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Environmental Science for European Refining

Review

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Foreword

The European Green Deal tackles all aspects of our industry, and it is no surprise that all of the articles in this edition of the Concawe *Review* are related to it.

In light of the zero pollution action plan and the proposed revision of the air quality standards, the first article evaluates the feasibility and the level of success of current and projected compliance concerning ozone, a secondary pollutant formed and removed via complex chemical reactions. In the second article, the author analyses how the lockdown measures implemented in 2020 to counter the spread of the SARS-CoV-2 virus have impacted air quality in selected European cities.

The European Commission is currently finalising its plan to achieve a 55% reduction in greenhouse gas (GHG) emissions by 2030. In this context, the third article summarises a Concawe Report which provides an outlook for the transport sector, modelling the evolution of different powertrains and the availability of different alternative fuels. With the growing and rapid electrification of passenger cars, some uncertainty has arisen as to whether the capacity for battery production will be able to meet the demand. The fourth article explores the optimal passenger car sales composition (internal combustion engines, hybrid electric vehicles, plug-in hybrid electric vehicles and battery electric vehicles) for minimising well-to-wheels GHG emissions as a function of battery production capacity available in 2030.

The two last articles relate to the Green Deal toxic-free environment and the REACH legislation. The correct evaluation of the persistence of our products in the environment is key to correctly evaluating their potential to do harm, and is part of the evaluation under REACH. The fifth article refers to a study, and a paper published in a peer-reviewed scientific journal, showing that temperature correction for historical biodegradation simulation tests should be hydrocarbon-specific, rather than follow a generic default correction as currently addressed in the ECHA guidance. The REACH regulation also promotes alternative methods to animal testing for the hazard assessment of substances. The final article summarises the achievements reached under Concawe's important Cat-App project, which aims to reduce the amount of animal testing required for hazard evaluation of our substances thanks to the identification of biological similarity through innovative in-vitro testing, high-throughput genomics and integrative data analyses.

I am confident that these articles will generate as big an interest to the reader as the passion of the scientists who have written them.

Jean-Marc Sohier
Concawe Director

Contents

Towards the adoption of the 2021 zero pollution action plan for air, water and soil, that has been announced by the European Commission (EC) as part of the European Green Deal, the EC is notably proposing to revise air quality standards to align them more closely with the World Health Organization (WHO) recommendations. This article focuses on ozone (O_3), for which the EU air quality limit values (AQLVs) have not been changed since the late 1990s, and assesses how current and projected compliance trends will change under the current EU AQLV as well as under lower limit values, and under different emission reduction scenarios.

The study highlights that any revision of the current AQLVs for O_3 should follow a two-step process where quantifying the environmental and human health risks associated with the concentrations of pollutants is as significant as assessing how these risks should be managed (i.e. in terms of technical feasibility, cost-effectiveness, control measures and level of success in improving compliance).

The major findings of this study are as follows:

- O_3 compliance with the EU AQLV (120 µg/m^3, not to be exceeded on more than 25 days) is currently fully achieved only in parts of Europe, with non-compliance remaining an issue in several areas in southern and eastern European countries.
- The vast majority of European countries are currently not able to meet the Ambient Air Quality (AAQ) Directive long-term O_3 objective of 120 µg/m^3 without any allowance for exceedances. In addition, reducing the threshold to the current WHO guideline value of 100 µg/m^3 results in a substantial EU-wide increase in non-compliance, with 94% of all monitoring stations in Europe being unable to achieve compliance in 2017 (i.e. the latest year for which O_3 data were available at the time the study was undertaken).
- Under current legislation, O_3 compliance will continue to improve from 2025 onwards. However, full compliance with the existing EU AQLVs will not necessarily be achieved in all EU countries.
- Further emission reduction measures, beyond the current legislation, that will mainly target NO_x and VOC emissions, will further improve O_3 compliance with the current EU AQLV. However, full compliance will still remain unachievable in some countries (e.g. Italy, Spain).
- A move to a threshold of 100 µg/m^3 (the current WHO air quality guideline value) or a move towards the AAQ Directive long-term O_3 objective (i.e. zero allowable exceedances at the current threshold) will essentially create an EU-wide compliance challenge for O_3. Under such a revision of the current EU AQLV, O_3 compliance will be far from technically achievable, regardless of the measures applied to control emissions.

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In response to the spread of the novel coronavirus SARS-CoV-2 in Europe since the beginning of 2020, the implementation of restrictive measures across countries to mitigate the rate of infection has led to a significant reduction in economic activity. This, in turn, has had a consequent impact on air quality.

This article uses up-to-date measured data from monitoring stations in selected European cities to quantify how the lockdown measures have impacted the concentrations of NO_2, PM and O_3. The major findings of the study indicate the following:

- NO_2 concentrations in 2020 appear to be at lower levels compared to those in 2019.
- NO_2 concentrations showed a significant drop during the first period of the national lockdown measures, in some cases falling by more than 50%. This could be attributed mainly to the lower NO_x emissions associated with road transport in the same period. During the subsequent deconfinement period, NO_2 levels were seen to increase. The second period of restrictive measures that then followed is not proven to have been as effective in reducing NO_2 concentrations as when similar measures were taken during the first lockdown period.
- The impact of the lockdown measures on PM concentrations was less pronounced than for NO_2 and did not show a consistent downward response. A variable response of PM levels was seen during all stages of the Covid-19 pandemic and the lockdown measures at national level. Compared with 2019 levels, PM concentrations in 2020 were, on average, found to be somewhat lower, although significant temporal variations were observed.
- The implementation of lockdown measures has had a different effect on O_3 concentrations, with the majority of cities analysed experiencing higher O_3 concentrations in 2020 compared with 2019 levels, especially during the period when the first national lockdown measures were in place.

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This article summarises the findings of a Concawe report which provides an outlook for the European transport sector by modelling elements such as the evolution of the different powertrains and the availability of different alternative fuels over a certain time frame. The outlook focuses on the 2018–2030 period and, through the definition of a baseline, its main objective is to inform stakeholders on current market and industry trends and 2030 target compliance, identifying key enablers for, and potential barriers to, boosting the penetration of renewable energy as well as improvements in the GHG intensity of the European transport sector.

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Recent forecasts for the rapid electrification of the road transport sector towards 2030 have given rise to considerable uncertainty associated with battery production capacity and whether it will be able to meet the growing demand for batteries in Europe. In view of this uncertainty and the potential implications for GHG emissions, this article explores the optimal passenger car sales composition for minimising well-to-wheels (WTW) GHG emissions as a function of battery production capacity available for the electrification of the new vehicle sales mix in 2030.

The options considered for the different levels of electrification of passenger cars include vehicles powered solely by internal combustion engines (ICEVs), hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs) and battery electric vehicles (BEVs). Within that context, a wide range of possible cases are explored based on a sensitivity analysis of key parameters including the utility factor of PHEVs (i.e. their share of electric driving), the carbon intensity of the electricity supply, the energy consumption of vehicles, and the use of low-carbon fuels. The results present a break-even analysis of different passenger car sales compositions in terms of the minimum achievable GHG emissions.

The findings indicate that, under a low/medium battery production capacity scenario (up to about 0.30 TWh/year) and moderate/high levels of utility factor (higher than 45%), a combination of 'HEV+PHEV' in new passenger car sales is deemed to be the most effective option to reduce GHG emissions. In the battery cap scenarios of up to 0.55 TWh/year in 2030, the PHEV with a moderate/high utility factor would be a key component of the optimal sales mix, with its share reaching 94% of new sales at a battery supply capacity of 0.30–0.35 TWh/year. In the scenarios considered, increasing the utility factor of PHEVs is the most immediate and accessible way to decrease GHG emissions in the short term. Increasing the contribution of low-carbon fuels in the fuel mix, and a decrease in the carbon intensity of the electricity mix will offer significant additional WTW savings, which are expected to be more significant in the period 2030+.

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The potential for a chemical to do harm is related to its persistence (P) in an environmental system. The persistence of chemicals is an important part of substance evaluation under REACH. It is assessed primarily using standardised OECD biodegradation simulation testing methods, which were historically performed at around 20°C. In 2017, ECHA altered its guidance to require biodegradation simulation data at 12°C, which is considered to be the average temperature in the EU. This means either performing the biodegradation simulation testing at 12°C or applying a mathematical correction, termed the Arrhenius equation, to adjust the biodegradation rates derived at other temperatures. However, there are serious drawbacks associated with this practice. First, the REACH P criteria were developed using degradation studies performed at room temperature on chemicals known to be persistent. Second, in a 2020 publication, Concawe showed that the use of ECHA's default 'temperature correction' would lead to an overestimation of persistence for petroleum hydrocarbons. The repercussions of overestimating persistence can be severe, including authorisation and/or restriction of the chemical in Europe. Concawe therefore encourages a more accurate study and substance-specific approach for temperature adjustment for petroleum hydrocarbons.

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One of the aims of the REACH regulation is to promote alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals. However, in practice it has proven to be challenging to obtain regulatory acceptance for the application of such alternatives alongside existing toxicology data to minimise or replace the standard required animal tests. At the same time, the alternative options currently proposed under REACH are not practically applicable to petroleum substances. Concawe's Cat-App project aims to address these challenges by developing a framework based on chemical-biological read-across, which integrates chemical compositional data with innovations in (i) in-vitro testing, (ii) high-throughput genomics and (iii) integrative data analyses and visualisation into a transparent workflow.

The practical work of the Cat-App project was completed in 2018, resulting in almost 3.5 million data points on 141 substances from 15 cell models. A final report was published in 2020, along with a peer reviewed publication in ALTEX (Vol. 38, No. 1, 2021), showing that a biological component can be added to the required similarity assessment which facilitates grouping substances for a more holistic rather than substance-driven assessment. In addition, it was shown that trends can be observed across the chemical space of these substances in line with the hypothesised dose [of the specific chemical constituents]-response [in terms of bioactivity] relationship, which can be used in combination with other available data to build read-across hypotheses and assessments.

Overall, this is expected to help address practical challenges with the regulatory assessment of UVCB substances, which may help to avoid unnecessary animal testing in the short term. In addition, if these data find regulatory acceptance for this purpose they can be further built upon and will ultimately help to develop alternatives to animal testing in the longer term, eventually putting the opportunities provided by REACH to innovate the conservative toxicology testing paradigm into practice.

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Understanding the process of setting air quality limit values and the associated compliance challenge—the ozone study

The European Commission is proposing to revise air quality standards to align them more closely with the World Health Organization (WHO) guidelines. This article focuses on O_3, and assesses how current and projected compliance trends will change under the current EU AQLV, as well as under lower limit values and under different emission reduction scenarios. It also highlights the need to follow a two-step process including both risk assessment *and* risk management when considering further close alignment of the current EU AQLVs for O_3 with the WHO guidelines.

Introduction

The European Commission (EC) recently completed the fitness check of the EU Ambient Air Quality (AAQ) Directives (Directives 2008/50/EC[1] and 2004/107/EC[2]). The EC drew on the experience from all Member States and various other stakeholders, focusing on the period from 2008 to 2018 (i.e. the period in which both Directives were in force) and finalised the process by publishing its Staff Working Document in November 2019.[3] The EC has concluded that, overall, the AAQ Directives have been broadly fit for purpose; however, the existing air quality framework remains subject to further improvements that would help in achieving the overarching ambition to fully meet all air quality limit values (AQLVs) for all pollutants and throughout the European Union.

Specifically, the fitness check identified several lessons learnt that should be considered in any follow-up decisions made by the EC. Among others, these include the following:

a) The EU AQLVs have been instrumental in driving a downward trend in exceedances, and in exposure of the population to exceedances. However, the current AQLVs are not as ambitious as established scientific advice suggests for several pollutants; the World Health Organization (WHO) is currently reviewing its air quality guidelines, and the EC is closely following this process.

b) AQLVs have been more effective in facilitating downward trends than other types of air quality standards, such as target values.

These important considerations have been taken into account by the EC in its Communication of the European Green Deal and its plan to adopt, in 2021, a zero pollution action plan for air, water and soil.[4] The EC has announced that it will draw on the lessons learnt from the fitness check of the AAQ Directives, and will notably propose to revise air quality standards to align them more closely with the WHO's recommendations,[1] [5, 6] which are lower than the limit values set in the AAQ Directives for the majority of regulated pollutants.

Ozone (O_3) is one of the 13 air pollutants for which AQLVs have been set under the current AAQ Directives. O_3 is a secondary pollutant which is not directly emitted into the atmosphere, but is formed (and removed) via complex chemical reactions that take place in the presence of sunlight and gas precursors (mainly nitrogen oxides (NO_x) and volatile organic compounds (VOCs)) emitted by both anthropogenic and biogenic sources. The EU AQLV for O_3 was set under Directive 2002/3/EC[7]—the 'Third Daughter Directive'—which is focused entirely on O_3. This introduced a 'target value' of 120 $\mu g/m^3$ for maximum daily 8-hour O_3 mean concentrations,[2] not to be exceeded on more than 25 days per calendar year averaged over three years, that should be met as of 1 January 2010.

[1] In the preface of the WHO *Air Quality Guidelines for Europe*, it states that '*It should be emphasised, however, that the guidelines are health-based or based on environmental effects, and are not standards* per se. *In setting legally binding standards, considerations such as prevailing exposure levels, technical feasibility, source control measures, abatement strategies, and social, economic and cultural conditions should be taken into account.*' As risk management is not considered in the WHO guidelines values, these are lower than the limits set in the AAQ Directives for the majority of regulated pollutants. https://www.euro.who.int/__data/assets/pdf_file/0005/74732/E71922.pdf

[2] The daily maximum 8-hour mean is the maximum of the valid 8-hour running means for that day. Calculation of all the 8-hour running means for a given day is a prerequisite.

In addition, a long-term objective was introduced for O_3 which refers to the same 'target value' of 120 µg/m^3 but without any allowance for exceedance days within a calendar year. The AQLVs set in this Directive reflected the risk assessment undertaken by the WHO in the late 1990s, and no changes were made when the Third Daughter Directive was replaced with Directive 2008/50/EC.

Since the establishment of the EU AQLV for O_3, significant further research has been undertaken on the health impacts of O_3. This was already partly reflected in the 2005 revision of the WHO's Air Quality Guidelines[5] in which the WHO reduced the O_3 guide value (i.e. the maximum daily 8-hour O_3 mean concentration) from 120 µg/m^3 to 100 µg/m^3. This represents a significant toughening of the guide value, which might be lowered further based on the outcome of the ongoing review of the WHO's air quality guidelines. It is therefore highly likely that, in the expected revision of the AAQ Directives, the current 'target values' for O_3 will be revised downwards and will be made binding (and get the same status as, for example, NO_2 and PM_{10}).

However, any decision for further close alignment of the current EU AQLVs for O_3 with the WHO air quality guidelines should not be made by only taking into account the environmental and human health risks presented by concentrations of air pollutants (risk assessment step). According to the WHO instructions, this should be a two-step process where the risk assessment step will be followed by an assessment of how these risks may be managed (risk management step). In practical terms, the risk management step should assess how emissions of pollutants and their precursors may be controlled, how emission limits are technically achievable, the associated cost, and the level of success in improving air quality.

Building on the important insights derived from an earlier Concawe study[8] with respect to the significance of the risk management step as part of the AAQ Directive revision process, Concawe worked with Aeris Europe to carry out a study that analyses the current compliance trends for O_3 in Europe, and how these would change in response to a potential lowering of the AQLV to the current WHO guideline value of 100 µg/m^3. In addition, the analysis of these trends is extended into the future (up to 2030) to also assess the implications of changing the EU AQLV under the current EU legislative emissions projections and under several emissions scenarios. The analysis covers the EU, with a special focus on five Member States (France, Germany, Italy, Poland and Spain) and the UK.[3] For brevity, this article uses illustrative examples from the analysis to demonstrate the results of the study.

[3] The United Kingdom left the EU on 1 February 2020 but will apply EU law until the end of the transition period.

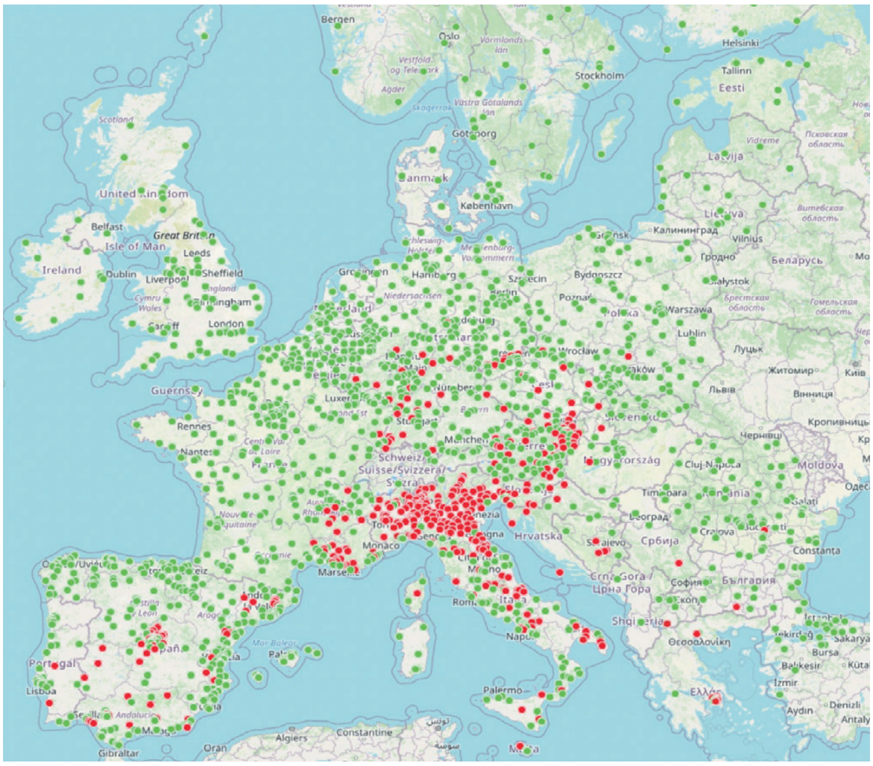
Understanding the process of setting air quality limit values and the associated compliance challenge—the ozone study

Current compliance trends for O_3

Based on available hourly measurement data from all European O_3 monitoring stations (~2,200 stations) taken from the European Environment Agency (EEA) Air Quality e-Reporting database,[9] the state of compliance in each Member State under the current AQLV of 120 µg/m^3 (with an exceedance allowance of 25 days) was analysed. The analysis covered both the latest year for which O_3 data were available (i.e. 2017) at the time when the study was undertaken, as well as historical years. Figure 1 shows the O_3 compliance picture in Europe in 2017 under the current AQLV.

Figure 1: Maximum daily 8-hour mean O_3 concentrations (µg/m^3) in Europe in 2017

- monitoring stations that measure concentrations below the target value of 120 µg/m^3 (not to be exceeded on more than 25 days) (compliant stations)
- monitoring stations that measure concentrations above the target value (non-compliant stations)

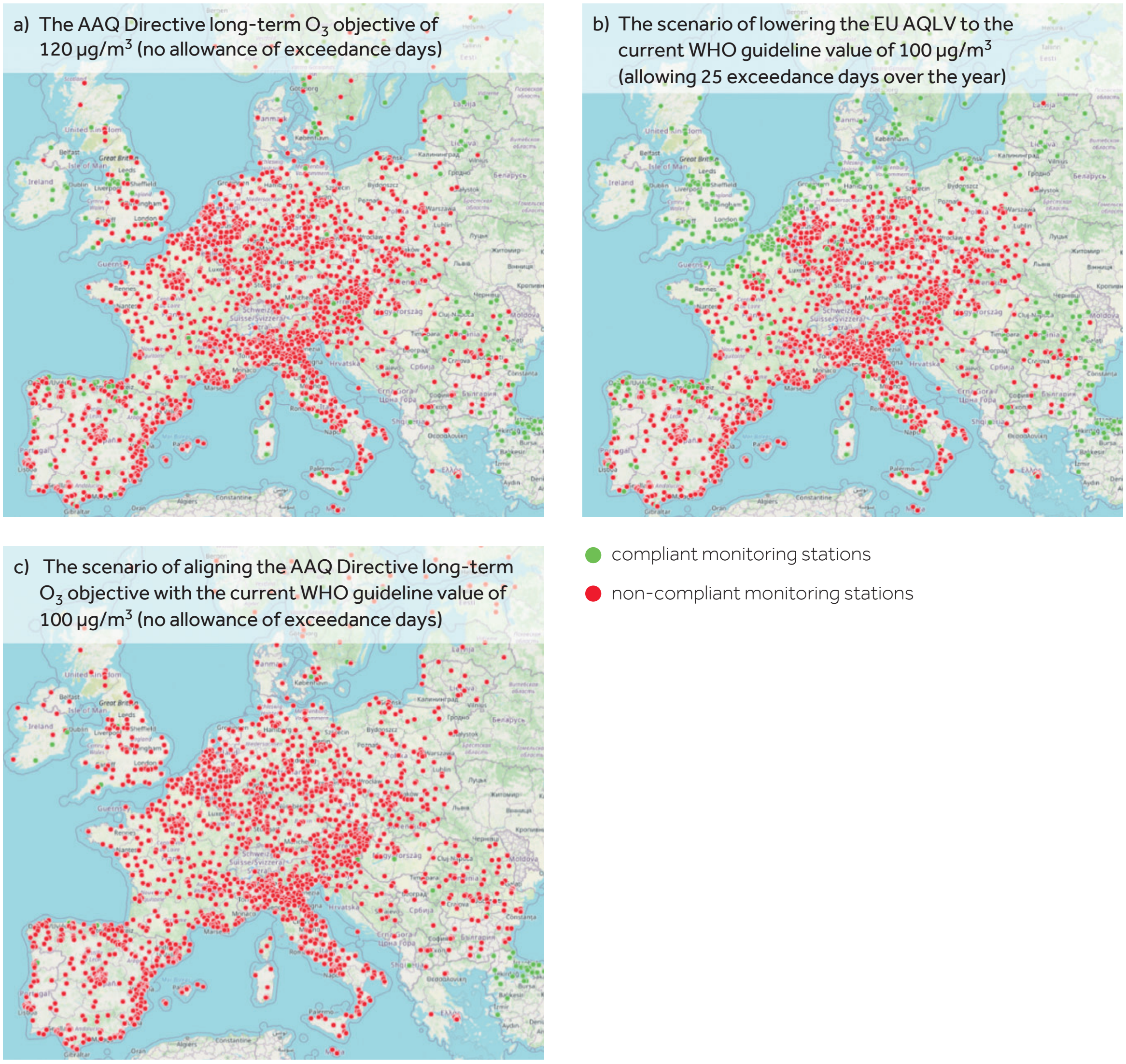


In 2017, approximately 81% of all stations measuring O_3 in Europe were compliant with the current EU AQLV. However, on the national scale, full compliance in all monitoring stations within a country is only achieved in approximately 35% of European countries, with 17 Member States and 5 other reporting countries[4] registering concentrations above the O_3 target value for more than 25 days. O_3 compliance also shows a strong spatial variability, with most of the non-compliant stations being found in southern and eastern European countries; this indicates the important role that meteorology plays on O_3 formation, especially during peak O_3 episodes which are strongly linked and favoured by warm, stagnant conditions which occur in this part of Europe. Ozone concentrations also show a strong inter-annual variation, with compliance ranging between 75–90% over the past five years.

[4] Andorra, North Macedonia, Bosnia and Herzegovina, Serbia and Switzerland.

However, the vast majority of the monitoring stations in Europe are a long way from fulfilling the long-term O_3 objective of 120 µg/m^3 without any allowance for exceedance days set in the AAQ Directive. In 2017, only 17% of all stations in Europe were compliant with the long-term O_3 objective of zero exceedances of 120 µg/m^3 (maximum 8-hour daily average)—see Figure 2a. In addition, a significant downward change in the AQLV raises notable compliance problems. For example, a reduction in the EU AQLV to the current WHO guideline value of 100 µg/m^3, while keeping the 25 exceedance days threshold, results in a substantial EU-wide increase in O_3 non-compliance (67% in Europe)—see Figure 2b. The non-compliance issues could be even more significant when the long-term O_3 objective is aligned with the current WHO air quality guideline value, as only 6% of all O_3 monitoring stations in Europe were able to achieve this value in 2017 (Figure 2c).

Figure 2: O_3 compliance in Europe in 2017 under three different scenarios



a) The AAQ Directive long-term O_3 objective of 120 µg/m^3 (no allowance of exceedance days)

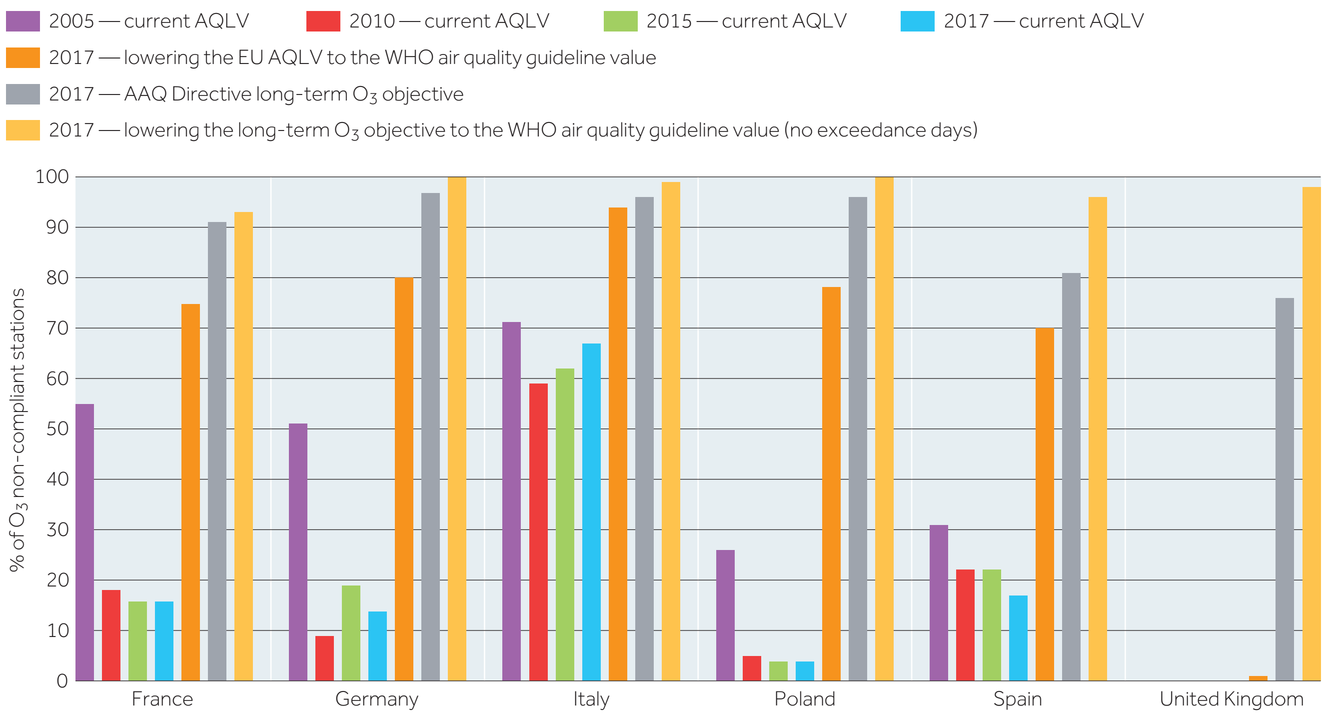
b) The scenario of lowering the EU AQLV to the current WHO guideline value of 100 µg/m^3 (allowing 25 exceedance days over the year)

c) The scenario of aligning the AAQ Directive long-term O_3 objective with the current WHO guideline value of 100 µg/m^3 (no allowance of exceedance days)

Understanding the process of setting air quality limit values and the associated compliance challenge—the ozone study

Analysing the O_3 compliance trends at a national scale, in the six countries (i.e. five EU-27 Member States and the UK) used for a more detailed focus, the results show that over the years from 2005 to 2017, O_3 compliance has generally improved. However, full compliance with the current EU AQLV is currently achieved only in the UK, with non-compliance in 2017 ranging from 4–70% in the other five countries (Figure 3). A move to a limit value of 100 µg/m^3, or a move towards zero allowable exceedances at the current or lower AQLV, creates a significant non-compliance problem. These findings provide an important illustration of the need to include the risk management step in any AQLV setting revision process.

Figure 3: Percentage of O_3 non-compliant monitoring stations in six European countries (five EU-27 Member States and the UK) under the various scenarios



Another important finding that can be derived from the analysis is that O_3 compliance does not show a similar spatial pattern in all areas within a country. This can be more evident in the major urban areas where, in most cases, the analysis shows that O_3 concentrations could impose compliance issues in contradiction to the general compliance improvement at the national scale. This is mainly attributed to reductions in NO_x emissions in urban areas, mainly due to the implementation of measures to mitigate road transport emissions, which could eventually favour the formation of O_3.

