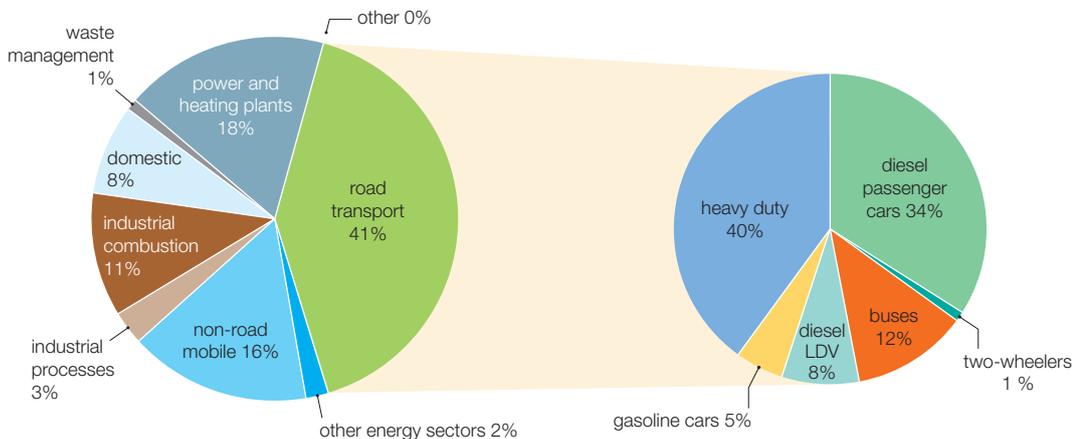




Figure 2 Sources of NO<sub>x</sub> emissions in 2015



(WLTP), for use on the chassis dynamometer, and the Real Driving Emissions (RDE) procedure for on-road use. Going forward, these tests will be used to certify vehicles, so there is much interest in how they will compare with the current NEDC certification test and in whether or not new Euro 6b+ vehicles will meet emissions limits under the new procedures. It is expected that the challenges will include:

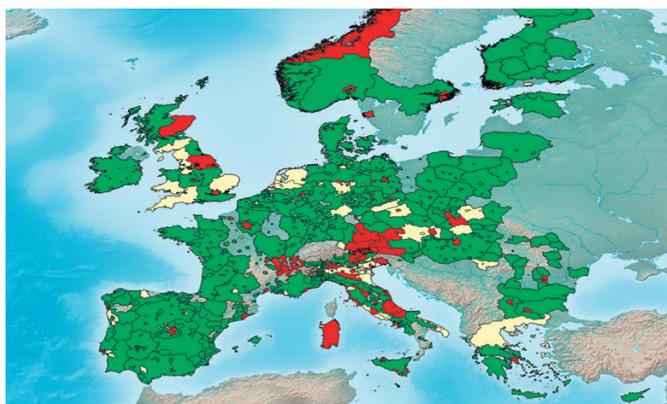
- urban driving conditions under which selective catalytic reduction (SCR) after-treatment technologies may not rapidly reach an efficient operating temperature;
- high load conditions under which exhaust temperatures may become too high for lean NO<sub>x</sub> traps technologies to be effective, and high flow rates at high load which may diminish performance of smaller SCR volume solutions; and

- low temperatures which may limit the use of exhaust gas recirculation (EGR)—another method used to reduce NO<sub>x</sub> emissions.

One of the enablers to being able to carry out testing of more real-world on-road driving has been the development of portable emissions measurement systems (PEMS) which are able to measure gaseous and particle number (PN) emissions under real driving conditions. The RDE test protocol was adopted in 2016 together with the not-to-exceed (NTE) limit for NO<sub>x</sub>, published in the first two packages of EU legislation.<sup>[5,6]</sup> Two extra Euro 6 vehicle stages will be introduced as a consequence: Euro 6d-temp as of September 2017 with a NO<sub>x</sub> conformity factor (CF) of 2.1; and the full Euro 6d as of January 2020 with a NO<sub>x</sub> CF of 1.5 or less. The limits apply to both an urban por-

Figure 3 Attenuation of air quality standards for NO<sub>2</sub>

(a) 2010



(b) 2030 projection







The main conclusion from this study is that Euro 6d compliance is expected to be possible with the right combination of engine and after-treatment systems.

Some of these after-treatment systems have been tested in another programme which Ricardo has been running for Concawe, as described below.

### Concawe RDE test programme

Three modern diesel vehicles (see Table 2) were installed on a chassis dynamometer and tested over the NEDC, WLTC and US06 drive cycles. On-road RDE tests were also carried out on these vehicles. All the testing was carried out at and around Ricardo's facility at Shoreham-by-Sea in the UK. The test vehicles were purchased second-hand from the German market but all of them had been driven for around 5,000–10,000 km and were equipped with modern after-treatment systems with different configurations.

The CD and RDE testing was conducted on a market diesel fuel which fully met the EN590 requirements. Selected properties are shown in Table 3.

### Chassis dynamometer and real driving emissions test cycles

Three chassis dynamometer drive cycles were tested, two European and one from the USA. Unusually, during the current European regulatory phase, Euro 6c, two cycles may be used: the legacy NEDC (Figure 5a), which has only moderate transient character, and the newly

**Table 2 Technical details of the test vehicles**

	Car A	Car B	Car C
Emissions class	M1	M1	M1
Size category	C	D	E
Emissions certification	Euro 6b	Euro 6b	Euro 6c
Year of registration	2016	2015	2016
Cylinders/valves	3/12	4/16	4/16
Displacement (litres)	1.50	1.97	1.95
Output (kW)	85	140	143
Emissions controls	High Pressure EGR, LNT, DPF, SCR	High & Low Pressure EGR, urea-SCR <sup>*</sup> , ASC	High & Low Pressure EGR, urea-SCR <sup>*</sup> , SCR/ASC

\* Car B used closed-loop control for urea (aq) dosing, Car C open-loop control

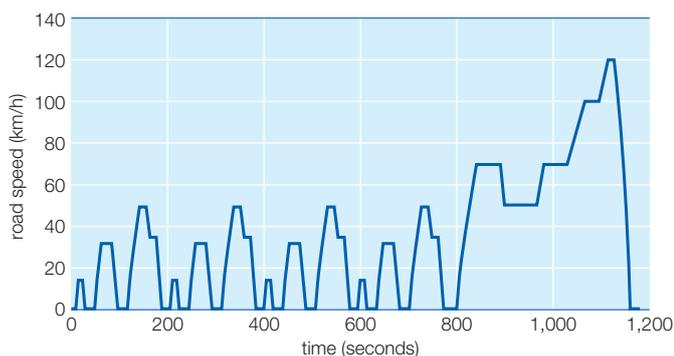
**Table 3 Test fuel properties**

Property	Method	EN590 min.	EN590 max.	Fuel
CN	EN ISO 5165	51	-	53
Density (kg/m <sup>3</sup> )	EN ISO 12185	820	845	822
Sulphur (mg/kg)	EN ISO 20846	-	10	7.9
Viscosity at 40°C (mm <sup>2</sup> /s)	ASTM D445	2	4.5	2.28
FAME (v/v%)	EN 14078	-	7	4.1
IBP (°C)	ASTM D86	-	-	160
T50 (°C)	ASTM D86	-	-	255
T95 (°C)	ASTM D86	-	360	344
FBP (°C)	ASTM D86	-	-	355

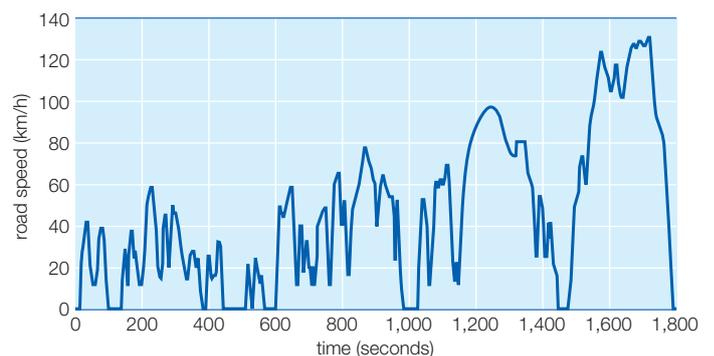
developed WLTC (Figure 5b) which contains a mix of far more realistic driving characteristics and a range of speeds. A third, US cycle, the US06, which was developed to specifically highlight the impacts of high speed,

**Figure 5 Chassis dynamometer test cycles**

(a) NEDC



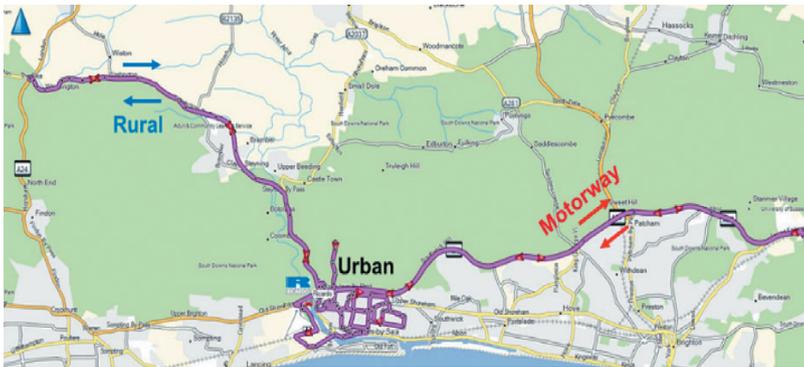
(b) WLTC



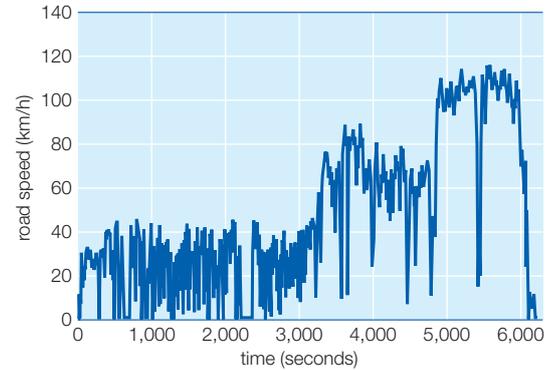


**Figure 6 The Ricardo RDE route**

**(a) Map of the RDE route**



**(b) Speed/time plot (eastbound route)**



rapid acceleration and speed variability on emissions was also tested but is not discussed here. The NEDC lasts ~20 minutes and covers ~11 km, and the WLTC lasts ~30 minutes and covers ~23 km.

