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Foreword

As the September 2023 edition of the Concawe *Review* was being finalised, a number of reports discussed the decrease in the biodiversity of the planet. Because the biodiversity contained in different ecosystems can function as a natural carbon sink, its loss could accelerate climate change. The restoration and preservation of ecosystems and biodiversity is one of the key priorities of the European Green Deal, and solutions to limit climate change should not have a negative impact on biodiversity. The first article of this *Review* summarises the findings of a study that Concawe launched with Fraunhofer Institute to quantify the potential impact of the use of biomass, as per Imperial College Consultants' study, on biodiversity. The authors compared different methodologies to quantify the biodiversity state, and evaluated the quantity of miscanthus, as a representative for energy crops, that could be used without negative impact on biodiversity.

July 2023 is reported to have been the hottest July ever, providing further evidence of climate change and the need to implement good solutions. The second article of the *Review* summarises a study that Concawe has launched to assess the real-word energy performance and emissions of plug-in hybrid electric vehicles in a range of usage scenarios (e.g. different battery capacities, recharging frequencies, trip distances, etc.) based on experimental data. The Russian invasion of Ukraine and the resulting sanctions on Russia have highlighted Europe's dependence on strategic resources such as oil and gas, but also on batteries and materials required for renewable energy and the electrification of transport (lithium, cobalt, graphite, rare earth elements, etc.). The European Commission is currently working on a plan for strategic resources, and although numerous battery 'gigafactories' are being built, several articles indicate that a constrained supply of batteries may be unable to meet Europe's 2030 requirements. This article builds on the analysis of the emissions of PHEVs to determine the optimal use of battery capacity to minimise greenhouse gas emission in a battery-constrained world.

The last two articles reflect the origins of Concawe's name, CONservation of Clean Air and Water in Europe. The issues that justified the creation of Concawe in 1963 are just as relevant today, especially with the zero pollution objective of the European Green Deal. The third article presents the results of a modelling study assessing how concentrations of key air pollutants in 2030 and 2050 would compare with the new WHO air quality guidelines and interim targets under different scenarios. The fourth article presents the LNAPL (light non-aqueous phase liquids) Toolbox developed by Concawe—a web-based set of tools which aims to help sites manage their historic hydrocarbon releases to soil and groundwater.

Jean-Marc Sohier

Concawe Director

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Biodiversity impact assessment of future biomass provision for biofuel production

Restoring and preserving biodiversity is widely acknowledged as crucial in the mobilisation of biofeedstocks for biofuels. Following Concawe's joint study with Imperial College Consultants on the potential availability of advanced biofeedstocks (as included in RED II, Annex IX, 2019/319) in the EU-27 + UK by 2030 and 2050, there remains a need to better understand the impact of their use for biofuels on biodiversity. Therefore, a study with Fraunhofer Institute was launched, with the objective of assessing the biodiversity impact of the cultivation of energy crops for biomass production in marginal (unused, abandoned and degraded) lands.

For the study, Miscanthus was chosen as a representative energy crop, and the analysis was conducted for Germany and Bulgaria as representative countries. Fraunhofer employed two recognised methodologies to quantify biodiversity: 1. Biodiversity Impact Assessment (B.I.A) and 2. Potentially Disappeared Fraction of species (PDF). For both methods, in addition to the base case set for unused, abandoned and degraded lands, a sensitivity analysis was conducted for degraded lands to cover their different definitions and characterisations of their current biodiversity state. For the analysis, the data from the 'high biomass availability' scenario in the Imperial College study were used.

Applying the B.I.A method, which is more rigorous compared to PDF, it is concluded that cultivating Miscanthus may have a positive biodiversity impact on degraded lands due to their severely eroded soil. As a result, in Germany and Bulgaria combined, using up to 23% of their marginal lands' biomass potential can lead to biodiversity improvements, while higher utilisation rates up to 50% do not cause any harm. Finally, for both methods, biodiversity change is strongly dependent on the reference state of the land. Therefore, a widely accepted definition, especially for degraded land, needs to be established to address the current uncertainties concerning the characterisation of these lands, and to prevent inaccurate biodiversity conclusions.

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Evaluation of plug-in hybrid vehicles in real-world conditions by simulation and their contribution to mitigating greenhouse gas emissions in a battery-constrained environment

Assessing the real-world energy performance and emissions of plug-in hybrid electric vehicles (PHEVs) is complex: it depends on their usage (trip distance, recharging behaviour), which results in different combined uses of their thermal and electric propulsion.

This article summarises the results of a Concawe study in which vehicle simulators were calibrated using experimental data (in-lab and onroad), allowing a comprehensive range of uses to be evaluated, spanning vehicle configurations, battery capacity, outside temperature and driving profiles. The results were synthesised through a method that weights each simulated use case according to its probability, based on statistics of daily distance travelled and temperature. The assessment was made for a wide range of battery capacities and recharging frequencies, and provided the real-world share of electric drive, CO₂ emissions, and fuel and electricity consumptions of PHEVs according to these two key parameters. It concluded that, in an environment where the supply of batteries will very likely be constrained, PHEVs should be fostered to minimise greenhouse gas emissions providing that they are recharged at least every five driving days.

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Revising EU ambient air quality standards — the implications for compliance in Europe towards 2050 40

This article presents the results of a modelling study carried out to examine how concentrations of key air pollutants (i.e. nitrogen dioxide (NO_2) , particulate matter (PM) and ozone (O_3)) would vary under different emission reduction scenarios, and to assess how these might compare with the new WHO air quality guidelines and interim target metrics which are the basis for the proposed new ambient air quality standards under the revised EU Ambient Air Quality Directive.

The study uses a similar methodology to that supporting *The Second Clean Air Outlook* published by the European Commission in 2021 by considering three emission scenarios: a Current Legislation (CLE) trend scenario and two scenario assumptions about maximum emissions reduction potential (i.e. MTFR and MTFR + 1.5 LIFE). The study also considers some illustrative emission reduction scenarios that were simple cases where emissions from key sectors were set to zero in turn. The purpose was to determine whether emissions from any of the sectors had, individually, a dominating effect on future air quality.

The results of the study indicate that, overall, the outlook for 2030 and for 2050 is that air quality in Europe will improve. Larger improvements will result if consumption is reduced, as well as controls put in place and measures extended to agriculture. The majority of air quality monitoring stations will register short-term and long-term average concentrations that fall within the range of interim target values set out in the recently updated WHO air quality guidelines. However, even under the most ambitious MTFR + 1.5 LIFE scenario, air quality in Europe is unlikely to meet the WHO guideline values by 2050 at many locations in Europe covered by the current monitoring networks.

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The Concawe LNAPL Toolbox

The Concawe LNAPL Toolbox is a web-based tool that provides essential information to the LNAPL remediation community. LNAPL, or light non-aqueous phase liquids, are typically historic hydrocarbon releases into soils and groundwater, such as liquid fuels, crude oil and condensates. The toolbox offers a range of complexity with more than 20 different tools, including infographics, nomographs, calculators, mobility models, videos and checklists. These tools are organised into three tiers, with Tier 1 offering basic graphics and essential information, Tier 2 providing simple quantitative models and calculators, and Tier 3 featuring access to, and explanations of, more complex tools. The Toolbox is designed to address six key questions that are important to environmental consultants and regulators managing LNAPL sites, including determining the amount of LNAPL present, estimating migration and persistence, assessing risk over time, determining the effectiveness of LNAPL recovery, and estimating natural source zone depletion (NSZD).

The Concawe LNAPL Toolbox is one of the first completely online web-based tools for managing LNAPL-impacted sites. It is accessible on the web via an internet browser or by downloading the Toolbox code for use on a personal computer.

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Abbreviations and terms

Concawe reports and other publications

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Phase 1 of a new study, undertaken with Fraunhofer Institute in collaboration with Imperial College Consultants, has been completed to assess the biodiversity impact of the cultivation of energy crops for biomass production in marginal (unused, abandoned and degraded) lands

Phase 1: Biodiversity in marginal lands

Introduction

Sustainable biomass feedstock availability and its impact on biodiversity, the protection and recovery of which is one of the main pillars of the European Green Deal as shown in Figure 1, have been raised by different stakeholders as a justification for minimising the role of biofuels in the decarbonisation of the transport sector.

Figure 1: The European Green Deal¹



In 2021, Concawe contracted Imperial College London Consultants to conduct a study on biomass availability for every EU country + UK by 2030 and 2050.^[1] To comply with the sustainability standards, the study was focused on the advanced biofeedstocks (non-food or feed crops) listed in Parts A and B of Annex IX in the Renewable Energy Directive II (RED II). The future biomass potential was estimated for three different biomass mobilisation scenarios:

- Low scenario: farming and forest practices kept at 2020 levels.
- Medium scenario: improved agricultural/forest management in selected countries in the EU with high biomass availability.
- High scenario: strong management practices and increased availability through research and innovation in all EU countries.

According to the findings of this study, the total theoretical sustainable biomass availability potential by 2050 ranges from 408 to 533 Mtoe, depending on the applied scenario. The amount of sustainable biomass that can be used for biofuels production after deduction of the quantities of biomass allocated to other bioenergy sectors such as power and heating as given in the Impact Assessment by the EU Commission^[2] amounts to 101–252 Mtoe. This amount of sustainable biomass (as listed in RED II Annex IX, parts A and B) is shown to be more than sufficient to satisfy the potential demand for biofuels in the transport sector in 2050 according to Concawe's low-carbon scenarios.^[3]

¹ https://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:52019DC0640&from=ET

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Nevertheless, to guarantee the availability of such biomass for biofuels, additional R&D efforts and the implementation of improved management practices in forestry and agriculture will be required. The supply chain also needs to be developed to mobilise these very important volumes of biomass to the transformation points.

An important element for the acceptance of sustainable biofuels potential is the premise of not harming, or guaranteeing a minimal impact on biodiversity. Biodiversity has been considered in the study on biomass availability by Imperial College London Consultants, based on two principles:

- 1. Conservation of land with significant biodiversity values.
- 2. Land management minimising the effects on biodiversity.

However, Concawe wanted to fine-tune this assessment and better understand how biomass removal for biofuels production affects the biodiversity of natural habitats. We therefore decided to commission a study with Fraunhofer, in collaboration with Imperial College London Consultants, to evaluate more precisely and quantify the impacts on biodiversity.

Scope

In this study on the impact on biodiversity, published in 2022, Fraunhofer Institute focused on assessing the impact on the biodiversity of unused, abandoned and degraded lands as a result of the cultivation of energy crops (choosing Miscanthus crop as a representative example). The definitions of these types of marginal land, as given in RED II, are:

- Unused land: areas which, for a consecutive period of at least five years before the start of cultivation
 of the feedstock used for the production of biofuels, bioliquids and biomass fuels, were neither used
 for the cultivation of food and feed crops or other energy crops nor any substantial amount of fodder
 for grazing animals.
- Abandoned land: unused land, which was used in the past for the cultivation of food and feed crops but where the cultivation of food and feed crops was stopped due to biophysical or socioeconomic constraints.
- Degraded land: land that, for a significant period of time, has either been significantly salinated or presented significantly low organic matter content and has been severely eroded.

This study on the impact on biodiversity focused on Germany and Bulgaria as representative examples of two EU countries with high biomass potential but with significant differences in infrastructure, policy drivers and innovation.

Biodiversity assessment methods

The impact on the biodiversity of a land is defined as the change in the biodiversity quality between the final (after land use) and the pre-use (reference) state. Currently there is no accepted method of reference to quantify the biodiversity quality. For this reason, Fraunhofer used two different recognised biodiversity assessment methods:

- 1. Biodiversity Impact Assessment (B.I.A.), a method by Lindner (Fraunhofer's methodology).
- Potentially Disappeared Fraction of species (PDF), according to Chaudhary & Brooks (International Institute of Applied Systems Analysis (IIASA²) methodology)

Biodiversity Impact Assessment (B.I.A.) method by Lindner (Fraunhofer's methodology)

The B.I.A. method developed by Fraunhofer quantifies the impact on biodiversity quality using different land-use parameters of various importance. The biodiversity quality calculated with this method can become region-specific by multiplying it with a region-specific weighting factor (ecoregion factors). The different ecoregions in Germany and Bulgaria are shown in Figure 2.