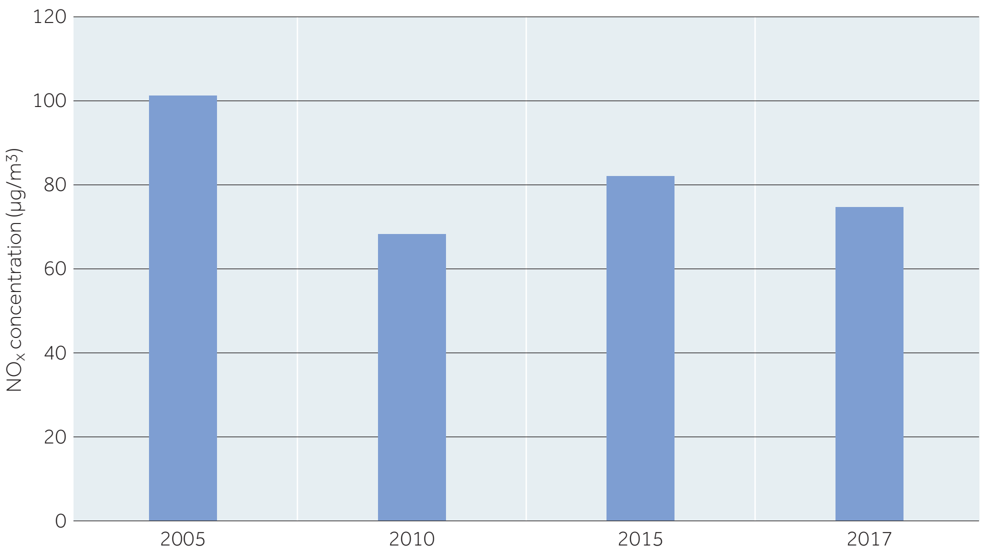
Ozone formation is mainly driven by emissions of NO_x and VOCs through complex photochemical reactions, and in areas where NO_x concentrations are significantly high (i.e. in urban areas and cities) O_3 formation is dominated by NO_x. In such areas, a reduction in NO_x emissions will have a counter-effect on O_3 formation, causing O_3 levels to increase.[10,11] In Madrid, for example, O_3 non-compliance remains an important issue from 2010 onwards, in contrast with earlier years (2005) when full compliance with the current EU AQLV was achieved (Figure 4).

Figure 4: O_3 compliance in Madrid from 2005 to 2017

- monitoring stations that measure maximum daily 8-hour mean concentrations below the target value of 120 µg/m^3 (not to be exceeded on more than 25 days) (compliant stations)
- monitoring stations that measure concentrations above the target value (non-compliant stations)

In 2010, around 30% of the monitoring stations measuring O_3 in Madrid were not able to achieve compliance with the current EU AQLV, while in 2017 the proportion of O_3 non-compliant stations increased to 50%. On the other hand, NO_x concentrations in Madrid showed a downward trend, with concentrations in 2017 being 26% lower compared to 2005 (on average over Madrid) (Figure 5). It should be noted that 2015 and 2017 were two of the warmest years in Europe,[12,13] which could favour O_3 episodes. This fact, in combination with the effect of NO_x on O_3 formation, could explain the increased number of O_3 non-compliant stations in 2015 and 2017 compared to 2010.

Figure 5: Annual mean NO_x concentrations in Madrid, 2005–2017



Long-term O_3 compliance assessment

Modelling approach

To predict how O_3 concentrations will project into the future (i.e. 2030), as well as to assess the practicability of achieving compliance with current and lower ambient air quality limit values, a modelling approach was taken using the AQUIReS+ model.[14] The model uses a gridded emission inventory and source-receptor relationships[15] that relate a change in emission to a change in concentration. These data are derived from regional chemical transport models (EMEP,[16] CHIMERE [17]) used in air quality studies. The model takes into account the local environment, traffic and topographical characteristics of each monitoring station. Model predictions are compared with data from the EEA Air Quality e-Reporting database[9] to ensure that the model performs well and accurately reflects concentrations of pollutants over historic years.

Ozone concentrations at the monitoring stations were predicted under different emissions scenarios. The following section provides an overview of the scenarios examined, and the modelling results are presented in the section that follows thereafter.

Emissions scenarios

a) Current legislation baseline

The starting point of the modelling part of the study are the emissions under a current legislation (CLE) scenario. This is an official EU projection of how emissions (based on multiple sector contributions) will evolve over time. The CLE scenario takes account of economic growth and the progressive impact of European legislation currently in force. Projections are made in five-year steps (2015–2020–2025–2030). The geographic distribution of emissions is accounted for at a fine scale, and national emissions for the EU Member States (EU-27 + UK) are calculated by spatial aggregation.

The CLE scenario is described in the Thematic Strategy on Air Pollution (TSAP) Report #16, published by IIASA.[18,19,20] The focus of that report is on $PM_{2.5}$, NO_x, SO_2, NH_3 and NMVOCs (non-methane volatile organic compounds). For simplicity, the many source emissions are aggregated into 10 different sectors according to the SNAP (Selected Nomenclature for sources of Air Pollution) method.

b) Maximum Technically Feasible Reductions (MTFR) scenario

A second scenario used in policy planning is the Maximum Technically Feasible Reductions (MTFR) scenario. This is historically named and refers to the case where emissions from stationary sources are reduced by using all available technical measures. It gives a reference point for both 'minimum emissions' and 'maximum costs' for these sources. It is important to note that not all sources are included, and non-technical measures can also be used to reduce emissions. The implementation of non-technical measures would require specific political will, and their feasibility is not considered. Foreseen plant closures, such as the phasing out of some older fossil-fuelled power stations, are accounted for in the CLE scenario.

In addition to the MTFR scenario, and since O_3 formation strongly depends on NO_x and NMVOC emissions, two additional MTFR-based emissions scenarios were considered explicitly for the purposes of this study:

i) NO_x-MTFR: implementation of all available technical NO_x abatement measures only; and
ii) VOC-MTFR: implementation of all available technical NMVOC abatement measures only.

Under both of these scenarios, the emissions of the remaining pollutants were assumed to remain below the levels projected under the CLE scenario.

c) Removal of NMVOC emissions

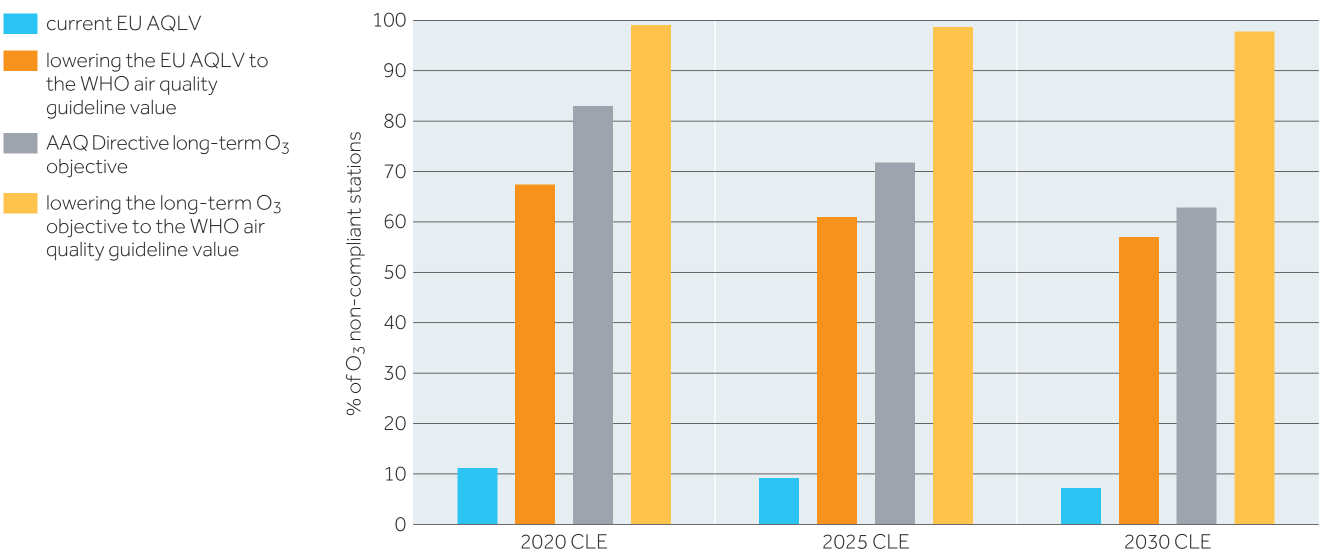
As the reduction of NMVOC emissions limits the formation of O_3, and can partially offset any increase in O_3 concentrations due to NO_x emissions reductions, especially in urban areas, an additional scenario was considered which assumes the removal of all NMVOC emissions from human activities. This scenario, however, is extreme and should be considered only as a sensitivity test.

Results

Figure 6 shows how O_3 compliance at a European level is projected into the future, from 2020 onwards until 2030, under the current CLE scenario, and how this changes depending on the AQLV that is set.

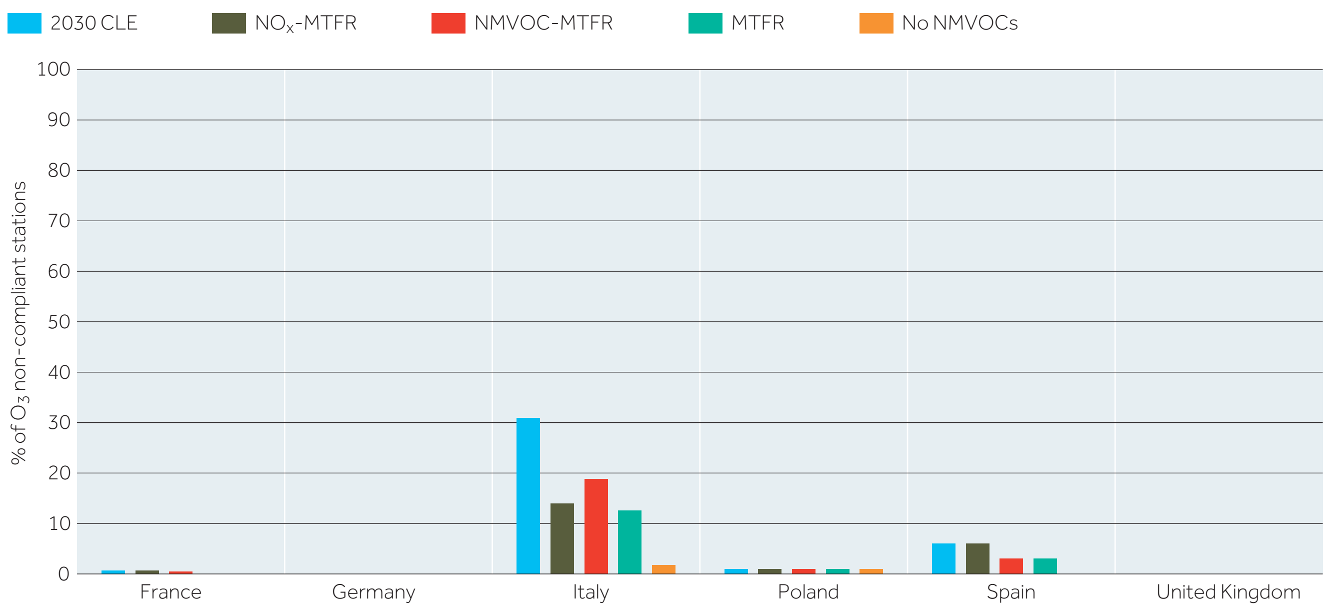
Under the CLE scenario, a slight O_3 compliance improvement with the current EU AQLV is predicted in Europe over the period. However, even in 2030, full compliance with the current EU AQLV is not predicted to be achieved as a remaining 7% of monitoring stations are found to record exceedances. Reducing the current AQLV clearly has important implications for making compliance more challenging in Europe, even in 2030. A lowering, for example, of the limit value to the current WHO level (100 µg/m^3), or a move towards zero exceedance days, is predicted to result in substantial EU-wide compliance issues with more than half of the O_3 monitoring stations measuring concentrations above the limits in all cases examined; this could increase by up to 97% in Europe if the EU AAQ Directive long-term O_3 objective is aligned with the current WHO air quality guideline value for O_3 (100 µg/m^3 and no exceedance days).

Figure 6: Predicted percentage of O_3 non-compliant monitoring stations in Europe under the CLE scenario



At a national scale, the projected future O_3 compliance trends are consistent with the predicted results across Europe. Analysing, for example, the projected O_3 concentrations in the six countries used for a more detailed focus in this study (i.e. five EU-27 Member States and the UK), the results show that under current legislation, Germany and the UK are predicted to achieve full compliance with the current EU AQLV for O_3 in 2030, and in France and Poland only a limited number of monitoring stations will remain non-compliant (Figure 7). The adoption of all available MTFR measures could eventually lead to full compliance in France and Poland. On the other hand, southern European countries (Italy, Spain) are predicted to have significant compliance problems with O_3 in 2030 under the current legislation. In Italy, for example, around 30% of the O_3 monitoring network is predicted to be non-compliant with the current EU AQLV in 2030 (Figure 7). The application of MTFR measures will reduce O_3 concentrations in both countries, although neither country will achieve full compliance. In Italy in particular, to arrive close to full compliance (~98% of its monitoring network), an extreme scenario of removing all NMVOC emissions from anthropogenic sources would be needed.

Figure 7: Predicted percentage of O_3 non-compliant monitoring stations in six European countries, with the current EU AQLV (120 µg/m^3 not to be exceeded on more than 25 days) in 2030 under the different scenarios examined

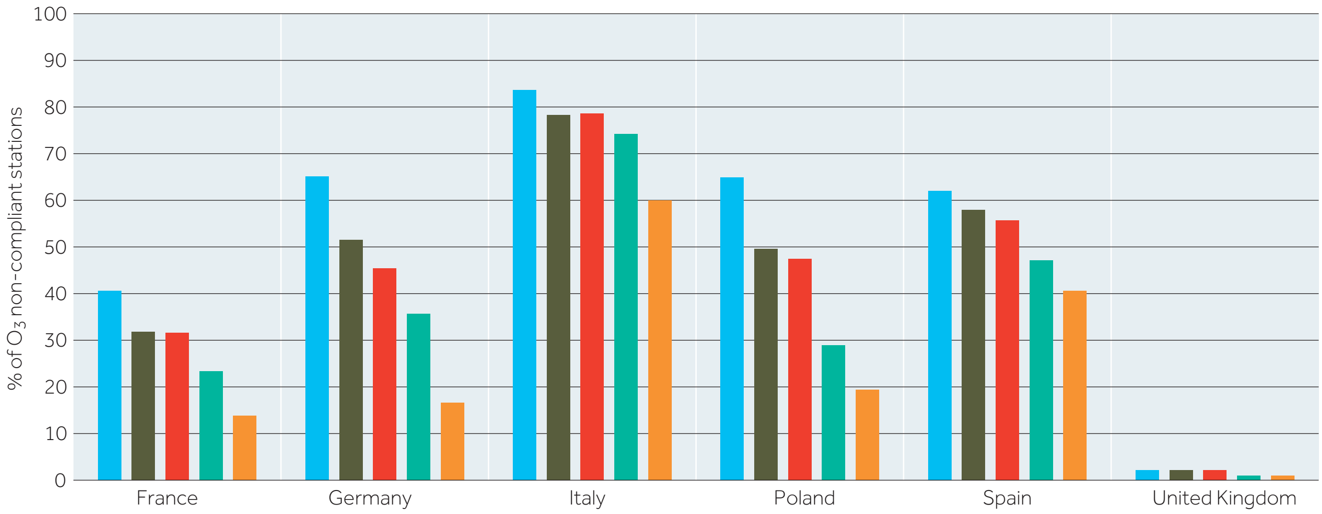


Any downward change of the current EU AQLV, either towards a reduction in the number of allowable exceedance days in order to achieve the EU AAQ Directive long-term O_3 objective, or a reduction in the current threshold of 120 µg/m^3 to align with the WHO air quality guideline value, will pose essential non-compliance problems in 2030 even with maximum abatement measures in place (Figure 8).

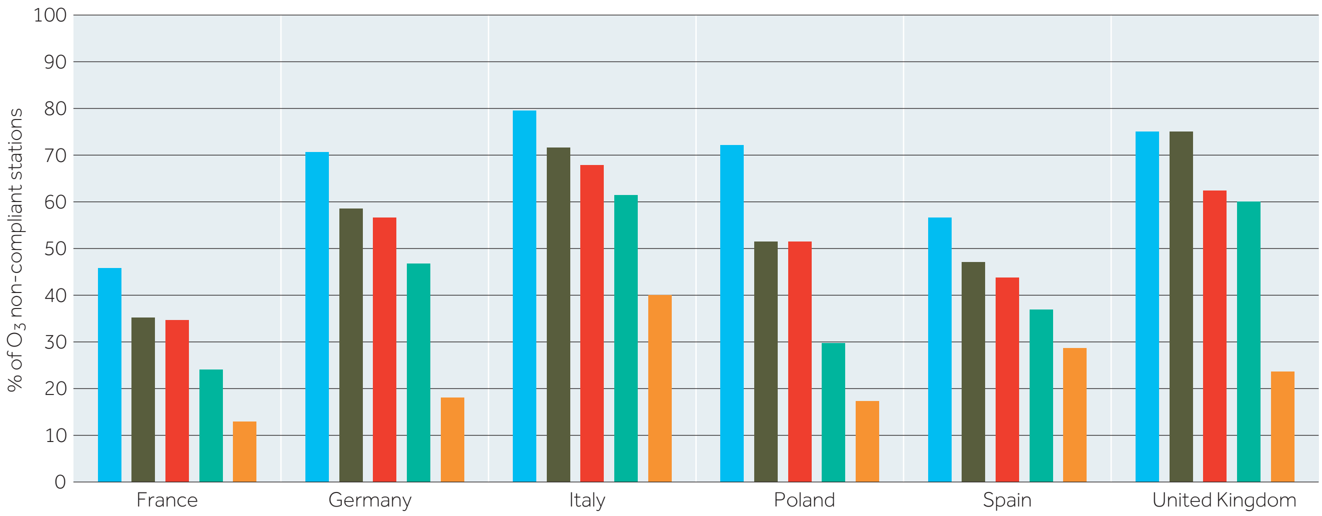
Figure 8: Predicted percentage of O_3 non-compliant monitoring stations in six European countries in 2030 under the different scenarios examined

2030 CLE | NO_x-MTFR | NMVOC-MTFR | MTFR | No NMVOCs

a) The current EU AQLV lowered to the WHO air quality guideline value of 100 µg/m^3 (not to be exceeded on more than 25 days)



b) The current EU AQLV being aligned with the AAQ Directive long-term O_3 objective of 120 µg/m^3 (no allowance of exceedance days)



Under the current legislation, by lowering, for example, the concentration threshold to the current WHO guideline value of 100 µg/m^3 (with 25 allowable exceedance days), the proportion of monitoring stations that are non-compliant exceeds 40% in five of the Member States examined (in the UK, the number of non-compliant O_3 monitoring stations is only around 2%). The application of all available technical measures to reduce emissions of O_3 precursors (i.e.the NO_x-only and NMVOC-only MTFR scenarios) as well as the application of all available MTFR measures is predicted to significantly reduce O_3 concentrations in all Member States, thereby improving compliance. However, even with MTFR measures, full compliance with the 100 µg/m^3 threshold (even if the 25 allowable exceedance days are maintained) will be far from technically achievable (Figure 8a). Similar results are also predicted when the AAQ Directive long-term O_3 objective of 120 µg/m^3 (without the exceedance days allowance) is considered as the EU AQLV, with the UK experiencing a significant increase in non-compliance[5] (Figure 8b). These are important findings, as they reflect the need for the inclusion of a risk management process in setting AQLVs, bearing in mind that technical achievability may prevent several countries from meeting a new EU AQLV even if cost and social considerations are not barriers.

It should be noted that since O_3 formation depends strongly on the meteorological conditions, the predicted results are subject to some uncertainty. This arises from the fact that the modelling simulations do not take into account any changes in meteorology, as their only focus is to assess how O_3 concentrations will change in the future due to changes in emissions. However, the projected future trends in O_3 compliance, even though they are subject to some uncertainty due to meteorology, are still dominated by the changes in emissions.[21,22] The compliance picture is not, therefore, expected to change significantly due to meteorology. Another point of uncertainty may also arise from the fact that the analyses focus on how the already-agreed measures, as well as measures beyond the current legislation, to reduce emissions of O_3 precursors from anthropogenic sources would affect O_3 concentrations in the future. However, VOC emissions from biogenic sources also play a significant role in O_3 formation. Several studies have indicated that, despite biogenic VOC emissions being a subject of high uncertainty, the increased temperature in a future climate will result in higher biogenic VOC emissions that will enhance O_3 formation.[23,24,25,26] This might, therefore, offset the potential effectiveness of measures to reduce anthropogenic emissions of O_3 in future efforts to achieve compliance.

[5] This indicates that O_3 compliance in the UK is mainly subject to exceedances above the number of allowance days that is currently set, rather than absolute concentrations above the limits.

Conclusions

The zero pollution action plan for air, water and soil that the EC will adopt in 2021 as part of the European Green Deal includes, among others, a proposal for revising the current air quality standards and aligning them more closely with the WHO recommendations. The WHO's guidelines for the majority of regulated pollutants are lower than the limit values set in the current AAQ Directives.

An earlier Concawe study highlighted the importance of following a two-step process of firstly assessing the environmental and human health risks presented by concentrations of air pollutants (risk assessment step) and secondly, assessing how these risks may be managed (risk management step) when binding AQLVs are set. The current study builds on the earlier study, and focuses on O_3, for which the current EU AQLV reflects a risk assessment undertaken by the WHO in the late 1990s without further changes; a revision of the AQLV is therefore highly possible.

The study analyses the current O_3 compliance trends in Europe and how these would change in a potential lowering of the AQLV. In addition, the study uses modelling to analyse how these trends are extended into the future (up to 2030) under several potential emission reduction scenarios. The analysis covers the EU, with a special focus on six European countries (France, Germany, Italy, Poland, Spain and the UK). The results of these analyses are summarised below:

- Full compliance with the EU AQLV (120 µg/m^3, not to be exceeded on more than 25 days) is currently achieved (based on the 2017 EEA data) in nine Member States, with non-compliance issues mostly found in southern and eastern European countries.
- The vast majority of the European countries are currently not able to meet the AAQ Directive long-term O_3 objective of 120 µg/m^3 without any allowance for exceedances. In addition, they are unlikely to be able to achieve compliance if the EU AQLV is lowered to the current WHO guideline value of 100 µg/m^3 (either keeping the 25 exceedance days threshold or not).
- The current emissions legislation, as described under the CLE scenario, will be effective in reducing O_3 concentrations from 2025 onwards and improving compliance. However, full compliance with the existing EU AQLVs will not necessarily be achieved in all EU countries. The country variation in terms of O_3 compliance remains significant in the future, with countries in southern Europe still experiencing significant non-compliance issues (e.g. 30% of monitoring stations in Italy are non-compliant in 2030 under the CLE scenario).
- Reductions beyond the already-legislated emission reduction measures, and towards MTFR, will further improve O_3 compliance with the current EU AQLV. However, full compliance still remains unachievable in some countries (e.g. Italy, Spain), despite the significant economic investment that will be required for implementing all MTFR measures.
- A move to a threshold of 100 µg/m^3 (the current WHO air quality guideline value) or a move toward the AAQ Directive's long-term objective for O_3 (i.e. zero allowable exceedances at the current threshold) will essentially create an EU-wide compliance challenge for O_3. Under such a revision of the current EU AQLV, O_3 compliance will be far from technically achievable, regardless of the measures applied to control emissions.

The above findings provide an important illustration that moving to a binding EU AQLV which will be closely aligned to the WHO air quality guideline value (with potentially less or even zero allowable exceedance days) is highly likely to be infeasible in large parts of Europe. It is therefore essential that all consequences of changing the AQLVs embedded in the AQ Directive are considered from the perspective of implementation by including a risk management step in the AQLV revision process.

It should also be noted that the analyses focus on how already-agreed measures, as well as measures beyond the current legislation, to reduce emissions from anthropogenic sources would affect O_3 concentrations in the future. However, VOC emissions from biogenic sources also play a significant role in O_3 formation. Even though they are subject to a high degree of uncertainty, biogenic VOC emissions are predicted to increase in the future and enhance O_3 formation, therefore offsetting the effectiveness of anthropogenic emission reduction measures.

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How Covid-19 lockdown affected air pollution in Europe — a multi-city analysis

Introduction

Concawe has undertaken a city-level analysis to quantify the ways in which the Covid-19 lockdown measures have had an impact on air quality in Europe. This article presents the results of the analysis for particulate matter ($PM_{2.5}$), nitrogen dioxide (NO_2) and ozone (O_3).

Following the emergence of the novel coronavirus SARS-CoV-2 in late 2019, when the first case was reported in the city of Wuhan in China, the Covid-19 pandemic outbreak has had significant health and economic consequences for the world.[1] As of January 2021, SARS-CoV-2 has globally infected more than 100 million people and caused more than 2 million deaths.[2] In Europe, more than 19 million cases and 450,000 deaths have been reported, with the UK, France, Spain and Italy being the most affected countries.[3]

After the virus had spread across Europe, most European countries began to introduce lockdown measures, starting in mid-March 2020, to mitigate the infection rate. Depending on the level of Covid-19 impact in each country, as well as country-specific situations and response capacity, European governments began, and continue, to adopt different types of interventions including partial or full closure of national/international borders, various restrictions on travel, closure of schools, and numerous economic responses as well as restrictions on social mobility. These efforts to prevent the virus spreading have inevitably led to a significant drop in emissions of air pollutants from several sectors, most notably from road transport and aviation.[4]

The changes in air pollutant emissions resulting from the sudden decrease in economic activities, and the subsequent impact on air quality, have been the objective of several studies during the past year since the Covid-19 pandemic started. For example, Guevara *et al.*[5] used a bottom-up approach that considered a wide range of information sources (e.g. open access and near real-time measured activity data, proxy indicators, etc.) and prepared an open-source dataset of daily, sector- and country-dependent emission reduction factors for Europe associated with the Covid-19 lockdowns. Their estimates showed average emissions reductions of 33% for NO_x, 8% for NMVOCs, and 7% for SO_x and $PM_{2.5}$ across 30 European countries (EU-27 plus UK, Norway and Switzerland). For all pollutants except SO_x, more than 85% of the total reduction was attributed to road transport. In addition, all studies conducted so far[6,7,8,9,10,11,12] agree that there has been a profound reduction in NO_2 concentrations[1] as a consequence of the implemented lockdown measures, while for $PM_{2.5}$ a consistent reduction cannot yet be seen because the response of $PM_{2.5}$ emissions and PM formation during the lockdown is more complex. On the other hand, the majority of studies indicate an increase in O_3 concentrations during the lockdown, which is mainly attributed to the titration effect of NO_x emissions.

Among the different initiatives that have been undertaken over the past year to study how the lockdown measures implemented in Europe have impacted air quality, the European Environment Agency (EEA) launched an online data viewer which includes hourly data for PM and NO_2 as measured by approximately 3,000 monitoring stations across European countries during the period 2018-2020.[13]

1 There have been exceptions which show that, in some cases, the reduction in NO_x levels was less obvious (i.e. German Federal Environment Agency study: https://www.cleanenergywire.org/news/diesel-driving-bans-table-lockdown-shows-low-effect-german-nox-levels-state-sec). This could be explained by the fact that the reduction in emissions from road activity might relate more to newer vehicles with more advanced NO_x control technology, and not to older vehicles or vehicles that emit more NO_x and were still operating (e.g. delivery vans).

Based on the hourly measured concentrations, the data viewer provides daily, weekly and monthly average concentrations of these pollutants at a city level, which allows the user to track the changes occurring as a result of the lockdown measures.

Data from the EEA's data viewer have been used as the basis for a city-level analysis that Concawe has undertaken to quantify how the lockdown measures have impacted air quality in Europe. This article presents the results of the analysis for $PM_{2.5}$ and NO_2 concentrations in five European cities (Athens, Brussels, Madrid, Milan and Paris). Like most of the research studies undertaken to date, the analysis covers the first lockdown period, from March to June 2020. However, the analysis was extended to assess the impacts of the relaxation of measures during the summer period, as well as the re-implementation of lockdown measures during autumn-winter 2020 to prevent a second wave of the virus, on concentrations of $PM_{2.5}$ and NO_2. In addition, the analysis was further extended to assess the response of O_3 concentrations to the imposition of lockdown measures. Since the EEA's data viewer does not currently include data for O_3, Concawe used hourly data taken directly from the EEA's Air Quality e-Reporting database.[14] The main findings of the analyses for each pollutant are presented in the following sections.

It should be noted that, because Covid-19 restriction measures have been developed and implemented differently among European countries, the results that follow provide a means for a qualitative assessment of the effects of the lockdown measures on air pollutant concentrations, as well as an indication in quantitative terms of the spatial/temporal patterns and the magnitude of changes in concentrations. However, a direct quantification of the impact of Covid-19 restriction measures on pollutant concentrations cannot be derived from these data as other factors may play a role. For example, meteorological variability[2] is one key factor that determines the transport and fate of air pollutants, and will subsequently also have an impact on air pollutant concentrations and their variability from one year to another. A more detailed analysis will be needed to provide an in-depth assessment of the influence of these factors.

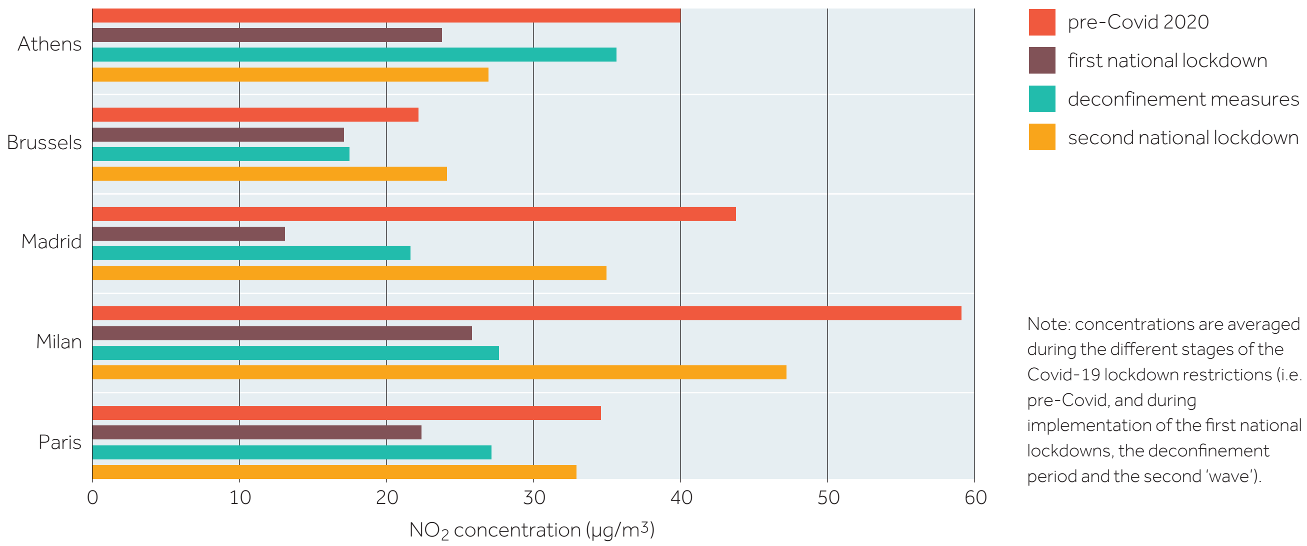
NO_2 concentrations

Figure 1 on page 23 shows the trends of NO_2 concentrations in 2020 in the five European cities considered. The concentrations are averaged over the different stages of the Covid-19 pandemic and lockdown measures at the national level (i.e. before the Covid-19 pandemic began, and during the lockdown period, the relaxation of lockdown measures, and the second wave of the virus). It should be noted, however, that the implementation date,[3] as well as the types of measures introduced, may differ between countries.