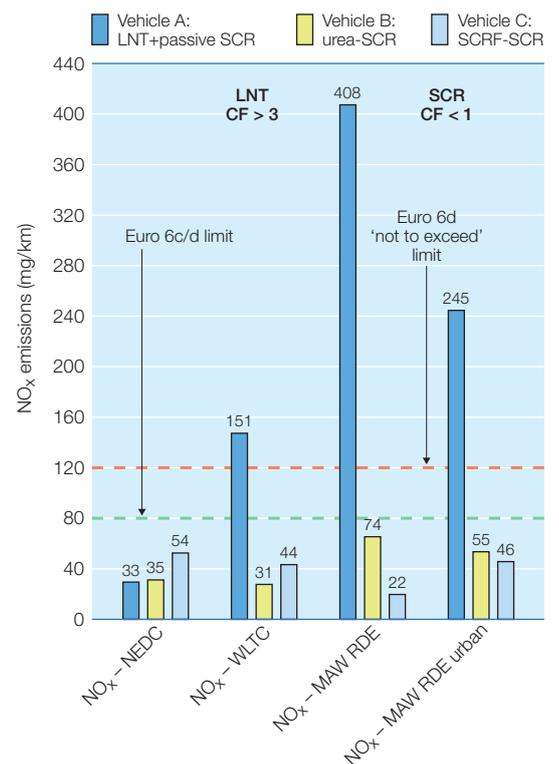
The RDE route used is illustrated in Figure 6a. The route commences with urban operation wholly in 20 and 30 mi/h (32–48 km/h) zones. Rural and motorway phases are conducted on major roads to the west and east of Ricardo’s site, respectively. The requirements of the test are achieved without introducing artificial stop periods, and urban severity is achieved through moderate hill climbs and multiple T-junctions. Hill climbs and descents are also present in both rural and motorway sections. The total test time is around 105 minutes and cold start emissions were included in the analysis.

### NO<sub>x</sub> emissions

For NO<sub>x</sub> emissions, two of the vehicles (B and C) gave results well below the Euro 6 limit (shown by the green dotted line on Figure 7), while for vehicle (A) only the NEDC results were below the limit (Figure 7). Vehicles B and C were both equipped with urea-SCR systems and both high and low pressure EGR, and were certified to Euro 6b and Euro 6c respectively. These vehicles used an active urea dosing strategy that responded to engine-out NO<sub>x</sub> levels in real time. Vehicle A was a Euro 6b vehicle equipped with a lean NO<sub>x</sub> trap (LNT) and passive SCR. NO<sub>x</sub> emissions from the LNT-passive SCR car (A) increased with cycle duty and exceeded the Euro 6 limit over the WLTC and during both the

urban and total RDE cycles. It is notable that the non-urea-SCR car (A) produces around half of the NO<sub>x</sub> in the urban portion of the RDE than it does in the full RDE, whereas vehicle B produces similar NO<sub>x</sub> over urban and whole RDE and vehicle C produces higher NO<sub>x</sub> over the urban section of the RDE. The urea-SCR

**Figure 7 NO<sub>x</sub> emissions from vehicles A, B and C under the various test cycles**





vehicles (B and C) appear to have the capability of reducing tailpipe NO<sub>x</sub> via urea-SCR activity irrespective of the engine-out level, whereas the Euro 6b LNT vehicle was not optimized to handle high engine-out NO<sub>x</sub> levels associated with high exhaust gas flow rates and temperatures, which are conditions encountered in non-urban driving. The dominance of high-temperature operation in these cycles limited NO<sub>x</sub> storage and reduction via the LNT. The extended heat-up time of the larger catalyst volume in the urea-SCR-only vehicle may explain why vehicle B has lower performance than vehicle C in the urban section.

Three Euro 6 diesel passenger cars with differing exhaust aftertreatment technologies have been tested over the NEDC and WLTC chassis dynamometer test cycles as well as over the RDE test cycle. The test results show that state-of-the-art diesel passenger cars are capable of meeting near future NO<sub>x</sub> emissions requirements of moderate RDE testing commensurate with Euro 6d. Combinations of emissions control technologies, for example long- and short-route EGR, large-volume SCR and possibly LNT will be required. Vehicles equipped with urea SCR systems can reduce tailpipe NO<sub>x</sub> by reactive urea reductant dosing varying the urea-reductant consumption, and can therefore produce acceptable NO<sub>x</sub> emissions even over high-duty drive cycles. Future work will involve investigation of emissions under more severe test cycles and a wider range of temperatures, and will also involve updating the urban air quality study using the results obtained from these studies.

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### Acknowledgements

Concawe would like to acknowledge the staff from Ricardo at Shoreham-by-Sea, UK for carrying out the study and test work, and Coryton Advanced Fuels, UK for blending the fuels for this programme.

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6. EU (2016b). European Commission Regulation (EU) 2016/646 of 20 April 2016 amending Regulation (EC) No 692/2008 as regards emissions from light passenger and commercial vehicles (Euro 6).



# Concawe Safety Management Group: strategy review

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**A broad survey and subsequent review of Concawe's SMG strategy points to a number of topics that will be key areas of focus for the SMG in the coming year with a view to further improving safety performance in the European downstream oil industry.**

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The Safety Management Group (SMG) chaired by Harald Hess of OMV, serves as the technical management committee on all issues relating to personal and process safety in the refining and marketing of petroleum products. Its mission is to promote excellence and efficiency in the development of personal and process safety as part of sustainable development in the downstream oil industry in Europe. The SMG aims to assist enhancing member company safety performance; develop and maintain effective communications with member companies, industry organisations, the public and regulatory authorities on safety matters; and facilitate access to information on the latest developments in the practice of personal and process safety management.

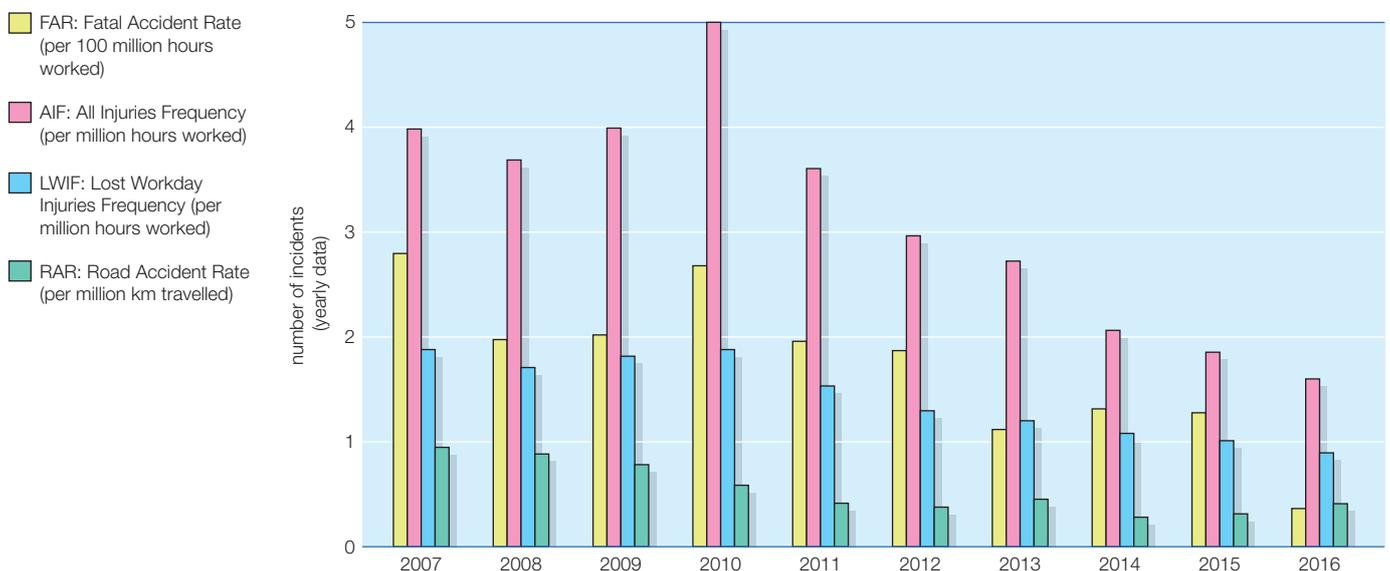
Since 2009, the SMG has continued to review its charter and agreed to follow and respond to developments in EU legislation relevant to safety management and industrial risk, and to maintain appropriate direct links with the European Commission. It contributes to the enhancement of member company safety performance by identifying areas of safety management and performance where members share the need for improvement. Through information analysis and exchange, the SMG proposes a collective approach to resolving problems where it may be beneficial to do so. It strives to develop and maintain effective communi-

tions between member companies and with other industry organisations with interests in safety, such as CEFIC, IOGP and the European Process Safety Centre, as well as with regulatory authorities.

While improvements in European downstream oil refining industry safety performance have been evident over the years since publication of the first Concawe report in 1993, the SMG considered, in 2016, that a focus on 'behaviour-based safety management' would support the next step change in safety performance in the sector. An SMG strategy survey was launched, aimed at all Scientific Committee and SMG members, as well as company safety staff, to identify what is valued in the current SMG offering and to assess whether any changes in current scope would improve its value to member companies.