Figure 2: Ecoregions in Germany and Bulgaria



As the concept behind this method is to quantify biodiversity quality as a consequence of land use, this method can be successfully implemented to calculate the biodiversity value of marginal lands in 2050 after their use for biomass production but not for the current (reference) state. To quantify the current biodiversity status, the hemeroby concept is deployed. Hemeroby is a land classification system used to assign biodiversity values to lands depending on the degree of anthropogenic interaction that takes place.

² International Institute for Applied Systems Analysis (IIASA) is an independent international research institute with National and Regional Member Organisations in Africa, the Americas, Asia and Europe. https://iiasa.ac.at/

The structure of the hemeroby framework together with the definition of its classes is shown in Table 1. The classification of the marginal land types in the hemeroby list, based on their definitions in RED II and other agricultural directives, was indicated by Fraunhofer and is presented in Table 1. Although the definitions between the hemeroby system and the directives match well for abandoned and unused lands, degraded land can take a broad spectrum of definitions, with hemeroby level V being considered as the best fitting one (set as the base case), and levels IV and VI to be alternative matching options that were considered in this study as part of a sensitivity analysis.

Hemeroby Class	Class name	Different types of land use; indicative examples, to be defined by measurements
I	Natural	Undisturbed ecosystem, pristine forest, no utilisation
II	Close-to-nature	Close-to nature forest management, no thinning
III	Partially close-to-nature	Intermediate forest management (moderate thinning, natural assemblage of species); highly diversified agroforestry systems, low input
IV	Semi-natural	Semi-natural forest management (regular thinning, exotic species); close-to-nature agricultural land use, extensive grassland, orchards, highly structured cropland with low input
V	Partially distant-to-nature	Mono-cultural forest; intermediate agricultural land use with moderate intensity, short rotation coppices
VI	Distant-to-nature	Distant-to-nature agricultural land use
VII	Non-natural artificial	Long-term sealed, degraded or devastated area

Table 1: Fitting of unused, abandoned and degraded lands to the different hemeroby classes according to their definition in RED II and agricultural directives by the EU Commission

Base case

(classification by Fraunhofer as being the most fitting):

- Unused land: Hemeroby class II
- Abandoned land: Hemeroby class III
- Degraded land: Hemeroby class V

Sensitivities

(to capture uncertainty in the classification):

- For unused and abandoned lands, the hemeroby levels II and III fit quite well ⇒ No sensitivity
- Degraded land however showed a broader spectrum of definition ⇒ Sensitivities to levels IV and VI

Potentially Disappeared Fraction of species (PDF) according to Chaudhary and Brooks (IIASA methodology)

This method, developed by IIASA, quantifies the effect on biodiversity in terms of the potentially disappeared fraction of species (species lost per m²) based on the type and intensity of land use. For this reason, species-area relationships are used to calculate species loss for every ecoregion and land use. To make values specific to the two countries, region-specific factors are used. It should be noted that, compared to the B.I.A. methodology, this method is less rigorous as it requires less detailed input data.

Table 2: Land classification according to the PDF method

For the calculation of the current biodiversity state, degraded lands are classified as: Base case = natural habitat/regenerative vegetation (according to original methodology); Sensitivity case 1 = intense cropland; Sensitivity case 2 = light urban area (sensitivities suggested by IIASA's representatives in an ad-hoc meeting)

Broad land use type	Management type	Details	
Natural habitat None		Little or no human disturbance (pristine state).	
Regenerating secondary vegetation	None	Little or no human disturbance.	Base case Best fitting
Managed logged forests	Minimal use (Reduced impact logging (RIL) forests)	Forests managed with RIL techniques designed to minimise impacts on biodiversity.	classification for degraded land
	Light use (Selectively logged forests)	Forests where only selected commercially valuable trees are harvested at a time such that the disturbance is not enough to markedly change the nature of the ecosystem.	
	Intense use (Clear-cut forests)	Forests with extractive use, with even-aged stands and clear-cut patches. The disturbance is severe enough to change the nature of the ecosystem.	
	Minimal use	Extensively managed or mixed timber plantations in which native understorey and/or other native tree species are tolerated, which are not treated with pesticide or fertiliser, and which have not been recently (< 20 years) clear-felled.	
Fightation forests	Light use	Monoculture timber plantations of mixed age with no recent (< 20 years) clear-felling.	•
	Intense use	Monoculture timber plantations with similarly aged trees or timber plantations with extensive recent (< 20 years) clear-felling.	
Pasture	Minimal use	Pasture with minimal input of fertiliser and pesticide and with low stock density (not high enough to cause significant disturbance or to stop regeneration of vegetation).	-
	Light use	Pasture either with significant input of fertiliser or pesticide, or with high stock density (high enough to cause significant disturbance or to stop regeneration of vegetation).	
	Intense use	Pasture with significant input of fertiliser or pesticide, and with high stock density (high enough to cause significant disturbance or to stop regeneration of vegetation).	-
Cropland	Minimal use	Low-intensity farms, typically with small fields, mixed crops, crop rotation, little or no inorganic fertiliser use, little or no pesticide use, little or no ploughing, little or no irrigation, little or no mechanisation.	
	Light use	Medium intensity farming, typically showing some but not many of the following: large fields, annual ploughing, inorganic fertiliser application, pesticide application, irrigation, no crop rotation, mechanisation, monoculture crop. Organic farms in developed countries often fall within this category, as may high-intensity farming in developing countries.	-
	Intense use	High intensity monoculture farming, typically showing many of the following features: large fields, annual ploughing, inorganic fertiliser application, pesticide application, irrigation, mechanisation, no crop rotation.	
	Minimal use	Extensive managed green spaces; villages.	
Urban	Light use	Suburban (e.g. gardens), or small managed or unmanaged green spaces in cities.	Sensitivity analysis:
	Intense use	Fully urban with no significant green spaces.	land classification



The primary drawback of this method is that no differentiation in the current (reference) biodiversity quality between degraded, abandoned and unused lands can be considered. For this method, the closest land use type to all these lands is either the natural habitat or the regenerating secondary vegetation class (see Table 2 on page 8), which implies that even where there is minor human interference biodiversity loss will occur. After an ad-hoc discussion with IIASA's representatives, their recommendation was to run sensitivity analyses considering degraded land as intensive cropland, as well as light urban area classes.

Biodiversity assessment results

To assess the impact that Miscanthus cultivation for biomass production has on the biodiversity of unused, abandoned and degraded lands, the B.I.A. and PDF methods described above were applied. As previously mentioned, B.I.A. has the potential to give more precise results as it is based on more detailed input data compared to PDF. For the analysis with both methods, the production yields of biomass from Miscanthus in 2050 given by the high biomass availability scenario of Imperial College Consultants were used in order to identify the largest positive or negative impact on biodiversity.

B.I.A. method

For the B.I.A. method, the biodiversity quality change is expressed by the biodiversity value increment (BVI), defined as follows:

BVI = biodiversity quality (current, 2020) - biodiversity quality (after land use, 2050)

Given this definition, a positive impact on biodiversity corresponds to negative values for BVI while the opposite happens in the case of biodiversity loss.

As described in the methodology, for the analysis using B.I.A., a base case was set, for which the current biodiversity status of degraded land is matched to hemeroby level V (partially distant-to-nature). Although this level seems to be the best fitting to the different definitions assigned to degraded land, due to the broad spectrum of these definitions, the hemeroby classes IV (semi-natural) and VI (distant-to-nature) were also considered in a sensitivity analysis as alternative options. For unused and abandoned lands, the definitions given in the directives are well established and there is no uncertainty regarding their matching with hemeroby levels.

Base case

To conclude the impact of Miscanthus cultivation on the biodiversity of marginal lands, the biodiversity value increment per kg of Miscanthus in all the NUTS 3³ regions in Bulgaria and Germany is shown in Figure 3. It can be clearly seen from the figure that, in both countries, some regions demonstrate a negative BVI (which means a biodiversity improvement) while others show a positive BVI change (which means a biodiversity loss).

³ NUTS 3 regions = 'small regions for specific diagnoses' as defined in the European Union's NUTS (Nomenclature of territorial units for statistics) 2021 classification. https://ec.europa.eu/eurostat/web/nuts/background

This is explained by the fact that, in the regions that experience biodiversity improvements, degraded lands currently exist in which the cultivation of Miscanthus is shown to enhance local biodiversity. On the other hand, the opposite happens in areas that are rich in unused and abandoned lands; in these areas, such human interference leads to biodiversity losses.

Figure 3: Biodiversity value increment (BVI) per kg of Miscanthus (from 2020 to 2050) in all the NUTS 3 regions in Germany and Bulgaria as a result of Miscanthus cultivation in marginal (degraded, unused and abandoned) lands



To determine the maximum amount of biomass that can be sustainably produced from energy crops in Germany and Bulgaria combined, the cumulative biodiversity quality loss in marginal lands as a function of the biomass produced in the two countries is given in Figure 4. The highest amount of biomass produced annually in the two countries, as calculated in the high biomass availability scenario of Imperial College Consultants, is equal to 14.4 Mt.



Figure 4: Cumulative biodiversity quality loss (from 2020 to 2050, using the B.I.A. method) versus cumulative biomass production as a result of Miscanthus cultivation in marginal lands

Note: the cumulation goes through all the NUTS 3 regions in Germany and Bulgaria, starting with degraded and continuing with abandoned and unused lands.

BVI < 0 means biodiversity benefits. This concerns regions with degraded lands. BVI > 0 means biodiversity damage. This concerns regions with abandoned and unused lands.

The cumulative biodiversity loss curve starts with the areas that are rich in degraded lands, and by aggregating biodiversity benefits, the BVI expectedly decreases (biodiversity improves) up to a Miscanthus production of 3.3 Mt/year, which is equal to 23% of the total biomass that can be produced in the marginal lands of the two countries. Then, by adding the biodiversity losses of areas with abandoned and unused lands, the BVI curve starts to follow an upward trend and reaches a break-even point at 6.9 Mt/year (48% of the total biomass availability potential). Consequently, this is the maximum amount of biomass that can be produced in the two countries combined without harming marginal lands' biodiversity. Higher biomass production rates could potentially damage biodiversity.

While the quantity of Miscanthus that could be produced according to the high scenario (14 Mt/year) of the Imperial College Consultants study introduces a negative impact on the biodiversity of marginal lands in Germany and Bulgaria, this is not the case for the other scenarios: the low scenario, which corresponds to a production rate of 3 Mt/year, is possible with a positive impact on biodiversity, and the medium scenario, corresponding to a production of 7 Mt/y, can be achieved with no harm on biodiversity. As the low and medium scenarios have shown the potential to satisfy the demand for biofuels in the transport sector estimated in Concawe's low carbon scenarios, this study indicates that they can achieve it in a non-harmful or even restorative way for the biodiversity of marginal lands.

Sensitivity analysis

a) Hemeroby class VI (distant-to-nature)

For the two sensitivity cases, in which the distant-to-nature and semi-natural hemeroby classes were used to calculate the current biodiversity status in degraded lands, the impacts of biomass production on biodiversity in the two countries are shown in Figure 5. In contrast to the base case, the biodiversity is either not harmed (distant-to-nature case), even with the maximum production of the high scenario of the Imperial College Consultants study, or is always damaged regardless of the degree of biomass removal (semi-natural case).