[2] For example, the month of February 2020 was exceptionally warm in Europe: it was 1.4 °C above the second warmest February on record in 2016,[15] which led, for example, to lower NO_2 concentrations than normal in February, while in the month of November 2020, the predominant conditions were drier than average, with below average precipitation notably in the central and western part of the continent and parts of the Iberian Peninsula.[15] Thus, weather variability has a substantial influence on surface concentrations of pollutants.

[3] https://covid-statistics.jrc.ec.europa.eu/RMeasures

Figure 1: Daily NO_2 concentrations in 2020 in the five European cities analysed in the study



Note: concentrations are averaged during the different stages of the Covid-19 lockdown restrictions (i.e. pre-Covid, and during implementation of the first national lockdowns, the deconfinement period and the second 'wave').

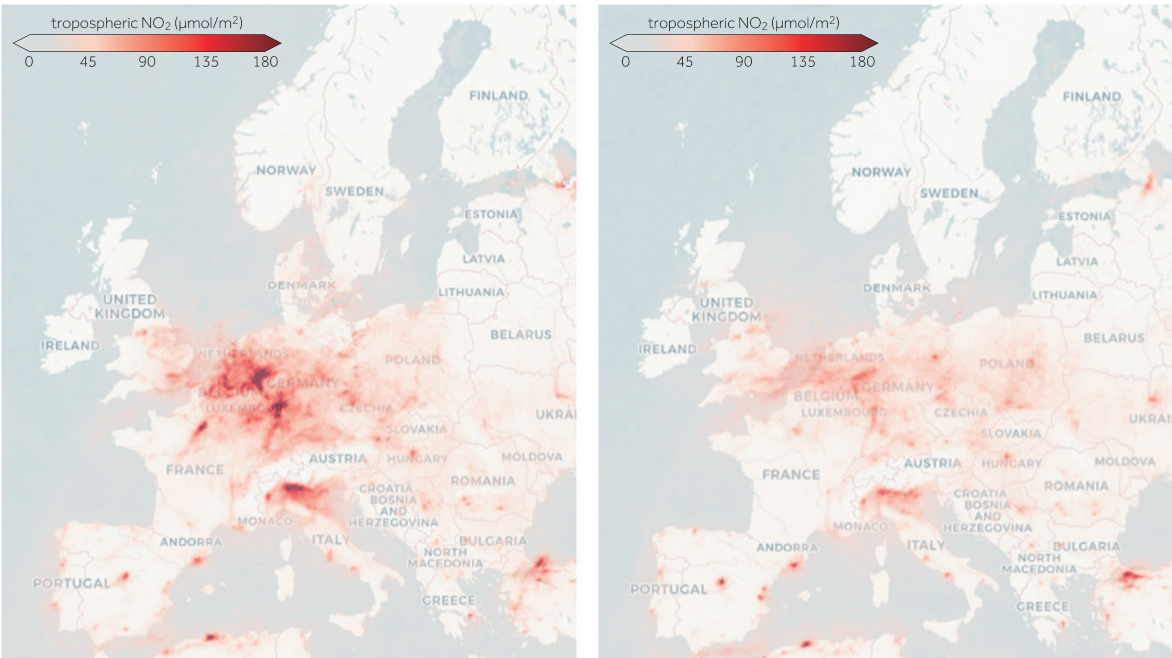
In all cities analysed, the results show that NO_2 levels were higher during the pre-Covid period (January to early March, 2020) compared to the periods that followed the Covid-19 pandemic. The analysis also confirms that, as seen in earlier studies, with the implementation of restriction measures during the first lockdown period, all cities experienced a significant reduction in NO_2 concentrations compared with pre-Covid levels. This reduction exceeded 20% in all cities, with Milan and Madrid experiencing reductions of up to 55% and 70%, respectively. The lower NO_2 levels can be largely attributed to the significant reduction in NO_x emissions from road transport which, in most European countries, amounted to a reduction of 50–80%. This was a result of the significantly lower levels of traffic congestion, which also had an indirect effect on NO_x emissions from vehicles by allowing the diesel exhaust treatment systems to operate at optimum temperatures. Following the deconfinement measures that began in May, NO_2 levels showed an increasing trend in all cities, but nevertheless remained lower compared with pre-Covid levels. The results also show that the re-implementation of restrictive measures to prevent the spread of the second Covid-19 'wave' was not as effective in reducing NO_2 concentrations as the measures taken during the first lockdown period. In most of the cities analysed, NO_2 concentrations continued to show an increasing trend, while in Brussels, NO_2 levels were comparable to those during the pre-Covid period. This trend could partially be explained by the fact that, during the first lockdown period, the restrictive measures were extremely strict and fairly uniform among European countries, while during the second Covid-19 'wave' period, restrictive measures varied more among countries, being less strict compared with the first period and eventually having a less profound impact on traffic congestion.[4]

[4] https://www.tomtom.com/en_gb/traffic-index/

A comparison of NO_2 concentrations in 2020 with those in 2019 shows the significant impact of the restrictive measures imposed in most urban areas across Europe. Figure 2 shows the average satellite-observed vertical columns[5] of NO_2 from 15–30 March 2020 (Figure 2b), a period which corresponds to the month when lockdown measures were introduced in most countries in Europe, in comparison to the same period in 2019 (Figure 2a).[16] The maps show that most of the urban areas in central and western Europe exhibited significant lower NO_2 pollution levels in the period from 15–30 March 2020 than in the same period in 2019, while the respective NO_2 changes in eastern Europe were less profound.

Figure 2: Average NO_2 pollution levels (tropospheric vertical column) in 2019 and 2020, measured by the TROPOMI system on board the Sentinel-5P satellite

a) 15–30 March 2019 b) 15–30 March 2020



Data source: Copernicus Sentinel-5P Mapping Portal, https://maps.s5p-pal.com

The differences in NO_2 concentrations at the city level, between 2020 and 2019, can be seen in Figure 3 on page 25, which shows how the annual mean NO_2 concentrations measured at the monitoring stations changed in 2020. A reduction in NO_2 concentrations in all cities is observed in 2020, compared with 2019 levels, reaching up to a 30% reduction in Brussels. However, the respective reductions show a significant temporal variation which depends on the stage of the Covid-19 pandemic.

[5] The TROPOspheric Monitoring Instrument (TROPOMI) derives information on atmospheric NO_2 concentrations by measuring the solar light backscattered by the atmosphere and the Earth's surface. In general, satellite measurements are characterised by high spatial resolution and can be suitable for monitoring polluting emission sources at a city level, while ground-based measurements have a spatial resolution which is constrained by the limited number of monitors and their proximity.

For example, in the two cities that were affected the most by very strict lockdown measures (Milan and Madrid), a significant drop in NO_2 concentrations was observed during March–May (when the first national lockdown was set) compared with 2019 levels. Levels remained low in 2020 but, as lockdown measures began to be relaxed around mid-May, the rate of reduction in NO_2 concentrations slowed down, and from July 2020 onwards NO_2 concentrations were similar to 2019 levels (Figure 4).

Figure 3: Annual mean NO_2 concentrations in 2019 and 2020 in the five cities analysed in the study

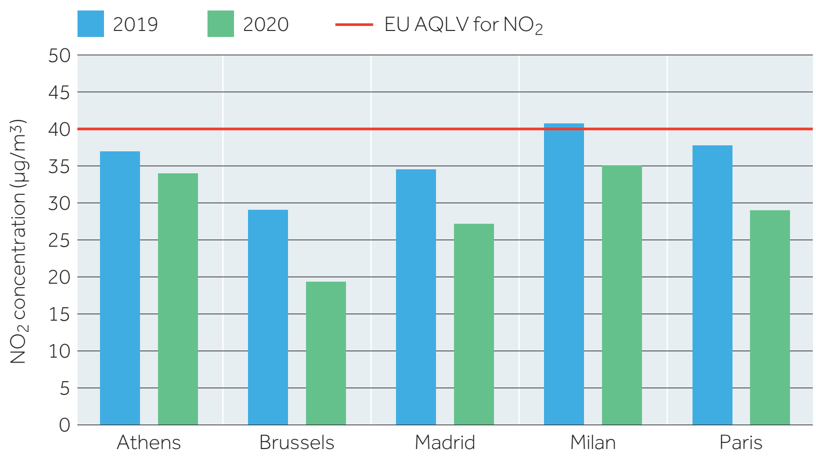
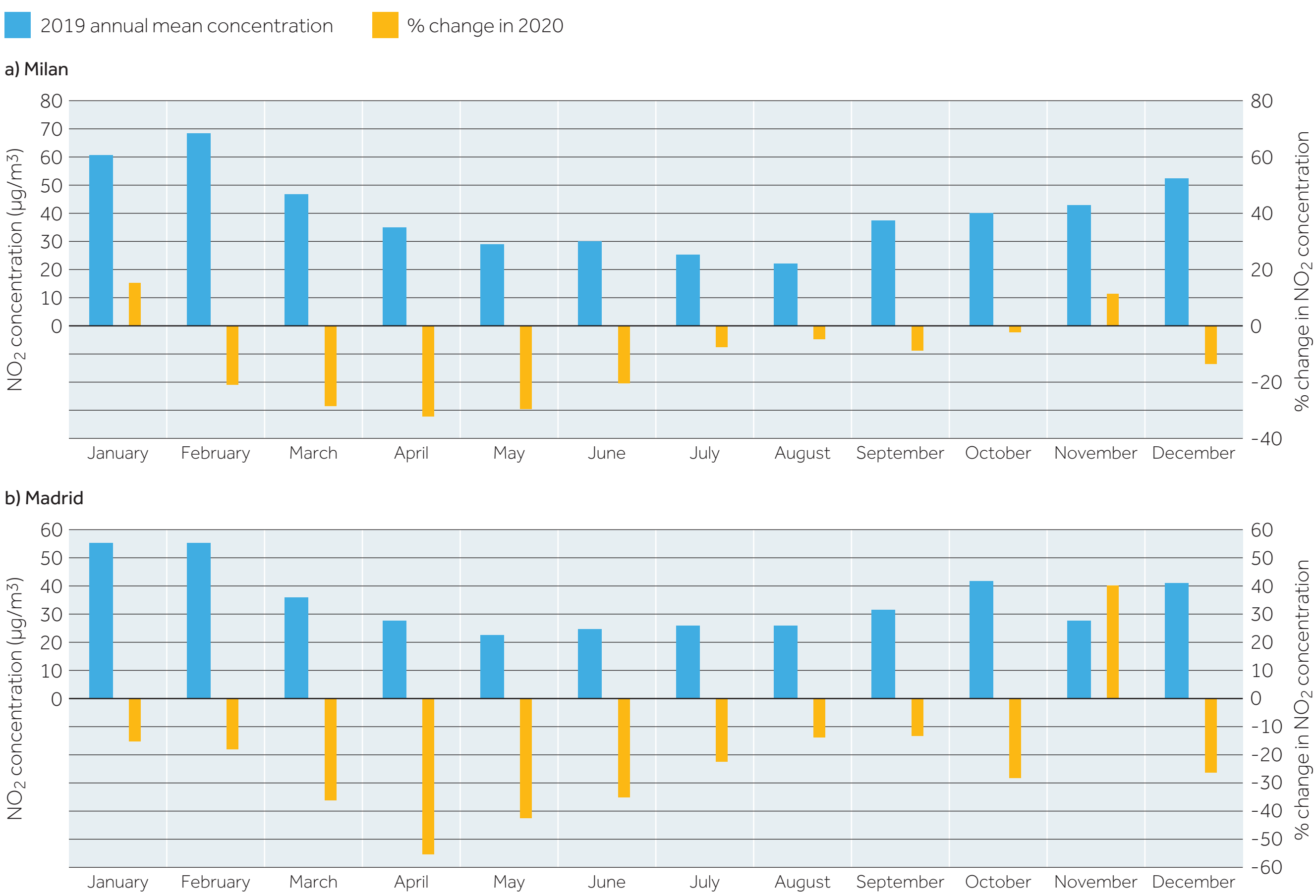


Figure 4: Monthly mean NO_2 concentrations in 2019 and the percentage changes in 2020

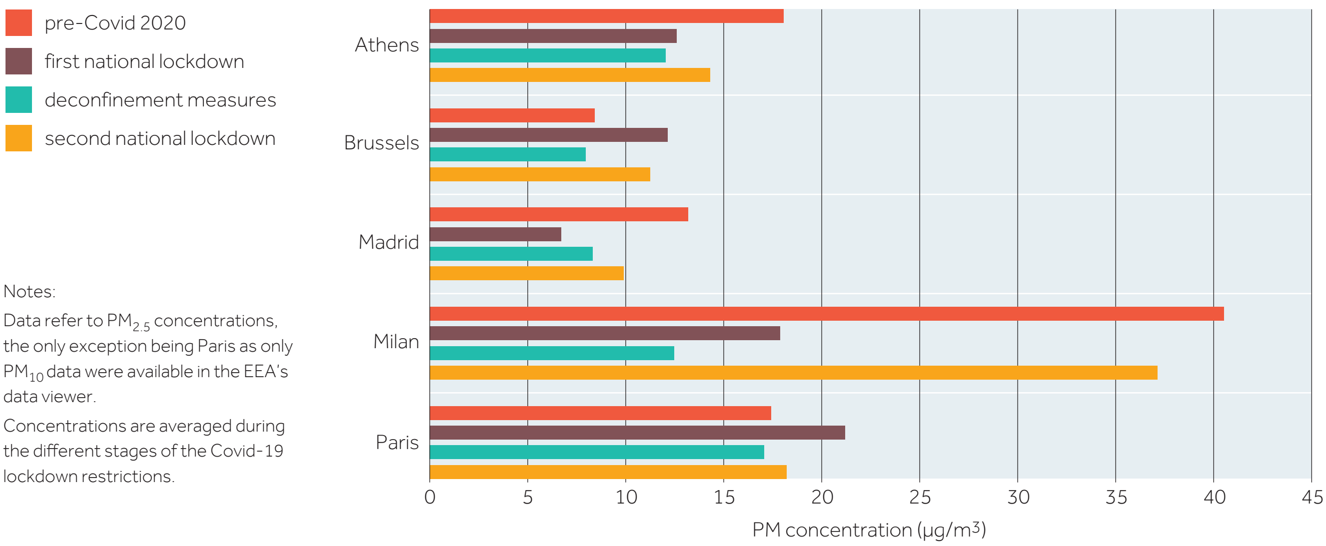
Note: negative values indicate a decrease.



PM concentrations

Figure 5 shows the trends in PM concentrations in 2020 in the five European cities analysed. As with NO_2, the concentrations are averaged over the different stages of the Covid-19 pandemic and the lockdown measures at the national level (i.e. before the Covid-19 pandemic, and during the lockdown period, during relaxation of lockdown measures, and during the second wave of the virus).

Figure 5: Daily PM concentrations in 2020 in five European cities analysed in the study



Notes:

Data refer to $PM_{2.5}$ concentrations, the only exception being Paris as only PM_{10} data were available in the EEA's data viewer.

Concentrations are averaged during the different stages of the Covid-19 lockdown restrictions.

A variable trend in PM concentrations among the cities analysed can be seen throughout 2020; the effect of the different stages of the Covid-19 pandemic on PM levels is less clear compared with the effects on NO_2. During the first period of the implementation of restrictive measures, Athens, Milan and Madrid experienced a significant drop in PM concentrations (a drop of up to 55% in Milan). This was the general response of PM at the majority of monitoring stations in Europe.[4] However, there are areas where PM responded to the restrictive measures in a different way. For example, in Brussels and Paris, higher PM concentrations (45% in Brussels, 20% in Paris) were measured during the first national lockdown compared with the pre-Covid period. This variable PM response continued after the relaxation of restrictive measures, while during the second Covid-19 'wave', when restrictive measures were reinstated, PM concentrations in most of the cities analysed reached similar levels to those in the pre-Covid period.

The somewhat less pronounced, and sometimes variable, effect of Covid-19 restrictive measures on PM concentrations has also been seen in earlier studies.[8,10] The high variability in PM concentrations can be explained by a number of factors, including:

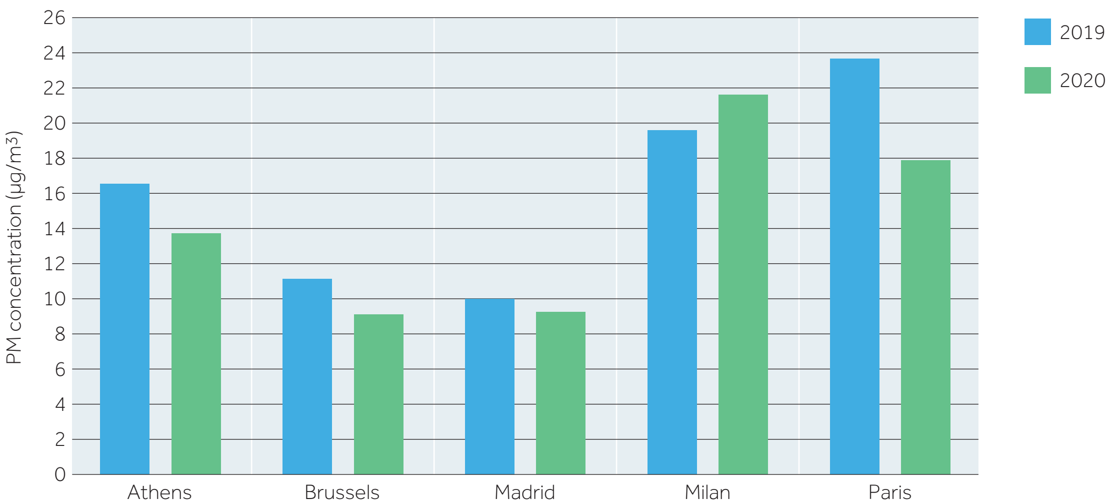
a) the complex chemical mechanism behind the formation of PM;

b) the chemical composition of PM, which may differ between the areas; and

c) the fact that PM is not directly linked to one emissions source; instead, multiple sources impact their levels, and each source may have a different response during the Covid period. For example, the reduction in road transport emissions may have resulted in lower PM emissions associated with this source, either due to lower primary PM emissions, or to lower NO_2 levels that could eventually form secondary PM. However, in several regions, as people had to stay at home for longer periods, there may have been an increase in primary PM emissions from domestic heating. In addition, the meteorological variability, as well as the contribution of emissions from natural sources, should not be neglected.

The lower impact of the restrictive measures on reducing PM levels compared to NO_2 can also be seen in Figure 6, which compares the annual mean PM concentrations in 2020 with those in 2019. In general, most cities registered lower PM concentrations in 2020 compared with 2019 levels, with Paris reaching a 24% reduction in PM levels. However, the reductions in PM concentrations were considerably less than the reductions in NO_2 concentrations; in Milan, despite the strict restrictive measures that were in place for a substantially long period, the measured PM concentrations in 2020 were higher by around 10% compared with 2019 levels.

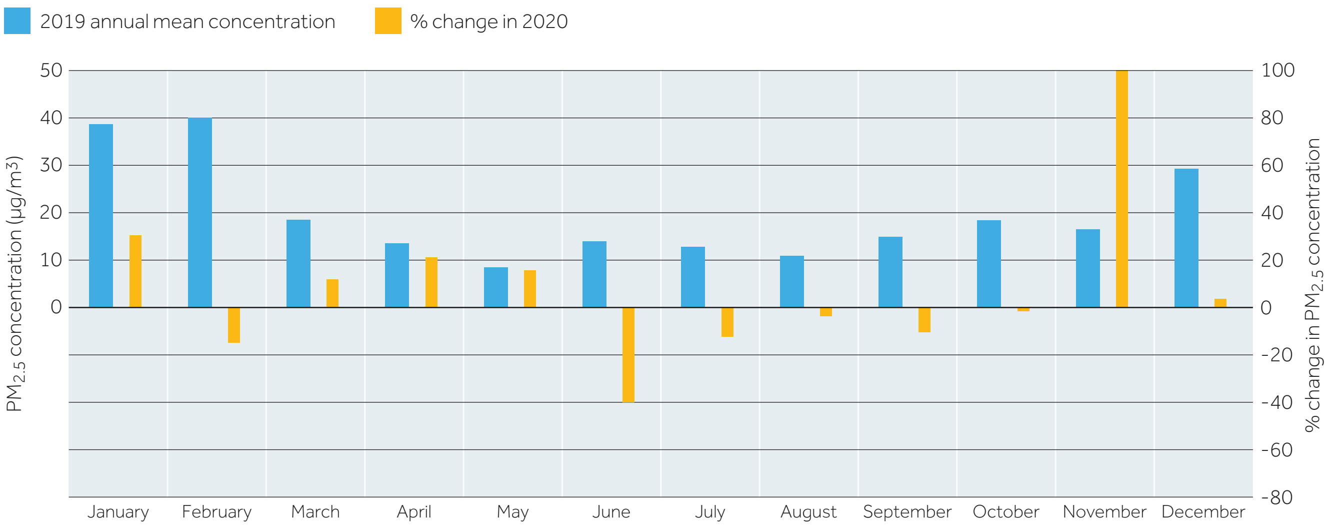
Figure 6: Annual mean PM concentrations in 2019 and 2020 in the five cities analysed in the study



Interestingly, in Milan, during the months when a national lockdown was imposed during the springtime, PM concentrations were constantly above the corresponding 2019 levels (Figure 7). With the relaxation of restrictive measures in summer (June–July), $PM_{2.5}$ concentrations in 2020 were found to be lower compared with 2019 levels. The fact that activities in several sectors did not reach pre-Covid levels, and that large parts of southern Europe experienced periods of high precipitation[21] that was well above the average, could explain this trend.

Figure 7: Monthly mean $PM_{2.5}$ concentrations in 2019 in Milan, and the respective % changes in 2020

Note: negative values indicate a decrease.

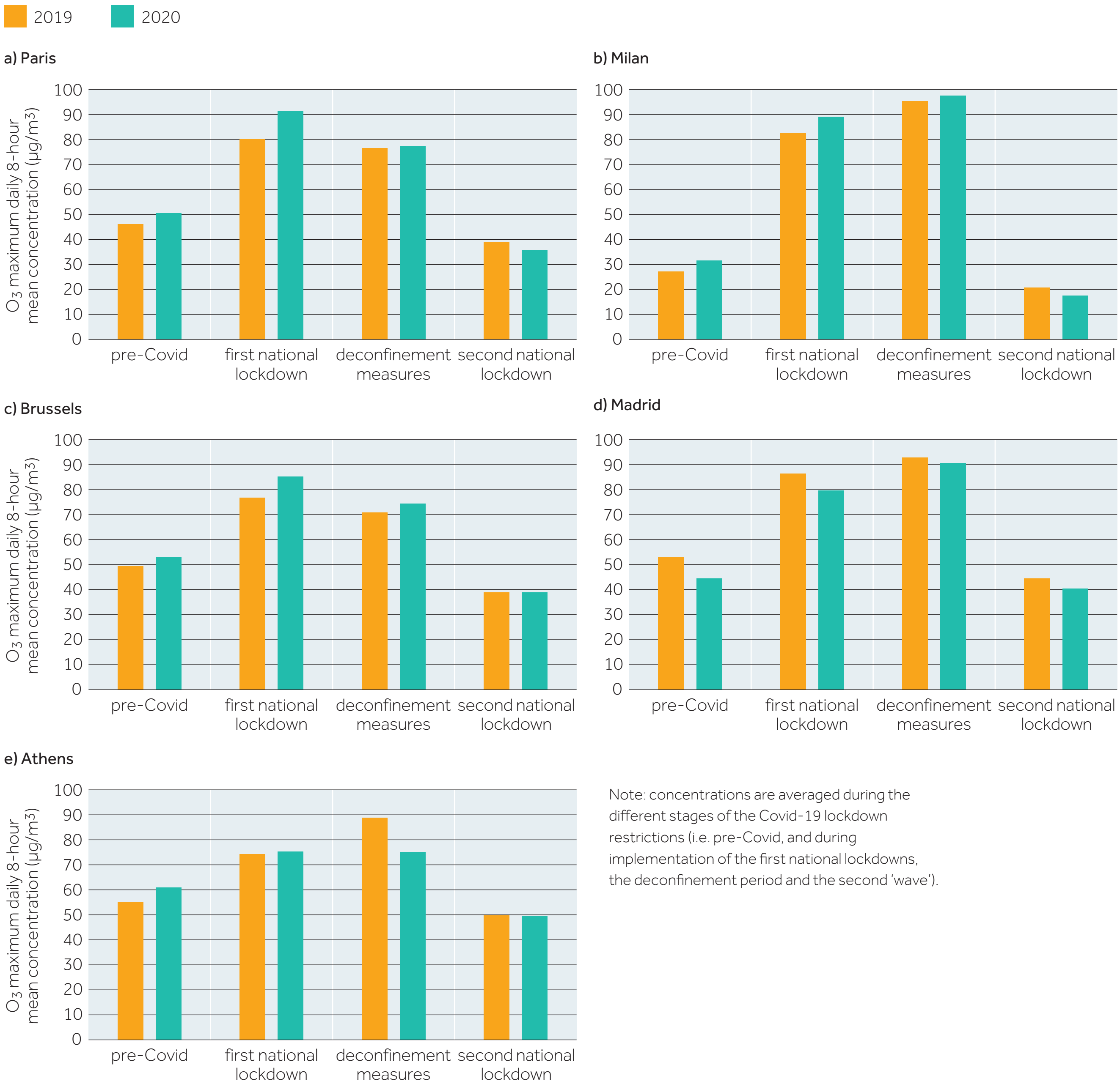


O_3 concentrations

The implementation of stringent lockdown measures, especially during the first 'wave' of Covid-19, did not seem to have a positive effect on O_3 levels. In the majority of the cities analysed in the study, O_3 levels were found to be higher in 2020 during the period when the first national lockdowns were set, compared to 2019 levels (see Figure 8 on page 29). The increase exceeded 10% in Brussels, while in Paris the increase reached approximately 15%. Similar results were also found in other studies.[9,11,17] The O_3 response can, to a large extent, be explained by the significant drop in NO_2 concentrations during the same period, which could, eventually, have favoured the formation of O_3. In general, O_3 formation is driven mainly by emissions of NO_x and VOCs through complex photochemical reactions, and depends on the VOC-NO_x ratio.[18] In most urban areas, where NO_x concentrations are in excess, O_3 formation is dominated by NO_x. In such areas, a potential reduction in NO_x emissions will result in counter-effects regarding O_3 concentrations, causing them to increase to higher levels.[19,20]

Trends in O_3 concentrations may also be enhanced by the meteorological conditions in these areas, as was the case during the first national lockdowns (March to April), when large parts of Europe exhibited significantly drier than average conditions.[21] In contrast, the Iberian Peninsula experienced significantly more precipitation during the same period, which could explain the somewhat lower levels of O_3 in Madrid during the first national lockdown compared with the corresponding 2019 levels.

Figure 8: Maximum daily 8-hour mean O_3 concentrations in 2019 and 2020 in the five European cities analysed in the study



Note: concentrations are averaged during the different stages of the Covid-19 lockdown restrictions (i.e. pre-Covid, and during implementation of the first national lockdowns, the deconfinement period and the second 'wave').

Conclusions

The novel coronavirus SARS-CoV-2 continues to spread around the world with severe implications for human health, as well as having major financial and societal impacts. In early 2020, the vast majority of European countries began taking measures to manage the outbreak. These measures had an impact on many of the upstream economic activities that drive emissions of air pollutants, thus affecting air quality. This study used up-to-date measured data, taken from the EEA's Air Quality e-Reporting database and online data viewer, to analyse the effects of the measures taken to avoid the spread of Covid-19 on concentrations of NO_2, PM and O_3 in selected European cities in 2020.

The results of these analyses are summarised as follows:

- On average, NO_2 concentrations in 2020 were measured to be lower than those in 2019 in all cities analysed in the study. The reduction ranged between 10% (Athens) and 35% (Brussels).
- NO_2 concentrations were significantly reduced in March-April, when the first restriction measures were put in place. The extent of the reductions varied considerably among cities, and were dependent on the types of measures implemented, with reductions exceeding 50% being observed in some cases (Milan and Madrid).
- The significant drop in transportation activity as a consequence of the lockdown measures, and the subsequent reduction in road transport NO_x emissions across Europe (i.e. around 50–80%) could, to a large extent, explain the lower NO_2 levels observed during that period.
- With the relaxation of restrictive measures starting in May, all cities experienced an increase in NO_2 concentrations, while the re-implementation of restrictive measures aimed at preventing the spread of the second Covid-19 'wave' was not as effective in reducing NO_2 concentrations as when similar measures were taken during the first lockdown period.
- The impact of lockdown measures on PM concentrations was less pronounced than for NO_2, and did not show a consistent downward response. A variable response of PM levels was seen during all stages of the Covid-19 pandemic and the lockdown measures at national level. Compared with 2019 levels, PM levels in 2020 were, on average, found to be somewhat lower, although significant temporal variations were observed. The variable changes in PM emissions from different sources as a result of the lockdown measures (i.e. decreases in road transport emissions, increases from domestic heating) and the sensitivity of PM to meteorological variables could explain this variable trend in PM concentrations.
- The implementation of lockdown measures has had a different effect on O_3 concentrations, with the majority of cities analysed experiencing higher O_3 concentrations in 2020 compared with 2019 levels, especially during the period when the first national lockdown measures were in place.