The strategy review found that the annual safety statistics report was the most valued SMG deliverable. It provides member companies with a benchmark against which to compare their performance, so that they can determine the efficacy of their safety management systems, identify shortcomings and take corrective actions. The report also demonstrates that responsible safety management in the downstream oil industry results in a low level of accidents despite the hazards intrinsic to its operations.

**Figure 1 Safety performance indicators for the European downstream oil industry, 2007–2016**





*The strategy review found that the annual safety statistics report was the most valued SMG deliverable, providing member companies with a benchmark against which to compare their performance.*

The 2016 safety statistics report, published in June 2017, received input from 38 Concawe member companies representing approximately 99% of the European refining capacity. There were two fatalities in the industry in 2016. While this is the lowest number of annual fatalities since Concawe began compiling industry records in 1993, we must consider this to be two fatalities too many. Lost workday injuries fell from 546 to 501, a drop of approximately 8%. The number of Tier 1 and 2 process safety releases continues to decline but the rate of decline per annum appears to be slowing.

The structure of the twenty-third annual safety report was revised to focus on incidents in 2016 and included a comparison with data from the past 10 years. A new concise format and executive summary made the key messages accessible while maintaining all historic data for reference in the appendix.

Also highly valued in the 2016 strategy review survey were the one-day workshops/theme days that allow in-depth analysis and learning from topics of interest on

an annual basis, bringing science back into the SMG. It is important that each workshop/theme day has appropriate follow-up to realise further growth in knowledge and application.

The SMG's annual Safety Theme Day entitled 'Human Factors and Situation Awareness' took place on 31 May 2017.

As many member companies find continuing improvement in safety performance difficult to achieve through management systems, standardised processes and competency training, attention is turning to the role of human behaviour in safety incidents. This event aimed at raising awareness of human psychology and sharing practical approaches to implement improvements in situational awareness.

Participants benefited from the broad experience of three expert guest speakers from within and beyond the downstream oil sector:

- Professor Rhona Flin, a psychologist conducting research on human performance in high-risk industries;
- Pekka Erkama, an ex-pilot and human factor consultant optimizing human performance and managing human errors; and
- Simon Monnington, a chartered human factors specialist and human factor advisor at BP.

The Safety Theme Day provided the opportunity for maximum interaction with speakers and participants to share their own experiences in the field. Feedback from the 12 companies present was extremely positive, and the event was described as 'inspirational'.



*Delegates at the 2017 Safety Theme Day workshop; the topic was 'Human factors and situation awareness'.*



*Carol Banner joined Concawe as Science Executive for safety in February 2017.*

Armed with a raft of ideas for implementation across all levels from corporate leadership to engineering design to front line staff and contractors, participants left the event energised. As a spin-off, some companies are currently planning internal situation awareness training sessions. As one participant commented, 'a good comprehension of human factors will be essential for the future of oil refining and this day will certainly contribute to that.'

The safety consulting network function is also a valued SMG activity. It is used regularly by SMG members posting queries on safety matters. These are normally reacted upon on the same day or within a week. In 2017, the SMG moved to a SharePoint® system and is making use of the discussion board functionality which facilitates the exchange and retrieval of discussion topics.

In addition to exploring the benefits and applicability of 'behaviour-based safety management' for the refining sector, the strategy review recommended establishing a system enabling Concawe members to learn from sector-specific incidents that have occurred in member companies.

In the first quarter of 2017, a Learning from Incidents (LFI) task force was set up by the SMG. Its initial task was to establish a scope and deliverables, something that has proved to be challenging given the breadth of the subject and differences in company safety cultures. Two rounds of surveys and several teleconferences later, the terms of reference have been agreed and work was started on the first of four key deliverables in the first quarter of 2017. The LFI task force, chaired by Ana Berrocal of CEPSA, will focus on what is learnt from incidents and how we learn from incidents, rather than on the details of incidents per se. The aim is to share best practice in learning from incidents, consider the importance of human behaviour as a cause of incidents, and share information and experience in influencing such behaviour.

The 2016 strategy review has shaped and focused SMG activities in 2017. Looking ahead, there are plans to gather additional data about Tier 1 process safety events in the 2017 annual safety report, the question-

naire for which will be available to member companies in January 2018. The aim is to provide a better understanding of the causes of process safety events, in the same way that Concawe has been collecting cause category data for personal safety incidents since 2013. In parallel, the LFI task force is planning to deliver best practice in three areas:

- effective recommendations and actions following an incident investigation;
- measuring implementation of recommendations/ actions and evaluating change; and
- maximising individual learning from remote incidents

The strategy review also indicated that an increase from 0.1 to 0.5 FTE would be the optimal requirement for Concawe secretariat support for the SMG. To address this, Carol Banner joined Concawe as Science Executive for safety in February 2017. Carol has more than 20 years' experience with Shell and has in recent years led systems improvement for safety reporting and learning from incidents. She currently divides her time between the SMG and coordinating updates of the Concawe REACH dossiers.

Chair Harald Hess of OMV has explained that, since the strategy review, the SMG has started working on the subjects that had been considered most valuable to member companies, and has tried to share the activities and their results more visibly, including outside the SMG. Carol is driving the increased activities with high energy and a very positive momentum, constantly fostering the collaboration between the SMG members. There has already been considerable interest and participation by member companies in activities related to 'behaviour based safety' (for the theme day) and the recently installed LFI task force. These topics will remain focus areas of the SMG for next year. The SMG will also continue to further improve the annual safety report in terms of data completeness, quality and data collection, and will put a special focus on more granularity of the process safety chapter which should provide more insight into incident categories, trends and patterns as a basis for further activities to bring process safety management to the next level.



# New web-based Concaawe water use/effluent quality survey

A new water use/effluent quality survey is launched to efficiently record refinery discharges and address EU initiatives on the sustainable use of water resources.

## Background

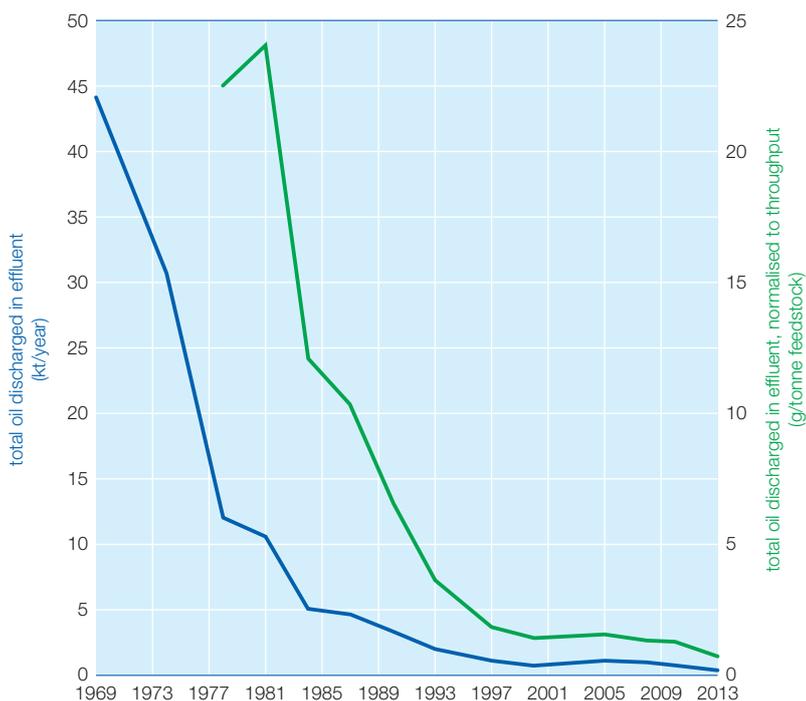
Since the founding of Concaawe in 1963, great progress has been made towards improving water quality in Europe. Refineries have played their part in this, with substantial reductions in discharges and improvements in effluent quality leading to large reductions in the quantities of pollutants discharged to surface waters. This is clearly illustrated by Figure 1 below, which shows a large reduction in the discharge of oil in water from 1969, when the first Concaawe survey of refinery effluent discharge was completed, to the most recent survey in 2013.

In recent years the development and implementation of EU legislation, including the Water Framework Directive (2000/60/EC), the Industrial Emissions Directive (2010/75/EC), the European Pollution Release and Transfer Register Regulation (EC 116/2006) and REACH (EC 1907/2006), has led to a growing need for data on refining sector water use and effluent quality. In particular, additional data on water use and consumption is needed to address legislative initiatives under the 2012 Blueprint to Safeguard Europe's Water Resources

and the 2016 EU initiative on the circular economy. For example, the latter includes a legislative proposal on water reuse, known as the 'Water is too precious to waste' initiative (EC, 2017), which promotes treated wastewater reuse to build resilience against an anticipated increase in the frequency and severity of drought events. As a result of such initiatives, industrial stakeholders will face increased pressure to maximise water reuse and reduce freshwater consumption, e.g. during the revision of Best Available Techniques (BAT) reference documents (BREFs).

While early Concaawe surveys primarily addressed the discharge of oil in effluents, the survey has expanded since 2005 to take into account the growing number of substances that are subject to EU-wide discharge limits or environmental quality standards. In addition, the survey has been adapted to capture data on water treatment processes, freshwater consumption and water reuse. With the increased size and complexity of the survey, however, the use of spreadsheets for data entry has become difficult, leading to an increased risk of data entry errors or partial completion.