Figure 5: Cumulative biodiversity quality loss (from 2020 to 2050) versus cumulative biomass production, as a result of Miscanthus cultivation in marginal lands for (a) Hemeroby class VI and (b) Hemeroby class IV, used for the calculation of the current biodiversity value in degraded lands



b) Hemeroby class IV (semi-natural) Positive values: always potential harm to biodiversity



Potentially Disappeared Fraction of species (PDF) method

For the PDF method, similarly to B.I.A., the biodiversity quality change is expressed as the deviation of the potentially disappeared fractions from the current state to the future:

PDF = PDF (current, 2020) - PDF (current, 2050)

This means that a negative PDF value implies a biodiversity improvement, whereas a positive PDF value implies a biodiversity loss.

As elaborated in the methodology, a base case and two sensitivity cases were established for the application of this second biodiversity assessment method. For the base case, an analogy between the natural habitat class used for the PDF method and the current status of degraded lands was considered. For the sensitivity cases, after an ad-hoc meeting with IIASA and following their indications, it was noted that, due to the broad spectrum of definitions usually given to degraded land, there could be an analogy between the degraded land and the intensive cropland or the light urban area class of the PDF concept.

Base case

For the base case, using the PDF method, regardless of the type of marginal land being considered, even very small amounts of biomass produced have a negative impact on biodiversity quality (positive PDF values). This is not necessarily related to any vulnerability of those lands, but to the inherent inadequacy of this method to provide a representative land-use classification for the initial status of marginal lands. As the closest characterisation in the PDF concept is the natural habitat class (zero interaction with humans), the consequence (see Figure 6) with this method is that even the smallest interference results in a biodiversity loss.

Figure 6: Cumulative biodiversity quality loss (from 2020 to 2050, using the PDF method) versus cumulative biomass production in marginal lands



Note: the cumulation goes through all the NUTS 3 regions in Germany and Bulgaria, starting with degraded and continuing with abandoned and unused lands.

Sensitivity analysis

In the two new sensitivity cases shown in Figure 7, the current human presence is more intense compared to the natural land class assumed for degraded lands in the base case. It therefore follows that the biodiversity quality is of a much lower standard, and using these lands for biomass production up to a certain limit may have a positive impact on biodiversity.

Figure 7: Cumulative biodiversity quality loss in Germany and Bulgaria combined (from 2020 to 2050, using the PDF method) versus cumulative biomass production in marginal lands, with degraded lands to be identified as (a) intensive croplands and (b) urban light areas



Conclusions

The primary conclusions from this study conducted by Fraunhofer Institute are summarised as follows:

- 1. The results show that, according to Fraunhofer Institute's B.I.A. method (base case), the cultivation of Miscanthus for biomass production on degraded lands can lead to a biodiversity improvement.
- 2. Using the Fraunhofer Institute's B.I.A. method (base case) and the Imperial College's biomass availability potential results, the study shows that, in the marginal lands of Germany and Bulgaria combined:
 - Up to 3.3 Mt biomass (23% of the biomass availability potential in these lands and 5% of the total biomass potential for bioenergy coming from the agricultural sector as calculated by Imperial College, and equivalent to the quantities produced in their 'low scenario') can be produced that could improve the biodiversity in marginal lands in the two countries.
 - Up to 6.9 Mt of biomass (almost half of the biomass availability potential in these lands and 11% of the total biomass potential for bioenergy coming from the agricultural sector as calculated by Imperial College, and equivalent to the quantities produced in their 'middle scenario') can be produced without harming the biodiversity in marginal lands in the two countries.
- 3. Both the B.I.A. and PDF methods show that different conclusions can be drawn with different definitions of the current state of land (especially for degraded land). A detailed inventory and definitions of the state of land need to be developed at the EU level.

This study also demonstrates the importance of establishing a method of reference to quantify the impact on biodiversity of biomass production and the need to have a better definition of the precise status of the lands in Europe.

As a next action, Concawe is aiming to conduct another study in which the focus of biodiversity impact assessment will be shifted from unused, abandoned and degraded lands to forests. According to the Imperial College biomass availability analysis, 40–45% of the estimated biomass potential for bioenergy in Europe in 2050 comes from forests; this demonstrates the importance of assessing the imprint that biomass production leaves on the biodiversity of these habitats.

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Introduction

Context

Transport-related greenhouse gas (GHG) emissions represent approximately one quarter of total GHG emissions in the European Union (EU).^[1] In the context of targeting carbon neutrality in 2050, as set by the EU Green Deal,^[2] reducing transport-related GHG emissions represents both an important stake and challenge. The present study focuses on passenger cars only. When considering each vehicle individually, there are several ways to consider their GHG emissions:

- The tank-to-wheels (TTW) approach focuses only on the tailpipe emissions.
- The well-to-wheels (WTW) approach is more complete and considers the GHG emissions related to the production of the energy carriers.
- The life-cycle assessment (LCA) approach is holistic and also considers the GHG emissions related to the production of capital goods that are necessary for the transport system (e.g. vehicles, energy system infrastructure, etc.).

The LCA approach is the most pertinent one as it presents the most relevant assessment of the impact on the climate. Nevertheless, the TTW and WTW approaches should also be considered because they are currently regulated in Europe (TTW for the vehicles according to the CO_2 standards^[3] and WTT with combustion for the fuels according to the EU Renewable Energy Directive (RED II)^[4]). For example, a solution that would have a high performance in the LCA scope but a poor performance in the TTW scope would probably face significant barriers to its development in the EU market.

In this context, plug-in hybrid electric vehicles (PHEVs) represent an interesting option as they seem to address the challenges associated with low GHG emissions at each stage (TTW, WTW and LCA).^[5] Furthermore, they can relieve some of the (time) pressure on the implementation of fast charging infrastructures for battery electric vehicles (BEVs) so as to make their rollout feasible in a shorter time frame. However, it is believed that the assessments currently available in the literature may need to be updated:

- **TTW**: As of today, TTW CO₂ emissions are assessed based on the Worldwide Harmonised Light Vehicle Test Procedure (WLTP) which does not necessarily consider the real-world emissions of the vehicle; this could affect PHEV credibility in the future for at least the following three reasons:
 - i) Some PHEVs are purchased due to tax incentives but are rarely plugged in (especially company cars).^[6]
 - ii) Some journeys are much longer than the Worldwide harmonized Light-duty Test Cycle (WLTC) over which the CO_2 emissions are assessed. It is therefore possible that, in some cases, the internal combustion engine (ICE) runs for a larger proportion of the total distance travelled than expected in the regulation. According to German statistical studies,^[7] only 2% of daily trips are longer than 100 km, but they account for 26% of the mileage driven. These 'rare but long trips' may have a significant impact on the real-world fuel consumption and TTW emissions of PHEVs, which need to be assessed properly.
 - iii) The PHEV has a higher weight than a conventional hybrid electric vehicle (HEV) or pure ICE vehicle a downside for fuel consumption and CO₂ emissions if they are not charged.

Assessing the real-world energy performance and emissions of plug-in hybrid electric vehicles (PHEVs) is complex: it depends on their usage (trip distance, recharging behaviour), and on the different combined uses of their thermal and electric propulsion. This article presents the results of a Concawe study designed to assess the realworld potential for plug-in hybrid vehicles in a battery-constrained environment.

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- WTW and LCA: Several WTW and LCA studies, such as those led by Ricardo^[8] or by IFPEN,^[5,9] rank the PHEV among the best solutions in terms of CO₂ emissions. This is especially true if they use renewable fuels. In some favourable cases, PHEVs can even have lower CO₂ emissions than BEVs over their life cycle as their battery is smaller; this will of course be highly dependent on the driver's behaviour in charging the vehicle, as well as on the carbon intensity of the energy sources. While these studies may have encouraging outcomes for PHEVs, they do not address the question of the real ratio of all-electric drive from PHEVs (raised above, also called the 'utility factor', UF), which may be a limiting factor in the applicability of the study conclusions.
- Systemic aspects: More recently, Concawe developed a study on optimal electrification scenarios for passenger cars, which aimed to minimise their WTW CO₂ emissions under the constraints of battery availability.^[10] It was concluded that, under limited battery availability, PHEVs are the preferred option before BEVs for minimising the WTW CO₂ emissions of new passenger cars, even under conservative UFs ranging between 20% and 50%. This result is explained by the fact that, as long as the overall battery availability is limited, it is more efficient to electrify trips by spreading smaller batteries among many users who use their full capacity than by allocating large batteries to few users who generally use only a small fraction of their full capacity on a daily basis. However, the question remains as to whether the real-world UFs are beyond the 20%–50% threshold identified in this study.

Scope and objectives

If it is understood that PHEVs fuelled by renewable fuels and low-carbon electricity are an interesting option in terms of CO_2 emissions over their life cycle, this technical option also offers the opportunity to reduce the consumption of liquid fuels. This is particularly interesting in the frame of the outcomes of Concawe's work,^[11] which mentions that liquid fuels for road transportation could be 100% low-carbon by 2050, but with a consumption of liquid fuels that could be up to approximately one third compared to today's level to be compliant with the GHG emissions trajectory designed by the European Commission in its 1.5 TECH scenario from 'A Clean Planet For All'.^[12] Hence, for PHEVs fuelled by renewable fuels to be a viable solution in the long term, they need to prove that they can compete with a third of the consumption of liquid fuels as a first approximation (and still comply with this in real-world operation).

In addition to CO_2 emissions and energy consumption, air quality is also an important factor for road transportation. PHEVs are often seen as an asset for air quality as they allow electric drive in urban areas. However, the intermittent electric drive of PHEVs (and hybrids in general) can present additional challenges for tailpipe emissions control due to multiple exhaust after-treatment heating phases during a drive cycle — which are not necessarily well monitored in the current vehicle homologation process. In this context, the aim of this study was to assess the energy performance and emissions of state-of-the-art PHEVs in real-world conditions.

More specifically, this study intends to assess the life-cycle GHG emissions of PHEVs in real-world conditions, including their sensitivity to the behaviour of the driver regarding recharging, to the battery capacity, to the trip distance, to the fuel used (e.g. fossil fuel vs low-carbon renewable fuel) or to the carbon intensity of the electricity mix. This part of the study was built on experimental results detailed in other articles^[13,14] by using simulations. It is the objective of the present article to explain the method used for this part of the study and the results obtained.

The present article provides a detailed description of the following aspects of the study (see also Figure 1):

- The experimental data, used as inputs to the calibration of the vehicle simulator—see *Experimental* data on page 18;
- The calibration of a non-dimensional, physical vehicle simulator and its validation against experimental data (1)—see *Simulation platform set-up* on page 20;
- The projection of the simulation results over a design of experiments (DoE) see Simulations over a Design of Experiments (DoE) on page 22;
- The mathematical methods used to extract patterns from the simulation results database, allowing the energy performance characteristics of PHEVs (CO₂ emissions, fuel and electricity consumptions, and UF) to be obtained from any combination of usage parameters (initial state of charge (SoC) of the battery, trip distance, driving style and profile (urban, extra-urban, highway) and ambient temperature) (3) see *Analytical model rendering* on page 23;
- The statistical data representative of real-world usage, particularly in terms of vehicle-kilometres travelled (VKT) and outside temperature (2)—see *Statistics of use: Representativeness of each use case* on page 25;
- The forecasted energy performance of PHEVs in real-world usage, as a function of their battery capacity and recharge frequency (4)—see *Weighted average outputs* on page 29;
- Subsequently, the results obtained in this study were able to support the development of a vehicle life-cycle GHG emissions interactive platform—see pages 36–37.



Figure 1: Simulation workflow for PHEV energy performance real-world assessment



Methods and data

Experimental data

Two PHEVs complying with Euro 6d standards were evaluated on a chassis dynamometer (Figure 2) and on-road (Figure 3) using the same road profile, complying with RDE requirements (Figure 4). The two vehicles differ only by their powertrain, one being diesel fuelled, and the other being gasoline fuelled (see Table 1 for the main characteristics of the selected vehicles). The two vehicles, a Mercedes C300e (diesel) and a Mercedes C300e (gasoline), were tested under various conditions, including charge-depleting (CD) and charge-sustaining (CS) modes (i.e. tests starting with a fully charged battery and a discharged battery, respectively), with various fuel compositions including traditional fossil-based fuels (B7, E10), 100% renewable hydrotreated vegetable oil (HVO) and 100% renewable gasoline blended with 20% v/v ethanol (E20). The set of measurements included fuel and electricity consumption, CO_2 and regulated pollutant emissions (NO_x , CO, HC, PN23, PM) as well as non-regulated pollutant emissions such as PN10, CH₄, NH₃ and N₂O.