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Concawe's transport and fuel outlook towards the EU 2030 climate targets (baseline and sensitivity analysis)

A new Concawe report identifies key enablers and potential barriers associated with boosting the penetration of renewable energy and improving GHG intensity in the European transport sector towards 2030. This article summarises the findings of the report, which aims to provide stakeholders with an informed view on current trends and the parameters that may need to be enhanced in order to meet current 2030 objectives.

Objective

This article summarises the findings of a Concawe report[1] which provides an outlook for the European transport sector for the 2018–2030 period. The main objectives of the outlook are to:

- conduct a thorough assessment of the progressive penetration into the EU vehicle fleet of energy efficiency measures and different powertrain technologies, combined with the market-based availability of alternative fuels and energy carriers; this will define the baseline towards 2030;
- assess the potential of various renewable alternative fuels, with a focus on biofuels and electricity which, when combined with different powertrains, could contribute to reducing greenhouse gas (GHG) emissions and fossil fuel demand in the EU transport sector, taking into consideration factors such as availability of supply, technology readiness and existing fleet constraints;
- explore the potential of the EU transport sector to integrate renewable fuels and reduce GHG emissions towards 2030, and compare the baseline versus the EU targets (currently in revision) for carbon dioxide (CO_2) standards in vehicles, along with the Renewable Energy Directive 2 (RED II) and Fuel Quality Directive (FQD);
- perform a sensitivity analysis on key parameters identified to show the individual impact on reaching these targets; and
- inform the currently ongoing process of defining future RED II targets for road transport (to be agreed in 2021).

The baseline modelled in the Concawe report is based on statistics, market-based projections and the best educated view of the experts involved in the working group for both the fleet modelling and the outlook on alternative fuels. This could be complemented by additional reports in the future, assessing the impact of different scenarios on GHG emissions and energy demand in EU transport for the same time frame, taking into account alternative and accelerated scenarios to meet higher-ambition targets triggered by the recently published European Green Deal[2] and 2030 Impact Assessment,[3] which will have an impact on future RED II / FQD targets.

The analytical tool

To conduct the analysis, an analytical fleet-based model has been used which projects the evolution of the fleet composition as well as the corresponding fuel demand towards 2020+. In recent years, the paradigm in road transport has changed drastically as a result of different pieces of legislation aimed at accelerating the transition to a lower GHG-intensive transport sector in Europe. As a consequence of legislation such as the CO_2 regulations for cars and heavy-duty vehicles, as well as the RED I/II targets, the development and progressive penetration of different forms of electrification and new powertrains in road transport, as well as the announcement and build-up of alternative fuels-related projects beyond the conventional crop food-based biofuels, are likely to change the previous trends in energy consumption and GHG emissions in transport.

1 https://www.concawe.eu/wp-content/uploads/Rpt_21-2.pdf

2 https://ec.europa.eu/info/strategy/priorities-2019-2024/european-green-deal_en

3 https://ec.europa.eu/clima/sites/clima/files/eu-climate-action/docs/impact_en.pdf

As a consequence of this change in trends, a major update of the fleet model has been conducted to enable a scientifically sound, market-based baseline definition. The main assumptions are presented throughout the report, defining current trends and allowing the exploration of different projections and sensitivities.

The fleet model is based upon historical road fleet data (for both light- and heavy-duty vehicles), updated with recent statistics aggregated at the European level (EU-27 + UK, Norway and Switzerland). Once the calibration has been conducted up to 2018, projections for the vehicle fleet are conducted towards 2030, including the effects of key parameters such as the potential composition of new sales in 2030 (meeting the CO_2 regulatory targets for both passenger cars and heavy-duty vehicles), scrappage rates or expected efficiency improvements in different powertrains. The modelled fleet composition leads to a road transport fuel demand and provides the basis upon which the introduction and availability of alternative fuels are explored (market-based in the case of liquid/gaseous fuels, as well as IEA projections in the case of electricity) to assess the total contribution of renewable energy and GHG emissions in transport. In addition, current and future estimates of both the total energy requirements and alternative fuel penetration have been included for other transport modes (aviation, rail and maritime sectors) and compared with the current RED II targets.

Due to rapid developments in technology and their potential impact on the current assumptions and projections, this baseline could be updated periodically as market trends change. The baseline is also complemented in the present report by sensitivity analyses of key individual parameters, allowing the reader to understand their impact on the RED II targets and providing both information and material for further investigation in several research areas where energy and transport compositions interact. Furthermore, the baseline is used to explore alternative scenarios which will be published in due course to complement the results presented in the report.

Due to simplifications made and estimates used, the fleet model should be considered as a 'scenario tool': it will not lead to an optimised strategy but instead looks at a variety of scenarios for fleet and fuel development. The assumptions made should not, therefore, be considered as a forecast of, or commitment to, the future availability of vehicle technologies or vehicle features.

Results

The analytical tool is used to simulate different parameter combinations of vehicle and fuel (including renewable fuel) technologies to assess fuel demand scenarios, looking at:

- vehicle fleet mix;
- fossil fuel demand and diesel/gasoline balance;
- total renewable energy demand (including conventional and advanced biofuels); and
- the demand for renewable energy in transport needed to achieve the RED II and FQD targets.

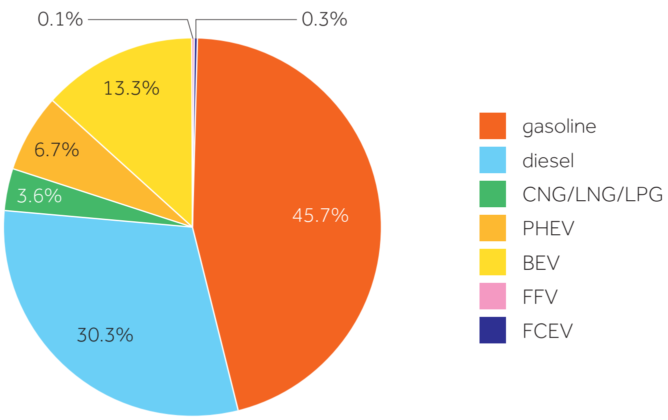
Fleet evolution/energy demand

Calibrated for the year 2018 (including historical trends), the updated baseline models the evolution of the fleet towards 2030, and includes the following:

- Improvements in terms of the energy efficiency of conventional powertrains (internal combustion engines (ICEs)), running on either gasoline or diesel-like fuel, as well as the projections in terms of new sales, activity levels or scrappage rates of old vehicles.
- The progressive penetration of new types of powertrains towards 2030, especially in the heavy-duty segment: as a result of the update, the model now integrates natural gas-powered vehicles using both compressed and liquefied fuels (CNG/LNG), as well as different levels of electrified vehicle (EV) powertrains moving from different levels of hybridisation with ICEs (hybrid electric vehicles (HEVs) to plug-in hybrid electric vehicles (PHEVs), battery electric vehicles (BEVs) or hydrogen fuel cell electric vehicles (FCEVs)).
- The composition of new sales in 2030 (Figure 1) has been defined based on market trends and experts' views, in compliance with the current 2030 CO_2 intensity targets for new sales in road transport (expressed in NEDC terms for comparison purposes):
    - **Passenger cars:** 95 g CO_2/km in 2021 and a further 37.5% reduction by 2030 (equivalent to about 59 g CO_2/km NEDC in 2030 baseline).

      In line with the JEC Tank to Wheels (TTW) v5 report,[4] it is worth noting that, for passenger cars, a representative medium-size (C-segment) vehicle has been selected as the reference for the best available technology for 2025 onwards; this cannot, therefore, be considered as being fully representative of all new registrations.

Figure 1: Shares of new car registrations in 2030 per powertrain in the baseline

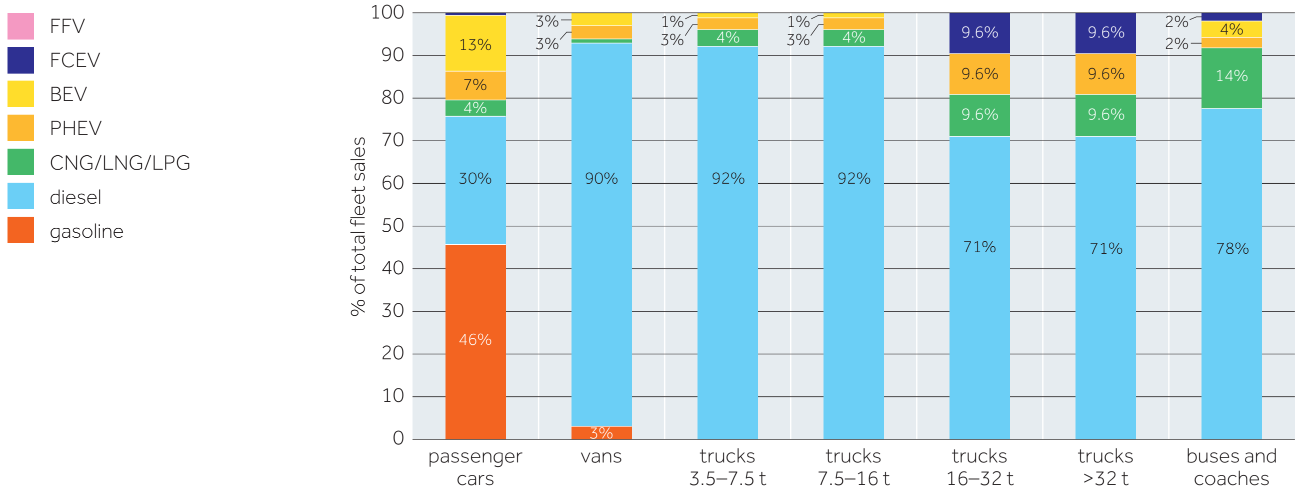


    - **Light commercial vehicles (vans):** 147 g CO_2/km in 2020, and 31% less CO_2-intensive (TTW) in 2030 than in 2020/2021 (equivalent to ~100 g CO_2/km modelled in the 2030 baseline).
    - **Heavy duty vehicles:** 30% reduction in emissions by 2030, compared to 2019 (for trucks >16 t in g CO_2/tkm) and a value of 536 g CO_2/km as the average for heavy-duty commercial vehicles in 2030.

[4] https://ec.europa.eu/jrc/en/publication/jec-tank-wheel-report-v5-passenger-cars

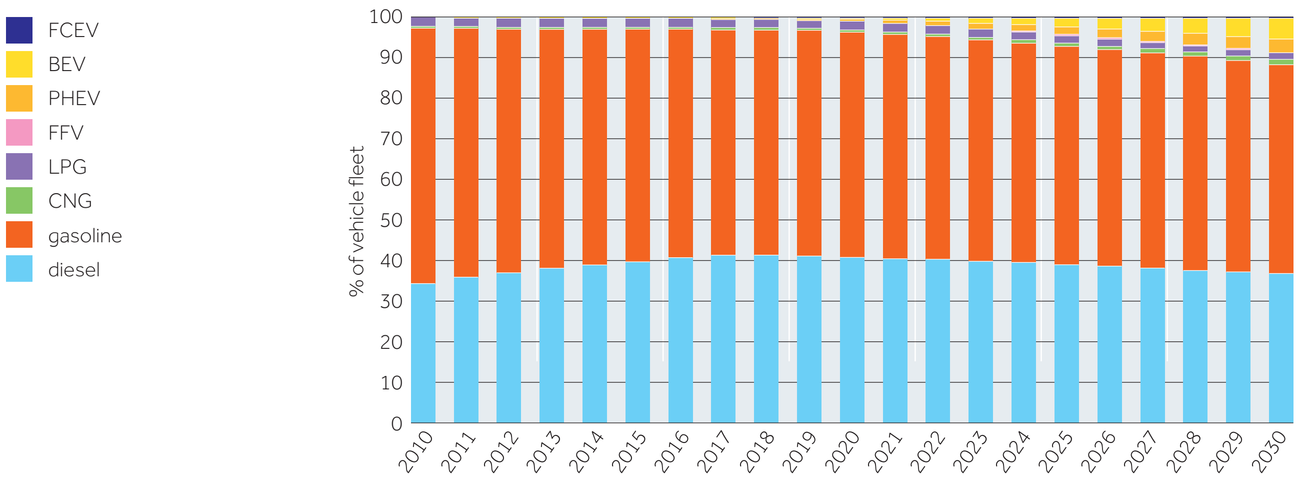
Overall, the share of alternative vehicles (including PHEVs, BEVs, FCEVs and CNG/LNG/LPG-powered vehicles) in new sales for road transport accounts for ~24% of passenger cars (versus ~4% in 2018), 7% of vans (versus 1.9% in 2018), 8% of heavy-duty trucks <16 t (versus 2.2% in 2018), 29% of heavy-duty trucks >16 t (versus 0.5% in 2018), and 23% in the case of buses and coaches (versus 4.7% in 2018) (see Figure 2).

Figure 2: New fleet sales mix in 2030 required to meet the CO_2 emissions targets



- As a result of both the evolution of the existing fleet and the penetration of alternative powertrains in new sales, the composition of the European passenger car fleet includes more than 280 million cars on the road in the baseline: ~12% of these vehicles are not expected to be running on either conventional gasoline or diesel in 2030 (versus the current ~3% in 2018) (Figure 3).

Figure 3: Examples of fleet model output: powertrain types in fleet stock — passenger cars



- As a result of the composition of the fleet and the fuel efficiency improvements towards 2030, the total energy demand in road transport has been estimated as 239 Mtoe/year. In addition to the road transport segment, the evolution of the aviation, rail and maritime sectors (international extra-EU trips considered) generally increases in activity towards 2030, representing an additional ~80 Mtoe/year, resulting in an estimated ~318 Mtoe/year energy demand for the whole EU transport sector in the 2030 baseline.
- The composition of the road transport fleet along with the projected energy demand in other transport modes defines how this total energy demand is split between the different types of fuels (liquid, gaseous, hydrogen or electricity — see Figures 4 and 5), which will define the basis for the fuel composition/availability assessment described on the following pages.

Figure 4: Total energy use per fuel or energy carrier

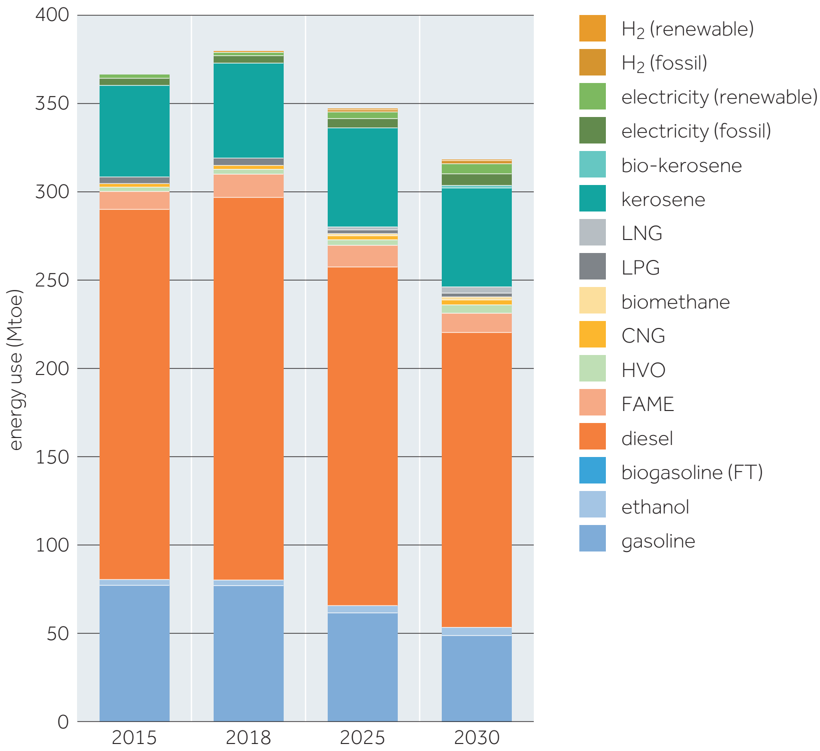
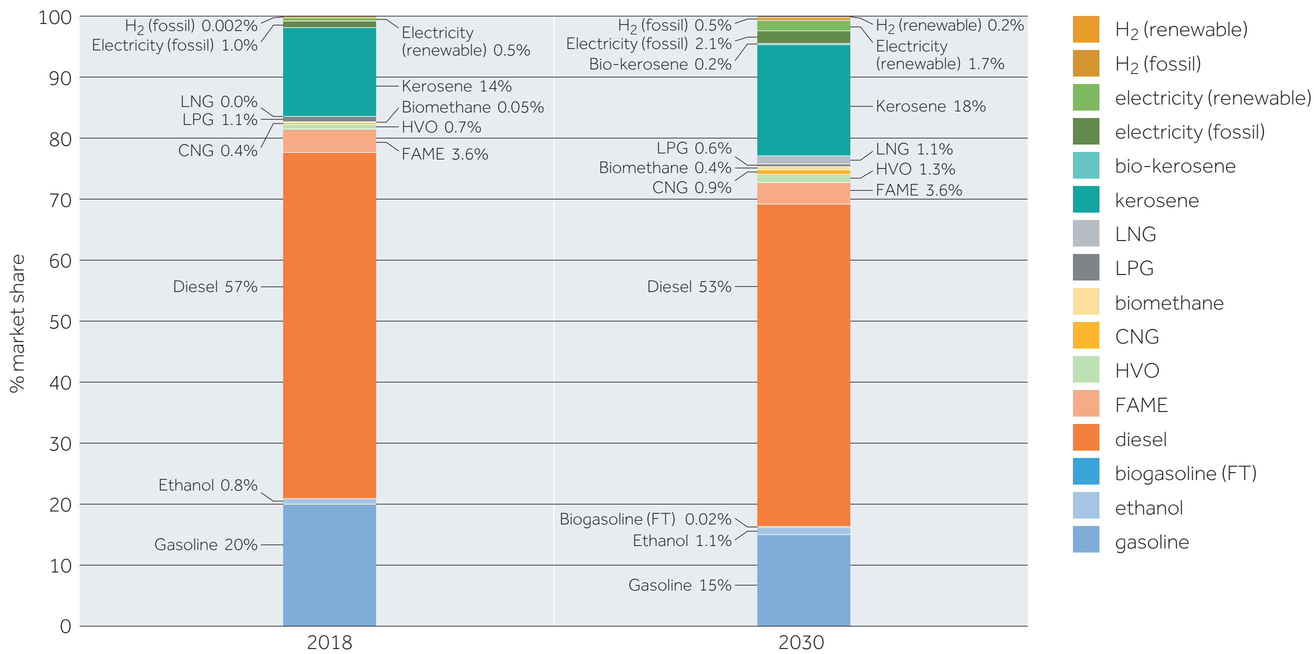


Figure 5: Percentage of market share per type of fuel (2018 vs 2030)



Energy supply and alternative fuel availability

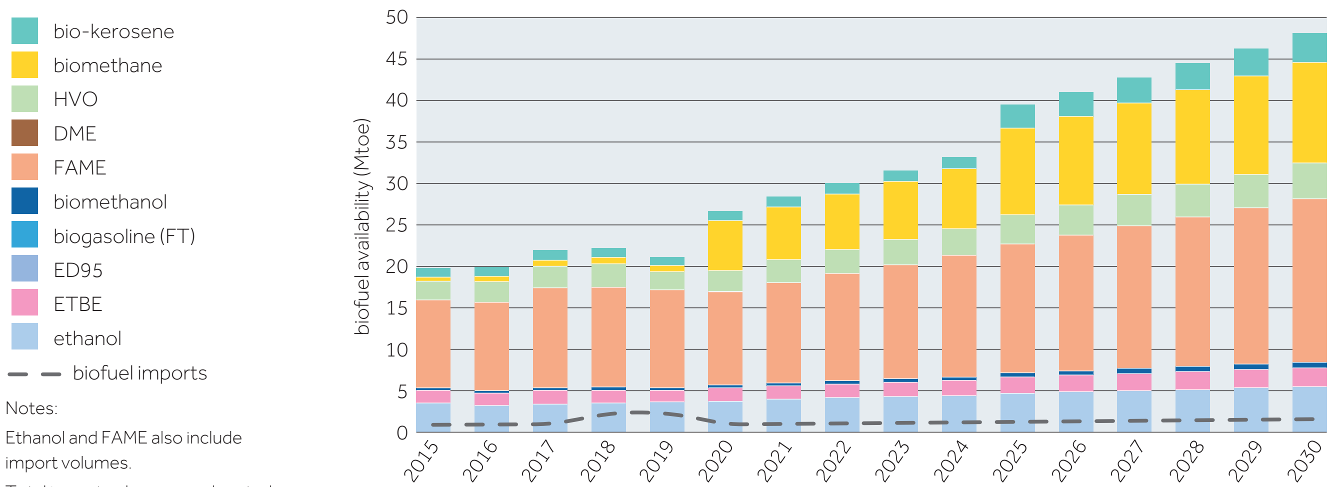
For the purposes of this fuel outlook, alternative fuels (according to Directive 2014/94/EU, Article 2) are defined as *'Fuels or power sources which serve, at least partly, as a substitute for fossil oil sources in the energy supply to transport and which have the potential to contribute to its decarbonisation and enhance the environmental performance of the transport sector. Liquid, gaseous and electricity are included in this categorisation'*. The penetration of alternative fuels in transport could be either unlimited (drop-in fuels) or constrained by certain blending walls regardless of their potential availability.

The updated baseline scenario includes the currently standardised grades for biofuel blends (B7, E5 and E10) that are widely used as road fuels in Europe, and considers the future availability of a number of different alternative fuels that will progressively become available in Europe during the 2020–2030 time frame. This availability has been assessed following a market-based approach, extracting aggregated data from the STRATAS[5] proprietary database, purchased for the purpose of this study and updated with recent developments. This database maps the status of alternative fuel production facilities in Europe (including those in operation and under construction, and planned installations already announced). The market-oriented baseline considers the following:

Liquid and gaseous (excluding H_2) fuels

The baseline is founded on an updated outlook for production plants currently in operation, under construction, and recently announced in Europe (based on the STRATAS 2017 database mapping facilities worldwide, updated with recent announcements in Europe), maximising the current utilisation rate of existing plants towards 2030. New types of fuels like dimethyl ether and ED95, and a small proportion of power-to-fuel plants (currently at demonstration scale) are also included in the scope of the study. The volumes of these fuels produced are also complemented by imports, keeping the same ratio of domestically-produced vs imported fuel volumes in 2030 as it is today (Figure 6).

Figure 6: Estimated availability of various biofuel types in Europe



Notes:

Ethanol and FAME also include import volumes.

Total import volumes are denoted by the dashed line on the figure.

[5] https://www.stratasadvisors.com

As a conclusion to this update on alternative fuels, it is worth noting the following:

- The current (installed) capacity for alternative fuel production is still very much based on food crop biofuels and, despite recent announcements about newly built plants in Europe, including facilities for the production of second-generation biofuels, the market-based signals seem to show only a modest ramp-up, at least regarding those projects announced in the public domain.
- Fully utilising the existing (installed) capacities in 2018 would be able to deliver an additional volume of ~11 Mtoe/year (100% utilisation is considered at the end of the 2030 period). This evaluation is based on the technical production potential and may not result in actual production outputs for a certain year as market conditions affect the real outputs of plants.
- When all existing and new facilities are considered, the 2030 baseline reports a maximum technical availability of ~47 Mtoe/year (based on the maximum installed capacity), of which only ~21 Mtoe/year are deemed to be used in transport as a result of the energy demand modelled. This is due to the fact that the energy demand for alternative fuels is determined by factors such as the demand for different powertrains, constrained by the existing blending walls in case of oxygenate-derived fuels, or the competition with other sectors in the case of biomethane availability.

Therefore, the total fuel use in transport is lower than the maximum technical availability reported by the installed capacity, and some surplus volumes may exist which will either be diverted to other sectors or exported out of Europe. This 'excess' concept (volumes not used in road transport to meet the modelled demand) would become especially relevant in the case of biomethane (as detailed in the related sensitivity case).

Electricity and hydrogen (as final fuels)

The projections for renewable electricity in the European mix are defined according to the IEA projections (45% in 2030), extensively detailed in the JEC WTT v5 report (Section 3.4), and the energy requirements would be defined by the fleet composition. Due to the foreseen electricity demand in transport in the 2030 baseline (~12 Mtoe/year of electricity, mainly in road and rail modes, representing about 4% of the current gross generation capacity in the EU27 + UK, Norway and Switzerland), as a simplification, no limitations on the EU electricity generation capacity have been assumed at this stage. A deep analysis on the feasibility of the integration of this electricity demand in transport within the whole EU economy (including other sectors such as domestic households, industrial sites, etc.) is part of a holistic energy system modelling process, and is beyond the scope of the present analysis.

Regarding the demand for hydrogen (as final fuel) modelled in the 2030 baseline, assuming a mix between natural gas and electrolytic hydrogen production in 2030, no assumptions on potential availability limits are considered. Hydrogen production for transport applications is limited in the 2030 baseline (2.1 Mtoe/year of total demand), where the majority stems from road transport (2.0 Mtoe/year) and the remainder from rail. Based on the current pace of development of renewable hydrogen in Europe, an increase in renewable hydrogen was assumed for road and rail applications (25% in 2030).

RED II targets (baseline and sensitivity analysis)

Baseline

As the RED II 'framework on additionality in the transport sector' (Article 27, point 3) is in the process of being fully defined by the Commission, this study explores the impact of two different interpretations when this concept of renewable electricity is applied to the transport sector. The results of the baseline, in terms of the percentage of equivalent renewable energy versus the RED II 14% minimum sub-target in road and rail transport by 2030, are presented below:

1. Interpretation 1 (Additionality criteria on renewable electricity in transport): RES-T 15.6%
2. Interpretation 2 (Additionality criteria on total renewable installed capacity): RES-T 17.0%

Note that the difference between both interpretations is mainly due to the current electricity consumption in rail transport, which helps to meet the RED II target. In both cases, all the sub-targets are met with the exception of Annex IX part A (min 3.5%) which, with the current market trends/ announcements, is deemed unlikely to be accomplished. When the compliance with RED II regulation is explored (for the detailed assumption see Section 5.3 of the Concawe report), the 2030 baseline shows the following:

- The multipliers boost the contribution of electrically-driven powertrains and the role of biofuels in transport in compliance with RED II up to a total of 15.6% (Interpretation 1) and 17.0% (Interpretation 2) in the baseline.
- The impact of these multipliers is significant and deemed to represent ~5–6% of renewable energy content within the current baseline (without multipliers, the absolute renewable energy share would represent 10.3% (Interpretation 1) and 11.1% (Interpretation 2)).
- Renewable electricity use in transport represents 3.9% (Interpretation 1) and 5.4% (Interpretation 2) of the total renewable energy in transport (RES-T) target (with multipliers) while the contribution of biofuels is ~11.5% (5.3% of which corresponds to advanced biofuels).
- Based on both the expected availability and blending walls, the share of first-generation (crop-based) biofuels remains below the imposed cap (max 7%).
- Regarding advanced biofuels, while the physical cap in Annex IX part B of RED II is respected (1.7%), the minimum requirement in part A is not reached (2.2% vs the 3.5% minimum defined in RED II).
- Based on these results, additional investments/support for alternative fuels (including liquid, gaseous and electricity) will be required to realise their potential towards 2030, versus current trends/publicly announced projects.
- The penetration of biomethane in the different transport sectors is deemed to have a significant impact when meeting the 2030 targets. The baseline assumes a higher biomethane content in all transport sectors (20%) versus the natural gas grid which would need to be confirmed, meeting the additionally criteria, to realise the potential GHG savings across the whole economy (instead of shifting emission reductions from one sector to another).

Sensitivity analysis

Complementing the baseline, additional sensitivities on key individual parameters have been explored (Table 1). While these are not intended to represent alternative scenarios, they show interesting trends and conclusions which could help to identify areas for further research and development, and to boost the penetration of renewable energy in transport towards a higher 2030 RED II goal.

Table 1: Summary of the sensitivity analysis considering a change in model parameters

Case	RED II % interpretation 1	RED II % interpretation 2	Key outcome
Baseline	15.6%	17.0%	
30% BEV+PHEV in 2030 sales	16.4%	17.8%	Additional sales of 1.6 million new EVs in 2030 raises RED II by ~0.8%
5% bio-kerosene in 2030 aviation fuel	16.7%	18.1%	Raises RED II by 1.1%, but the realisation of feedstock potential gain could be at risk
Increased use of hydrotreated vegetable oil (HVO) to reach minimum 3.5% (RED Annex IX part A feedstock)	16.9%	18.4%	The use of feedstock detailed in Annex IX part A of RED II is about 60% higher than in the baseline
40% share of biomethane in total gas	16.8%	18.3%	Towards meeting all RES-T targets and biofuel feedstock sub-targets with Annex IX part A at risk (3.4%)
1.7% administrative cap on Annex IX part B feedstocks*	14.1%	15.6%	1.5% lower RED II compared to the baseline
E10 limited uptake (78% of fuel grades by 2030)	15.4%	16.9%	Slight reduction in RED II by 0.2%
Only E5 grade (theoretical assessment)	14.6%	16.1%	~1% reduction in RED II
Liquid biofuels in 2030: 20% in maritime and 10% in non-electric rail	16.0%	17.5%	Small increment of 0.5% in RED II
LNG trucks (>16 t segment) with dual-fuel high pressure direct injection (HPDI) technology in 2030	15.5%	17.0%	Very small decrease in RED II due to lower use of biomethane

* Case study exploring the potential impact of the current physical cap to an administrative one.