Figure 1 Concaawe survey data for effluent discharge from European refineries, 1969 to 2013



To address this issue the Concaawe refinery effluent Special Task Force (WQ/STF-34) has developed a new web-based data collection system for the 2016 reporting year. The new system will streamline data capture, provide sites with an immediate overview of their water use, and expedite the process of data analysis and reporting. In particular, the new survey will provide additional insight into water reuse, which is likely to become an increasingly important performance metric for refineries in future years given the European Commission focus on sustainable use of water resources.

The new web-based water use/effluent quality survey will be deployed to Concaawe member company refineries in the final quarter of 2017 along with training videos to demonstrate the process of data entry. As with previous surveys, the data gathered will be held in secure storage and only communicated outside the secretariat in the form of aggregated statistics, so that data cannot be attributed to individual refineries.



### Survey distribution platform

The survey will be hosted on a new Concawe survey platform, which has been developed to efficiently manage multiple surveys of refinery emissions and discharges. The survey operates within a secure (encrypted) browser protocol (https), with different access rights for platform administrators, survey administrators and refinery users. For each reporting refinery, data entry is managed by a focal point nominated by the member company, who is then responsible for coordinating and approving the site response. Where refineries comprise multiple sites (e.g. with separate water supplies and wastewater treatment facilities) the focal point can advise that a separate survey will be returned by each facility. The Concawe science executive responsible for the survey will be able to review the completion status of each survey via a control panel, and also view the data contained in each survey return for quality assurance/quality control (QA/QC) purposes.

### Survey design

Figure 2 shows the design concept for the new web-based survey. The survey allows users to build a simplified process flow scheme for their refinery, incorporating the major intakes, effluents, outfalls and water uses. A site water balance is calculated based on the reported annual flow data and can be viewed alongside a Sankey<sup>1</sup> diagram to identify any data entry errors. The new survey design also provides users with a summary report of water use and discharge data to facilitate QA/QC prior to survey submission.

### Intakes, effluents, outfalls and discharges

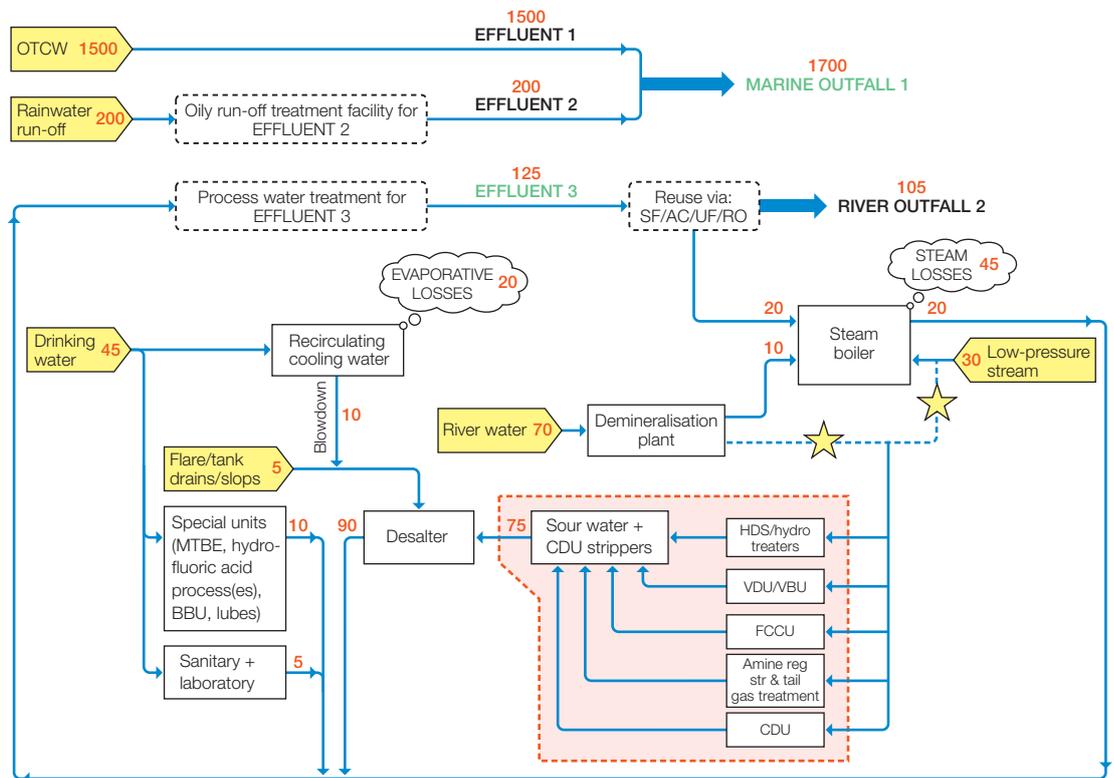
When completing the water use/effluent quality survey users first enter data on feedstock capacity and throughput, which is used to normalise substance discharge data. They then define the site intakes, effluents and outfalls. In accordance with previous surveys,

Figure 2 Simplified flow scheme for refinery water use illustrating the design concept for the new web-based survey

The new Concawe web-based survey allows users to build a simplified flow scheme for the refinery and append discharge data to monitored effluents and outfalls (shown in green).

**Key**

- water intakes
- water uses
- water uses
- 155** volume/year data
- flows to various uses that are returned as aggregated sour/CDU waters
- aggregated sour/CDU waters
- EFFLUENT/OUTFALL** monitored effluent or outfall (discharge data appended)



<sup>1</sup> A Sankey diagram is a specific type of flow diagram, in which the width of the arrows is shown proportionally to the flow quantity.



effluents are defined as treated wastewaters or flows that do not require further treatment prior to discharge. Outfalls are the actual points of discharge to the water body, and may comprise more than one effluent stream if these are merged prior to discharge. When the effluents and outfalls have been defined the user can add details of the treatment processes applied to effluents, as well as discharge data for monitored effluents and outfalls.

### Water use and reuse

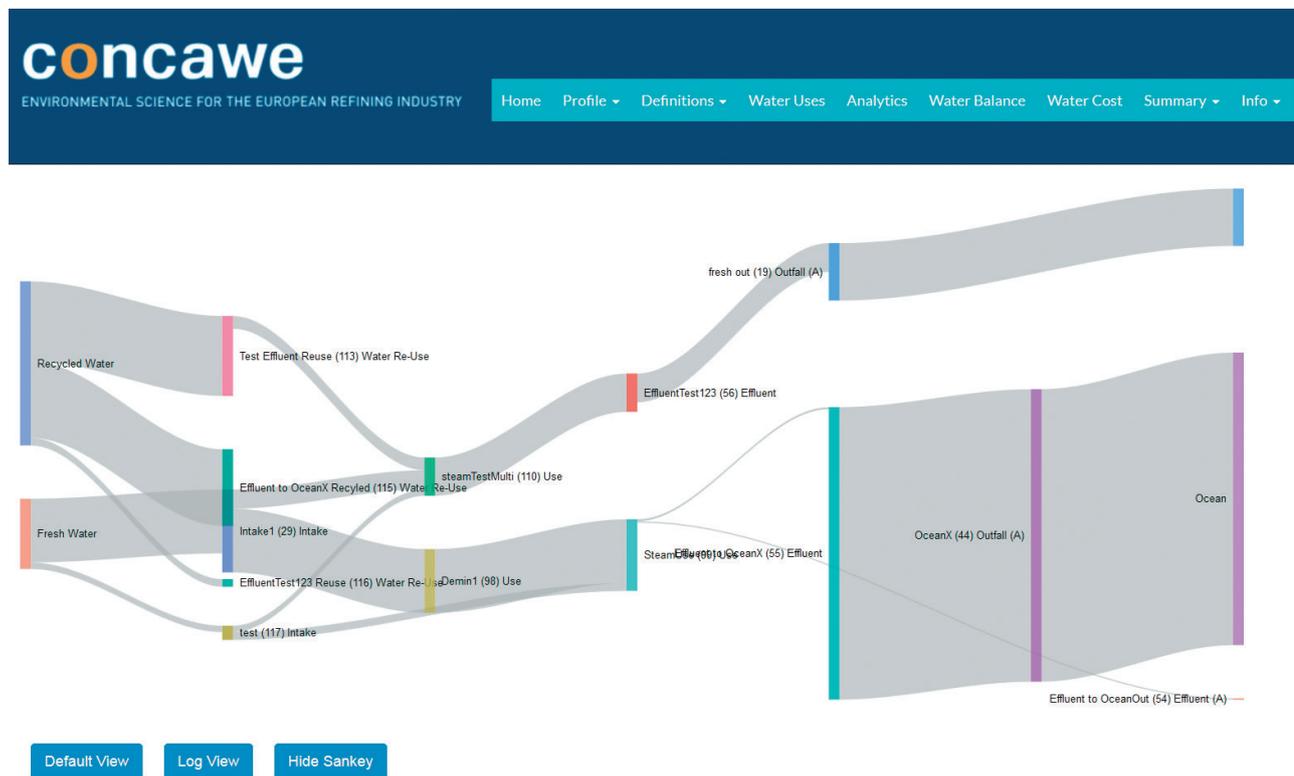
When the intakes, effluents and outfalls have been defined, users can add the major water uses to each intake to describe the routing of water through the refinery. A standard list of uses has been developed, containing water uses for which it is considered that annual use volume data may be available. Water can be routed through one or more uses before being assigned to one of the effluent streams. As data is entered, a

Sankey diagram is built, which describes the flow of water through the refinery (see Figure 3). The Sankey diagram makes it easier for the user to identify incomplete data entries, for example where an intake has been defined but is not linked to any effluent.

In addition to the standard intake types, the new survey allows the following special intake types to be defined, which provide data on the **efficiency of site water use**:

- **Rainwater intake:** used to specify whether the annual rainfall volume is known, whether rainfall is included in the reported effluent volume data, and whether captured rainwater is used on-site.
- **General reuse intake:** used to show where water is recovered from an effluent stream for reuse.
- **Sour/crude distillation unit (CDU) water intake:** used to report the annual volume returned to the sour/CDU water stripper (comprising aggregated flows from production units not reported individually in the survey).