Figure 2: The chassis dynamometer set-up with one of the tested vehicles



Figure 3: Vehicle set-up for on-road tests using a portable emissions measurement system



A significantly higher fuel consumption was observed in the on-road tests than in the chassis dynamometer tests, despite being driven on the same test cycle. This discrepancy is accounted for in the simulation models for an improved fit with real-world data.



Figure 4: Vehicle speed profiles (RDE compliant) measured during chassis dynamometer and on-road tests



Table 1: Main specifications of selected vehicles, and CO_2 emissions in charge-sustaining mode^a (i.e. empty battery at start of test) and weighted between CD mode (i.e. full battery at start of test) and CS mode,^b according to the current regulation

	C300e EQ	C300de EQ			
Regulation	Euro 6d-temp				
Fuel type	Gasoline	Diesel			
Test mass (kg)	1,885	1,970			
WLTP CO ₂ (g/km)	CS: 146 ^a Weighted: 31 ^b	CS: 140 ^a Weighted: 30.5 ^b			
Thermal engine	2.0L 4cyl 155 kW turbo direct injection	2.0L 4cyl 143 kW turbo direct injection			
Transmission	9-speed automatic transmission				
Battery	13.5 kWh 365 V				
Electric motor	90 kW				
Hybridisation	P2 parallel hybrid architecture				
Aftertreatment system	2*three-way catalyst close coupled + gasoline particulate filter underfloor	Diesel oxidation catalyst + selective catalytic reduction filter + selective catalytic reductor close coupled			
Mileage (km)	4,000	14,000			



Simulation platform set-up

The simulations were carried out using Simcenter Amesim[™] software. These models transcribe the physics of all devices present in conventional vehicles (combustion engine, transmission, etc.) and electric vehicles (battery, traction engine, power electronics, etc.). The simulation sketch used in this study is provided in Figure 5 for illustration purposes.



Figure 5: Detailed Simcenter Amesim[™] sketch of a P2 hybrid powertrain

A component dedicated to hybrid architectures (ECMS: Equivalent Consumption Minimisation Strategy) was used to determine the optimal management strategy for internal combustion and electrical energy to minimise fuel consumption. It was calibrated to fit the experimental behaviour characterised on pages 18 and 19, as illustrated in Figures 6 and 7 on page 21.

Figure 6: RDE test cycle simulation for CD mode (on the left) and CS mode (on the right)



Figure 7: Comparison between the experimental and simulation results for the gasoline and diesel PHEVs, in CD and CS modes

measured simulation



c) Charge-depleting mode, diesel PHEV (B7)



b) Charge-sustaining mode, gasoline PHEV (E10)









After calibration, the simulator was fully capable of reproducing the behaviour of the tested PHEVs, at any temperature between -2°C and +35°C, for a range of driving profiles and trip distances, and under any state of charge of the battery. The simulator also provides an extension to accommodate any battery capacity between 2 kWh and 35 kWh (knowing that the tested vehicles were equipped with a 13.5 kWh battery) as well as a non-plug-in HEV (which is basically 120 kg lighter and working only in CS mode as it cannot be recharged). Although this amounts to a significant range of configurations that can be simulated, the results cannot be extrapolated to any other PHEV having, for example, other engine or electric power, or other energy management strategies.

Projection over a comprehensive range of cases

Simulations over a design of experiments (DoE)

A set of simulation results was generated over all possible vehicle use conditions, aiming at extending the simulation results over a broad range of usage (i.e. not only over a specific RDE cycle). The calibrated simulator referred to above was thus used to provide projections for a wide range of driving conditions and styles, weather temperatures, battery sizing and conditioning, etc.

The simulation matrix has five dimensions, which are summarised in Table 2: ICE type (2 levels); PHEV mode (3 levels); driving cycle (24 levels); battery capacity (3 levels); and outside temperature (3 levels). This results in 1,296 possible combinations, all of which were simulated. In practice, more than 3,000 simulations were performed, and provided detailed results, because several shorter driving cycles required repetition to empty the battery and allow the transition from CD mode to CS mode to be observed.

Table 2: Simulation DoE dimensions and features

Dimensions explored	Number of variations	Values
ICE type	2 combustion modes	Gasoline, diesel
PHEV mode	≥3 initial SoC	CD 95% until 15% depletion + CS hot + CS cold
Driving cycle	5+19 speed profiles	WLTC, ARTEMIS x 4 [Road Type 1–>4] x [Road Conditions 1–>7]
Battery capacity	3 capacities	7 kWh, 13.5 kWh, 25 kWh
Outside temperature	3 initial T°	-2°C, 23°C, 35°C

Notes: Road Type 1->4 refers to: inner city; outer city; extra urban; and highway. Road conditions include: jammed circulation; moderate driving; increasingly dynamic patterns, even harsh ones; and finally speeding.

Analytical model rendering

Although simulation can provide any result from any situation once it is properly calibrated, it remains a time-consuming process that cannot be generalised to each practical application. As the study intended to aggregate day-to-day PHEV users' patterns over a whole population, it was necessary to design a simpler analytical method by using the previously generated database. Instead of rerunning simulations, a mathematical post-processing method was developed to bring the results together.

The concept behind the mathematical process developed in this study consists of identifying the asymptotic (lowest) values of energy consumption for each speed profile, to which overconsumptions (i.e. deviations) are then added, knowing that the latter correlate with thermal conditioning. Once consumptions over any clustered cycle can be calculated, they can be summed into a sequence of identified speed profiles, provided as a cycles list and respective mileages, along with the vehicle characteristics and weather conditions. Thereafter, in a loop pattern, a temperature deviation profile and then consumptions can be successively estimated for each segment. Eventually, the addition of all segments indicates the total amounts of electricity and fuel required in this specific use.

To validate the mathematical approach, the same driving cycle was calculated in the physical simulator (Amesim) and with the mathematical equations at -2°C, 10°C, 23°C and 35°C. The results are compared in Figure 8 which shows a good fit between the two sets of results. It can therefore be concluded that the mathematical model is predictive in the range of modelled ambient temperatures [-2°C, 35°C].



Figure 8: Simulation vs mathematically assessed driving sequence for the complete range of ambient temperatures

Note

The values on top of the bars are the % difference between the results of the two simulation methods



Results over generalised usage

Due to the degrees of freedom induced by the architecture of PHEVs, they are extremely versatile, being equally capable of operating almost exclusively on electrical or chemical energy depending on the conditions of use. It is therefore necessary to assess the actual behaviour of PHEVs by:

- evaluating the sensitivity of technologies to the conditions of use; and
- assigning a weighting to each condition according to its representativeness.

Thanks to the simulation work, it was proposed to:

- consider the sensitivities of technologies (particularly to ambient temperature);
- consider a wide range of use cases through statistics;
- consider a broad range of recharging frequencies; and
- vary the battery capacity.

Capturing the sensitivity of technologies: assessment of results on a large matrix

Based on the analytical model described above, each individual use case was simulated as a combination of:

- v conditions of daily VKT and associated driving patterns, 24 cases [4:400 km]
- t conditions of ambient temperature, 20 cases [-2:36°C]
- r conditions of recharge interval, 11 cases [0.5:10 days]
- **b** conditions of battery sizing, 10 cases [2:35 kWh]

Figure 9 on page 25 shows the results of simulations made for one given value of battery capacity (15 kWh) and recharge frequency (every day) for the gasoline PHEV. A total of 480 combinations of temperature/daily mileage were considered.

The simplified mathematical model reproduces the behaviour of the physical model, and therefore also of the vehicles evaluated experimentally. A plateau of high UF values (>95%) is observed for short distance trips (<20 km) as a PHEV recharged every day is able to handle these distances almost completely in allelectric mode. In such cases, a low fuel consumption is consistently observed and a high electrical consumption is stated. A sharp increase in power consumption in cold ambient conditions is observed as a consequence of battery and cabin conditioning. As trips become longer, the battery SoC decreases, resulting in a sharp decrease in the UF. Consequently, the average electrical consumption decreases and the average fuel consumption increases sharply with trip distance, and even more at low temperature due to the decrease in the electric range caused by the battery and cabin heating.



Figure 9: Example of results for one given battery capacity and recharge frequency









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The same simulations were performed for every battery size (2 to 35 kWh) and recharge interval (0.5 to 10 days), for both diesel and gasoline vehicles, leading to around 53,000 use cases simulated, including variations in technology sizing, and in environmental and driving conditions.

Statistics of use: representativeness of each use case

As seen above, the most influential parameter on the behaviour of a PHEV for a given charging interval is the daily distance travelled. Furthermore, as is the case for highly electrified vehicles in general, the electrical consumption of PHEVs is particularly sensitive to ambient temperature conditions.

This following text focuses on the statistical distributions of use observed for these two influencing parameters, extracted from the literature. These statistical distributions are then used to weight the different use cases according to their probability.

Ambient temperature

Through the Geco air application, IFPEN has collected daily mobility data from thousands of nonprofessional drivers. The frequency of temperature recorded during each trip (weighted by distance) is shown in Figure 10. This distribution is approximated by a gamma distribution law (equation (1)), as illustrated in Figure 11:

$$P(t;k,\theta) = \frac{(t-t_0)^{k-1} e^{\frac{t-t_0}{\theta}}}{\Gamma(k)\theta^k}$$
(1)

To study the climatic sensitivity, this same distribution is shifted by an offset of $+10^{\circ}$ C and -10° C to arbitrarily represent warmer and colder climate conditions. The average temperatures thus reproduced are close to the average Australian (22°C) and Swedish (2°C) temperatures, respectively.



Figure 10: Distribution of the ambient temperature while driving (weighted by distance travelled)





- central case (France)
- colder case
- warmer case
- T<t = share of kilometres driven up to t°C

Daily vehicle mileage travelled

The UFs defined by the WLTP protocol for the type approval of PHEVs come from mobility studies determining the daily distances operated. Assuming daily charging, they represent the possible percentage of the distance covered in all-electric mode by a fleet according to the vehicle's electric range.

Other data are available in the literature, in particular from mobility surveys in Germany.^[15] Figure 12 represents the log-normal distribution (see equation (2)) from the German mobility survey by Plötz *et al.*^[15] for the 'medium' vehicle class (yellow curve in the left graph, 'Median trips scenario'). From there, two other scenarios were designed, corresponding to shorter and longer trips (blue and orange curves). The bar graphs on the right hand side allow the reader to visualise the corresponding share of trips (top) and the share of mileage driven (bottom) according to the trip distance.

$$Prob(d;\mu,\sigma) = \frac{1}{d\sigma\sqrt{2\pi}} \exp\left(-\frac{\ln(d)-\mu}{2\sigma^2}\right)$$
(2)

Figure 12: VKT distribution retained for the current work



Share of daily trips (%)





Driving pattern (a function of VKT)

The type of route also has an impact on energy (electricity and fuel) consumption levels and UF. In the IFPEN database, as illustrated in Figure 13, the share of kilometres travelled in slow urban, urban, rural and motorway conditions is determined as a function of VKT. For the sake of simplification, the driving order adopted was always from the slowest (slow urban) to the fastest (motorway).





Resulting probability matrix

Assuming that temperature and trip distance are independent, the probability of a pair (VKT-ambient temperature) is obtained by the multiplication of the laws previously established for the VKT and the ambient temperature. Therefore, considering the driving temperature distribution in France and the daily vehicle mileage from literature (German mobility survey in this instance), a probability matrix is determined which makes it possible to ascertain the probability of each situation in real-world conditions (see Figure 14 on page 29).