The sensitivities explored indicate the following:

- Increasing the share of EVs (BEVs+PHEVs) from 20% in the baseline to a higher level of 30% in 2030 sales raises the RES-T by ~0.8%. It calls for the registration of 4.8 million new EVs, one-third of which are expected to be PHEVs.
- The penetration of renewable fuels in aviation plays a key role when meeting the targets, especially due to their contribution in the numerator (not in the denominator) and the ad-hoc multipliers defined by RED II for the sector. A 5% share of renewable jet fuel in the total EU aviation pool (equivalent to multiplying the capacity defined in the baseline by five) increases the RES-T share by 1.1%. This sensitivity case assumes additional biofuel capacity without jeopardising the volume of advanced feedstocks dedicated to road transport. In the case of feedstocks and/or future installed capacity competition, the realisation of this potential gain could potentially be at risk.
- Reaching the administrative mandate of 3.5% on Annex IX part A feedstocks is estimated to require an increase from 0.8 to 2.4 Mtoe of Annex IX part A feedstocks being diverted to, for example, $HVO_{equivalent}$.[6] This volume is about three times that used in the baseline and would require new additional HVO capacity, well beyond the current installed capacity and public market plans/imports levels in Europe.
- By assuming a higher share of 40% for biomethane diverted from other sectors to transport (and replacing fossil CNG and LNG), an increment of 1.2% would be expected for RED II. With this assumption, the Annex IX part A[7] share reaches 3.4% with the use of multipliers in the numerator, approaching the minimum requirement of 3.5%. It is important to note that, beyond RED II, biomethane is mainly used as an energy source in non-transport sectors, so any increase in the use of biomethane in transport may not imply an additional GHG reduction versus the baseline unless the whole energy system is considered and new ad-hoc additional capacity is added for the specific purpose of meeting future transport demand (otherwise there may be a potential risk of shifting GHG emission reductions among sectors).
- Applying a 1.7% administrative mandate on Annex IX part B feedstocks reduces the RES-T share to 14.1% when multipliers are used in the numerator. In this case, the RES-T target of 14% and all biofuel feedstock sub-targets are met.
- Limiting ethanol penetration in the fleet by assuming a slow penetration of E10, modelled through the historical ramp-up of E10, leads to a slight decline of 0.2% in RES-T share, compared to the baseline.
- Limiting ethanol penetration through the extrapolation of historical E5 data and excluding E10 from gasoline fuel grades resulted in ~1% decline in RES-T share. This theoretical case shows the impact and importance of full E10 penetration in the fleet model.
- Assuming a higher share of liquid biofuels in rail (10% of non-electric in 2030) and maritime (20% of total fuel in 2030) raises the RES-T share by ~0.5%.
- Assuming a full penetration of dual-fuel LNG trucks by 2030 would slightly reduce the RES-T share by only 0.1% compared to baseline.The use of dual-fuel LNG trucks with HPDI technology reduces the demand for LNG and, thus, the room for additional biomethane uptake, compared to the baseline.

[6] As a simplification, this sensitivity case does not consider an increase in the use of Annex IX part A feedstocks used for FAME production as the B7 blending wall is reached (higher blends, B10, or a different repartition of feedstocks to different final and/or blending fuels may offer different alternatives to comply with this sub-target).

[7] According to the STRATAS database all biogas (and SNG) feedstocks are considered as Annex IX part A.

A look into GHG emissions

At the time of publication of this article, a revision of the FQD is being undertaken by the European Commission. The results of the assessment of GHG emission reductions in the road transport[8] baseline are explored in the Concawe report, and indicate the following (see also Table 2):

- In 2020: The total GHG emissions from the road sector (GHG_{road}) was estimated to be 1,097 Mt CO_2eq and the total energy consumption from both fossil and renewable energy sources was estimated at 297 Mtoe.
- In 2030: The GHG intensity calculations showed that the total road GHG emissions reached 857 Mt CO_2eq and the total energy from both fossil and renewable energy sources was 238 Mtoe. The results show an emission factor of 85.8 g CO_2eq/MJ.

  In absolute terms, derived from the composition of the fuels in transport and the fuel production pathways modelled in the JEC WTT v5 report, the total GHG emissions in the whole transport sector have been estimated in 1,146 Mt CO_2eq/year at the EU level in 2030 (~18% decline in the 2018–2030 period).
- Based on the above, the 2030 baseline estimates a reduction in the GHG intensity of road transport fuels in 2030 of 8.8% versus 2010. The results of the 2030 baseline are intended to be used to inform the ongoing revision of the FQD. As a result of this process, new criteria could be defined, impacting the present outcome of the analysis. If so, the present outlook will be updated accordingly in due course.

Table 2: Baseline results for GHG intensity reduction in road transport fuels

Year	GHG emissions (Mt CO_2eq)	Energy use (Mtoe)	Emission factor (g CO_2eq/MJ_{fuel})	GHG intensity reduction from 2010
2030	857	238	85.8	-8.8 %

Important note

The 2018 baseline does not represent any individual company's views and is the result of a consensus prior to the publication of the EU's 2030 Impact Assessment. The modification of various parameters (some of them already explored as sensitivities in this analysis) or any additional policy considerations (e.g. the use of renewable fuels of non-biological origin (RFNBO), electrolytic hydrogen, and e-fuels versus electricity) could have an impact, and could effectively enable a higher penetration of renewable energy in the transport sector.

Conclusion

A key conclusion that can be derived from the initial assessment using this baseline is that, since the composition of the fleet and fuel contribution is founded on market-based outlooks and expert judgment, it is considered the best starting point for understanding and exploring potential scenarios towards 2030. Concawe's outlook has not, therefore, been back-calculated from the RED II and FQD targets. It is intended to provide the reader and various stakeholders with an educated market and industry view on where the current trends could lead the sectors, and to help identify key parameters to be further enhanced when meeting the current 2030 objectives. (Note that the revision of the 2030 targets under the EU's current Impact Assessment is not included in the baseline and will be explored in future publications).

[8] This section is not intended to be used as a direct comparison with the FQD targets as it is only focused on road (e.g. gas oil used in non-road mobile machinery, which is included in the FQD, is not considered here) but gives a good indication of the potential GHG reductions based on the WTT intensity considered/described in the Appendixes of the Concawe report.

The optimal vehicle electrification level in a battery-constrained future

In light of the EU's commitment to reduce greenhouse gas (GHG) emissions in Europe, there is considerable uncertainty as to whether battery production capacity will be able to meet the growing demand for batteries in Europe towards 2030. This article summarises the results of a study that explores the optimal passenger car sales composition that would minimise well-to-wheels GHG emissions as a function of battery production capacity.

Introduction

As part of the European Green Deal, the European Union (EU) has committed to significantly reduce its greenhouse gas (GHG) emissions. A cut of 55% in 2030 compared to 1990 levels has been agreed by the European Commission, the European Parliament and the Council, to which passenger cars should contribute with a reduction of at least 37.5% in their CO_2 emissions between 2021 and 2030 (currently under revision and with the level of ambition likely to be raised in June 2021). This raises the obvious question for automotive manufacturers, energy providers, customers, regulators and other stakeholders: what is the best way forward to minimise GHG emissions from passenger cars?

For a given usage,[1] three main drivers play an important role in addressing this challenge:

1. The fleet mix, with four main technologies discussed in this instance (given in increasing order of electrification): vehicles powered solely by an internal combustion engine (ICEVs), hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs) and battery electric vehicles (BEVs).
2. The energy mix used for transport, i.e. the share of liquid and gaseous fuels or electricity used.
3. The carbon intensity of different combinations of feedstocks and conversion technologies used to supply energy carriers.

With a focus on the role of the fleet mix, many studies have been performed using a life-cycle assessment (LCA) approach to compare the merits of each of these four technologies.[2] Most of these studies carried out back-to-back comparisons of the life-cycle emissions of ICEVs vs BEVs expressed in terms of g CO_2eq/km or tonnes of CO_2eq along the whole lifetime of the vehicle in use, and concluded that, on an average C-segment basis in Europe, and using the average energy mix forecasted for the 2020–2030 time frame, BEVs would emit less GHG than ICEVs when no low-carbon fuels are considered.[3] The same conclusion in favour of BEVs is generally given when comparing HEVs with BEVs in an average European environment. The comparison of PHEVs with BEVs has received much less attention and there is no unanimous agreement in this regard. For example, IFPEN[2] concluded that PHEVs would emit less than BEVs over their life cycle, based on the assessment that the former has smaller batteries than the latter, which results in significantly lower GHG emissions over the vehicle life cycle, while keeping a high share of electric driving (referred to as the utility factor). However, ICCT[3] came to the opposite conclusion in their assessment that the real-world utility factor of PHEVs is overestimated by homologation measures, and is more likely to be in the range of approximately 20% for company cars and 50% for private vehicles, as users (especially those of company cars) do not charge them regularly enough. This results in higher CO_2 emissions in real use than those calculated during the homologation process. It is a fact that the LCA approach is often affected by many uncertainties, and the utility factor of PHEVs is among the most discussed topics along with the GHG emissions related to battery production.

1 For example, the number of cars sold each year, the mileage driven by each car, the occupation rate of the vehicles, etc.

2 For example, see Yugo (2018)[1] among many others.

3 This is an average result at the European scale, and does not necessarily apply in every European country as it depends on the energy mix of each country.

Notwithstanding the relevance of the aforementioned LCA studies, when a back-to-back comparison of, for example, an HEV with a BEV leads to the conclusion that the latter should replace the former in terms of sales, those studies all make the important — while often implicit — assumption that a bigger battery would be available to equip each and every new BEV vehicle sold.

But what if that was not the case? In such a scenario where, in 2030, the raw material availability and battery manufacturing capacity are still constrained, would it be preferable to allocate all the available materials/batteries to BEVs, with the consequence of having the rest of the sales as ICEVs? Or would it be more efficient for mitigating GHG emissions to spread the available batteries in different portions among HEVs, PHEVs and BEVs? [4]

The purpose of the present work is to answer the question, *'What would be the optimal sales mix to minimise GHG emissions from passenger cars in a battery-constrained environment in the same 2020–2030 time frame, according to a number of different analysts?'* (see the section entitled *Batteries: forecasted demand and production capacities* on pages 46–48). To answer this question, we need to move away from the back-to-back LCA comparison paradigm described above, and shift to a systemic view that takes account of constraints on battery availability, such that batteries allocated to BEVs may result in batteries no longer being available for HEVs and PHEVs, leading to an increase in sales of ICEVs.

To address this question, the authors performed an optimisation of the sales mix to reduce well-to-wheels (WTW) CO_2 emissions of passenger cars for different levels of battery production capacity. At this stage it is worth noting that, for each level of battery production capacity, it is assumed that the GHG emissions related to vehicle production are not influenced by the composition of vehicle sales, as all of the batteries produced are fully allocated to all vehicles sold that utilise electrified powertrains (xEVs).[5] This assumption results in a significant simplification compared to the full LCA method and justifies the use of a simpler WTW approach.

It could be argued that this study will be of limited use, being that automotive manufacturers should already be in the process of minimising the CO_2 emissions of their vehicles sold in a — potentially — battery-constrained environment. However, this is only partly true. As with any private corporation, vehicle manufacturers aim to maximise profits under certain constraints (reaching their CO_2 targets being a particularly important constraint). This means that they also have to account for vehicle costs, customer acceptance, long-term strategy, investments, etc., which makes optimisation far more complex — and different — from the work presented here. Manufacturers also have to face non-optimal regulations, for example the fact that GHG emissions are regulated only on a tank-to-wheels (TTW) basis and not on a WTW basis, or the fact that low-emission vehicles can benefit from double counting (super-credits).

4 With the underlying assumption that HEVs, PHEVs and BEVs all use the same lithium-ion (Li-ion) battery technology.

5 In a simplified approach, the emissions related to the production of vehicles is the sum of the emissions from the production of the car and those from the production of the batteries. As the number of cars and batteries produced is constant for each level of battery production whatever the fleet mix, one concludes that the emissions related to the production of vehicles does not depend on the fleet mix. To be more accurate, one should also account for the number and type of powertrains produced, which varies with the fleet mix. However, this was assumed to have a negligible effect on the life-cycle emissions.

These regulations can result in a suboptimal sales mix, in terms of minimising the global GHG emissions of passenger cars. For these reasons, the ultimate purpose of this article is to open a debate with automotive manufacturers and regulating authorities to identify, and hopefully also eliminate, any barriers that could lead to suboptimal WTW CO_2 emissions from passenger cars.

Batteries: forecasted demand and production capacities

How likely is it that the next decade is going to be battery-constrained with respect to passenger cars? To assess the likelihood of this assumption, Concawe has collected data from the literature regarding forecasted demand and production capacities, and observed whether there are any gaps between the two.

Forecasted demand

There are considerable uncertainties regarding the demand for batteries used for transport in 2030, as this depends heavily on the level of electrification of the vehicles sold, which in turn depends on regulations, customer preferences, vehicle manufacturers' strategies, etc. Added to this, the share of electrified vehicles has evolved quickly in recent years, and forecasts are somewhat sensitive to this dynamism.

Batteries Europe ETIP forecasts an annual demand of 0.44 TWh of batteries by 2030, in a context where the global demand for batteries would be multiplied by 14 between 2018 and 2030, initially driven by demand in China (1.12 TWh).[4] McKinsey & Company has also shared forecasts which anticipate demand ranging between approximately 0.3 and 0.7 TWh/year in 2030.[5]

In the work presented here, the most extreme case regarding battery demand assumes that 100% of new vehicle sales will be BEVs by 2030, with an annual sale of 16 million passenger cars in Europe,[6] all of them being equipped with a 50 kWh battery. This results in a demand scenario of 0.8 TWh/year of batteries, which is already in the upper range of the aforementioned scenarios, without taking into account the demand from other sectors such as heavy-duty transportation or energy storage.

Forecasted production capacities

The forecasts regarding battery production capacities face the same level of uncertainty as for the demand:[6]

- Batteries Europe ETIP reports that there are a total of 25 announced projects for Li-Ion factories in Europe, ranging from pilot plants to 'gigafactories' which, if realised, will add approximately 0.5 TWh/year to total production capacity in Europe by 2030.[4]
- PV Europe mentions an expected 0.3 TWh/year of battery production capacity by 2029, with large uncertainties, and refers to the meta-study, 'Batteries for electric cars: Fact check and need for action' commissioned by VDMA and carried out by the Fraunhofer Institute for Systems and Innovation Research ISI, which suggests that production capacities of 0.3 to 0.4 TWh/year could be achieved by 2025.[7]
- Volkswagen recently announced its plan to build six battery cell factories in Europe by 2030, corresponding to a production capacity of up to 0.24 TWh/year.[8]
- Tsiropoulos *et al.*, on behalf of the Joint Research Centre of the European Commission, evaluated that European battery production capacity could be sufficient to meet a domestic demand for 2–8 million BEV sales[9] — far from the expected annual sales of 16 million passenger cars.
- A recent report by Ultima Media predicts that the rising demand for EVs, the introduction of regulations supporting local battery production, and the number of factories under construction or announced will lead to considerable growth in European battery manufacturing capacity of up to 0.95 TWh/year by 2030.[10] However, the report indicates that there is no guarantee that all of the announced capacities or stated ambitions can be realised.

For the sake of comparison, in the second half of 2020, the global battery capacity deployed in all newly sold passenger xEVs combined (HEVs, PHEVs and BEVs) amounted to 0.093 TWh/year, out of which 0.037 TWh/year were used in Europe.[11] This is far from the levels of battery manufacturing capacity projected in the high-BEV demand scenario.

A battery-constrained environment?

In spite of all the uncertainties, the trends collected for battery production and demand undoubtedly show that we will be living in a battery-constrained environment during the next decade, as the demand that would result from a high-BEV electrified scenario could not be met by the forecasted production capacity. Even when reaching the 2030 horizon, meeting the overall battery demand remains highly uncertain; not only does the forecasted production capacity vary widely, but the demand from other sectors, such as heavy-duty vehicles and energy storage, could add to the demand originating from passenger cars. Recycling of batteries could help to alleviate this constraint, but the role of recycling is expected to be limited in this decade due to the level of technology development still required and because demand is expected to grow too fast to allow recycled batteries to have a significant share of sales by 2030.

[6] The figures presented here are from different sources and are not necessarily consistent; they should not, therefore, be combined in an attempt to derive a total future value for battery production capacity.

Even though an accelerated demand for batteries could incentivise the expansion of battery production capacity in the future, it is expected that, within the time frame up to 2030, battery supply in the EU would need time before it is able to keep pace with the accelerated demand due to the potential constraints on both raw material availability and production capacity.

The EU's ambition is to become a global leader in sustainable battery production and use by developing its own production capacity.[12] It may still need to rely on imports from other regions for some of its battery requirements, but Europe considers local battery production to be a strategic goal, according to the strategic plan supporting the European Battery Alliance.[12] Hence, it is assumed that Europe will not rely on imports as an important source of battery supply, not least considering its ambitious target of 100% sourcing from its local battery production capacity.[10] It is, therefore, fully justifiable to conduct a study under an assumption of battery constraints, and to investigate the best sales mix in this environment to minimise GHG emissions from passenger cars.

Method and key assumptions

To deal with uncertainties surrounding battery supply capacity, and the potential implications for GHG emissions, a linear programming model was developed to explore the optimal passenger car sales composition, minimising WTW GHG emissions as a function of battery production capacity. The model determines the optimal mix among all feasible combinations of powertrains. The scope of the analysis is limited to ICEV, HEV, PHEV and BEV powertrains; the potential impact of fuel cell electric vehicles (FCEVs) is ignored in the 2030 passenger car fleet mix. Furthermore, the modelling framework does not aim to evaluate the impact of other barriers that could hinder the penetration of xEVs (e.g. the availability of recharging points in Europe). In addition, any impact of possible competition among different transport modes in utilising battery resources is ignored, mainly due to the expected centrality of electric passenger cars in the battery market towards 2030.[13]

The main question in the optimal framework is how to make the best use of a certain level of battery production cap (TWh/year) to minimise WTW GHG emissions of newly registered cars EU-wide in 2030. In this framework, the analysis explores the optimal vehicle sales mix to minimise GHG emissions subject to the following constraints:

- Battery supply cap, ranging from 0.0–0.8 TWh/year, being the upper limits for the total battery supply used in the xEVs sold.
- Annual sale of 16 million passenger cars per year (based on Yugo *et al.,* 2021).[6]

The main assumptions and input parameters used to calculate WTW GHG emissions are summarised in Table 1 (for vehicles) on page 49, and Table 2 (for energy carriers, i.e. liquid fuels and electricity in this instance) on page 50. TTW emissions in g CO_2eq/km are calculated based on the energy consumption of vehicles (MJ/km) and fuel emission factors (g CO_2eq/MJ). Vehicle energy consumptions (MJ/km based on the Worldwide Harmonised Light Vehicle Test Procedure (WLTP) cycle) for the base case were derived from 2025+ figures in the JEC TTW study v5.[14] In a higher-energy consumption case, a 50% increase is applied to the energy consumption of all powertrains to show the sensitivity of results.

It is worth noting that a C-segment passenger car is used as the reference vehicle in this study. The efficiency data should therefore be considered as an estimate, as it is not fully representative of all new registrations.

Table 1: Key assumptions for the selected vehicles

	ICEV	HEV	PHEV-f (fuel mode)	PHEV-e (e-mode)	PHEV (average)[b]	BEV
Vehicle mileage (km/vehicle/year)	12,000	12,000	4,800[b]	7,200[b]	12,000	12,000
Battery size (kWh)	--	2	--	20	--	50
Energy consumption (MJ/km, WLTP)[a]						
Baseline: Gasoline + Electricity	1.41	1.03	1.15	0.52	0.77	0.45
High: Gasoline + Electricity	2.11	1.54	1.73	0.79	1.16	0.67
Low-carbon fuel illustration: Diesel + Electricity	1.30	1.08	1.14	0.51	0.76	0.45
WLTP/NEDC[d] **emission ratio (g CO_2/km)**	1.15	1.32	--	--	1.00[c]	1.26

Notes:
All data for energy consumption and utility factor are based on the WLTP cycle.
[a] Data source: JEC TTW study v5.[14]
[b] Assuming 60% utility factor.
[c] Data source: Tsiakmakis *et al.*, 2017.[15] The conversion factor of 1.0 is applied to the PHEV in its combined mode.
[d] NEDC: New European Driving Cycle.

The average vehicle mileage is assumed to be 12,000 km/year for all vehicle types. For PHEVs, the annual mileage in electric-driving mode (e-mode) is determined by the utility factor. The JEC TTW v5 data suggests that, with an increased battery size allocation of about 20 kWh for PHEVs, the range using electric drive should be approximately 90% of the distance travelled by 2030 (WLTP). In addition, the estimated WLTP function, based on ICCT (2020)[3] and UNECE (2017),[16] shows that a WLTP range of 100 km returns a utility factor of about 90%. In Concawe's evaluation, an average battery size of 20 kWh is assumed for the PHEV with a 100 km WLTP e-driving range (assuming a depth-of-discharge level of about 70–75%). An average battery size of 2 kWh is assumed for full HEVs. The battery size for the BEV with a WLTP range of 400 km is 50 kWh.

Table 2: Key assumptions for the energy carriers

FUEL	Combustion emission factor [a] g CO_2eq/MJ (TTW)	Well-to-tank (WTT) emission factor [a] g CO_2eq/MJ	Biogenic credits [a] g CO_2eq/MJ
Gasoline (fossil-based)	73.4	17.0	0.0
Ethanol (E100)	71.4	44.2	-71.4
Gasoline (E10)	73.3	18.9	-4.9
Diesel (fossil-based)	73.2	18.9	0.0
FAME (B100)	76.2	38.7	-76.2
HVO	70.8	27.6	-70.8
Diesel (B7)	73.4	20.2	-4.9
B7(50%) + HVO(50%) [b]	72.1	23.9	-37.9
Electricity [c]			
Base (2030 EU mix)	0.0	21.0	0.0
Low (Wind)	0.0	0.0	0.0
High (2019 EU mix)	0.0	76.4	0.0

Notes:

[a] Data source for liquid fuels: JEC WTW study v5,[17] assuming total theoretical combustion of the fuel.

[b] Assuming 50% share of hydrotreated vegetable oil (HVO) in energy term to replace diesel fuel (B7 fuel grade).

[c] Source: EEA, 2020.[18]

A range of sensitivity analyses have been conducted around the following key parameters:

- **Utility factor:** varies from 30% to 90% with the base case being at 60% (all using the WLTP cycle).
- **Total sales:** changes in annual vehicle sales within +/- 25% around the baseline sale of 16 million cars (i.e. 12 million cars in the low case and 20 million cars in the high case).
- **Electricity supply carbon intensity (g CO_2eq/MJ):** ranges from 0 (e.g. from wind-generated electricity, excluding emissions from infrastructure) to 76.4 g CO_2eq/MJ as of 2019 (average value) in the high case, with the base case value of 21 g CO_2eq/MJ representing indicative intensity levels that would allow the EU to achieve a net 55% reduction in GHG emissions by 2030, compared with 1990.[18]
- **Vehicle energy consumption (MJ/km):** 2025+ numbers in the JEC TTW report v5 are considered as the base case assumption for 2030, and a 50% increase in fuel consumption is considered for the sensitivity analysis.
- **Use of low-carbon fuels:** HVO is considered as a partial replacement for the 50% of diesel passenger car sales in 2030. (It is important to note that other low-carbon fuel alternatives such as pyrolysis gasoline from waste resources can also be considered in the sensitivity analysis. However, for simplicity in the current analysis, HVO is considered as the illustrative case for low-carbon fuels because of its higher replacement potential for fossil fuels[6]).

Results

The optimal sales mix to minimise GHG emissions

Figure 1 displays the optimal sales composition for different levels of battery supply cap in 2030 when the utility factor is above 45%. The corresponding minimised WTW GHG emissions at each level of battery cap is shown by the diamonds and can be read on the right axis. The results show that, below the battery cap of 0.30 TWh/year, the combination of 'PHEV+HEV' would be the most effective option towards a low-carbon sales mix when pursuing the ultimate goal of reducing GHG emissions (WTW). When the available battery capacity rises to 0.55 TWh/year, the PHEV would still be the most attractive technology, with its share remaining higher than the BEV. For battery supply capacities greater than 0.55 TWh/year, BEVs would have the dominant share over PHEVs in all the sensitivity cases explored. Overall, the PHEV appears to be a key technology for decarbonising transport, as it is present in all the partially electrified scenarios, from a 0.05 TWh/year to a 0.75 TWh/year battery production cap. PHEVs are excluded from the optimal sales mix in only two cases: the non-electrified case (ICEVs only, with no battery production — a scenario that would not comply with future TTW CO_2 emissions limits) and the 100% BEVs case (enabled by a battery production capacity of 0.8 TWh/year, assuming the annual sale of 16 million passenger cars per year). The sensitivity analysis with respect to a change in annual sales of +/-25%, as demonstrated in Figure 2 on page 52, confirms the key contribution of PHEVs in the optimal fleet sales mix: the higher the vehicle sales, the higher the expected contribution of PHEVs to decarbonising the new sales mix.

Figure 1: Optimal vehicle sales mix minimising WTW GHG emissions subject to a battery supply cap in 2030 when the utility factor is greater than 45%

Note: WTW emissions are calculated at a 60% utility factor.

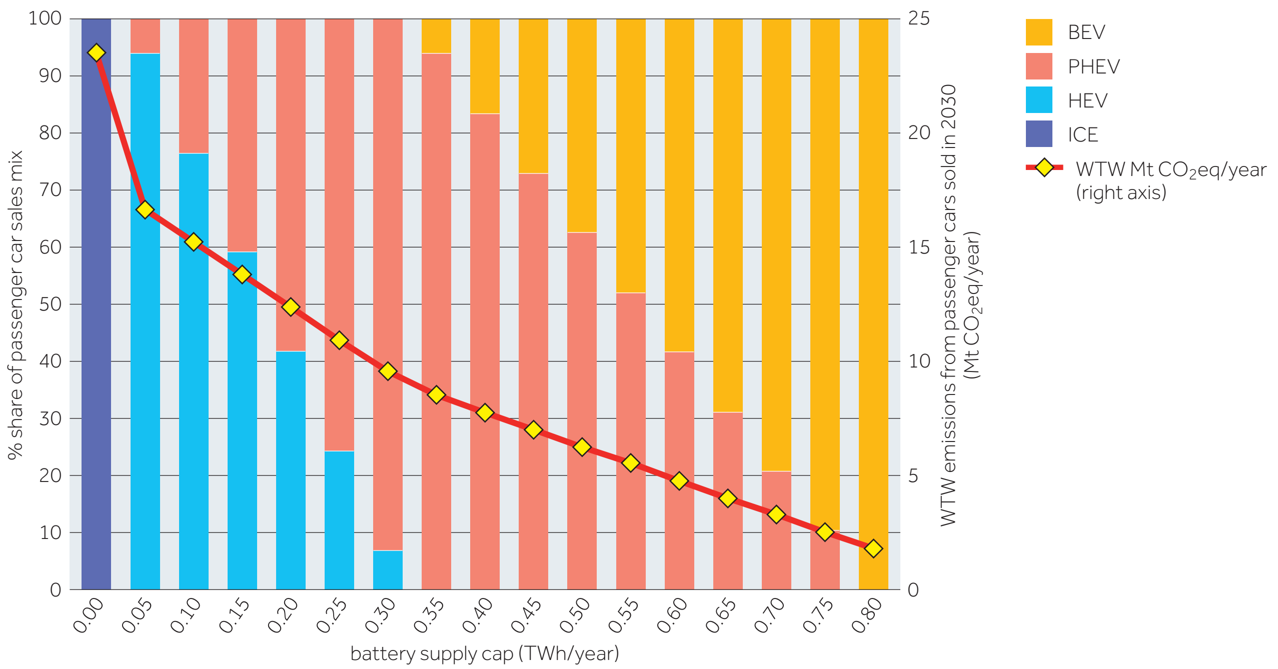
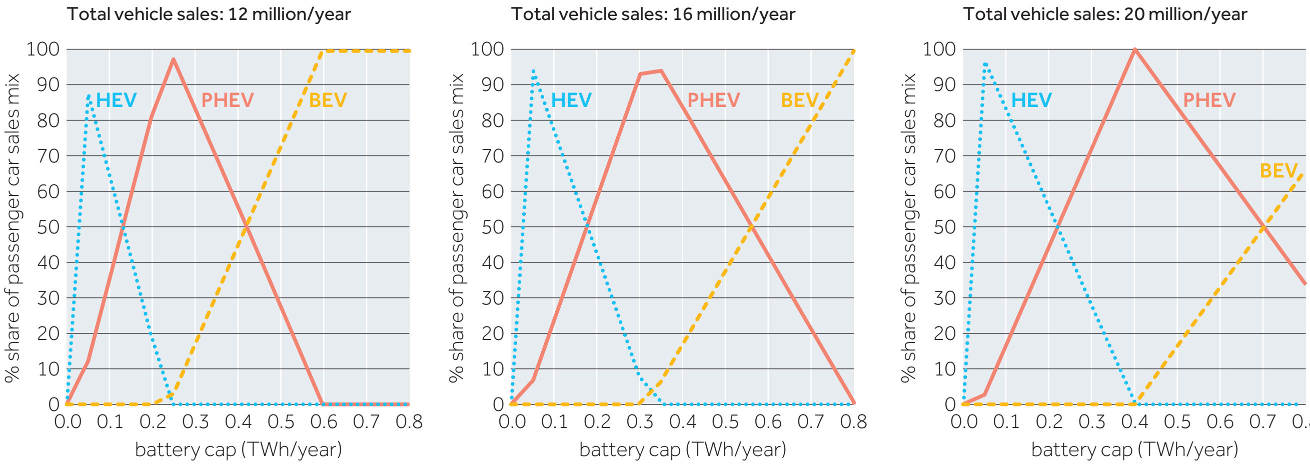
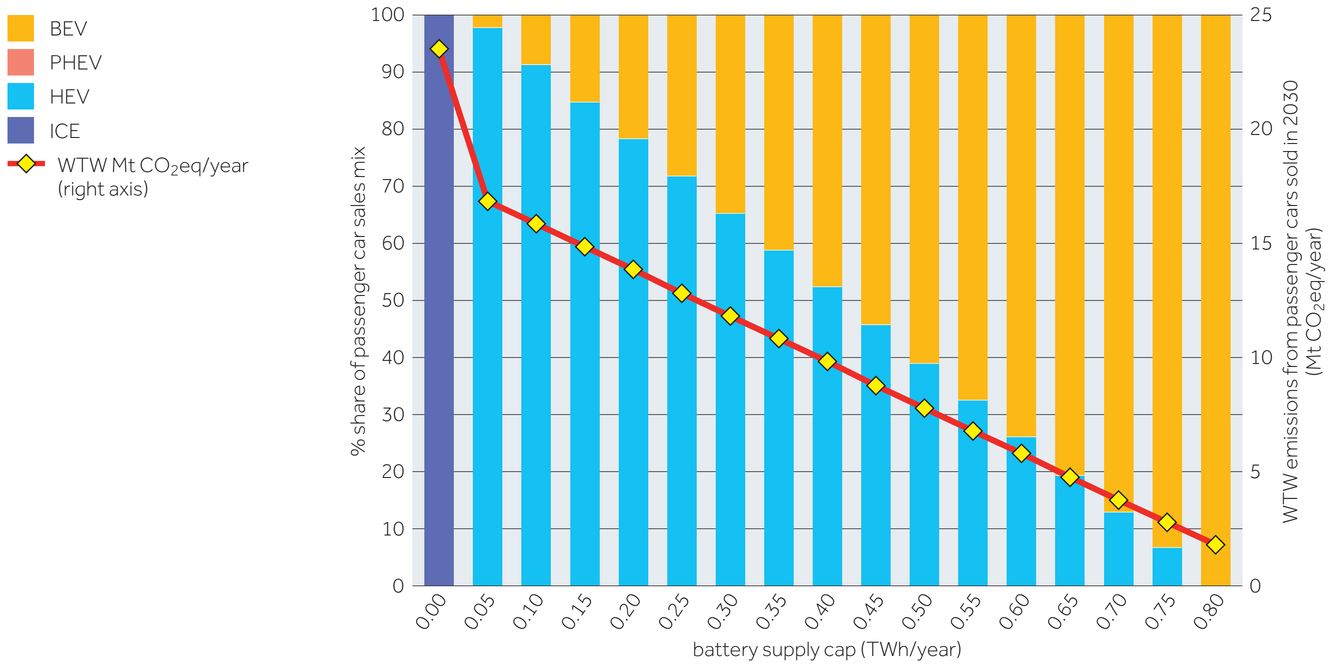


Figure 2: Optimal share of xEVs in 2030 sales: impact of total sales volume



The sensitivity analysis around the utility factor of PHEVs showed that the optimal mix remains unchanged for utility factors above 45%. It indicates that, in the battery cap scenarios up to about 0.55 TWh/year in 2030, the PHEV with 100 km electric driving range would be the key component of the optimal solution, with a share of the sales mix higher than 50%. However, when the utility factor of PHEVs is too low (below 45%), the optimal sales mix would include BEV+HEV (with no PHEV playing a role), as shown in Figure 3.