Figure 3 Example Sankey diagram from the new web-based survey, showing water flows for a hypothetical refinery





### Water intake, treatment and discharge costs

To address the growing regulatory focus on water pricing (e.g. WWAP, 2017), the 2016 survey captures the total cost of water intakes, the total cost of water treatment and the total cost of discharges. Users are also requested to specify which costs are included in these totals to allow for meaningful aggregation of the data. The cost data will be analysed to provide an improved understanding of how changes in water supply costs could impact the European refining sector.

### Survey outputs

When the survey has been completed, a printable summary report of water use and discharge data can be viewed. The summary includes standard Carbon Disclosure Project (CDP), Global Reporting Initiative (GRI) and IPIECA sustainability metrics for water use, as shown in Table 1. The summary also includes mass loadings for all reported substances and the complete water balance Sankey diagram.

### Analysis and reporting of 2016 survey data

A statistical analysis of the data returns will be completed to provide an improved understanding of how European refineries manage water resources. The data will also be used to assess trends in discharge quality over time, and the performance of different water treatment technologies. As with previous surveys, Concawe reports and publications will be published to highlight key findings and provide the scientific understanding needed for effective decision making.

### References

EC (2017). *Water is too precious to waste*. European Commission, DG Environment (online). <http://ec.europa.eu/environment/water/reuse.htm>

WWAP (2017). *The United Nations World Water Development Report 2017. Wastewater: The Untapped Resource*. United Nations World Water Assessment Programme. Paris, UNESCO. [www.unesco.org/new/en/natural-sciences/environment/water/wwap/wwdr/2017-wastewater-the-untapped-resource](http://www.unesco.org/new/en/natural-sciences/environment/water/wwap/wwdr/2017-wastewater-the-untapped-resource)

**Table 1 Standard CDP, GRI and IPIECA sustainability metrics for water use**

	Metric	Unit
GRI water use metrics	Total Water Withdrawal (GRI EN8)	m <sup>3</sup> /year
	Total Water Discharged (GRI EN21)	m <sup>3</sup> /year
	Total Water Recycled + Reused (GRI EN10)	m <sup>3</sup> /year
	Percent Recycled + Reused / Total Withdrawal (GRI EN10)	%
CDP water use metrics	Water Consumption by Barrel of Oil Equivalent (BOE)	m <sup>3</sup> /metric tonne
	Water Withdrawal Volume by Source	m <sup>3</sup> /year
	Water Discharge Volume by Body	m <sup>3</sup> /year
	Total Water Withdrawal (GRI EN8)	m <sup>3</sup> /year
	Total Water Recycled + Reused (GRI EN10)	m <sup>3</sup> /year
	Percent Recycled + Reused / Total Withdrawal (GRI EN10)	%
IPIECA water use metrics	Total Freshwater Withdrawals	m <sup>3</sup> /year
	Total Freshwater Discharged	m <sup>3</sup> /year
	Total Freshwater Consumed	m <sup>3</sup> /year
	Total Freshwater Consumed per unit of production	m <sup>3</sup> /unit production
	Total Water Recycled + Reused (GRI EN10)	m <sup>3</sup> /year
	Total Petroleum Hydrocarbons Discharged	metric tonne/year

Note that the GRI metric GRI EN10 is also used within CDP and IPIECA reporting metrics.



# The EU refining industry and the challenge of the IMO global sulphur limit for bunker fuels

As refineries face the prospect of a 0.5% m/m global sulphur limit in marine fuel oil by 2020, a number of studies have been carried out to assess the challenges they will face in meeting the demand for lower-sulphur marine fuels.

The International Maritime Organization (IMO) has set a global limit for sulphur in fuel oil used on board ships of 0.5% m/m from 1 January 2020. This is the biggest single specification change to ever hit the refined product market, and could cause a major disruption in supply, demand and market strains. The shipping, bunkering and refining industries are all interlinked with respect to this change, and the response by one industry will affect decisions made by others.

This article describes the regulatory situation, shares the current knowledge of experts speaking on the topic and gives an overview of a technical study being carried out using linear programming and supervised by Concawe's Refinery Technology Support Group.

## Regulatory developments

The IMO's Marine Environment Protection Committee (MEPC) was established in November 1973 with the responsibility of coordinating IMO activities aimed at the prevention of ship-source pollution. To better address marine pollution, the International Convention for the Prevention of Pollution from Ships (MARPOL) was adopted in 1973.

### MARPOL Annex VI

Several amendments to MARPOL have been made since its adoption, of which the most significant was

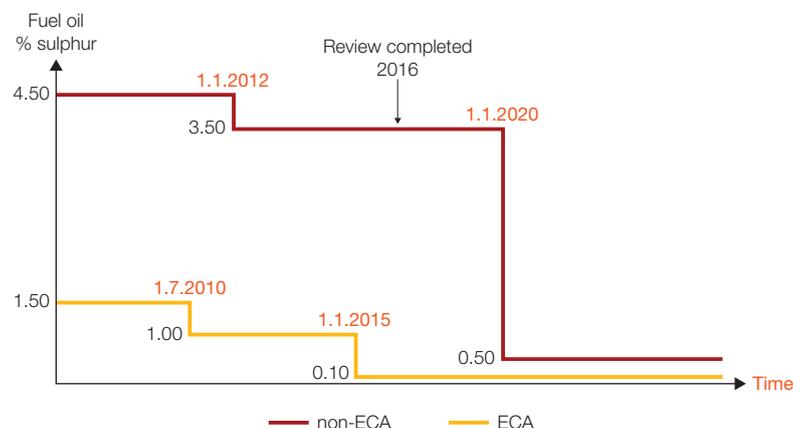
the Protocol of 1997 which introduced the new Annex VI. Adopted in 1997, Annex VI came into force in May 2005, and applies to all ships trading internationally involving countries that have endorsed the convention. It expanded MARPOL's scope to include air pollutants contained in ship exhaust gas, and 88 states out of 197 have so far ratified the Protocol of 1997 (Annex VI). Recognizing the harmful effects of sulphur oxide (SO<sub>x</sub>) emissions, Regulation 14 of Annex VI sought to reduce emissions by limiting the sulphur content of bunker fuels. It also mandated the monitoring of sulphur content in residual fuel oils supplied for use on board ships. Initially, it set a global limit on the sulphur content of marine fuels at 4.50%, and designated the Baltic Sea as the first Sulphur Emission Control Area (SECA) where a sulphur content limit of 1.50% in marine fuels was mandated.

Stricter regulations were adopted in a modified Annex VI in 2008 under Resolution MEPC.176(58), within which Regulation 14 states that the sulphur content of any fuel oil used on board ships shall not exceed 0.50% m/m from 1 January 2020. However, a provision was adopted which requires the IMO to review the availability of low-sulphur fuel oil for use by ships, to help Member States determine whether this new global cap on sulphur emissions from international shipping could potentially be deferred until January 2025. In addition, in 2010, MARPOL redesignated SECAs as Emission Control Areas (ECAs), adding a provision to include special limits for SO<sub>x</sub>, nitrogen oxides (NO<sub>x</sub>) and particulate matter (PM) within these areas.

### Latest developments

At the 70th session of the IMO's MEPC held in October 2016, it was decided that the 0.50% limit should apply from 1 January 2020. This decision was supported by a study prepared by the IMO's hired consortium of consultants, led by CE Delft, which concluded that sufficient quantities of compliant marine fuels would be available by 2020. A complementary study performed by EnSys Energy and Navigistics Consulting was more cautious, highlighting the uncertainties, difficulties and risks of limited availability.<sup>1</sup>

Figure 1 Regulation 14: fuel oil used on board ships



<sup>1</sup> EnSys Energy-Navigistics Consulting *Supplemental Marine Fuel Availability Study* submitted to the IMO, July 2016. Available from: <https://www.ensysenergy.com/downloads/supplemental-marine-fuels-availability-study-2>



Ships may meet SO<sub>x</sub> emission requirement by using approved equivalent methods, such as exhaust gas cleaning systems (EGCS) or 'scrubbers', which aim to remove sulphur oxides from the ship's exhaust gases before they are released into the atmosphere. Where such an equivalent arrangement is adopted, it must be approved by the ship's Administration (i.e. flag State).

#### Implementation and enforcement

The IMO has no regulatory or enforcement power, i.e. it develops and adopts regulations that must then be ratified by its member countries. Implementation is the remit and responsibility of the Administrations (referred to as flag State Control—the country where a ship is registered) and port/coastal State Control (PSC—the country in whose waters the vessel is sailing, anchored or docked). Ensuring the consistent and effective implementation of the 2020 0.50% sulphur limit should be considered a high priority.

The daunting task of providing uniform, international enforcement across the high seas lies with the IMO's MEPC and Pollution Prevention and Response (PPR) Sub-Committee. The PPR has the responsibility to develop enforcement of the 0.50% global sulphur cap to achieve the environmental benefits sought through Regulation 14. The scope of work, proposed to be completed during PPR sessions in 2018 and 2019 includes:

- considering the preparatory and transitional issues, as well as the impacts on fuel and machinery systems; and
- verification, control mechanisms, actions, safety implications, standard format for non-availability and any consequential regulatory amendments and/or guidelines necessary to address issues raised and to ensure compliance and consistent implementation.

#### Availability

MARPOL Annex VI Regulation 18.2 on fuel oil availability requires each Party to 'take all reasonable steps to promote the availability of fuel oils which comply with [Annex VI] and inform the [IMO] of the availability of compliant fuel oils in its ports and terminals'. Parties are also required to notify IMO when a ship has presented evidence of the non-availability of compliant fuel.