$\label{eq:Figure 14:Matrix of use cases, probability function of ambient temperature and daily mileage$





Daily mileage statistical distribution in real use



Continuous surface of probability



Probability medium (%)



Weighted average outputs

For each combination of battery capacity and recharge frequency, weighted average values are calculated taking into account each individual use case over the whole range of VKT and ambient temperature, and its representativity.

Thus, for a given battery capacity and charging interval combination, mean scores representative of the actual use are obtained, resulting from the weighting of the energy performance in each use case, weighted by its representativeness and its distance. This was done for each combination of battery capacity and recharge interval, so that the evolution of energy performance parameters in real-world conditions as a function of these two key parameters could be obtained. Figure 15 on page 30 shows the weighted average outputs over the full range of variations for recharge interval and battery capacity. This figure is key to understanding the sensitivity of real-world average energy performance (fuel and electrical consumptions and UF) of PHEVs to both the technological sizing and the final user behaviour.



Figure 15: Weighted average fuel consumption, CO_2 emissions, electricity consumption and UF over the full range of variations for battery capacity (from 2 kWh to 35 kWh) and recharge frequency (from twice a day to every 10 days) — gasoline PHEV





Recharge every X day(s): twice a day 1 2

- 3

- 4

5

- 6

7

8

- 10

9





d) Weighted average utility factor



Discussion

Impact of battery capacity and recharge interval on PHEVs - key results

Figure 15 illustrates the influence of the dimensioning of the battery according to the frequency of recharging:

• Frequent recharging of PHEVs is a necessary condition for a high electrification rate: recharging every day enables the potential to reach an average weighted fuel consumption of 2.25 I/100 km and a UF of around 77% with a gasoline PHEV equipped with a 15 kWh battery. Recharging every three days induces a fuel consumption of 4.85 I/100 km (+116%) and a UF of around 48% (-29 points).

- A weighted average UF of 50% is reached at around 6 kWh of battery capacity, and 80% is reached at around 18 kWh of battery for an every-driving-day recharge.
- The first few kWh of battery capacity are the most effective in reducing the weighted average fuel consumption: considering 1 recharge/day, the gain in increasing the battery capacity above 20 kWh is low. For instance, adding another 15 kWh to the vehicle, leading to a 30 kWh PHEV, would increase the UF by only 10 points, from 77% to 87%, if recharged every day; in contrast, the same 15 kWh battery could electrify 77% of the mileage of another PHEV, which is more efficient if the total amount of available batteries is constrained.^[10]

Shifting from an individual vehicle evaluation to a systemic perspective

To shift from the individual vehicle evaluation performed in this work to a systemic perspective, it is necessary to link this work to the conclusions drawn by Shafiei *et al.* (2022).^[10] In their study, Shafiei *et al.* could not evaluate the UF of PHEVs by themselves and had to draw from the literature based on data from UNECE (2017)^[16] and ICCT (2020),^[6] as shown in Figure 16. It is interesting to compare these UFs with those obtained in this work, shown here in the case of the gasoline PHEV (Figure 16). It can be observed that the UF calculated for a recharge frequency every day is 4 to 8 points lower than the one given by the WLTP. It can also be seen that the UF calculated for a recharge every five days follows closely the UF suggested by the ICCT.







- - recharge every five days (c)

Note:

Relationship between PHEV all-electric range and battery capacity according to Shafiei *et al.*, 2022.^[10]



Based on the UFs extracted in UNECE (2017)^[16] and ICCT (2020),^[6] Shafiei *et al.* (2022)^[10] calculated the optimal allocation of batteries to passenger cars that would minimise their WTW GHG emissions, under various levels of battery supply to Europe ranging between 0 to 1.2 TWh/year. Figure 17 on page 33 shows one of the major findings of their work: under a constrained supply of batteries, it is better to allocate batteries to PHEVs first to minimise WTW GHG emissions; and only once the battery supply is less constrained do BEVs start to be part of the optimal solution, firstly along with PHEVs, and eventually alone. This conclusion reflects the fact that (i) in the frame of a highly decarbonised electricity grid (assumed for 2030 in their work), electrifying the driven mileage leads to reduced WTW GHG emissions, and (ii) to maximise the electrification of the driven mileage, it is more efficient to share smaller batteries used at their full capacity in all vehicles (enabled by PHEVs under a constrained supply of batteries) rather than to allocate underutilised bigger batteries to a few vehicles (which would occur if a BEV strategy is adopted too early).

The question remains as to whether Europe will actually experience a constrained battery supply in 2030. Regarding the demand aspects, according to Shafiei et al.,^[10] supplying 0.95 TWh/year of batteries for passenger cars in Europe would enable all of them to be electrified, providing that their individual battery capacity is lower than 60 kWh. According to Strat Anticipation (2022),^[17] the demand for batteries in the EU for electrified light vehicles would be 0.894 TWh/year in 2030 (for BEVs equipped with a 78 kWh battery and sales which are not fully electrified), starting from 0.123 TWh/year in 2022, and through 0.365 TWh/year in 2025. Regarding the supply aspects, there have been significant differences in announced, revised and realistic output forecasts for battery production facilities ('Gigafactories') in the EU. For example, according to Strat Anticipation,^[17] the EU's planned output for battery production in 2025 went down from 0.45 TWh/year (evaluated Q4 2021), through 0.392 TWh/year (evaluated February 2022) to 0.224 TWh/year, therefore requiring 0.141 TWh/year of imports; for 2030, the EU's planned output was 0.80 TWh/year in Q4 2021, rose to 1.037 TWh/year in February 2022, and dropped to 0.609 TWh/year, therefore requiring 0.285 TWh/year of imports. It is unclear where the imports would come from, but they are unlikely to come from North America as its planned production output is also lower than its demand, resulting in an import balance; and forecasts of China's planned production output indicate that China will barely meet its internal demand.

In brief, it appears highly likely that the battery supply for passenger cars in Europe will be constrained for the next 10 years (i.e. not sufficient to enable 100% of passenger car sales to be BEVs) and, under these conditions, Shafiei *et al.*^[10] concluded that a vehicle sales mix oriented towards PHEVs would be optimal in minimising WTW GHG emissions.

Figure 17: Optimal vehicle sales mix minimising WTW GHG emissions subject to a constrained battery supply in 2030



Additionally, Shafiei *et al.*^[10] looked further into the influence of the UF on the results of their optimisations. They found that, below a certain UF, called the 'break-even utility factor', PHEVs were no longer efficient in minimising WTW GHG emissions, and therefore the structure of the passenger car sales mix shifted directly from HEVs to BEVs without going through PHEVs (Figure 18, left). Conversely, above the break-even utility factor, PHEVs play an important role in the transition between HEVs and BEVs to minimise WTW GHG emissions, and the structure of the passenger car sales mix remains mostly unaffected whatever the utility factor above the break-even point (Figure 18, centre and right).

Figure 18: Optimal vehicle sales mix minimising WTW GHG emissions as a function of battery supply to Europe in 2030 for three levels of UF (20%, 40% and 90%), with the break-even point being 30%

Results assume fixed battery sizes of 1.54 kWh (HEV), 12.5 kWh (PHEV) and 58.4 kWh (BEV). (Source: adapted from Shafiei et al., 2022^[10])





Shafiei *et al.*^[10] generalised this approach and calculated the break-even utility factor for a variety of combinations of battery capacities for PHEVs and BEVs (shown as a function of their all-electric driving range in Figure 19). It can be seen that PHEVs with smaller batteries (e.g. PHEV 20) have a lower break-even utility factor: this is because smaller batteries can be shared with more vehicles that are more likely to use them at their full capacity, resulting in an efficient electrification of the overall mileage. For the same reasons, BEVs with smaller batteries (e.g. BEV-200) require PHEVs to have a bigger break-even utility factor.



Figure 19: Break-even utility factor of PHEVs for various combinations of battery capacities for PHEVs and BEVs

The results published by Shafiei *et al.*^[10] can be bridged with the work undertaken in this study: as the models developed here give the real-world utility factors as a function of the PHEV battery capacity and their recharge frequency, they can be compared to the break-even utility factor. In Figure 20 on page 35 it can be observed that a PHEV recharged every driving day or every two driving days always has a utility factor above the break-even point, whatever the battery capacities of the PHEVs and the BEVs. This means that, under limited supply of batteries to Europe, it is always preferable to roll out PHEVs first (before BEVs) providing that they are recharged at least every two driving days. If the PHEVs are recharged only every five driving days, the conclusion is somewhat different: for the PHEVs having a smaller battery (PHEV 20 and PHEV 40), the real-world utility factors are still above the break-even point.

Notes:

The values following 'PHEV' and 'BEV' relate to their all-electric driving range. Error bars show the sensitivities with

respect to the carbon intensity of the electricity supply mix ranging from 0 to 76.4 gCO₂e/MJ. Source: adapted from Shafiei *et al.*, 2022^[10]
This means that 'small PHEVs' (with a battery capacity lower than 8.6 kWh) are a no-regret option: even if they cannot be recharged very often (notwithstanding that the more often they are recharged, the better), they will always manage a deeper cut in WTW GHG emissions compared to a 'BEV-only' strategy. For the PHEVs having a bigger battery (PHEV 60 to PHEV 100), the results are more contrasted if they are recharged every five driving days as they depend on the BEVs against which they 'compete': if the BEVs have a smaller battery (less than 60 kWh or 400 km driving range), these become more efficient in minimising WTW GHG than those PHEVs; but if the BEVs batteries are bigger than 60 kWh, then the PHEVs become more efficient again, whatever their battery capacity.







Note:

The values following 'PHEV' and 'BEV' relate to their all-electric range. Source: adapted from Shafiei *et al.*, 2022^[10] with additional data from this work.

Conclusions

Two Euro 6d PHEVs were selected to allow a relevant comparison between gasoline and diesel internal combustion engines. These vehicles were tested on a chassis dynamometer and on-road, both with standard and renewable fuels, in CD and CS modes.

Two simulators for the gasoline and diesel PHEVs were set up, calibrated and validated. A DoE was performed under various conditions (temperature, driving cycles, initial battery SoC, battery capacity) to extend the energy performance findings of these two vehicles, i.e. the CO₂ emissions, UF, and fuel and electricity consumption. Finally, a simplified mathematical model was established and validated, allowing the energy performance parameters to be estimated for any combination of use. This work established that the energy performance of PHEVs is heavily dependent on the conditions of use (temperature, trip distance, recharging frequency and battery sizing), as the ratio of use of each of the two energy sources available on board is extremely variable.



A weighting methodology based on available real-world statistics was implemented on the parameters of ambient temperature and daily distance travelled. Furthermore, the recharging frequency and battery capacity factors, which depend on end users and manufacturers, respectively, were also varied (but not weighted as too few statistics are available) so as to provide insights via a sensitivity analysis. The study shows that frequent recharging of PHEVs is a necessary condition for a high electric drive rate: for a gasoline PHEV with a battery of 15 kWh, recharging every day leads to an average fuel consumption of 2.25 l/100 km and a utility factor of 77%, whilst recharging every three days leads to a fuel consumption of 4.85 l/100 km (+116 %) and a utility factor of 48% (-29 points). By comparison, the non-rechargeable gasoline HEV with a 2 kWh battery evaluated under the same conditions shows an average fuel consumption of 7.3 l/100 km and a utility factor of 24%. Compared to this reference HEV, the gasoline 15 kWh PHEV allows a consumption reduction of 69% if it is recharged every day and a reduction of 34% if it is recharged every three days. Furthermore, it is observed that the first kilowatt-hours of battery capacity are the most effective in electrifying the PHEVs: for instance, adding another 15 kWh of battery capacity to the vehicle, leading to a 30 kWh PHEV, would increase the UF by only 10 points, from 77% to 87%, if recharged every day; alternatively, the same 15 kWh battery capacity could have electrified 77% of the mileage of another PHEV, which is more efficient if the total amount of available batteries is constrained

Shafiei *et al.*^[10] concluded that, as long as the PHEVs' UFs are above their break-even points, they are part of the optimal vehicles sales mix minimising WTW GHG emissions in a scenario where the supply of batteries to the EU is constrained. The real-world assessment performed here confirms that, for a typical driving profile, the PHEVs' UFs are always above the break-even point when recharged every driving day or every two driving days. In addition, 'smaller' PHEVs with an all-electric driving range of 40 km or less are always above their break-even UF even if recharged down to every five driving days.