Figure 3: Optimal vehicle sales mix minimising WTW GHG emissions subject to a battery supply cap in 2030 when the utility factor is below 45%



With the optimised market share of different powertrains within the total new sales and corresponding NEDC TTW emissions intensities (calculated based on the WLTP/NEDC ratio presented in Table 1 on page 49), the average EU-wide new passenger car emissions (in NEDC TTW g CO_2/km) can be calculated and compared with the emission target of 59 g CO_2/km by 2030. Assuming the state-of-the-art efficiency figures for passenger cars in 2030, and regardless of the level of utility factor, the analysis shows that the optimised fleet mix in Figures 1 and 3 under the battery production capacity constraint above 0.05 TWh/year would be fully compliant with the emission target of 59 g CO_2/km by 2030.

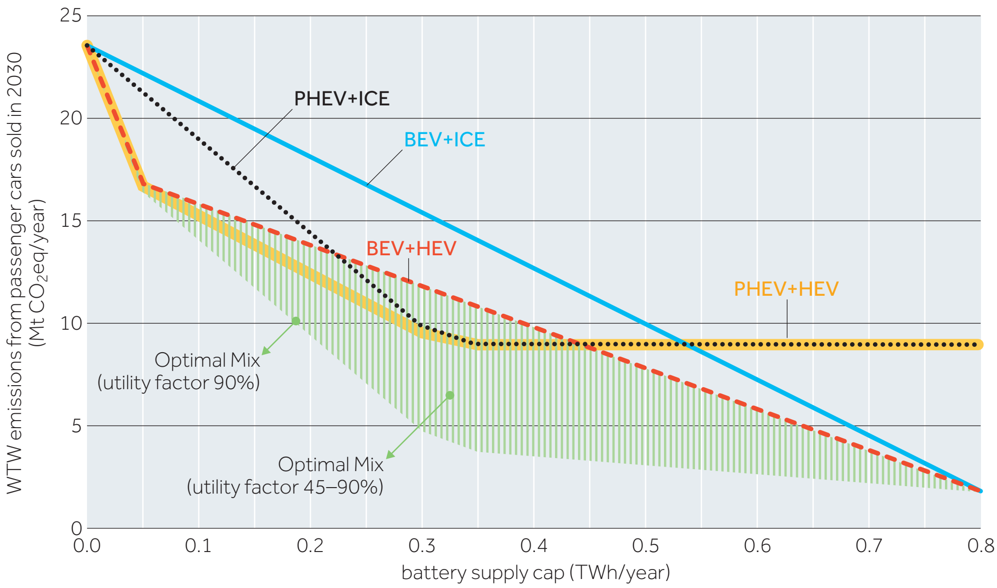
Pairwise comparisons of different sales mix scenarios

This section summarises the outcomes of comparing the following cases in pairs to evaluate which sales mix would be preferable in terms of WTW GHG emission reductions:

- **BEV+ICE:** the vehicle choice set is restricted to BEVs and ICEVs.
- **BEV+HEV:** the vehicle choice set is restricted to BEVs and HEVs for a battery supply cap above 0.05 TWh/year.
- **PHEV+ICE:** the vehicle choice set is restricted to PHEVs and ICEVs.
- **PHEV+HEV:** the vehicle choice set is restricted to PHEVs and HEVs for a battery supply cap above 0.05 TWh/year.
- **Optimal Mix:** the sales mix is optimised without exogenous constraints on the vehicle choice set.

In all of the above cases, the WTW GHG emissions of passenger cars are minimised subject to the battery supply cap constraints. Figure 4 demonstrates the key comparisons and break-even points, mainly under the baseline conditions defined in Tables 1 and 2.

Figure 4: Minimum WTW GHG emissions subject to battery supply constraints and break-even analysis of different sales combinations



Note: the green shaded area on Figure 4 presents the sensitivity of the 'Optimal Mix' case with the utility factor ranging from 45% to 90%.

A more detailed comparison of the minimum achievable emissions in different cases, including a comprehensive sensitivity analysis around the utility factor, is presented in Figure 5 on page 55. The key messages from the findings are expressed as follows:

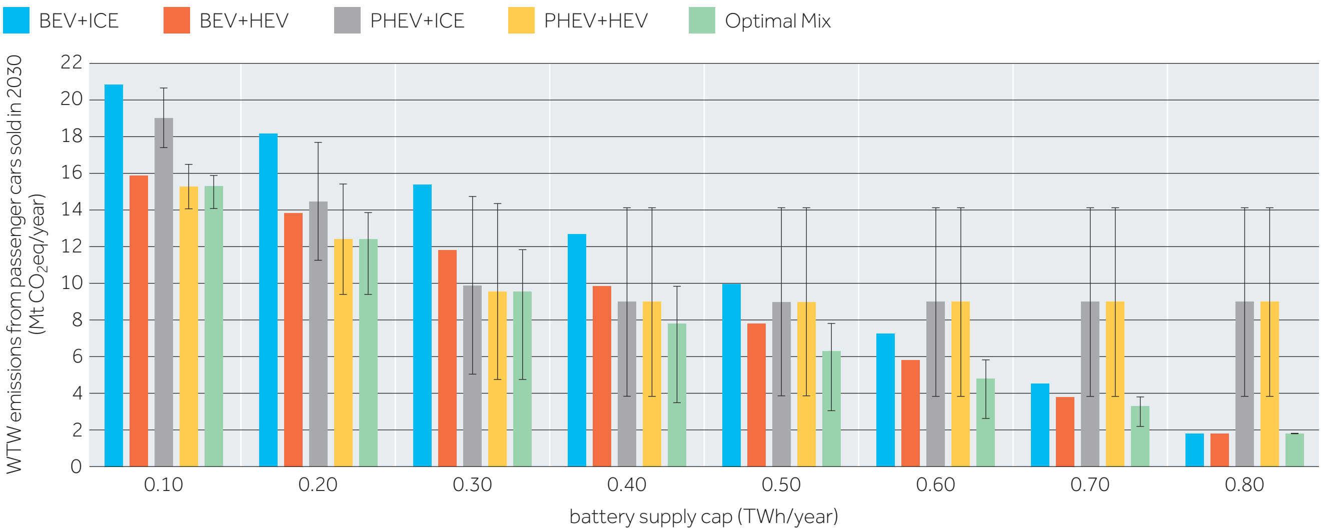
- Among the sales combination cases that fully utilise the available battery supply cap, the sales mix restricted to only BEV+ICE appears to be the worst combination when reducing GHG emissions, almost throughout the whole battery cap range explored, initially with a substantial gap compared to the other cases (see the blue line in Figure 4 on page 53). The gap is narrowed by increasing the battery supply up to the break-even point of 0.8 TWh/year with 'Optimal Mix'.
- Assuming the base case utility factor of 60% for PHEV, the BEV+ICE case could be advantageous over both the PHEV+ICE and PHEV+HEV cases (which would not fully utilise the available battery cap) only if the battery supply cap exceeds 0.55 TWh/year. This advantage is reduced as the utility factor for PHEV increases.
- The green shaded area on Figure 4 represents the optimal sales mix as described in Figure 1 (page 51) for a utility factor above 45%. The upper line of the green shaded area, resulting from the optimisation model for utility factors below 45%, is equivalent to a pure BEV+HEV case.
- For utility factors above 45%, the PHEV+HEV case appears to be the most effective option to reduce GHG emissions for a battery cap below 0.35 TWh/year.
- The emissions level would reach a floor in the PHEV+ICE and PHEV+HEV cases for the battery supply cap exceeding 0.32 TWh/year. The reason for this is that the whole new passenger car mix would be composed of 100% PHEVs.
- The green shaded area on Figure 4 shows the sensitivity of the minimised emissions with respect to the utility factor, changing from 45% to 90%: in these scenarios, it appears that increasing the utility factor of PHEVs is the most efficient way forward to decreasing GHG emissions from passenger cars.
- It is worth noting that a sales mix case involving PHEV+BEV would not be a feasible option for the battery cap below ~0.35 TWh/year (not shown in this instance). For the battery cap over this level, the results for this case are represented by the 'Optimal Mix'. This means that a sales mix made of PHEV+BEV would minimise GHG emissions for a battery cap above ~0.35 TWh/year.

The impact of the utility factor in different cases

Figure 5 on page 55 summarises the results of a sensitivity analysis around the utility factor for all considered sales mix cases. According to the Figure, for a battery cap below ~0.35 TWh/year, PHEV+ICE would be a more effective strategy than BEV+ICE regardless of the utility factor considered (i.e. 30–90%). For the higher levels of battery cap up to ~0.70 TWh/year, only upper utility factors could make PHEV+ICE preferable. For the battery cap below ~0.35 TWh/year, the baseline results for PHEV+HEV are identical to the 'Optimal Mix' solution. The error bars are, however, narrower in the optimal sales mix solution because PHEVs with low utility factors are excluded from the 'Optimal mix'.

Figure 5: Comparison of minimised GHG emissions subject to a battery supply cap in different sales mix scenarios (error bars show the sensitivities with respect to the utility factor).

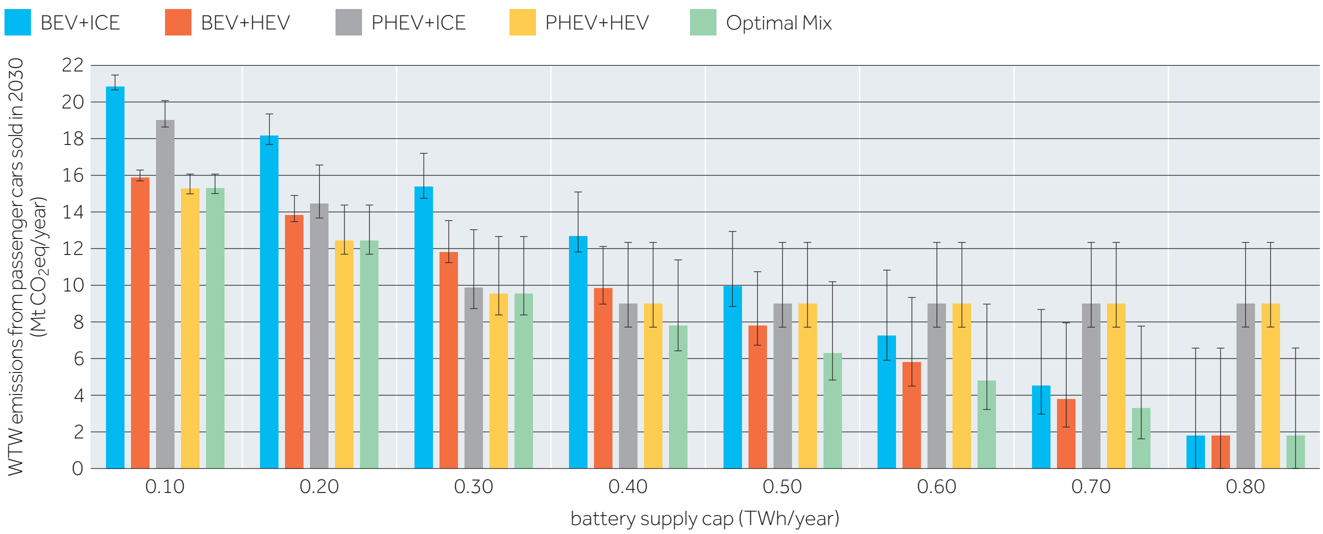
Note: The composition of 'Optimal Mix' is defined in Figure 1 (page 51) and Figure 3 (page 52).



The impact of electricity supply carbon intensity

Further sensitivity analysis around electricity supply emission factors ranging from 0 g CO_2eq/MJ to 76.4 g CO_2eq/MJ (the average emission intensity of EU electricity generation mix in 2019) shows that the above conclusion about the role of the PHEV would still be valid (see Figure 6). The main difference is that, under the upper emission factor of 76.4 g CO_2eq/MJ, the break-even utility factor (for changing the optimal fleet mix as defined in Figures 1 and 3) increases to 52%, compared to 45% in the baseline analysis.

Figure 6: Comparison of minimised GHG emissions subject to a battery supply cap in different sales mix scenarios (error bars show the sensitivities with respect to the carbon intensity of the electricity supply mix ranging from 0 to 76.4 g CO_2eq/MJ)



The impact of higher fuel consumption and low-carbon fuels

Further sensitivity analysis showed that assuming higher energy consumptions for vehicles according to Table 1 on page 49 (i.e. 50% higher MJ/km) would not change the optimal sales mix. Hence, owing to the unchanged sales mix, the total emissions of the new cars would go up proportionally by 50% compared to the baseline. Such differences are shown in Figures 7 and 8 for different levels of battery supply cap, utility factors and electricity supply emission intensity.

Figure 7: The impact of higher energy consumption and use of low-carbon fuels on the minimised GHG emissions under the 'Optimal Mix' case (error bars show the sensitivities with respect to the utility factor)

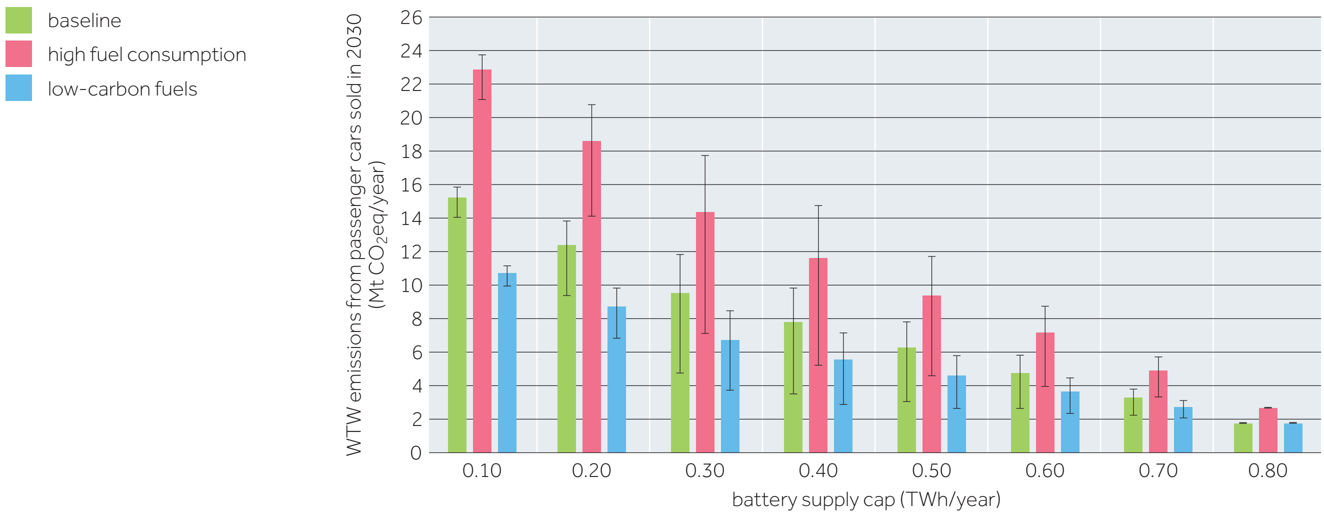
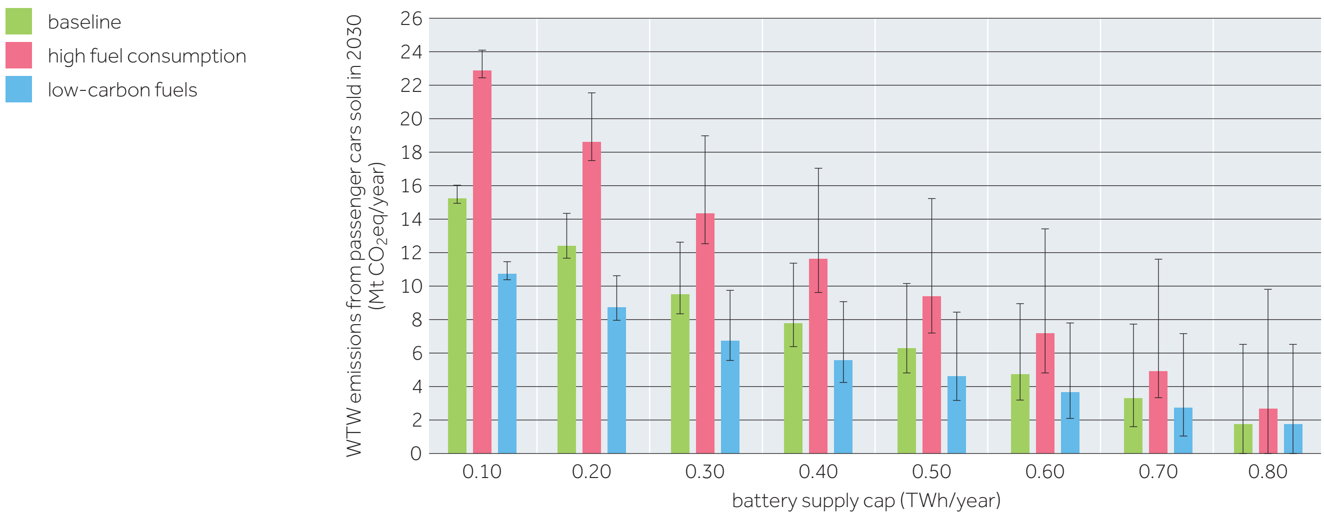


Figure 8: The impact of higher energy consumption and use of low-carbon fuels on the minimised GHG emissions under the 'Optimal Mix' case (error bars show the sensitivities with respect to the carbon intensity of the electricity supply mix ranging from 0 to 76.4 g CO_2eq/MJ)



Figures 7 and 8 also demonstrate the impact of considering the assumed illustrative example of low-carbon fuels in a 2030 time frame scenario (i.e. with HVO having a 50% energy share in total liquid fuel use, as explained in Table 2 on page 50) as replacement for diesel fuel in new sales. The sensitivity analysis around the share of HVO shows that it cannot change the optimal sales mix within the assumed range of utility factor and electricity supply carbon intensities. However, it results in lower WTW emissions from the same sales mix as in the baseline condition.

It is important to note that more optimistic scenarios for the share of HVO in total liquid fuels (as an illustrative example of low-carbon fuels) would be in favour of HEVs, especially when the carbon intensity of the electricity supply is high. For instance, further sensitivity analysis shows that, assuming an extreme case of a 100% HVO share of fuel used in diesel-fuelled vehicles, together with a high carbon intensity of the electricity supply (i.e. 76.4 g CO_2eq/MJ), would lead to the 100% HEV share being the optimal case in minimising WTW emissions.[7]

Conclusions

This study addressed the key question in a future battery-constrained environment, i.e. how to make the best use of a certain level of battery production towards minimised WTW GHG emissions of EU-wide newly registered passenger cars in 2030. To deal with the uncertainties relating to battery supply capacity and the potential implications for GHG emissions, the study explored the optimal passenger cars sales composition that would minimise WTW GHG emissions as a function of battery production capacity. A wide range of possible cases were defined based on the sensitivity analysis around the key parameters, including the utility factor of PHEVs, the carbon intensity of the electricity supply, vehicle energy consumption and the use of low-carbon fuels. Other considerations such as the total cost of ownership are not considered in this analysis which focuses only on strategies to minimise WTW GHG emissions.

The findings confirm that individual comparisons of powertrains (e.g. 1 BEV vs 1 PHEV) are not always relevant, and a systemic analysis optimising the whole sales mix, given the amount of limited battery supply resources, leads to different conclusions. The findings indicate that under a low/medium battery production capacity and moderate/high levels of utility factor, a combination of HEV+PHEV sales is the most effective option for reducing GHG emissions. In addition, in the battery cap scenarios up to about 0.55 TWh/year in 2030, PHEVs with 100 km electric-driving range would be the key component of the optimal sales mix, with its share reaching the maximum of 94% at the battery supply capacity of 0.3–0.35 TWh/year. In the scenarios considered, increasing the utility factor of PHEVs is the most immediate and accessible way to decrease GHG emissions in the short term. Increasing the contribution of low-carbon fuels in the fuel mix and a decrease in the carbon intensity of the electricity mix will offer significant additional WTW savings, which are expected to be more significant in the period 2030+.

[7] This assumes that a 100% HVO share of fuel used changes the optimal sales mix only in the case of very high electricity carbon intensity. In all other cases (including baseline electricity carbon intensity) its main impact is on the significant reduction in total emissions (from HEVs and PHEVs).

However, when the utility factor of PHEVs is too low (below 45%), HEVs and BEVs would replace them in the optimal sales mix. Table 3 provides a recap of the main findings for the optimal passenger car sales mix and break-even points with respect to battery production capacity, providing a clear message for an open debate with automotive manufacturers and regulatory authorities, which will be especially relevant in the 2030 time frame.

Table 3: Passenger car sales mix minimising WTW GHG emissions with break-even points

Note: the vehicle type mentioned in parentheses represents the dominant option within each sales mix.

	BATTERY PRODUCTION CAPACITY CONSTRAINT (TWh/year)					
PHEV UTILITY FACTOR	**Low 0.05–0.15**	**Medium 0.15–0.3**	**High 0.3–0.4**	**High 0.4–0.55**	**Very high 0.55–0.8**	**Relaxed >0.8**
Low: ≤45%	BEV+HEV (HEV)			BEV+HEV (BEV)		BEV
Medium/high: >45%	HEV+PHEV (HEV)	HEV+PHEV (PHEV)	PHEV+BEV (PHEV)		PHEV+BEV (BEV)	BEV

Notes:
Current capacity in 2021: 0.037 TWh/year.
Range of expected capacity in 2030: 0.3–0.95 TWh/year.

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Regulator-suggested 'temperature correction' of biodegradation rates leads to overestimation of persistence for hydrocarbon substances

Since 2017, the European Chemicals Agency (ECHA) has required that all new biodegradation simulation tests be carried out at 12°C, and now also requires that half-life criteria resulting from studies previously undertaken at higher temperatures be 'temperature-corrected' to 12°C using a generic mathematical equation know as the Arrhenius equation. This article outlines why, in Concawe's view, the use of such a generic approach to adjusting biodegradation rates for petroleum substances is not appropriate, and why a more nuanced, hydrocarbon-specific appproach would be justified.

Background

Biodegradability testing indicates whether a chemical will degrade or persist in the environment

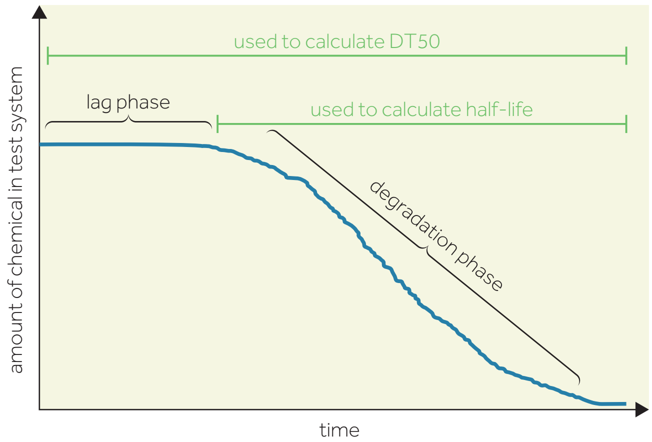
Biodegradation—the breakdown of chemicals by microbes in water, soil and sediment—is a major pathway for the removal of chemicals from the environment. The ubiquity of microbes and their metabolic diversity gives them the collective ability to utilise a stunning array of chemicals as carbon and energy sources. Humans have taken great advantage of the ability of microbes to degrade chemicals to clean waste water in water treatment facilities, to remediate contaminated sites, etc.

Environmental protection requires limiting the accumulation of chemicals in the environment so that they do not reach harmful levels. This potential to accumulate is referred to as the persistence (P) of the chemical and is estimated mostly by the biodegradability of that chemical. A chemical that biodegrades does not accumulate in the environment. However, it is a challenge to establish the biodegradability of a chemical in a clear standardised fashion for regulatory purposes.

Biodegradation testing is required for chemical registration under REACH. These tests involve introducing the chemical into an environmental medium (water, soil or sediment) and observing the microbially-mediated degradation of the chemical. The microbes in the test system are typically taken from environmental samples and consist of a variety of organisms. It is the diversity and density of microbes that affects the probability of an intrinsically biodegradable chemical to have a positive test outcome. For example, if the microbial density is too low, even if there are organisms that can degrade the chemical (known as competent degraders) there would be too few of them to observe biodegradation within the test time frame. Similarly, if there are too few different types of microbes, the diversity of the microbial population would be so low that the chances of a competent degrader being present would also be low.

There are several standardised OECD guideline methods for testing biodegradability of a chemical in different environmental media, with biodegradation simulation tests being used for P assessment. In these simulation tests, a relatively pristine environmental sample with its microbiota is incubated with the test chemical. Biodegradation is typically monitored directly by measuring the chemical in the test system over time (see Figure 1 on page 61). In an OECD simulation test system, there is normally a lag phase where there is no biodegradation and the chemical concentration is stable. During the lag phase, the microbial population adjusts to the presence of an available chemical for consumption, allowing the competent degraders of the test chemical to increase in population. At this point, the competent degraders begin to break down the chemical to a measurable degree. The rate at which the chemical degrades is often reported as a half-life, or the amount of time needed for 50% of the chemical to degrade during the degradation phase shown in Figure 1. An alternative metric is the DT50, which includes the lag phase when calculating the amount of time needed for 50% of the chemical to degrade.

Figure 1: Typical biodegradation curve in a biodegradation test



For regulatory designation of persistence, half-life criteria under REACH have been set for soil, sediment and water, as shown in Table 1. There are specific OECD simulation test methods (OECD 307, 308 and 309) which generate half-life values in these compartments for direct comparison with the criteria.

Table 1: Persistence criteria under REACH

Environmental compartments	Persistent (half life, days)	Very persistent (half life, days)
Marine water	60	60
Fresh or estuarine water	40	60
Marine sediment	180	180
Fresh or estuarine sediment	120	180
Soil	120	180

Biodegradation is a function of both the nature of the test substance (physicochemical properties, bonding, etc.) and the environmental parameters in which it is found (temperature, organic loading, etc.). The set-up of a simulation test can, therefore, greatly alter the perceived biodegradability of the test substance. The rate of biodegradation, or the half-life, will vary depending on the microbes involved and the environmental parameters. If the environment is unsuitable for the competent degraders, for example too saline, too hot or too cold, biodegradation will be slower than under optimal conditions. As mentioned above, the parameters of a biodegradation test should reflect common environmental circumstances under which the guidelines were developed. For convenience, OECD simulation and other similar tests have, historically, been performed largely at room temperature (20–25°C), and so the half-life criteria in Table 1 to designate persistent chemicals were based on experimental data also generated at this temperature range.