Notifications of non-availability of compliant fuel oil are reported on the IMO Global Integrated Shipping Information System (GISIS) database. This shows that, since the introduction of a 0.10% sulphur limit in the Baltic and North Sea ECAs on 1 January 2015 (Revised Annex VI, Regulation 14.4), there have been 9 notifications of non-availability in EU ECAs out of a total of 84 notifications from all ECAs globally. Even though compliant fuels are assumed to be available at all times due to the limited demand, it can be seen that instances of non-availability are numerous; hence the necessity to anticipate the necessary actions prior to the introduction of a global cap of 0.50% m/m sulphur in 2020.

#### The basics of refining in simple and complex refineries

The function of the oil refinery is to convert crude oil into the finished products required by the market in the most efficient and, hence, the most profitable manner. The four basic operations are:

- 1) fractionation or distillation;
- 2) converting or chemically transforming certain cuts into products of higher commercial value;
- 3) treating, i.e. removing/transforming all unwanted components; and
- 4) blending of finished cuts into commercially saleable products.

The methods employed vary widely from one refinery to another, depending on the crude processed, the nature and location of the market, the type of equipment available, etc. The choice of methods will depend on individual strategic decisions taken by the refiners over time.

Refineries in the EU range from simple (hydroskimming) to very complex; the complexity often reflected in the use of deep conversion units such as delayed coker, solvent deasphalting or hydrocracking units. A detailed design engineering study performed by Amec Foster Wheeler<sup>[1]</sup> lists performance levels for these typical units. Table 1 on page 19 shows the average yields from the EU refining industry (LP simulation).

Table 1 demonstrates that the challenges faced by refineries due to decreasing demand for heavy fuel oil (i.e. fuel used inland as well as bunker fuel used at sea)



**Table 1 Average yields from the EU refining industry (Wt%)**

	Typical refineries		Concawe LP simulation		
	Hydroskimming	Highly complex	2014 calibration	2020, no specification change	2020, global sulphur cap
Gasoline cut	18%	25%	23%	19%	20%
Distillates	45%	51%	52%	55%	58%
Bottom of barrel	29%	9%	16%	14%	10%

following the global cap will be very different from one refinery to another. Therefore, while an overall impact assessment may be possible, the local impact of the global sulphur cap could be very different; refiners will face huge difficulties because they will be unable to reduce their heavy fuel oil yields whereas demand will temporarily disappear. However, EnSys believe that the expected short-term nature of this phenomenon is likely to deter many refiners from making major investments.<sup>2</sup> They also expect refinery investment to be restricted because of the perception commonplace today that the wide price differentials between light and heavy fuel oils will induce a rapid take-up of scrubbers. The likely effect of this could be a reversion of demand away from 0.50% sulphur fuel oil and back toward 3.50%.

Refiners acting in strict compliance with competition law do not share their strategic decisions upfront, so the future remains uncertain.

### Concawe modelling study: marine fuel supply in 2020

#### Modelling methodology

The study was carried out using Concawe's EU-wide refining model, which uses the linear programming technique to simulate the whole of the European refining industry. It encompasses the EU-28 members plus Norway, Switzerland and Iceland. The modelling of Europe is segmented into nine regions, each of which is represented by a composite refinery having the com-

bined processing capacity of all the refineries in the region, as well as the complete product demand slate relevant to that region.

#### Main hypothesis

The first step in this type of study is to assemble a set of assumptions that will essentially be common to all cases, and to describe the expectations in terms of crude and feedstocks slate, product demand (quantity and quality), refinery configurations and plant capacities, and all other relevant constraints that need to be taken into account. The main features and assumptions relevant to this study are summarised as follows:

- 'Scrubbed marine fuel' equals 14% of the demand (initial hypothesis from EnSys), although this is currently under discussion and likely to be reviewed downward due to scrubber uptake at ~-50% of expectations one year ago; the current assessment is 400 ships/year (Exhaust Gas Cleaning System Association).
- About 25 million tonnes/year of residual marine fuel (RMF) to switch from 2.9% sulphur (no specification changes) to 0.50% sulphur (global sulphur cap).
- No non-compliance considered for the EU demand (compliance is expected to be high in EU waters but, on average, low in other parts of the world; experts show figures around 70% compliance).
- Middle distillate imports and heavy fuels exports allowed as per 2014 real data.
- Crude slate with fixed ratios according to 2014 data.

<sup>2</sup> '2020: Refining Industry Perspective—Ability to Meet Demand and Quality'. Presentation by Martin Tallet, President, Ensys Energy, at the S&P Global Platts 14th Annual Bunker and Residual Fuel Conference, 20–21 June 2017.



**Table 2 Evolution in demand for the primary products (tonnes per year)**

	2014	2020*	Evolution
LPGs	44	57	13
Aromatics	13	13	0
Gasoline	83	74	-9
Jet	55	60	5
Diesel	205	202	-3
Heating oil	53	49	-4
Marine gasoil	10	18	7
Low-sulphur fuel oil	16	10	-6
Marine fuels (RMF)	36	31	-5
Bitumen, lubes, wax	26	22	-5
<b>TOTALS:</b>	<b>542</b>	<b>536</b>	<b>-6</b>

Middle distillate demand: steady

Bottom of the barrel demand: -21%

\* Source: WoodMackenzie forecast.

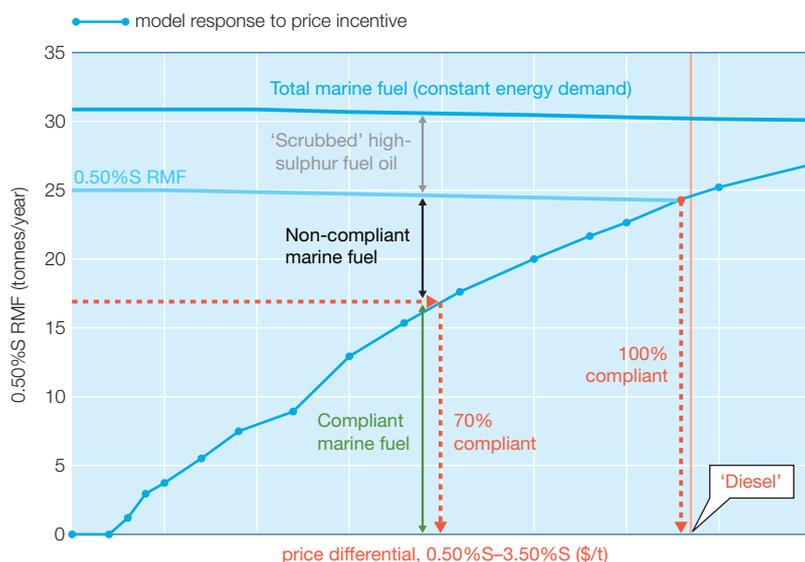
Note: figures may not add up exactly due to rounding.

**Modelling results—an overview**

Without additional capacities, the model could not find a feasible solution to produce sufficient marine fuels to meet demand at the new sulphur specification. The main bottlenecks were hydrogen manufacturing units (HMUs) and sulphur recovery units (SRUs).

Allowing for investments in these units, Concawe incentivised the model to produce 0.50% sulphur RMF by increasing the differential price for 3.5% sulphur RMF. Figure 2 shows the step by step analysis.

**Figure 2 Step-by-step analysis of the results of the Concawe modelling study**



The model shows a highly constrained system, as the model hardly reaches the 0.50% sulphur RMF demand (evaluated at 25 million tonnes/year). It also shows a potentially significant gap between demand and production, which may be an indication of the level of 'non-availability' of compliant fuel. On an open and balanced market driven by supply-demand, which is the case for petroleum products, the differentials between products is a fine equilibrium between the product demand and the incentive for the refiner to produce.

**Evolution towards distillates**

Figure 2 may also indicate that, as refiners increasingly blend more and more distillate molecules to increase the production of 0.50% sulphur RMF, the price differential (0.50%–3.50%) may increase to reach the 100% compliance case.

The demand for high-sulphur marine fuels (burned in ships equipped with scrubbers) in 2020 is around 6 million tonnes/year; maximum density and viscosity remain constant, but sulphur content goes up from 2.90% to 3.90%.

The blending of 0.50% sulphur marine fuel (25 million tonnes/year in 2020) results in multiple products, which can be divided into two categories:

- Heavy fuels at 0.50% sulphur:
  - Will most likely represent 30–50% of the demand.
  - Quality: pour point and sulphur will be maximised, density will be around 0.97 and viscosity ~25 cSt@100°C.
- Distillate type:
  - Will most likely represent 50–70% of the demand
  - Quality: pour point will be around 0°C and sulphur maximized, density will be around 0.87 and viscosity ~6 cSt@100°C.

In 2020, the ship operator/owner will order marine fuel containing 0.50% sulphur. The refiner/supplier will then supply the fuel at a quality which will depend on its own process and economic incentives. The study indicates that the range of quality will vary from heavy fuel (having either a very low sulphur crude slate or having residue desulphurisation capabilities) to a much lighter marine fuel with properties very similar to those of distillate



fuels (such as marine gasoil). Refiners might be tempted to bring to the market a very light fuel to supply the demand for 0.50% sulphur RMF if the differential vs distillate makes this practical. This will be the individual refiner's decision.

### Preliminary conclusions

Full compliance with the 0.50% sulphur limit for marine fuels across the EU28+3 refining system by 2020 will not be straightforward:

- SRU and HMU capacities are seen as a constraint by the Concawe model (both the EnSys-Navigistics Supplemental Study and the CE Delft IMO study (their Tables 92 and 93) also highlighted major deficits of H<sub>2</sub> and SRU capacity).
- Main conversion and hydrotreating units will need to be maintained at a high throughput.
- The model indicated that there will need to be a strong incentive for refiners to supply the demand for marine fuel at 0.50% sulphur.
- A key uncertainty will be world region trade flows (middle distillates imports and HSFO exports).
  - Hence, the ongoing collaboration with EnSys, who are performing simulations with their 'World Model', will be of benefit in providing Concawe with new input based on a broader simulation.