Outlook: from tank-to-wheel to life-cycle emissions — a vehicle LCA interactive tool

The TTW CO_2 emissions evaluated in this work do not offer a complete picture of the GHG emissions emitted during the life of a vehicle. To achieve this, a broader analysis of the vehicle's life cycle needs to be determined by considering not only the TTW emissions of the vehicle during its use, but also the WTT emissions related to the energy sources (electricity and fuel production) and, finally, the production and end of life of the vehicle itself, including the battery. Such an assessment is based on many parameters, for example: the CO_2 intensity of electricity production; the CO_2 WTT emissions and associated recycled CO_2 from different fuel production pathways; the CO_2 emissions related to the production of the vehicles, particularly the battery; the lifetime of the vehicles; etc. Given the quantity of possible pathways, assumptions and their variability, it is impossible to have a consensus on the definition of a baseline (around which sensitivities can then be run).



For this reason, a dynamic LCA GHG tool has been developed, allowing users to configure any possible combination of parameters and to compare the life-cycle emissions of PHEVs with those of other types of vehicle electrification, i.e. HEVs and BEVs (Figure 21). This tool is supported by the energy performance model developed in this article (which provides the TTW CO_2 emissions, the energy consumption and the UFs), which also integrates the WTT and life-cycle emissions as a function of the selected configurations.

Figure 21: Screenshot of the on-line vehicle LCA simulator (accessible at https://www.carsCO2comparator.eu)



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Introduction

Ambient air quality is quantified using the concentrations of pollutants associated with emissions from anthropogenic and biogenic origin. The pollutants may be emitted directly from sources (primary pollutants) or formed in the atmosphere by chemical reactions (secondary pollutants). Air quality is then judged as being good or poor according to how these concentrations compare with ambient air quality (AAQ) standards which will eventually determine the compliance status (i.e. compliance = concentrations at or below AAQ standards). Due to successful policies to reduce man-made (anthropogenic) emissions, the trend is for air quality to improve. At the same time, the AAQ standards are periodically reviewed to ensure that they continue to be relevant and appropriate and in close alignment with the latest scientific findings.

The EU Ambient Air Quality Directives^[1,2] came into force in 2008. They formalised AAQ standards from earlier regulations and, in particular, recognised advice from the World Health Organization (WHO) on the importance of airborne particulate matter (PM) in terms of its impact on human health. The 2005 version of the WHO *Air Quality Guidelines*^[3] served as reference for the present day AAQ standards set in 2008.

Since 2005, important developments on air quality monitoring and epidemiological health studies have taken place. The existing AAQ Directives^[1,2] required systematic monitoring of air quality across Europe, as it had been recognised that too little was known about key pollutant concentrations, particularly $PM_{2.5}$ and NO_2 . As a result, a comprehensive network of measurement stations has been established across Europe.^[4] In addition, many epidemiological studies have been carried out to better investigate the relationship between exposure to air pollution and population health. Using this data, the WHO concluded that the effect of air pollution on health was underestimated in certain respects and therefore, in 2021, the WHO air quality guidelines were revised downwards.^[5]

The WHO guidelines provide two levels of advice. The guideline metrics themselves are as protective of population health as possible. However, recognising that ambient air pollution in many, if not most, areas exceeds these guideline metrics, interim target values are provided for policy makers to consider. The progressive step between each interim target value provides a quantifiable gain in public health. Policy measures that lead to stepwise improvements in air quality can then be judged to provide positive health benefits. A long-term objective would be to attain the guideline metrics. For most of the regulated pollutants, the European standards set in the existing AAQ Directives fall within the range of interim targets suggested by the 2021 *WHO global air quality guidelines*^[5] (Table 1).

The European Commission is currently in the process of revising the AAQ Directives, and its current proposal for a revised Directive^[6] is considering these developments, as it sets lower AAQ standards for 2030, while it points to a post-2030 perspective for a full alignment with the 2021 WHO air quality guidelines, whilst also getting on track towards alignment with future WHO guidelines to achieve the zero pollution vision by 2050.

of the European Air Quality Network, and to assess how these might compare with the air quality guidelines and interim target metrics set out in the recently updated WHO global air quality quidelines (2021). The study uses a similar methodology to that supporting The Second Clean Air Outlook published by the European Commission in 2021 by considering a number of emission scenarios. Overall, it is predicted that air quality in Europe will improve, and that both shortand long-term average concentrations will fall within the range of the WHO interim target values. However, even under the most ambitious scenario, air quality in Europe is unlikely to meet the WHO guideline values by 2050 at many locations in Europe covered by the current monitoring network.

This article summarises the

results of a Concawe study to predict future concentrations of

key air pollutants (O₃, NO₂, PM)

at selected measuring stations

Author

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Table 1: Comparison between current EU air quality standards (2008) and the latest WHO air quality guidelines (2021) The proposed new EU AAQ standards for $O_{3,*}$ NO₂, PM_{2.5} and PM₁₀ (to be met by 2030) are highlighted with the red boxes

		EU Air Quality Directives			WHO Air Quality Guidelines					
Pollutant	Averaging period	Objective	Concentration	Comments		Concentration			า	Comments
					I	nterim	target	s	AQG level	
					1.	2.	3.	4.		
PM _{2.5}	24-hour	Target value			75	50	37.5	25	15 µg/m³	99th percentile (i.e. 3–4 exc. days/year)
PM _{2.5}	Annual	Limit value	25 µg/m³		35	25	15	10	5 µg/m³	
PM _{2.5}	Annual	Indicative limit value	20 µg/m ³							
PM ₁₀	24-hour	Limit value	50 µg/m ³	Not to be exceeded on more than 35 days/year	150	100	75	50	45 µg/m ³	99th percentile (i.e. 3–4 exc. days/year)
PM ₁₀	Annual	Limit value	40 µg/m ³		70	50	30	20	15 µg/m³	
O ₃	Max. daily 8-hour mean	Target value	120 µg/m³	Not to be exceeded on more than 25 days/year						
O ₃	Max. daily 8-hour mean	Long-term objective	120 µg/m³	(averaged over 3 years)						
O ₃	8-hour	Target value			160	120	-	-	100 µg/m³	99th percentile (i.e. 3–4 exc. days/year)
O ₃	Peak season	Target value			100	70	-	-	60 µg/m ³	
NO ₂	Hourly	Limit value	200 µg/m ³	Not to be exceeded on more than 18 hours/year					200 µg/m ³	
NO ₂	Annual	Limit value	40 µg/m ³		40	30	20	-	10 µg/m³	
NO ₂	24-hour	Target value			120	50	-	-	25 µg/m³	99th percentile (i.e. 3–4 exc. days/year)
SO ₂	Hourly	Limit value	350 µg/m ³	Not to be exceeded on more than 24 hours/year						
SO ₂	24-hour	Limit value	125 µg/m³	Not to be exceeded on more than 3 days/year	125	50	-	-	40 µg/m³	99th percentile (i.e. 3–4 exc. days/year)
со	Max. daily 8-hour mean	Limit value	10 mg/m ³						10 mg/m ³	
со	24-hour	Target value			7	-	-	-	4 mg/m ³	99th percentile (i.e. 3–4 exc. days/year)
C ₆ H ₆	Annual	Limit value	5 µg/m³						1.7 µg/m³	Reference level
BaP	Annual	Target value	1 ng/m ³	Measured as content in PM_{10}						
Pb	Annual	Limit value	0.5 µg/m³	Measured as content in PM_{10}					0.5 µg/m³	
As	Annual	Target value	6 ng/m ³	Measured as content in PM_{10}					6.6 ng/m ³	Reference level
Cd	Annual	Target value	5 ng/m ³	Measured as content in PM_{10}					5 ng/m ³	
Ni	Annual	Target value	20 ng/m ³	Measured as content in PM_{10}					25 ng/m ³	Reference level

* The proposed target value for the maximum daily 8-hour mean O₃ concentrations in the EU's proposal for a revised AAQ Directive is set at 120 µg/m³ not to be exceeded on more than 18 days per calendar year (versus 3–4 exceedance days/year in the 2021 WHO air quality guidelines). (Source: EEA, 2021)

The alignment of AAQ standards with the WHO guidelines, and the need for new AAQ standards to be met to ensure compliance, would most likely involve the need for a meaningful reduction in anthropogenic emissions across Europe. This reduction will need to be achieved to avoid compliance problems in the future.

In this context, Concawe commissioned a study, to examine how future ambient air quality in Europe might compare with the new WHO guidelines and interim target metrics. The study simulates future air concentrations of key pollutants (O_3 , NO_2 , $PM_{2.5}$ and PM_{10}) at selected measuring stations of the European Air Quality Network and assesses the implications with respect to compliance. The study uses a similar methodology to that supporting *The Second Clean Air Outlook* (CAO2)^{1[7]} published by the European Commission in 2021. In particular, it considers the Current Legislation (CLE) trend and two scenario assumptions made in *The Second Clean Air Outlook* about maximum emissions reduction potential.^[8] The study also investigates which sector emissions might be most important in determining air quality. The geographic scope chosen is the EU-27. For brevity, the article discusses the results at European level. Further details of the analyses at a country level can be found in the full Concawe report.^[9]

Methodology

Air quality monitoring station simulations

The AQUIReS+ model^[10] has been used to forecast atmospheric concentrations of O_3 , NO_2 , $PM_{2.5}$ and PM_{10} at each selected monitoring station that is included in the European Environment Agency's (EEA's) Air Quality e-Reporting dataset.^[4] This ensures that the modelling is directly related to the individual measuring stations used to monitor compliance with AAQ standards. The model uses a gridded emission inventory and source-receptor relationships.^[11] These derive from regional chemical transport models (EMEP^[12]) used in air quality studies. The local environment, traffic and topographical characteristics of each station are also taken into account by the model during the predictions. A correlation between the EMEP model predictions and the hourly measurements made at each station is developed. The robustness of the correlation has been tested using hindcasting for several years of data.

It is assumed that this correlation can be used to predict the future measurements at the station from air quality predictions made using different assumptions about emissions. In more sophisticated evaluations^[10] of air quality response to emission changes, a confidence interval has been calculated for the predicted air quality metric at each monitoring station location. A detailed overview of the model evaluation and a description of the data sources and dataflows in the model are presented in earlier studies.^[10,13]

¹ At the time of writing this report, the European Commission has published *The Third Clean Air Outlook* (available at https://environment.ec.europa.eu/publications/third-clean-air-outlook_en). However, the data underpinning the activity scenarios that have been developed have not yet been made publicly available.

For each monitoring station, the requisite annual air quality metrics of each pollutant were calculated based on the hourly concentrations from the model. These metrics can take one of the two following forms:

- An upper limit value for a pollutant concentration, i.e. a value that should not be exceeded. In this study, these are annual average concentrations.
- An exceedance frequency limit: typically, this is the number of times a value can be exceeded in a
 prescribed time. This is appropriate to concentrations averaged over the short term, which can be
 variable. In this study, these are daily average concentrations and exceedances of a limit, and are
 counted over a year.

For annual average concentrations, the average of hourly values was evaluated and reported. In postprocessing, the calculated annual average for each station was compared to see if it was less than or equal to the WHO interim target or guideline value. If this comparison was true, then the station was counted as meeting the criterion at that threshold for that year.