Regulator-suggested 'temperature correction' of biodegradation rates leads to overestimation of persistence for hydrocarbon substances

The change

New standard from ECHA to change the temperature of biodegradability testing to reflect typical temperatures in Europe

Starting in 2013, ECHA began requesting biodegradation simulation testing at 12°C, and then in 2017 ECHA altered its guidance so that it required all new simulation testing to be performed at 12°C, which is the average temperature of European waters.[1] This is consistent with REACH Annex XIII requirements that biodegradation testing reflects relevant environmental parameters. However, there are some practical issues associated with this change. Testing laboratories will need to have appropriate incubators and protocols, since testing will no longer take place at room temperature. A more pressing concern is that the persistence criteria in Table 1 have been established based on data at 20–25°C. If the temperature at which biodegradation data are being generated is changed, the persistence criteria would also need to be adjusted to values appropriate at 12°C. Finally, it has been repeatedly shown in literature that changing the temperature of the microbial inoculum, i.e. temperature manipulation, will change its behaviour. For example, a river water sample taken at 5°C will not have the same microbial profile or activity if it is incubated at 20°C and vice versa. Thus the goal of having an environmentally-representative biodegradation test is thwarted if the temperature of the inoculum is greatly altered from its source. The guidance issued by ECHA should be clearer on the way the inoculum is gathered and used.

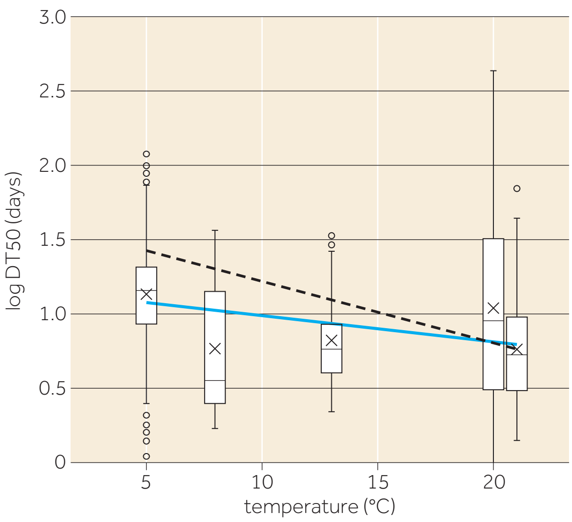
ECHA now also requires that biodegradation half-lives from any studies performed at higher temperatures be 'temperature corrected' to 12°C using a specific mathematical equation known as the Arrhenius equation. The Arrhenius equation shows an exponential relationship between chemical reaction rates and temperature (lower temperature = slower reaction rate, and so in this case longer half-lives and DT50s). The specific Arrhenius equation recommended by ECHA is derived from degradation data on pesticides, with the intention to adjust half-life data for exposure assessment. In Concawe's view, the use of the generic Arrhenius equation offered by ECHA is not appropriate for adjusting biodegradation rates for petroleum substances. The guidance allows for the use of chemical-specific corrections. A petroleum hydrocarbon-specific approach is justified in a Concawe article published in 2020 in the peer-reviewed journal *Science of the Total Environment*, entitled 'Is the Arrhenius-correction of biodegradation rates, as recommended through REACH guidance, fit for environmentally relevant conditions? An example from petroleum biodegradation in environmental systems' (Brown *et al.*, 2020).[2]

The issue

Use of the default Arrhenius equation to 'temperature correct' biodegradation half-lives greatly overestimates persistence for petroleum hydrocarbons

The goal of the Brown *et al.* paper was to determine the relationship between temperature and biodegradation rates for petroleum hydrocarbons from available biodegradation test data. Another publication[3] had already demonstrated in 2018 that the Arrhenius approach does not apply to the biodegradation of petroleum at low temperatures in seawater. Indeed, the biodegradation rates observed in that study are remarkably similar at -1.7, -1 and 5°C. In the Brown *et al.* paper, thanks to the large volume of petroleum hydrocarbon biodegradation data available in the literature, 993 data points on 326 hydrocarbon constituents across a temperature range of 5–21°C were available for consideration. The data were from tests in which the microbial inoculum was incubated within 5°C of their source temperature, meaning that they were 'temperature-adapted' and not 'temperature-manipulated'. The results (Figure 2) show that there is a correlation between temperature and DT50 when looking at 5–21°C, although the data are quite scattered. It would seem that the 5°C points are driving the correlation, such that if the 5°C data are removed, there is little correlation between DT50 and temperature. Still, the overall correlation (blue solid line) shows a lower effect of temperature on DT50 than ECHA's Arrhenius equation would predict (dashed black line). Thus, it is inaccurate to use the Arrhenius equation as described in the ECHA guidance to 'correct' DT50s for petroleum substances, as it would result in an overestimation of the DT50 (slower biodegradation rate). Furthermore, for the substances where a half-life instead of DT50 could be calculated, there was a poorer correlation with the Arrhenius prediction. This result truly undermines the use of the Arrhenius equation since half-lives are the metric for the persistence criteria under REACH. The direct impact of using the generic temperature correction method for petroleum substances is likely a higher number of hydrocarbons being concluded as 'persistent' when they would have been 'not persistent' if tested at 12°C.

Figure 2: Box plot of log DT50 (days) measured at different temperatures for all hydrocarbons available in the data set



Notes:

The box plot includes median, inner quartiles, min, max and outliers at different temperatures.

The crosses represent mean values.

The blue line shows the result of the simple linear regression ($y = -0.018x + 1.2$).

The dashed black line is the Arrhenius temperature dependency ($y = -0.042x + 1.7$) based using Ea = 65.4 kJ mol−1.[4]

It is not only petroleum substances for which the Arrhenius relationship has been shown to be inappropriate. Another recent publication looked at micropollutants and similarly concluded that the classic Arrhenius equation does not capture the effect of temperature on biodegradation rates with a temperature-manipulated system.[5] The authors explain that Arrhenius does not account for multiple enzyme systems that could have different temperature ranges existing in the same microbial community.

The explanation

Using the Arrhenius equation to 'temperature correct' biodegradation rates ignores the biological complexity of microbial systems

In the OECD simulation tests, many species make up the microbial community naturally found in environmental media. These microbial communities are adapted to their ambient temperatures. Different geographical locations with different temperatures may have different species (and thus different biodegradation capabilities) that are adapted to their ambient temperatures. When a microbial inoculum with its inherent microbial community is shifted to a different temperature from that of the source (temperature-manipulated), the relative populations of the microbial species in those communities shift. For example, those microbes that are more cold-tolerant may increase in relative density at a colder temperature. No new microbes are introduced. Since it is the same microbes (and same set of biodegradation capabilities) in this case, an Arrhenius-type relationship is expected. A soon-to-be-published study by the Danish Technical University sponsored by Concawe affirms that there is a reduction in biodegradation rate with temperature if one microbial community is used. Such a temperature-manipulated system is, however, of less environmental relevance, since it implies changing the temperature from which the microbial community comes. In the environment, the degradation process will take place at the same temperature to which the microbial community is adapted.

Competent degraders in an inoculum would normally have temperature optima that are in the range of their ambient temperature. Practically, this means that a microbial community adapted to a low temperature may perform as well as another microbial community at a higher temperature, as has been seen in the above-mentioned literature. This is particularly the case for hydrocarbons, which are ubiquitous in the environment, because many different organisms are capable of biodegrading them (not just one organism that performs well at one temperature).

Conclusions

Temperature adjustment of petroleum substance biodegradation data should be specific for petroleum substances

Concawe concludes that biodegradation rates for petroleum substances do not follow the generic Arrhenius relationship in ECHA's guidance. Based on the data analysed by Brown *et al.* the relationship between temperature and biodegradation rate for petroleum hydrocarbons is variable and weaker than predicted by the generic Arrhenius relationship. Substance-specific data for petroleum hydrocarbons should be used to avoid an erroneously long half-life calculation.

With ECHA's PBT (persistence, bioaccumulation and toxicity) guidance to either 'correct' biodegradation half-lives using the Arrhenius equation or to perform testing at 12°C regardless of the temperature at the inoculum source, biodegradation assessments lose their environmental relevance. Adjustment using the generic Arrhenius equation from ECHA would result in incorrect half-lives, which would be overly conservative. It will (and has) resulted in chemicals that are biodegradable in the environment being erroneously flagged as persistent and listed as Substances of Very High Concern (SVHC).[6] This is exacerbated by the lack of adjustment of the persistence criteria that were established at 20°C. Substances on the SVHC list can be subject to authorisation or restriction, greatly impacting the sale and use of those chemicals.

Through this article and further stakeholder engagement, Concawe is seeking to highlight the technical drawbacks and regulatory repercussions of ECHA's 'temperature correction' guidance. While Concawe agrees with the need for more accurate persistence assessment, a blanket 'temperature correction' does not solve the problem. As advocated in the Brown *et al*. paper, a nuanced approach to adjusting biodegradation results based on the inoculum source and the type of chemical would be more appropriate.

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Cat-App:[1] learnings from a multi-year research programme on alternatives to animal testing

One of the aims of the REACH regulation is to promote alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals. However, in practice it has proven to be challenging to obtain regulatory acceptance for the application of such alternatives alongside existing toxicology data to minimise or replace the standard required animal tests. At the same time, the alternative options currently proposed under REACH are not practically applicable to petroleum substances. Concawe's Cat-App project aims to address these challenges through ongoing research which helps to ensure that excessive animal testing is avoided and the opportunities provided by REACH to innovate the conservative toxicology testing paradigm can eventually be put into practice.

A 'twin challenge'

Because of the increasing and extensive need for animal testing as a default requirement to fulfil human health endpoints in the REACH dossiers, there is pressure to minimise laboratory animal use when complying with the REACH regulation. However:

1. it is challenging to justify the application of available alternative methods to avoid unnecessary animal testing under the regulation; while at the same time
2. the currently available alternative methods are not practically applicable to petroleum substances due to their inherent chemical complexity.

A rough calculation conducted by Concawe estimates that strict compliance with all data requirements in the petroleum substance REACH dossiers would incur a worst-case testing cost of more than €400 million for the current 168 actively registered substances, together with more than 25 years of testing and a need for around 1 million animals.[2, [1]] This is clearly undesirable from both animal welfare and cost perspectives. Furthermore, in terms of innovation, with an industry in transition, as well as from a timing perspective (it would take decades for these animal test programmes—and, therefore, the regulatory assessments—to be concluded), such an approach is not sustainable. In addition, the benefit that these extensive programmes will bring to better protect human health from the potential risks of exposure to petroleum substances is questionable. Both the hazards and risks are already assessed and carefully managed, based on a conservative application of available toxicological data on categories of petroleum substances from decades of testing under regulatory schemes, extensive research programmes and continuously growing expertise.

To address the needs of both regulators and the industry, there are opportunities under the regulation to avoid unnecessary animal testing and speed up the regulatory assessment. The two main approaches are the concept of data sharing (e.g. joint chemical dossier submissions through a consortium of companies registering the same chemical), and the application of alternative methods and approaches. The latter are described in Annex XI of the REACH regulation,[2] and the main tool described therein is the use of grouping and 'read-across'. The idea is that substances with similar molecular structures can be grouped together, and data on one substance can be applied via read-across to another one with a similar molecular structure for which no data are available.

This is a straightforward concept, until your substances contain thousands to millions of molecules ...

[1] New technologies to underpin CATegory APProaches and read-across in regulatory programmes.

[2] Figures previously published in Concawe (2019)[1] have been updated for this article based on the most recent number of registered substances and cost estimates (Spring 2021).

The aim of Cat-App

How can one apply grouping and read-across of data, when the similarity between the group members cannot be exhaustively proven—at least not by structural data, which is the main regulatory requirement? Petroleum substances are so-called UVCBs: substances which are of partly unknown or variable composition, complex reaction products, or of biological origin. In other words, these are substances that are challenging to assess, as they may contain thousands to millions of molecules and are variable in nature; for example, crude oil composition varies between fields and with production time, as well as due to the physical chemistry of boiling crude oil. This means that a substance will never be 100% the same if sampled from one day to another, and its composition can never be described with 100% accuracy. Having said that, petroleum substances are only made of hydrocarbons within a defined range of carbon chain length, and possess various chemical characteristics (aliphatics, naphthenics, aromatics) which constitute the hydrocarbon space of each substance. The constituents that matter from a hazard point of view, such as benzene and polycyclic aromatic hydrocarbons, can be identified and quantified. In addition, the compositions will not vary endlessly as they will need to meet product specifications which limit their boundary compositions. Nevertheless, from a regulatory perspective, it is not yet certain whether these minimal requirements — and the remaining uncertainty — are acceptable for describing UVCB substances.

The question is whether it matters when we do not exhaustively know the composition of the substance. What matters most, for regulatory purposes, is the confidence that we do not underestimate the potential hazards and risk of any substance and all of its constituents, i.e. describing and understanding the full chemical composition (the chemical space or, for a petroleum substance, its hydrocarbon space) is necessary for hazard assessment. Elaborated analytical research is enabling an increased understanding of the hydrocarbon space of petroleum substances. Because we know that the analytical composition of a substance drives its biological response, we can hypothesise that a group of complex petroleum substances within a globally similar hydrocarbon space will have a similar (global) biological response. The 'hydrocarbon space' now becomes a 'hydrocarbon-biological space', adding additional confidence in the grouping of substances with multi-dimensional data, to ultimately tackle the challenges described earlier with the application of read-across of data on petroleum substance UVCBs while not underestimating the potential hazards.

Such a framework, which Cat-App aims to achieve, will enable the most optimal use of the available toxicological information on petroleum substances by chemical-biological read-across, and will help to target additional animal testing in an informed way and only where really needed as a last resort, instead of blindly testing all substances where a data gap exists.

> ***Cat-App is based on the concept of chemical-biological read across***
>
> *The chemical space of a group of petroleum substances is defined by their hydrocarbon constituents with a specific range of carbon chain length and chemical characteristics. These constituents drive the biological responses of these substances, i.e. they define their biological space. Substances can therefore be grouped in both dimensions of the chemical-biological space, facilitating read-across supported by chemical and biological parameters.*

This general concept might sound straightforward, but we still find ourselves on an exciting bumpy road of defining and generating the necessary scientific evidence for this framework while not losing sight of the practical relevance in a regulatory context. The remainder of this article explains how the first phase of this journey, which started in 2015, was completed. It presents a selection of the data that best reflect the main findings so far, explaining why we are not yet at the journey's end, and describing the opportunities that exist to enable progress in the years ahead.

A multi-year international research consortium

In 2016, an article in a previous edition of the Concawe *Review* (Vol. 25, No. 2) described how the field of toxicological sciences was changing. In particular, the article described how a vision for toxicology testing in the 21st century, published by the US National Research Council [3] and known as Tox21c, *'has fuelled the discussion and changed the perspective on conservative animal-based toxicology studies, driven by animal welfare considerations and the revolutionary advances made in the field of biotechnology over the past decades. The main aim of Tox21c is to take advantage of these technological breakthroughs and move away from a regulatory testing paradigm that is currently still based on vertebrate animal models, following the '3R'* [4] *principle in toxicology testing: Refinement, Reduction and eventual Replacement of animal studies for research purposes'.* [5] Therefore, instead of studying observable outcomes in response to chemical exposures in an animal, such as the formation of a tumour 'in vivo',[3] one would eventually predict such an effect by studying the cellular or molecular mechanisms in the initiation and formation of a tumour 'in vitro'.[4] Unfortunately, as will be explained later, in-vitro assays are currently still not sufficient to fully *Replace* an animal test in order to predict toxicity in a human and meet regulatory requirements. Nevertheless, such types of mechanistic, or biological, responses observed after exposure of a cellular system to a substance provide highly valuable knowledge which can be smartly applied as supporting information to further *Refine* and *Reduce* required animal testing. These are the types of biological response data that are obtained from in-vitro assays, which are at the heart of the Cat-App framework.

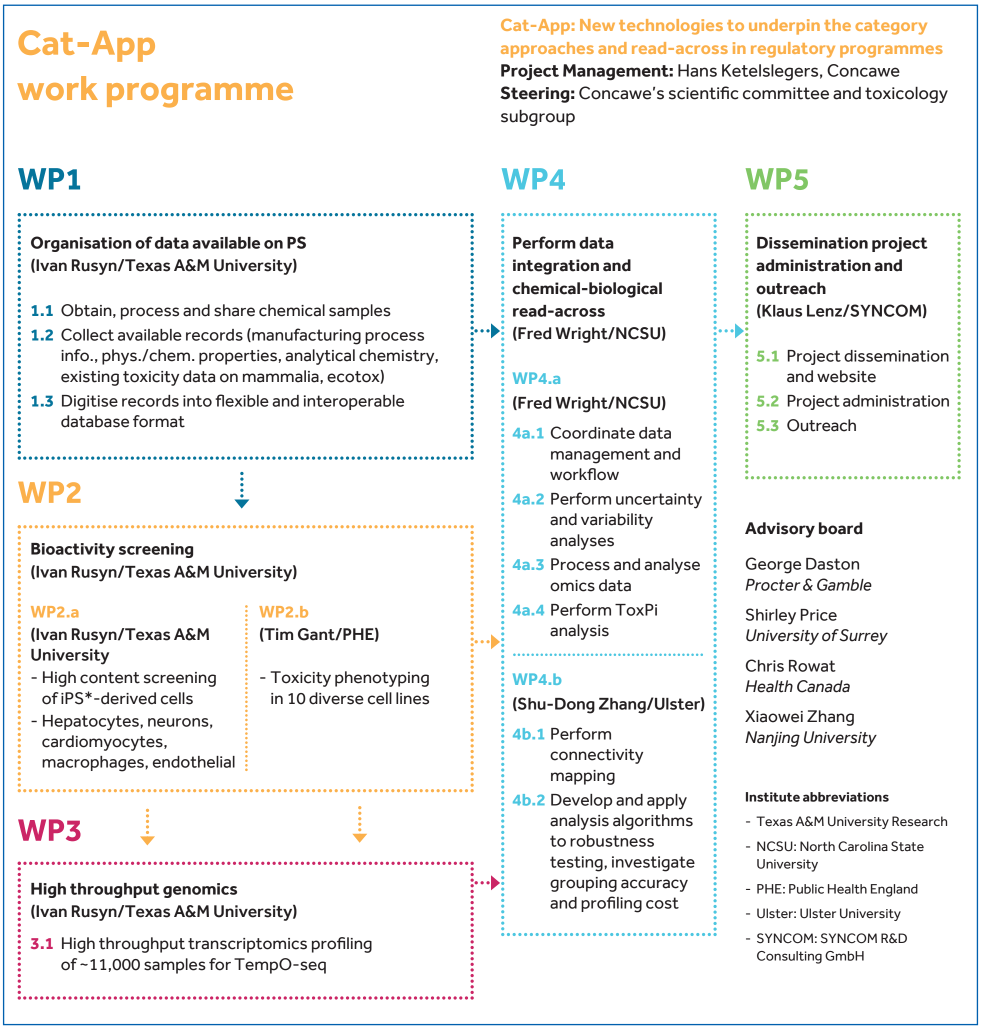
> *At the heart of the Cat-App framework are in-vitro data: mechanistic, or biological, responses observed after exposure of a (human) cell system to a substance which can be smartly applied as supporting information to further refine and reduce required animal testing.*

[3] In vivo: Latin for 'within the living', i.e. testing in a whole living animal.

[4] In vitro: Latin for 'in glass', i.e. testing the components of an organism isolated from their normal biological context (organs, cells, subcellular components, molecules such as DNA, etc.).

To develop this approach, Concawe established a research consortium in 2015 with multiple partners and scientific advisers from the US, UK, Canada, Asia and Europe. Participating organisations and their roles are shown in Figure 1.

Figure 1: Overview of the Cat-App research consortium



* Induced pluripotent stem cells

The work began in 2016, and was divided into five different work packages (WPs). WP1 collected samples, as well as any relevant existing data (e.g. phys-chem and analytical), from 141 petroleum substances. By extracting the biologically active fraction of the substance using dimethylsulphoxide (DMSO), this WP also coordinated the generation of petroleum substance extracts (PS-E[5]) which ensure that the lipophilic substances can be introduced into the aqueous environment of the in-vitro assays.

[5] In this article, the test samples are referred to as 'PS-E' to indicate the distinction from full petroleum substance UVCBs.

Cat-App: learnings from a multi-year research programme on alternatives to animal testing

This DMSO extraction approach is an established methodology, and the PS-E obtained using this method are used routinely for safety testing (e.g. mutagenicity) and chemical characterisation of the refinery streams.[6] Overall, the 141 PS-E tested in Cat-App represent the entire continuum of active petroleum substance registrations under REACH, from diverse manufacturing process categories. For statistical visualisation purposes, some categories were merged together, which lead to the 16 Cat-App-specific PS-E categories shown in Table 1.

Cap-App Work Package 1 was responsible for coordinating the generation of petroleum substance extracts (PS-E) which ensure that the biologically active fraction of the lipophilic petroleum substances can be introduced into the aqueous environment of the in-vitro assays.

Table 1: Cat-App-specific petroleum substance categories used in this project

Category	Abbreviation*	Number of samples in category
Petrolatums	P.LAT	3
Paraffin and hydrocarbon waxes/slack waxes	WAX (2)	10
Low boiling point naphthas (gasolines)	NAPHTHA	10
Other lubricant base oils/highly refined base oils	BO (2)	33
Kerosines/MK1 diesel fuel	KER (2)	10
Foots oils	FO	3
Other gas oils	OGO	4
Bitumens/oxidised asphalt	BIT (2)	5
Residual aromatic extracts	RAE	2
Treated distillate aromatic extracts	TDAE	2
Heavy fuel oil components	HFO	27
Unrefined/acid treated oils	UATO	4
Cracked gas oils	CGO	8
Vacuum gas oils, hydrocracked gas oils and distillate fuels	VHGO	10
Straight-run gas oils	SRGO	6
Untreated distillate aromatic extracts	UDAE	4

* The number in brackets represents the number of Concawe categories that were analysed together in Cat-App, which in total makes 20 categories.

Notes:

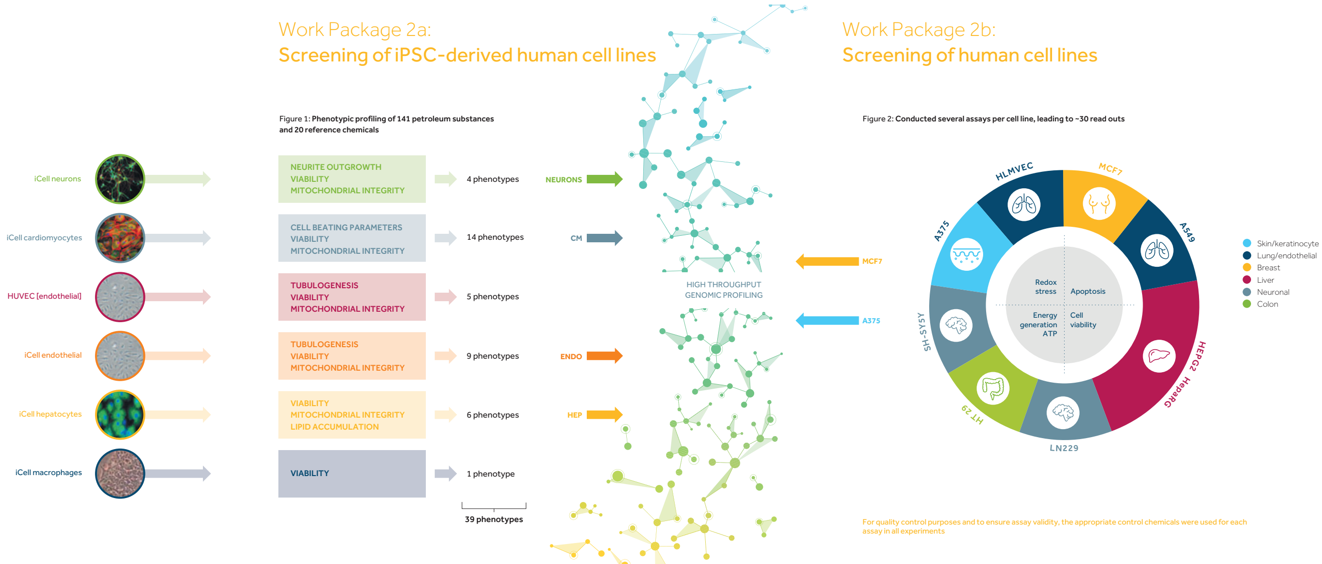
In some cases, closely related substances (PS-E) from different Concawe categories were grouped together solely for statistical and display purposes:

- HRBO was combined into OLBO (BO);
- slack waxes and paraffinic waxes were combined (WAX);
- bitumens were combined with the single substance oxidised asphalt (BIT); and
- a single MK1 was grouped with kerosine (KER).

Subsequently, in WP2, selected cellular systems were exposed to the PS-E of all 141 substances to measure their biological responses, or bioactivity, in these cell models. Cell type and vendor selections were based on the following considerations. Cells had to be of human origin and represent diverse organs/tissues. A number of more conventional, established cell models were used, as well as 'primary' cells, and so-called induced pluripotent stem cell (iPSC)-derived cells which are novel cell models that are more biologically active. All in-vitro models had to be reproducible (i.e. a particular cell/donor can be obtained from a commercial source) and suitable for the evaluation of both 'functional' and 'cytotoxicity' endpoints to enable an assessment of the specificity of the effects of test compounds. It was considered to be more important to have a strong screening assay which delivers consistent and reproducible responses regardless of its toxicological functionality, rather than have a model with a strong biological relevance, as the aim is to support grouping of substances based on a consistent response and not to predict the toxicological effects of a substance. Figure 2 provides an overview of all cell models used in Cat-App, and their in-vitro assays from which the biological response data were generated, i.e. bioactivity monitoring.

In WP2, selected human cell systems were exposed to the PS-E of all 141 substances to measure their biological responses, or bioactivity.

Figure 2: Human cell lines used for Cat-App bioactivity monitoring



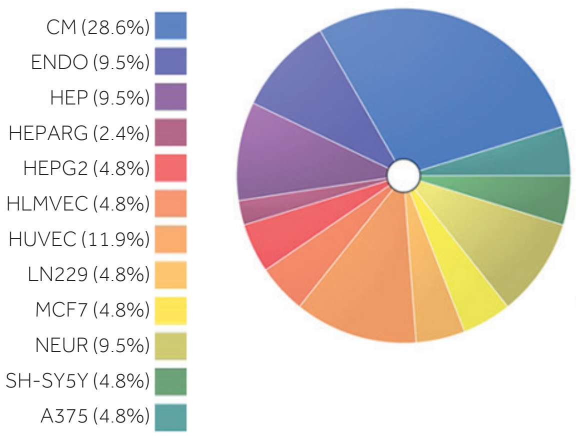
As can be seen in Figure 2, a number of assays which performed best in the biological monitoring experiments were subsequently selected for 'high content genome profiling'. This gene expression profiling, conducted in WP3, investigates the activity of genes, i.e. which genes are turned on or off in these cell systems in response to chemical exposure. It generates further mechanistic understanding behind the biological activity observed from the in-vitro assays. As will be further clarified later in the article, this additional mechanistic information is important for building further confidence in the generated in-vitro data, and as additional evidence in building grouping and read-across hypotheses.

The eventual application of chemical-biological grouping and read-across will require an integrated analysis of all the generated data. For this purpose, the statistical and visualisation tool called ToxPi [7] (Toxicological Prioritisation Index) was used. After running a quality control and uncertainty analysis on all data,[6] WP4 proceeded to run the tool on all assays which passed this control step. The principle behind ToxPi is that all assays (i.e. all biological activity measurements) in one cell model are grouped together in one slice of a pie chart, with weighting in proportion to the number of assays conducted per cell model, as shown in Figure 3.

The gene expression profiling, conducted in Work Package 3, investigates the activity of genes, i.e. which genes are turned on or off in these cell systems in response to chemical exposure, which adds further mechanistic insights into the observed biological responses.

Figure 3: ToxPi construction with bioactivity data

Note: acronyms refer to the cell types shown in Figure 2 on page 71.



Data from 43 assays across 12 cell lines were used to construct a ToxPi for each tested substance. The relative contribution of each cell type is shown on the pie chart.

The result is that each tested PS-E obtains its own bioactivity profile in the form of a ToxPi, integrating all data types (i.e. all cell models and assays). In addition to this overall integrated analysis, which thus compares overall bioactivity from all cell models across all petroleum substance categories, analyses of bioactivity profiles per cell model were also compared between the categories. In this case, the ToxPis for each substance tested were constructed with the pie reflecting a cell type, and each slice reflecting one assay type conducted on that specific cell model (no example is shown here but see, for example, Figure 5 in the next section).

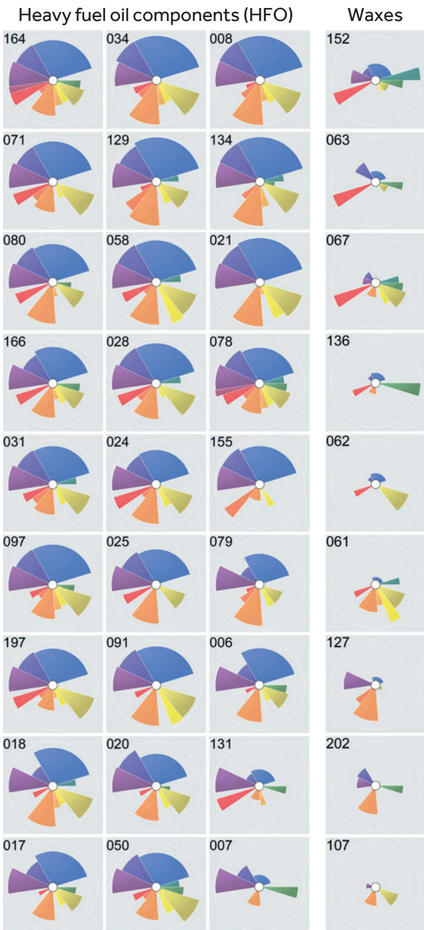
Each tested PS-E obtains its own bioactivity profile in the form of a ToxPi, integrating all data types. Substance-specific ToxPis are scored and ranked into the biological (Fig. 5) and chemical-biological (Fig. 6) spaces.

[6] Results of the quality control are not shown here, but can be found in the Cat-App report[8] which is available online at: www.concawe.eu/cat-app. In brief, 13 of the 15 cell lines used in the experiments were deemed to be of acceptable quality for further analyses. Data from 43 assays conducted in these cell lines were used in further analyses.