The crude slate ratios in the Concawe model are fixed, nevertheless it is intended that a sensitivity analysis will be performed based on simulations by EnSys who are evaluating the potential evolution for EU refineries based on world refining constraints and incentives.

The new marine fuels blending formulations should be treated with some caution, bearing in mind that the LP model is 'blind' with regard to issues such as compatibility, stability, lubricity and cold flow properties.

A key uncertainty is the rate of scrubber take-up, as this will have a dramatic influence on demand evolution and the decision-making process for refiners.

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### Reference

1. SINTEF (2017). RECAP Project: Understanding the cost of retrofitting CO<sub>2</sub> capture to an integrated oil refinery. Published 15 June 2017. See *Description of reference plants* by Amec Foster Wheeler. <http://www.sintef.no/recap>



# The low-dose benzene debate needs a sharp blade

.....  
**Concawe's ongoing research into the health effects of benzene aims to address recently published findings on the low-dose effects of benzene and the potential impacts on the EU refining industry.**  
.....

The health effects of benzene have been a major concern for regulators and health experts for many years. This has led to significantly lower regulatory threshold limits (such as occupational exposure limits, OELs<sup>1</sup>) and the implementation of corresponding risk management measures to reduce benzene concentrations and human exposure to benzene in the production, transport and use of petroleum products such as gasolines.

Over the past decade, a series of research papers has been published by a group of researchers at the University of California Berkeley who postulated effects of benzene at very low dose exposures (e.g. <sup>[1,2]</sup>). These low levels are relevant to current operations in the oil and gas industry and are currently (well) below the occupational exposure limits in most jurisdictions. However, the published findings on these low-dose effects have raised questions in the scientific community because the observations made are remarkable and report a relative increase in the intensity of the observed health effects at lower exposure concentrations; this is in contrast with the general rule in toxicology that 'the dose make the poison,<sup>2</sup> which implies that effects usually fade away as exposure concentrations get lower.

In these papers, the researchers pose that exposure to low concentrations of benzene (i.e. below 0.1 ppm) should be regarded as disproportionately hazardous. Because of these questionable findings and the potential impact on our industry, and since the scientific basis for the benzene OEL is presently under review in the EU, there is a need to verify the reported results in independent studies.

Concawe therefore has an ongoing research project which aims to shed new light on the reported benzene low-dose phenomenon. This project was initiated in 2016, starting with a re-analysis of the available evidence and the strength of the available data.

This first phase was completed in early 2017, with publication of the results in two peer-reviewed papers,<sup>[22,23]</sup> and indicates that the available data does not suggest an increased hazard from benzene at decreased exposure levels. These two papers have been shared with regulatory authorities to include in their (ongoing) assessments.

This Concawe review article on benzene is not intended to summarise the published papers from the Concawe project. It aims instead at providing the reader with a short overview of the scientific argumentation in the ongoing discussions on this topic as an example of an educational scientific debate; this is, incidentally, highly relevant in view of the ongoing OEL assessment for benzene in the EU, but also since the WHO's International Association for Research on Cancer (IARC) conducted a review on benzene in October 2017 in which it claimed that the low-dose effects of benzene are a major point of attention.

The following text is adapted from an article written by Prof. Dr Peter Boogaard (Shell, chair of Concawe's Toxicology Subgroup), which preceded the two Concawe publications mentioned above. The article, entitled 'The low-dose benzene debate needs a sharp blade', was published in a special section of the scientific journal *Chemico-Biological Interactions* (24 June 2017, e-publication ahead of print) and discusses the main aspects of the benzene low-dose debate in four major parts, addressing:

- metabolism of benzene;
- low-dose benzene measurement;
- low-dose benzene concentration calculation issues;
- the relevance of dermal exposure to benzene.

At the end of the article, the scientific debate is summarised and put into perspective.

## **No evidence exists that metabolism is different at low dose vs high dose benzene levels**

*Quantitative and qualitative differences in metabolism of certain compounds exist at low dose levels as compared to higher dose levels and this could potentially be due to the presence of a high-affinity, low-capacity enzyme. Indeed, the investigators reporting the low-dose phenomenon have postulated such an enzyme.<sup>[3,4]</sup> However, this hypothetical enzyme has not been found yet.<sup>[5,6]</sup> Typically, such high-affinity, low-capacity enzymes play some crucial role in maintaining homeostasis or some other crucial vital physiological process and is phylogenetically well preserved across species. Nevertheless, to the best of my knowledge, this type of enzyme has never*

<sup>1</sup> An occupational exposure limit (OEL) is an upper threshold limit below which no human health hazards are to be expected, i.e. the maximum allowed concentration level of a potentially hazardous substance which is used to manage potentially dangerous exposures in the workplace.

<sup>2</sup> According to the first rule of toxicology, 'All things are poison and nothing is without poison; only the dose makes a thing not a poison' — an adage (translated from German) by Paracelsus, considered 'the father of toxicology'. Paracelsus, *dritte defension*, 1538.



been found for benzene (nor similar dose-dependent metabolism) in any animal species, therefore it doesn't seem very likely that humans would possess it.

### **Benzene exposure levels used to explain hypothesized effects were solely estimated, not measured**

Another potential explanation could be found in the exposure assessment itself, that is if the claimed 'low dose' was actually not as low as it was deemed to be. The exposure data in the various publications go all back to a series of studies in China.<sup>[7,8,9]</sup> If you have a closer look at the exposure assessments as reported in later studies (e.g. <sup>[1,2,10]</sup>), it is clear that in most of these publications actual exposure measurements were not done. On the contrary, the exposures are based on previously reported studies and essentially there is only one paper that forms the basis for the exposure assessment which is subsequently used in the other publications.<sup>[11]</sup> A closer look at this particular study shows that the low concentrations are not actually measured but rather calculated. According to the original paper where the methodology was described, the limit of detection of airborne benzene was 0.20 ppm.<sup>[9]</sup> All exposure values lower than this limit of detection of airborne benzene were calculated from the measured concentration urinary benzene using a correlation between airborne benzene and urinary benzene. The authors claim that the correlation they applied to do this was corroborated by the data of Ghittori et al. from 1993.<sup>[12]</sup> The paper by Ghittori and co-workers is a typical methodological paper in which they show that urinary benzene correlates reasonably well with airborne benzene concentrations when both values are log-transformed ( $r = 0.559$  in 110 workers, both smokers and non-smokers;  $r = 0.763$  in the 63 non-smoking workers only). Ghittori and co-workers, however, did not report a limit of detection. The lowest values measured were reported to be approximately 0.1 ppm, but the scatter, especially at lower concentrations, is rather large. In any case, the 'low-dose' concentrations are not actually measured directly as clearly stated in the Thomas et al. paper:<sup>[11]</sup> "For each of the exposed individuals in the study, benzene exposure was estimated in terms of the average air-benzene level (in units of parts-per million). The exposure levels of the 42 subjects that were below the limit of detection were esti-

mated using un-metabolized urinary benzene levels, as previously described."<sup>[11]</sup> The McHale et al. paper<sup>[2]</sup> apparently uses the study population of the Lan et al. study<sup>[8]</sup> for which the exposure assessments were done according to Vermeulen et al.<sup>[9,13]</sup>

### **Low dose benzene levels that were used to proof non-linearity were calculated using linear statistical models**

If one has a look at the figures in the publication by Kim and co-workers where the dose related production of urinary metabolites is given as a function of the median value for airborne benzene concentration (Figure 4 in <sup>[11]</sup>), it is obvious that for most metabolites only the data points between 0.01 and 0.1 ppm benzene are not 'in line'. The most obvious reason seems to be that the airborne benzene concentrations related to these data points are calculated and not measured unlike the airborne benzene levels for the other data points, as explained above. The data are based on measured urinary benzene levels using a simple linear regression model: basically airborne benzene concentrations are linked to urinary benzene levels. In general, that is a valid approach, but, in my view, it is fundamentally wrong to use this linear equation subsequently to demonstrate non-linearity in metabolism for low exposure levels. If you assume that metabolism is different (i.e. essentially non-linear) at concentrations less than 1 ppm, you cannot use a linear regression between airborne benzene levels greater than 1 ppm and urinary benzene (or any urinary metabolite) to predict airborne benzene less than 1 ppm as the amount of un-metabolised benzene in urine is no longer independent under your assumption.