For the exceedance frequency, this involved calculating each daily average, or in the case of ozone the maximum daily 8-hour mean concentration. In post-processing, this value was then compared with each of the WHO interim target and guideline values in turn. If the prediction exceeded the WHO air quality guideline target value, then a counter was incremented. The annual result is the count of exceedances. The number of exceedances in one year for each station, for each target threshold, was evaluated to see if it was less than four, following that the WHO air quality guidelines use a 99% criterion for exceedance. If the condition was met, then the station was counted as meeting the criterion at that threshold for that year.

Detailed analyses of the results for all the above-mentioned metrics are provided in the Concawe report. In this article, the results for the ozone exceedance metric and the annual mean concentration metric for NO_2 and $PM_{2.5}$ are presented for brevity.

Emissions scenarios

The Second Clean Air Outlook scenarios

Three GAINS² scenarios developed for the European Commission's *The Second Clean Air Outlook*^[7] are used in this study. These represent the upper bound (CLE) and lower bound (MTFR) for expected emissions in the years up to 2050 without structural changes to the European economy, and a second lower bound (MTFR + 1.5 LIFE) that includes structural changes. The three scenarios are summarised on the following page.

² GAINS: Greenhouse gas and Air pollution Interactions and Synergies (http://gains.iiasa.ac.at)

- The baseline scenario (CLE): This is the expected trend in emissions in Europe between 2015 and 2050. This includes the impact of changes in European economic activity on emissions and the effect of current and pending legislation on abatement. The scenario differs in detail from that used to develop the revised NEC Directive (2016).³ Specifically, the CLE scenario assumes achievement of the EU energy efficiency target of 32.5% and a renewable energy target of 32% as agreed in the 'Clean energy for all Europeans' package⁴ until 2030, and implementation of the current policies on non-CO₂ greenhouse gas emissions.
- The Maximum Technically Feasible Reduction (MTFR) scenario: This is a scenario whereby emissions from all sectors, as described in GAINS, are reduced as far as technically possible, regardless of cost.
- The MTFR + 1.5 LIFE Scenario: The 1.5 LIFE scenario is an additional decarbonisation scenario of the EU energy and agricultural systems aligned with the objective of stabilising the global temperature increase at 1.5°C above pre-industrial levels. It assumes, inter alia, movement towards a more circular economy with reduced consumption of goods and energy, a move away from personal transport towards shared transport systems, reduced demand for energy in heating/cooling, and a dietary shift that reduces the demand for red meat and, consequentially, animal numbers and their need for forage provision. MTFR controls are applied to this 1.5 LIFE scenario.

Figures 1 and 2 provide an overview of the projected EU-27 emissions $load^5$ of $PM_{2.5}$ and NO_x , under the three CAO2 scenarios for the years 2030, 2040 and 2050. Each source sector is shown separately so that the contribution of each sector to the overall emissions can be clearly seen.

Figure 1: Sectoral PM_{2.5} emissions for the EU-27 under the three scenarios (CLE, MTFR and MTFR + 1.5 LIFE) developed for the European Commission's *Second Clean Air Outlook*



agriculture
waste management
non-road mobile
road transport
solvent use
fuel extraction
industrial processes
industrial combustion
residential combustion
energy sector

³ https://www.eea.europa.eu/policy-documents/directive-2016-2284-eu-national

⁴ https://energy.ec.europa.eu/topics/energy-strategy/clean-energy-all-europeans-package_en

 5 The figures provide an indication of the trends and relative contributions of NO_x and PM_{2.5} sectoral emissions, which is representative of all EU-27 countries. The absolute values, however, are country-specific.

Under the baseline scenario, $PM_{2.5}$ emissions are projected to decline significantly over the 10-year period from 2020 to 2030 (approximately 46%) (Figure 1). Residential combustion is expected to have the largest reduction of all sectors, amounting to approximately 70% by 2030, and 91% by 2050. It is also important to highlight that by 2050, industrial processes and agriculture are predicted to become the most significant sources of $PM_{2.5}$ emissions. $PM_{2.5}$ emissions are projected to continue their downward trend in 2040 and 2050, however the reduction rate is lower (60% reduction under CLE by 2050 compared to 2020). Under the maximum reduction scenarios, a larger decline is predicted for $PM_{2.5}$ emissions. By 2050, the additional reduction of $PM_{2.5}$ emissions compared to the baseline scenario is 33% for MTFR and 37% for MTFR + 1.5 LIFE.

 NO_x emissions also show a significant downward trend for the baseline scenario over the 10-year period from 2020 to 2030, with a 40% reduction by 2030 (Figure 2). Up to 2030, road transport remains the most important source of NO_x emissions; however, the sector is projected to have the largest reductions of all sectors, amounting to 65% by 2030. In addition, beyond 2030, it is forecast that road transport will no longer be the primary contributing sector, with the energy sector and industrial combustion becoming the dominant sources, accounting for 18% and 29% of NO_x emissions by 2050, respectively. NO_x emissions are projected to continue their downward trend in 2040 and 2050, although the reduction rate is lower (57% reduction under CLE by 2050 compared to 2020).



Figure 2: Sectoral NO_x emissions for the EU-27 under the three scenarios (CLE, MTFR and MTFR + 1.5LIFE) developed for the European Commission's Second Clean Air Outlook

Similarly to the overall trend of NO_x sectoral emissions, the additional reduction of NO_x emissions from road transport in 2040 and 2050 is lower, while as of 2040, no additional reduction is projected for NO_x emissions from road transport under MTFR, an indication that all available existing technical measures have been already applied to the maximum extent under the baseline scenario. Under the maximum reduction scenarios, a larger decline is predicted for NO_x emissions. By 2050, the additional reduction of NO_x emissions compared to the baseline scenario is 31% for MTFR and 48% for MTFR + 1.5 LIFE, respectively, with the largest additional reductions to be expected in the industrial combustion sector.

Sectoral emissions scenarios

In addition to *The Second Clean Air Outlook* scenarios described on pages 43–44, the study includes some additional sector-specific emission reduction scenarios (see Table 2). The purpose of these is to identify which emission reduction components of the common scenarios are having the greatest influence on ambient air quality.

Table 2: List of emissions reduction scenarios assessed in the study

Scenario	Description
Case (0)	<i>The Second Clean Air Outlook</i> (CAO2) — Current Legislation (CLE) Baseline: Expected trend in emissions with time, taking account of forecast economic activity and phasing in of legislation that affects emissions.
Case (1)	Removal of Energy Sector Emissions: Emissions of NO_x , SO_2 and particulate matter from large combustion plants used for power and energy products generation are set to zero.
Case (2)	Removal of Domestic-Commercial Emissions: Emissions of NO_x , SO_2 , PM, and volatile organic compounds (VOCs) from domestic, shop and office heating systems are set to zero.
Case (3)	Removal of Industry Combustion/Process and Solvent/Product Use Emissions: Emissions of NO_x , SO_2 , PM, VOCs and NH_3 from process industry, including the use of solvents (VOCs) in degreasing, ink and paint production, etc. are set to zero.
Case (4)	Removal of Road Transport Emissions: Emissions of NO_x , SO_2 , PM and VOCs from both private and commercial vehicles used for road transport are set to zero.
Case (5)	Removal of Non-Road Transport Emissions: Emissions of NO_x , SO_2 , PM and VOCs used in off-road applications (e.g. construction, agriculture) and on inland waterways are set to zero.
Case (6)	Removal of Agricultural NH $_3$ Emissions: Emissions of NH $_3$ from agriculture are set to zero.
Case (7)	CAO2-MTFR: Emissions from all sectors are reduced to the minimum technically possible according to the methods encoded in the GAINS EUROPE model.
Case (8)	'Beyond MTFR' — CAO2 MTFR + 1.5 LIFE: Emissions are reduced beyond the MTFR assuming major structural changes in the agricultural sector and in energy use aimed predominantly at reducing CH_4 , NH_3 and CO_2 emissions.

Notes: Case (0) is the Current Legislation (CLE) base case within which emission reductions are already mandated. Cases (1)–(6) are illustrative only. Cases (7) and (8) are reduction scenarios associated with *The Second Clean Air Outlook* (CAO2). Each scenario reduces emissions from a key emitting sector to zero. If the scenario produces a change in air quality that affects the comparison with the WHO air quality guidelines, this indicates which components of the GAINS scenarios are likely to be important.

The scenarios, including the baseline and maximal reduction scenarios, are presented in the order in which they were executed. The emission reductions are assumed to be applied in 2025 and for subsequent years.

EU-27 results

Presentation of results

The objective of this study is to evaluate how many of the monitoring stations would be likely to record a concentration, or an exceedance frequency, that is lower than each of the WHO interim target and air quality guideline values under the different scenarios examined. Therefore, the study results are calculated in terms of the number of stations where the pollutant metrics are at or below the interim target and guideline values set out in the WHO air quality guidelines. However, it is the converse that is of more direct interest. Therefore, the graphics presented on the following pages show the proportion (%) of stations where pollutant metrics exceed the WHO's interim target and guideline values.

The metrics considered in the study are:

- Ozone: The number of days in a year on which the average of the maximum daily 8-hour mean concentration exceeds a threshold value.
- NO₂: a) The number of days in a year on which the daily average concentration exceeds a threshold value.
 - b) The annual mean concentration versus a threshold value.
- PM_{2.5}: a) The number of days in a year on which the daily average concentration exceeds a threshold value.
 - b) The annual mean concentration versus a threshold value.
- PM₁₀: a) The number of days in a year on which the daily average concentration exceeds a threshold value.
 - b) The annual mean concentration versus a threshold value.

Detailed analyses of the results for all the above-mentioned metrics are available in the Concawe report.^[9] For brevity, the results for the ozone exceedance metric and the annual mean concentration metric for NO_2 and $PM_{2.5}$ are presented in this article.

Ozone exceedance

The current EU AAQ Directive sets a (non-binding) target of 120 μ g/m³ for maximum daily 8-hour O₃ mean concentrations, not to be exceeded on more than 25 days per year. This is evaluated as an average number of exceedances across three years in order to accommodate interannual variability in meteorology. The Directive also sets a long-term objective that foresees the number of exceedances falling to zero. In the proposed revision of the AAQ Directive, the maximum number of exceedance days is reduced from 25 down to 18 days, and the long-term objective is reduced down to 100 μ g/m³.

The WHO guidelines propose that all target thresholds be met as a 99th percentile of daily values, which is fewer than four exceedances per year. For ozone, the WHO suggests two interim targets (IT) with concentration values of 160 (IT1) and 120 μ g/m³ (IT2), respectively, and a guideline value of 100 μ g/m³. Although the second interim target of 120 μ g/m³ is numerically the same concentration as given in the EU Directive, the limit of fewer than four exceedances per year is much more restrictive than the 25 per year, averaged over 3 years.

The number of stations at which the predicted O_3 daily maximum 8-hour mean concentration exceeds the WHO interim target and air quality guideline values under current legislation is shown in Figure 3. Under current legislation, the results show that interim target 1 (160 µg/m³ not to be exceeded on more than four days) is not met by a small proportion of stations, and this proportion decreases in time (less than 5% in all European stations by 2050).







Interim target 2 ($120 \mu g/m^3$) is predicted to be exceeded by a substantial proportion of stations (80% of the stations in 2020) and this proportion decreases with time until 2040. However, even by 2050, more than half of the stations are not able to meet interim target 2 for the ozone exceedance.

The results predict that the WHO air quality guideline value ($100 \mu g/m^3$) is not met at more than 90% of stations in any forecast year. This proportion may change year by year depending on how climatic conditions affect ozone production. However, the number of stations not meeting both interim target 2 and the WHO air quality guideline will still remain significant. In particular, by 2050, around 95% of monitoring stations are predicted not to meet the WHO air quality guideline values, indicating that the full alignment of EU air quality standards with the 2021 WHO air quality guidelines by 2050 will be extremely challenging.

The results of the various emission reduction scenarios for O_3 exceedance for the year 2050, each also compared with current legislation, are shown in Figure 4. The results predict that the removal of VOC emissions from industrial production and solvent/product use (Case (3)) has the largest effect on increasing the number of stations meeting the WHO interim target and guideline values, being even higher than the effects under the MTFR and MTFR + 1.5 LIFE scenarios (Case (7) and Case (8), respectively). Removal of emissions from all other sectors are predicted to be ineffective.