Bioactivity-based grouping of petroleum substances

Once every tested substance, or PS-E, has its own bioactivity profile, these can be compared across the different categories of petroleum substances. The hypothesis here is that, globally, substances within one category will have similar bioactivity profiles, as they are chemically similar, while they will be different between different categories of petroleum substances. Figure 4 shows the bioactivity profiles of the individual substances tested in the heavy fuel oils (HFO) and waxes (WAX) categories as an example.

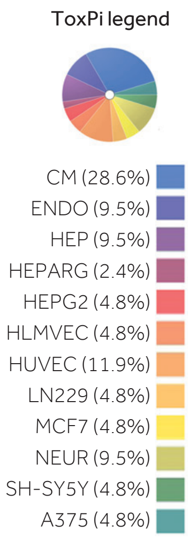
Figure 4: Supervised grouping of petroleum UVCBs based on the bioactivity profiling data (i.e. bioactivity data were grouped based on the existing Cat-APP categories)



ToxPi profiles are shown on the left for substances in the HFO and WAX Concawe categories.

As shown in the legend below, data from 43 assays across 12 cell types were used to construct a ToxPi for each substance tested.

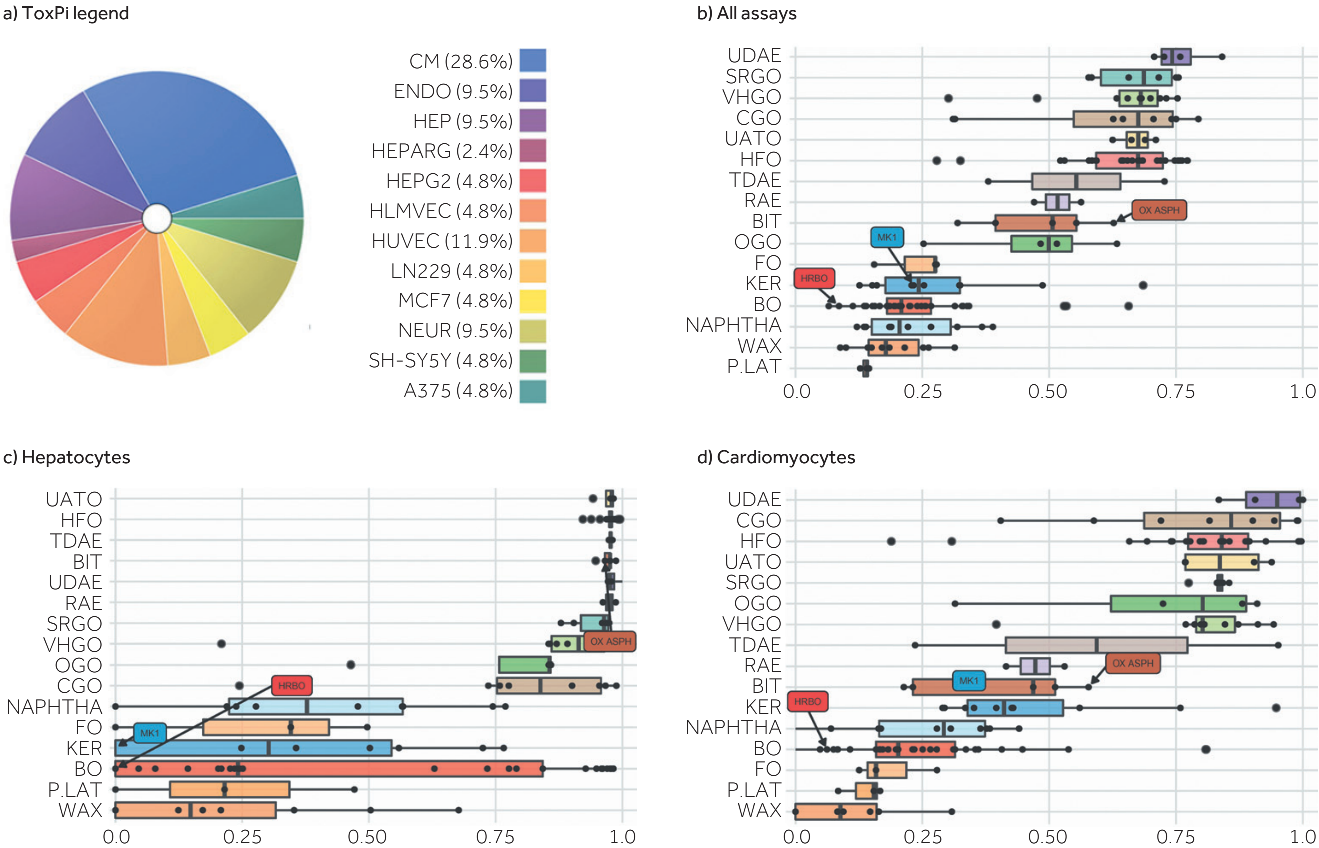
See Table 1 on page 70 for Cat-App-specific groups and acronyms.



In this example, it can be concluded visually that, for the HFO category, most of the PS-E exhibited very similar ToxPi profiles across all cell types, indicating an overall similarity in bioactivity (the left panel on Figure 4). Very different ToxPi profiles from those observed in the HFO category are apparent for the WAX PS-E (right panel on Figure 4). However, some variability among substances in each of the two categories displayed is also apparent. For example, two PS-E in the HFO category (bottom right) are quite different in the observations on cardiomyocytes (blue slice) and other cell types.

To further investigate this observed variability within a category, and to compare the bioactivity-based groups between each other, each ToxPi is scored, ranging from low (0) to high (1) bioactivity. Based on this scoring, all substances can then be ranked and compared to each other, as shown in Figure 5.

Figure 5: ToxPi analysis of the bioactivity data



Notes:

a) Data from 43 assays across 12 cell types were used to construct a ToxPi for each tested substance. The relative contribution of each cell type is shown here.

b) ToxPi scores based on all data for each Concawe category are shown as a box-and-whiskers plot, ranked from low to high bioactivity.

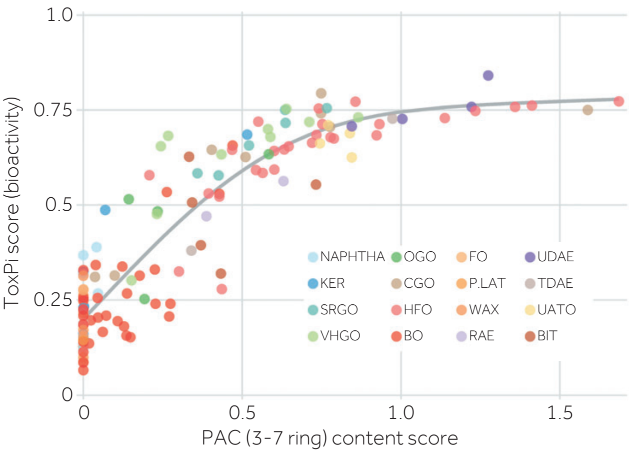
c–d) Separate ToxPi analyses were performed on the data from hepatocytes (i.e. liver cells; 5 assays) and cardiomyocytes (i.e. heart cells; 12 assays). See Table 1 on page 70 for an explanation of the acronyms and Cat-App-specific groupings. Individual substance data are presented in the supplemental material to House *et al.*, 2021.[9]

It is immediately visible that a clear gradient can be observed among the petroleum substance categories (Figure 5b). Overall bioactivities are higher for substances in the HFO, gas oils and aromatic extract categories, compared to, for example, petrolatums and waxes. This trend is well aligned with what is known from decades of toxicology testing on petroleum substances in our industry; the categories that exhibit higher bioactivity, now observed on current samples of petroleum substances, are the ones that are classified for specific hazards based on historical animal test data. The other side of the range can be explained similarly: categories which show almost no bioactivity in the current test samples are the ones that are not classified based on existing toxicological data. This separation is even more apparent when we zoom in to specific cell types: liver cells, shown in Figure 5c, are able to strongly separate the categories of substances into two broad bioactivity regions, whereas the cardiomyocytes (Figure 5d) show a gradient among the categories at the lower bioactivity spectrum. It is clear that, while a gradient of bioactivity exists between the Cat-App categories, there is also an appreciable degree of variability in bioactivity within each category. One explanation is that certain categories of petroleum substances were grouped together for statistical visualisation purposes (see Table 1 on page 70). An example is the merging of highly refined base oils (HRBO) with lubricant base oils (LBO). The HRBO is highlighted in the little red box in Figure 5, and it is obvious that these substances are at the very low end of the bioactivity spectrum. In addition, due to the inherent nature of petroleum substances (they are UVCBs) and due to the physical chemistry of refining, it is expected that these substances will form a continuum in the hydrocarbon space, i.e. they cannot be strictly separated by analytical boundaries. Based on this chemical overlap between categories, and the chemical variation within them, the observed overlap and variability in bioactivity can also be explained.

The observed overall trend is an important finding, and adds new current data to the weight of evidence and historical knowledge on petroleum substances. In addition to providing further confidence in these historical data, another hypothesis can be tested: it is known from the existing toxicology data on petroleum substances that observed effects are mostly driven by the levels of specific constituents in these substances — namely 3-7 ring polycyclic aromatic compounds (PACs). Can the observed variation in bioactivity be explained by the variability in 3-7 ring PAC content of each substance? To examine this, the relationship between bioactivity of the substances and the 3-7 ring PAC content in each substance was evaluated — see Figure 6 on page 76.

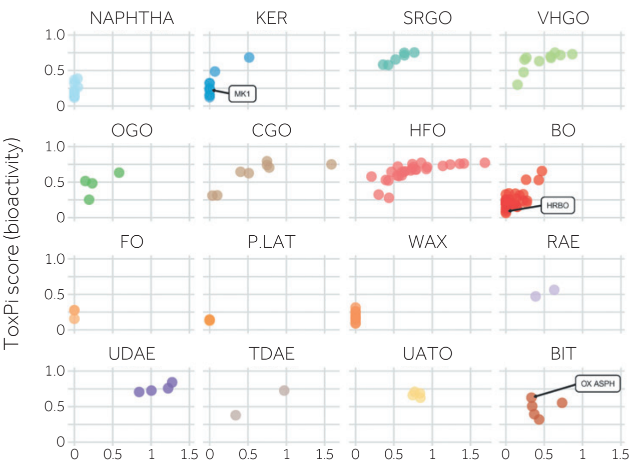
Figure 6: Relationships between the bioactivity-based ToxPi scores of PS-E and the PAH 3-7 ring content score of the petroleum UVCB used in Cat-App

a) Overall correlation plot



a) The chart shows the overall correlation plot with all substances included. The X-axis is the 3-7 ring PAC content score that was calculated by taking the sum of aromatic ring content (for 3 ring- through 7 ring-containing constituents) times the percent total weight of DMSO-extractable PACs determined by the PAC-2 Method. The Y-axis is the cumulative ToxPi score of each substance based on the bioactivity in 13 cell lines. Each substance is marked by a colour that corresponds to Concawe Cat-App-specific categories.

b) Separate plots for each Cat-App-specific category



b) The charts show the same information as above, but each plot contains the substances for a Cat-App-specific category. Note: for statistical visualisation reasons the Concawe categories were merged into 16 classes shown here by 16 colors. Subcategories are noted in the white boxes: MK1 (in KER), HRBO (in BO) and oxidised asphalt (in BIT). For further explanation of Cat-App-specific acronyms and groupings refer to Table 1 on page 70. See the supplemental material in House *et al.*, 2021[9] for cell-specific correlations.

Consistent with the hypothesis, as can be clearly seen in Figure 6, the overall fit for the ToxPi scores based on the bioactivity data from all 13 cell types showed a strong positive correlation (Spearman rho=0.89) with the 3-7 ring PAC content of each substance. The strong overall trend observed is that the higher the level of these constituents is in a substance, the higher the overall bioactivity; e.g. high 3-7 ring PAC-containing substances such as HFO or untreated distillate aromatic extracts (uDAE) show high bioactivity overall. On the other hand, these trends were not observed for the higher-refined substances, which contain low to negligible levels of 3-7 ring PACs, such as HRBO (highlighted in the LBO category), petrolatums, foots oils and waxes. In addition, clear trends can be observed not only overall but also within categories, but these data add further evidence that this can be explained by the variation in chemical composition of the substances even within petroleum substance categories. Overall, the results presented in this Figure corroborate the known relationship between the content of PACs, especially of the 3-7 ring type, in the petroleum refining products with their potential health hazard.

One important note is that these data cannot be interpreted as a quantitative indicator of the human health hazards of a substance. The ToxPi scores and ranking are helpful indicators of observed trends in the global biological response of substances between and within categories, in strong correlation with their (variable) analytical composition. This will not predict a human health hazard endpoint directly, but will help in underpinning the grouping of substances and read-across assessment in an overall integrative testing strategy, which maximises the efficient use of animals needed for toxicological assessments of petroleum UVCBs and reduces the overall time to complete the regulatory assessment of petroleum substances. Grouping and read-across hypotheses are needed to facilitate this, and a further understanding of the biological mechanisms underpinning the global bioactivity trends observed so far can help to build these.

Mechanistic underpinning of the bioactivity-based grouping of petroleum substances

To obtain this mechanistic information, gene expression changes were investigated in selected cell models which were exposed to the PS-E. Gene expression analysis, also called 'genomic analysis' or 'transcriptomics', investigates the activity of the genome (genes) in cells in response to chemical exposure, i.e. which genes are turned on or off and how strongly; this provides insights into how the biology works, and how it leads to the specific effects observed in earlier experiments. Of all cell models used in the bioactivity experiments, five were selected for genomic analysis based on the following criteria:

i. cells that have passed quality control analyses for bioactivity;
ii. cells that represent a diverse set of human tissues and/or organs; and
iii. priority was given to human iPS cells as these are (proven to be) biologically more active than the conventional cell models. As shown in Figure 2 on page 71, this led to the selection of four i-cell and two human cell line models for genomic analysis.

To get an initial idea of the gene expression activity across the different categories of petroleum substances, the transcriptomic data from all cell models were combined per substance and compared between substance categories. No obvious group-specific effects could be observed (data not shown here; see Concawe Report 24/20[10]). One explanation for this is that even the PS-E tested here contain a large number of constituents which all trigger the expression of various genes, and global genomic activity alone (i.e. just the number of affected genes in response to PS-E exposure) will not, therefore, be a good discriminator. However, when the category comparisons were conducted per cell model, more pronounced separation between categories could be observed in liver cells (Concawe, 2020). Since this effect was again similar to the effects observed in the bioactivity experiments, and correlated strongly with 3-7 ring PAC content, this was a first indicator of the biological mechanisms that will likely be key.

To further investigate this, the gene expression activity was compared between cell models to compare tissue and substance-specific effects. In addition, a more detailed analysis was conducted to understand which specific genes are affected and in which biological pathways (mechanisms) they are involved. As can be seen in the transcriptomic data shown in Figure 7, liver tissue is most responsive to exposure with PS-E.

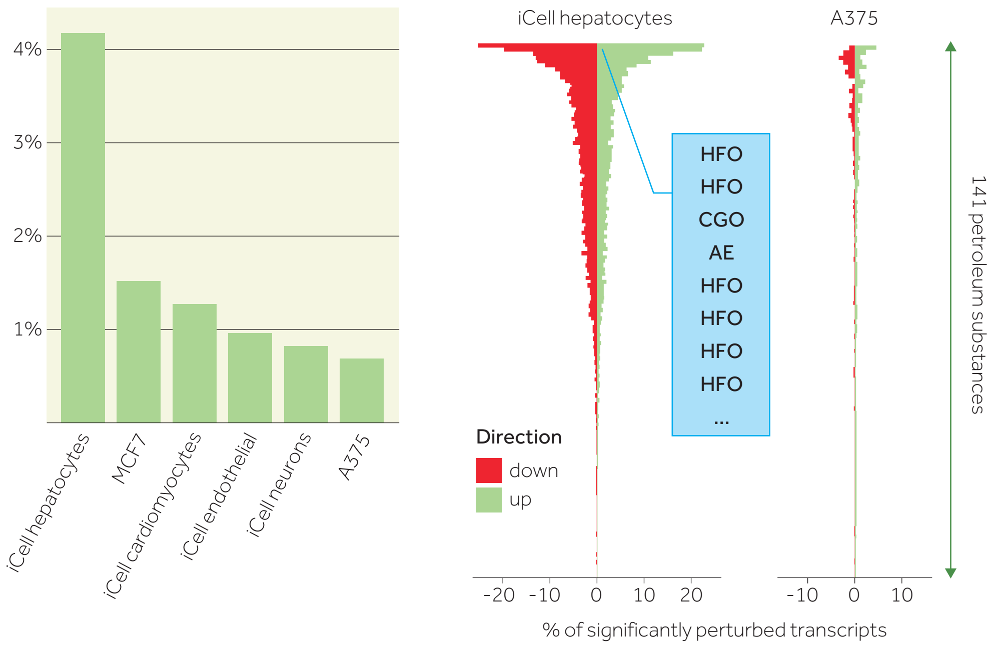
The most probable explanation for this is that liver tissue is more metabolically competent than other tissue. This is confirmed by the fact that PS-E with the highest PAH 3-7 ring content have elicited the most pronounced effects on gene expression. In addition, the functions of the genes and the biological mechanistic pathways in which they are involved all relate to metabolic processes and, specifically, to the metabolism of PACs.

Taken together, this information further underpins the PAC hypothesis for petroleum substances, namely that the level and type of polycyclic aromatic hydrocarbons drive the observed biological responses in human tissue.

Figure 7: Transcriptional effects of DMSO extracts of petroleum UVCBs (PS-E) on gene expression in six cell types

a) The fraction of transcripts affected by all substances

b) Substance and cell type-specific effects of the petroleum UVCBs



Notes:

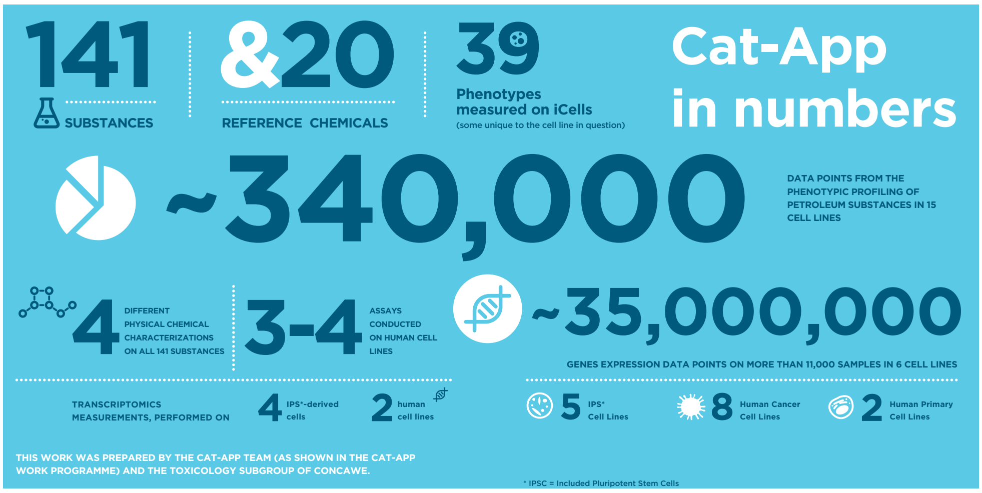
a) Near right: for each cell type, ~3,000 transcripts were evaluated across all 141 substances. For example, 4% represents the proportion of differentially expressed genes in the i-cell hepatocytes.

b) Far right: the i-cell hepatocytes and A375 cells, which represent the cell types that had the most and least pronounced UVCB-induced transcriptional effects, are shown as examples where substances are ranked by the total number of transcripts significantly affected by treatment. Colours represent the directionality of change. The top eight substances (indicated by their Concawe category) are shown in the insert for hepatocytes.

Addressing the 'twin-challenge'

After five years on this journey, Concawe has generated an enormous database with valuable biological information on its petroleum substances (Figure 8).

Figure 8: Infographic of the Cat-App work programme output



All data were published in Concawe Report number 24/20[10] in December 2020, and the initial part of the data was published in a peer-reviewed paper that made headline news in a renowned journal on alternatives to animal testing.[9] To present the scientific progress along the way, the project team organised annual meetings and multiple successful workshops, and presented the work in numerous lectures at international fora. The feedback on the programme, from the scientific community and key stakeholders, has been positive and constructive without exception. However, Concawe regrets that this scientific approach has not yet been accepted by the regulators, which undermines its impact and does not allow the potential benefits for human health testing and animal welfare that the work could bring.

The main aim of this project was to develop a framework which would be directly applicable to address the twin challenge: firstly, the need for animal testing is increasing as this testing strategy is still the default under REACH and, partly because of this, even the solid scientific evidence justifying the use of alternatives to animal data under REACH is proving difficult to get accepted. Secondly, the available alternatives under the regulation are not practically applicable to UVCBs, and this provides an additional challenge for petroleum substances.

It is therefore clear that petroleum substances, and UVCBs in general, warrant an additional approach addressing the specific need to underpin grouping and read-across, which moves away from the standard requirements based on molecular constituents. The main opportunity to make read-across work for complex substance such as UVCBs is to move towards an approach that is group-based and more holistic.

The following key learnings can be derived from the Cat-App programme:

1. The first learning from Cat-App is that, with these data, we can indeed add a biological component to the similarity argument to facilitate the grouping of similar substances. This is key, as manufacturing data, refining history or phys-chem/analytical parameters alone will not be sufficient to prove this grouping concept in the context of addressing the needs for hazard assessment of these substances. It also shows, now from a biological perspective, that petroleum substances form a continuum of substances without hard boundaries between groups.
2. Secondly, the bioactivity strongly correlates with the analytical composition of the substances, in particular the level and types of polycyclic aromatic hydrocarbons, which further underpins the PAC hypothesis for petroleum substances. This learning helps to add further granularity into the grouping exercise, helps to build read-across hypotheses and aids the selection of substances to be tested in the required animal studies.

Overall, it now shows, in multiple dimensions, that petroleum substances form a continuum in the hydrocarbon-biological space, while at the same time chemical-biological trends can be observed across and within the different categories of petroleum substances. This can help to address particular issues with UVCBs regarding unknown constituents and variability of substances, as further animal testing across a wider hydrocarbon space (holistic vs substance by substance approach) can be better targeted and prioritised. On the other hand, it could also help to justify where additional testing might not be immediately prioritised, and can perhaps eventually be addressed by other means in a weight-of-evidence approach applying all relevant available in-vivo and in-vitro data. This has the potential to significantly reduce animal testing, while not underestimating potential hazards, by adding additional biological information into the assessment.

But this is not the end of the journey. The main open issue is that much of this analysis is built around the PAC hypothesis, and from early interactions with authorities on these data, the question is being raised as to how we prove that we are indeed assessing the (biologically) relevant fraction of the substance, and that the remainder of the substance is not relevant in the eventual hazard assessment context. Within that hazard context, it has been deemed from a regulatory perspective that a predictive aspect in the analysis remains absent. However, it should be stressed again that the aim of the project is not to develop an alternative method to replace animal testing at this stage; in other words, Concawe is not aiming to predict toxicity (hazard). These points might not necessarily be a problem when considered purely from a grouping perspective. Nevertheless, they should be addressed when building read-across hypotheses to prove that any potential hazards are not overlooked. Concawe is currently working on a similarity approach to ensure that the entire chemical space of a particular group or groups of substances is assessed. At the same time, work is ongoing to provide further evidence that, for the PS-E, the relevant parts of the substances are tested in the in-vitro assays.

Concawe now has a major opportunity, as part of the organisation's human health strategy, to run Cat-App and other new approach methodologies (NAM) data on samples collected from the animal testing programme. This is being undertaken now, and will provide in-vitro data alongside the animal data from the same experiments, and can therefore lay the foundation for the development of true alternative screening assays. In addition, Concawe has completed, and is initiating, other NAM projects with different academic partners, including non-animal based in-vitro models that target specific hazard endpoints. Many data are already available, hence this is a critical point for Concawe to continue in its journey to make the best use of all of these data. Integration is key, as the combined data will help to further address the issues raised above, as well as helping to further develop these NAM approaches as acceptable alternatives under REACH.

Part of the reason why Concawe still finds itself on a bumpy road to the next stage in this project is that, at the moment, the data have not yet been formally evaluated in our REACH dossiers. As indicated earlier, the authorities have only seen part of the programme and have not yet reviewed the full published data. It is vital that the authorities and industry familiarise themselves with these types of data in a regulatory setting, to enable further development and progress towards the full replacement of animal testing in the longer term. The early applications described above should allow this and, in principle, ECHA should support this paradigm, being that one of the three main aims of the REACH legislation is to 'promote alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals.[11] Hence, it is now of critical importance to have the outcome of this project included into the dossiers.

There have been valuable learnings from this project so far, but the journey continues. It is vital that Concawe continues to push for the opportunities provided by REACH and, by extension, by the EU's Chemical Strategy for Sustainability (CSS), to put into practice the vision for toxicology in the 21st century and ensure that the necessary progress is made.

The animal testing programme that Concawe is conducting as part of its human health strategy for REACH compliance provides an outstanding opportunity to further develop in-vitro assays, as well as the Cat-App framework, which should eventually lead to a more sustainable testing and assessment paradigm.

Special thanks go to the various teams at Concawe, especially the Toxicology Subgroup, as well as Concawe's partners involved in the research consortium (see Figure 1 on page 69), for their innovative science and excellent insights over the past years.

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Abbreviations and terms

AAQ	Ambient Air Quality
AE	Untreated distillate, treated distillate, residual Aromatic Extracts
AQLV	Air Quality Limit Value
B7	Diesel fuel blend containing 7% biodiesel
BEV	Battery Electric Vehicle
BIT	Oxidised asphalt
BO	Other lubricant Base Oils/ highly refined Base Oils
Cat-App	Concawe project to investigate new technologies to underpin CATegory APProaches and read-across in regulatory programmes
CGO	Cracked Gas Oil
CLE	Current Legislation (Scenario)
CNG	Compressed Natural Gas
CSS	The EU's Chemical Strategy for Sustainability
CO_2	Carbon dioxide
CO_2eq	Carbon dioxide equivalent
DME	Dimethyl Ether
DMSO	Dimethylsulphoxide
DT50	Degradation half-time
E5	Petroleum fuel blend containing 5% ethanol
E10	Petroleum fuel blend containing 10% ethanol
EC	European Commission
ECHA	European Chemicals Agency
ED95	Diesel fuel blend containing up to 95% ethanol
EEA	European Environment Agency
EFSA	European Food Safety Authority
ETBE	Ethyl Tertiary Butyl Ether
ETIP	European Technology and Innovation Platform (Batteries Europe)
EU	European Union
EV	Electric Vehicle
FAME	Fatty Acid Methyl Ester
FCEV	Fuel Cell Electric Vehicle
FFV	Flexible Fuel Vehicle
FQD	Fuel Quality Directive
FT	Fischer Tropsch
GHG	GreenHouse Gas
H_2	Hydrogen
HEV	Hybrid Electric Vehicle
HFO	Heavy Fuel Oil
HPDI	High Pressure Direct Injection
HRBO	Highly Refined Base Oil
HVO	Hydrotreated Vegetable Oil
ICCT	International Council on Clean Transportation
ICE	Internal Combustion Engine
IEA	International Energy gency
IFPEN	IFP Energies Nouvelles (French Institute of Petroleum)
IIASA	International Institute for Applied Systems Analysis
iPSC	Induced Pluripotent Stem Cell
JEC	JRC-EUCAR-Concawe consortium
JRC	Joint Research Centre of the European Commission
KER	Kerosene
LCA	Life-Cycle Assessment
Li-ion	Lithium Ion
LNG	Liquefied Natural Gas
LPG	Liquefied Petroleum Gas
LBO	Lubricant Base Oils
MJ	MegaJoule
MTFR	Maximum Technically Feasible Reductions (Scenario)
NAM	New Approach Methodologies
NEDC	New European Driving Cycle
NMVOC	Non-Methane Volatile Organic Compound
NO_2	Nitrogen Dioxide
NO_x	Nitrogen Oxides
NRC	National Research Council (of the US National Academies of Sciences, Engineering, and Medicine
O_3	Ozone
OECD	Organisation for Economic Co-operation and Development
P	Persistence (of a chemical in an environmental system)

Abbreviations and terms

(continued)

PAC	Polycyclic Aromatic Compound
PAH	Polycyclic Aromatic Hydrocarbon
PBT	Persistent, Bioaccumulative and Toxic
PHEV	Plug-in Hybrid Electric Vehicle
PM	Particulate Matter
$PM_{2.5}$/PM_{10}	Particulate Matter with an aerodynamic diameter less than or equal to 2.5/10µm
PS	Petroleum Substances
PS-E	Petroleum Substance Extracts
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RED II	Renewable Energy Directive (Recast to 2030)
RES-T	Renewable Energy Sources in Transport
RFNBO	Renewable Fuel of Non-Biological Origin
SARS-CoV-2	Severe Acute Respiratory Syndrome CoronaVirus-2
SNAP	Selected Nomenclature for sources of Air Pollution
SNG	Synthetic Natural Gas
SVHC	Substances of Very High Concern
SO_x	Sulphur Oxides
TDAE	Treated Distillate Aromatic Extracts
ToxPi	Toxicological Prioritisation Index
TROPOMI	TROPOspheric Monitoring Instrument
TSAP	Thematic Strategy on Air Pollution
TTW	Tank To Wheels
TWh	TeraWatt Hour(s)
UDAE	Untreated Distillate Aromatic Extracts
UK	United Kingdom
UNECE	United Nations Ecocnomic Commission for Europe
UVCB	Substance which are of partly Unknown or Variable composition, Complex reaction products or Biological materials
VDMA	Verband Deutscher Maschinen und Anlagenbau (German Association of Mechanical and Plant Engineering)
VOC	Volatile Organic Compound
WAX	Paraffin and hydrocarbon Waxes/ slack Waxes
WHO	World Health Organization
WLTP	Worldwide harmonised Light vehicle Test Procedure
WP	Work Package
WTT	Well To Tank
WTW	Well To Wheels
xEV	Electrified vehicle (e.g. BEV, HEV, PHEV)

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