### **Dermal exposure, which is probably the most realistic exposure route given the occupational setting under evaluation, is completely dismissed**

Another question rose with regard to potential other routes of exposure, especially skin exposure. The Vermeulen et al. paper<sup>[9]</sup> explicitly states that dermal exposure is not expected to have contributed to the total exposure: "Preliminary analyses of dermal exposure data collected as part of the current study indicate that this route of exposure did not contribute substantially to the



total benzene and toluene doses received (unpublished data)". Actually, these data were published a couple of years later.<sup>[13]</sup> In this paper the authors describe the dermal monitoring of 70 individuals involved in 6 different tasks using dermal patches. However it is not reported how many persons that were monitored were involved in each of the tasks. In a number of individuals (3 for benzene and 5 for toluene), one or more of the patches indicated that dermal exposure might have occurred and, without exception, these persons were involved in the same task 'gluing'. The authors admit that dermal exposure might have been missed since only a very limited area of the skin was covered by the patches and the spatial distribution of dermal exposure was expected to be non-uniform. Nevertheless, because a strong association between airborne benzene and benzene in urine was found, it was concluded that inhalation was the predominant route of exposure. The authors then support the plausibility of their conclusion by quoting US EPA documentation on benzene that dermal absorption of benzene is usually negligible. However, the assumption by US EPA that dermal absorption of benzene is between 0.05 and 0.1% is dubious, if only since it is not specified what this percentage refers to: neat benzene on the skin, benzene vapour through the skin, dermal absorption as percentage of the inhaled amount. All of these aspects are important and it seems that this assumption is actually based on the IRIS documentation on dermal absorption of benzene, which is simply incorrect as I've argued before.<sup>[14]</sup> In fact, most regulatory authorities have assigned a skin notation to benzene, which implies that in occupational settings dermal uptake is more than 10% of the uptake by inhalation.<sup>[15]</sup> Assuming that it is less than 0.1% seems untenable. There are a few recent reviews on the dermal uptake of benzene<sup>[16,17]</sup> and there seems to be consensus that the dermal flux for benzene is between 0.2 and 0.4 mg/(cm<sup>2</sup>.h). Hence, if a flux of 0.3 mg/(cm<sup>2</sup>.h) is assumed—which is low, since the benzene is in glue, see below—and make the same assumption as was done in the paper that 10% of the surface of both hands (36 cm<sup>2</sup>) was contaminated, the estimated uptake would be 10.8 mg/h, or 86.4 mg of benzene over an 8-h working day, which is quite a bit higher than the ~ 0.5 mg that was suggested in the paper.<sup>[13]</sup> In addition, it should be realized that most assumptions for dermal uptake of benzene apply to neat benzene which is expected to be

different from benzene in glue. Available data indicate that aqueous benzene solutions behave similar to neat benzene, probably since the benzene is volatile and lipophilic. However, benzene dissolved in organic solvents (hexane, gasoline, and probably glue) has a more variable flux, but generally the organic matrix enhances skin penetration, which may be expected as the benzene won't evaporate as easily.<sup>[16]</sup> Hence, dermal uptake of benzene seems quite feasible to have occurred to some extent, especially during 'gluing'. This might explain one of the conclusions from the re-analysis of the data by McNally et al.<sup>[22]</sup> that "some aspect of exposure was not captured by a full shift air sample".

### **In summary: the low dose benzene debate, and why it would benefit from a sharp blade of Ockham's razor<sup>3</sup>**

Even if we ignore the arguments about the mysterious high-affinity, low-capacity enzyme as well as the potential dermal exposure that may have played a role, and we also disregard the fact that the lowest airborne concentrations are not actually measured, but just take the actual exposure data, as reported in the papers by Kim and co-workers,<sup>[8,9]</sup> at face value, the low-dose phenomenon is still not immediately obvious. Therefore, the original data from these studies as well as their modelling as performed by Kim et al.<sup>[7]</sup> were reanalyzed by Price et al.<sup>[18]</sup> Price and co-workers addressed several critical technical issues, such as the corrections applied for metabolite background levels and the calibration model applied to estimate airborne benzene concentrations for certain workers, and concluded that there was no statistically significant departure from linear metabolism at low exposure concentrations. Rappaport and co-workers reacted furiously to this critique<sup>[19]</sup> and Price and co-workers, in turn, reacted to the response by Rappaport et al.<sup>[20]</sup> providing additional analysis as to why both the original claim of low-dose specific metabolism and the rebuttal comments offered by Rappaport and co-workers remained highly implausible and speculative. One area of great attention arising from these public debates is the risk of conflict of interests that may occur for all stakeholders involved in these applied research programmes since these novel claims of increased risk of attracting leukemia by exposure to benzene at much lower levels than previously assumed to pose a carcino-

<sup>3</sup> Ockham's razor is a principle attributed to the 14th century philosopher William of Ockham, which states that, 'Entities should not be multiplied unnecessarily' — or in other words, when you have two competing theories that make exactly the same predictions, the simpler one making fewest assumptions is the better.



genic risk will most probably lead not only to increased benzene health-related litigation, but also to calls for regulatory action to further lower acceptable benzene exposures. Therefore, both the scientists conducting research and studies on behalf of industry and academic researchers, whose funding is generally provided by regulatory bodies and governmental institutes (US EPA, OSHA, NIEHS, NCI, NIOSH) and who act as expert-witness in benzene-litigation cases,<sup>[6, 11, 13, 19, 21]</sup> are likely to be subject to the risk of conflict of interest. As a result and in order to avoid any risk of conflict of interests, great care should be given by all involved stakeholders to develop conclusions that are built on correct and well supported scientific arguments.

It was therefore considered important that the data would be independently reanalyzed by two different research groups: Cox Associates and the UK Health & Safety Laboratory. The two research groups followed a very different approach in re-analysing the data but both came to the conclusion that, although the data reported in the studies that led to the hypothesis of the low-dose benzene phenomenon indeed do not exclude non-linear metabolism at lower concentration of benzene, the data are also fully consistent with the absence of any non-linearity in benzene metabolism at low doses. Since the absence of non-linearity does not require hypothetical enzymes or any other unproven assumption, it would be the preferable scientific stance according to Ockham's razor.

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# Abbreviations and terms



AC	Activated Carbon	LNT	Lean NO <sub>x</sub> Trap
AIF	All Incident Frequency (also known as Total Recordable Case Frequency; calculated from the sum of fatalities, LWIs, RWIs and MTCs divided by the number of hours worked expressed in millions of hours)	LP	Linear Programming (page 18)
AQ	Aqueous solution	LP	Low Pressure (Figure 3, page 15)
ASC	Ammonia Slip Catalyst	LPG	Liquefied Petroleum Gas
BAT	Best Available Techniques	LWI	Lost Workday Injury (a work-related injury that causes the injured person to be away from work for at least one normal shift)
BAT REF or BREF	BAT Reference document. Full title: 'Reference Document on Best Available Techniques for ...' (A series of documents produced by the European Integration Pollution Prevention and Control Bureau (EIPPCB) to assist in the selection of BATs for each activity area listed in Annex 1 of Directive 96/61/EC)	LWIF	Lost Workday Injury Frequency (the number of LWIs divided by the number of hours worked expressed in millions)
BBU	Bitumen Blowing Unit	MARPOL	International Convention for the Prevention of Pollution from Ships
BOE	Barrel of Oil Equivalent	MAW	Moving Average Window
CD	Chassis Dynamometer	MTBE	Methyl Tertiary Butyl Ether
CDP	Carbon Disclosure Project	MTC	Medical Treatment Case (i.e. injury)
CDU	Crude Distillation Unit	NCI	National Cancer Institute
CEFIC	European Chemical Industry Council	NEDC	New European Drive Cycle
CF	Conformity Factor	NIEHS	National Institute of Environmental Health Sciences
CN	Cetane Number	NIOSH	National Institute of Occupational Safety and Health
CO	Carbon monoxide	NO <sub>x</sub>	Nitrogen Oxides
CO <sub>2</sub>	Carbon dioxide	NO <sub>2</sub>	Nitrogen dioxide
DI	Direct Injection	NTE	Not-To-Exceed
DOC	Diesel Oxidation Catalyst	OBD	On-Board Diagnostic
DPF	Diesel Particulate Filter	OEL	Occupational Exposure Limit
ECA	Emission Control Area	OSHA	Occupational Safety and Health Administration
EGCS	Exhaust Gas Cleaning System	OTCW	Once-Through Cooling Water
EGR	Exhaust Gas Recirculation	PEMS	Portable Emissions Measurement System
EMROAD	RDE validation tool developed by the Joint Research Centre of the European Commission	PM	Particulate Mass/Particulate Matter
EN590	European Diesel Specification	PM <sub>2.5</sub>	Particulate matter with an aerodynamic diameter less than or equal to 2.5 µm
EU	European Union	PN	Particle Number
Euro 6	The European Commission's emission standards regulation for diesel vehicles	PSC	Port State Control
FAME	Fatty Acid Methyl Ester	QA	Quality Assurance
FAR	Fatal Accident Rate (the number of fatalities divided by the number of hours worked expressed in hundred millions)	QC	Quality Control
FBP	Final Boiling Point	RAR	Road Accident Rate (calculated from the number of accidents divided by the kilometres travelled expressed in millions)
FCCU	Fluid Catalytic Cracking Unit	RDE	Real Driving Emissions
FTE	Full-Time Equivalent	REACH	Registration, Evaluation, Authorisation and restriction of CHemicals
GISIS	IMO's Global Integrated Shipping Information System database	RMF	Residual or Refinery Marine Fuel ?
GRI	Global Reporting Initiative	RO	Reverse Osmosis
H <sub>2</sub>	Molecular Hydrogen	SCR	Selective Catalytic Reduction
HC	Hydrocarbon	SCRf	Selective Catalytic Reduction on Filter—an SCR catalyst combined with a DPF
HDS	HydroDeSulphurisation	SECA	Sulphur Emission Control Area
HMU	Hydrogen Manufacturing Unit	SF	Sand Filtration
HSFO	High Sulphur Fuel Oil	SMG	Safety Management Group
IARC	International Agency for Research on Cancer	SO <sub>x</sub>	Sulphur Oxides
IBP	Initial Boiling Point	SRU	Sulphur Recovery Unit
IDI	InDirect Injection	T50	Temperature (°C) at which 50% of the fuel is distilled off
IMO	International Maritime Organization	T95	Temperature (°C) at which 95% of the fuel is distilled off
IOGP	International Association of Oil & Gas Producers	UF	UltraFiltration
IPIECA	The global oil and gas industry association for environmental and social issues	US EPA	United States Environmental Protection Agency
LFI	Learning From Incidents	US06	United States transient test cycle used in the Supplemental Federal Test Procedure
		VBU	Vis-Breaking Unit
		VDU	Vacuum Distillation Unit
		WHO	World Health Organization
		WLTC	Worldwide harmonized Light-duty Test Cycle

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