Figure 4: O₃ exceedance for the EU-27— scenario comparison for the number of monitoring stations NOT meeting the WHO interim target and guideline values in 2050

NO₂ annual mean

The current EU AAQ Directive sets a limit value of 40 μ g/m³ for the annual mean value of NO₂, while the WHO air quality guidelines propose interim target values of 40 (IT1), 30 (IT2) and 20 μ g/m³ (IT3), and a guideline value of 10 μ g/m³.

The model results show that, under current legislation, there is a very small number of stations measuring NO_2 annual mean concentrations above interim target 1 (which is equal to the current AAQ standards) in 2025 (Figure 5) while as of 2030, all stations are predicted to meet this target. The number of non-compliant stations increases for interim target 2 and interim target 3. In particular for interim target 3, which is equal to the proposed new AAQ standards (to be met by 2030), around 8% of the stations are predicted not to meet the target in 2030, which reduces to ~2% by 2050. With respect to the WHO air quality guideline level, the model results show that nearly 37% of the stations are predicted to measure higher NO_2 annual mean concentrations in 2030. In 2050, it is predicted that annual concentrations would still be above the guideline at 11% of stations.



Figure 5: NO_2 annual mean for the EU-27—proportion of stations predicted NOT to meet the WHO interim target and guideline values under current legislation

WHO interim target (IT) and air quality guideline values





The results of the various emission reduction scenarios for NO₂ annual mean concentrations are shown in Figure 6 for the year 2050. In all scenarios, the interim target 2 annual mean concentration is met by all stations in 2050, while only a few stations (less than 1%) will not be able to meet interim target 3. In general, the removal of on-road (Case (4)) and non-road transport (Case (5)) emissions are predicted to have the largest effect among the sectoral emissions reduction scenarios. The predicted effect of the on-road transport emissions removal is actually similar to the effects associated with the MTFR scenario (Case (7)), and close to the effects of the MTFR + 1.5 LIFE scenario (Case (8)) which is predicted to result in the highest number of monitoring stations meeting the WHO air quality guideline. However, even in the case of removing all on-road transport emissions, around 7% of the monitoring stations in Europe in 2050 are still predicted to measure annual NO₂ concentrations above the WHO air quality guideline. In contrast, removal of emissions from the energy sector (Case (1)) is predicted to have the lowest impact.







PM_{2.5} annual mean

The current EU AAQ Directive sets an annual mean concentration of 25 μ g/m³ as the limit value for PM_{2.5}, while there is also a long-term objective that average concentrations should fall below 20 μ g/m³. In its revised guidelines, the WHO proposes interim targets of 35 (IT1), 25 (IT2), 15 (IT3) and 10 μ g/m³ (IT4), and a guideline value of 5 μ g/m³.

The number of stations at which the predicted $PM_{2.5}$ annual mean concentration exceeds the WHO interim target and guideline values under current legislation is shown in Figure 7. The results show that, as of 2025, interim target 2, which is equal to the existing EU AAQ standard, will be met at nearly all stations, while only a small proportion of stations (less than 5%) will be above the interim target 3 value in 2030. In 2050, almost all stations are predicted to meet interim target 3.

When assessing the compliance status with respect to interim target 4, the results predict that a substantial portion of stations will observe concentrations above the target value. In 2030, around 27% of stations will not be able to meet interim target 4, while in 2050, 10% of stations will still have concentrations above $10 \,\mu\text{g/m}^3$. It should be noted that, in its proposal for a revised AAQ Directive, the European Commission sets a new AAQ standard for PM_{2.5} annual mean concentration (to be met by 2030) that is equal to the WHO's interim target 4.



Figure 7: $PM_{2.5}$ annual mean for the EU-27—proportion of stations predicted NOT to meet the WHO interim target and guideline values under current legislation



With regard to the WHO air quality guideline value, the results show a significant non-compliance issue as the vast majority of stations are predicted to observe annual $PM_{2.5}$ concentrations above the guideline value. In particular in 2030, almost 87% of the stations do not meet the guideline value of 5 µg/m³, only slightly decreasing to 75% in 2050. The above results indicate that full alignment of the EU AAQ standards with the 2021 WHO air quality guideline by 2050 will be extremely challenging.

The results of the various emission reduction scenarios for $PM_{2.5}$ annual mean concentrations are shown in Figure 8 for the year 2050. Meeting the WHO's interim target 4, and the air quality guideline value in particular, is predicted to be challenging. In all sectoral emissions reduction scenarios assessed, the removal of NH_3 emissions from agriculture (Case (6)) is predicted to have the largest effect, being larger even than the effects associated with the maximum emission reduction of the MTFR (Case (7)) and MTFR + 1.5 LIFE scenarios (Case (8)). However, even under this theoretical scenario, a considerable proportion of stations is predicted to still record $PM_{2.5}$ concentrations above the WHO air quality guideline value (24%). The respective proportion of stations predicted not to meet the WHO air quality guideline value ranges from 37% to 73% in the remaining scenarios considered.



Figure 8: PM_{2.5} annual mean for the EU-27— scenario comparison for the number of monitoring stations NOT meeting the WHO interim target and guideline values in 2050



Conclusions

The ongoing review of the EU Ambient Air Quality Directive^[1,2] aims to set lower ambient air quality standards in order to align them more closely with the WHO air quality guidelines that were recently revised^[3] towards lower values.

In this context, Concawe commissioned a study to carry out sets of forward predictions for air concentrations of key pollutants (O_3 , NO_2 , $PM_{2.5}$, PM_{10}) across the European monitoring network for the period of 2015 to 2050, and to assess how these might compare with the new WHO air quality guidelines and interim target metrics. The study uses a similar methodology to that supporting *The Second Clean Air Outlook* (CAO2)^[7] published by the European Commission in 2021, by considering three emission scenarios: a Current Legislation (CLE) trend scenario and two scenario assumptions about maximum emissions reduction potential (i.e. MTFR and MTFR + 1.5 LIFE). The study also considers some illustrative emission reduction scenarios that are simple cases where emissions from key sectors are each set to zero in turn. The purpose of this is to determine whether emissions from any of the sectors are predicted to have, individually, a dominating effect on future air quality.

The results from the modelled scenarios show the following:

- Air quality in Europe, represented by the pollutants and metrics tested and determined across the air quality monitoring network, improves over time towards the 2050 horizon. This is due to the reduction in emissions already legislated within the economic outlook of *The Second Clean Air Outlook* which will result in almost full compliance for PM_{2.5} and NO₂ with the current EU AAQ standards across Europe from 2025 onwards.
- Under the current legislation pathway, the forecast air quality is largely consistent with the most ambitious
 of the WHO interim target criteria. However, the study shows that air quality in Europe in 2050 will not
 meet the guideline criteria set out in the 2021 WHO air quality guidelines. However, air quality is not
 uniform over Europe, and variability occurs within countries (see the Concawe report^[9] for details).
- Additional improvements in air quality are predicted under the two maximal emission reduction scenarios, namely MTFR and MTFR + 1.5 LIFE. In particular, the MTFR + 1.5 LIFE scenario results in improved air quality overall, compared to MTFR alone which mainly benefits particulate matter concentrations. However, neither of these two scenarios is effective enough to ensure that the WHO guideline values will be met by 2050 for all pollutants assessed.
- The sensitivity calculations, in which emissions from individual sectors were each set to zero in turn, show that agricultural emissions have a strong effect on PM_{2.5} concentrations. Road transport emissions lose importance with respect to their effect on NO₂ after 2030 because of the drop in older vehicles within the fleet, while non-road emissions for transport and construction play a growing role as their contribution becomes larger relative to on-road emissions. Further reductions in process industry emissions have a relatively small impact on ozone and particulate matter, which would be consistent with reductions in VOC emissions. Eliminating emissions from large industrial producers of energy—traditionally the source of air pollution—has very little effect on the air quality predictions. Finally, the results show that there is no single sector emission that has a dominant effect on how air quality at monitoring stations will compare with the WHO interim target and guideline criteria.

Overall, the outlook for 2030 and 2050 is that air quality in Europe will improve. Larger improvements will result if consumption is reduced as well as controls put in place and measures extended to agriculture. The majority of stations will register short-term and long-term average concentrations that fall within the range of interim target values set out in the recently updated *WHO global air quality guidelines* (2021). However, even under the most ambitious MTFR + 1.5 LIFE scenario, air quality in Europe is unlikely to meet the WHO guideline values by 2050 at many locations in Europe covered by the current monitoring networks.

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The Concawe LNAPL Toolbox

A new web-based Toolbox for understanding light nonaqueous phase liquids (LNAPLs) consists of a unique collection of useful tools, calculators, data and resources to help LNAPL scientists and engineers better understand how to manage LNAPL at their sites.

Background

LNAPL stands for 'light non-aqueous phase liquids' or hydrocarbons that exist as a separate undissolved phase in the subsurface at some sites with legacy releases of fuels. They are referred to as 'light' because most petroleum hydrocarbons are less dense than water. Because LNAPLs can sustain dissolved groundwater plumes for long time periods, it is important to understand how much LNAPL may be present at site, whether the LNAPL can migrate, whether it can be recovered, how the LNAPL composition changes over time, how long it may persist, and how quickly the LNAPL body is attenuating.

Understanding LNAPL behaviour is complex. Concawe, with the support of GSI Environmental, has therefore compiled a unique collection of useful tools, calculators, data and resources to help LNAPL scientists and engineers better understand how to manage LNAPL at their sites. This has led to the development of the Concawe LNAPL Toolbox, a wide-ranging but easy-to-use web-based toolbox designed to deliver key LNAPL knowledge to the LNAPL remediation community.

Author

Markus Hjort (Concawe)

The LNAPL Toolbox is intended to be a clear, transparent tool that regulators can use to validate site information that is given to them, and to learn about LNAPL so that they are able to make informed decisions using sound science. The Toolbox uses a three-tiered approach that provides access to more than 20 different LNAPL tools (key infographics, nomographs, calculators, mobility models, videos, checklists and other formats) with different levels of complexity, activation energy and time requirements. The three tiers of complexity are:

- Tier 1: Simple and quick graphics, tables and/or background Information
- Tier 2: Middle level quantitative methods and/or tools
- Tier 3: Gateway to complex models

In terms of content, the Toolbox is designed to address six questions via six different sections:

- 1. How much LNAPL is present?
- 2. How far will the LNAPL migrate?
- 3. How long will the LNAPL persist?
- 4. How will LNAPL risk change over time?
- 5. Will LNAPL recovery be effective?
- 6. How can one estimate natural source zone depletion (NSZD)?

The Concawe LNAPL Toolbox is publicly available on the internet (see Figure 1 on page 57) using a web browser (https://lnapltoolbox.concawe.eu/lnapl_toolbox) or by downloading the Toolbox code for use on a personal computer (https://github.com/concawe/LNAPL-Toolbox-).

Figure 1: Excerpt from the home page of the Concawe LNAPL Toolbox (https://lnapltoolbox.concawe.eu/lnapl_toolbox/)



The Concawe LNAPL Toolbox

Quick user guide

Once a user enters the Toolbox, either through the web or by using the downloadable version, they can engage with the Toolbox in the following steps using Table 1:

- Step 1: Determine the question you would like to learn more about (column 1).
- Step 2: Decide on the level of effort you would like to apply (columns 2 through 4):
 - Tier 1: a few minutes (approximately)
 - Tier 2: a few hours (approximately)
 - Tier 3: learn about more complex tools
- Step 3: Go to the appropriate tab using the buttons on the home page or the navigation bar.

Table 1: Concawe LNAPL Toolbox organisation and structure

Key LNAPL questions	Tier 1 Quick info	Tier 2 Models/tools	Tier 3 Gateway to complex tools
How much LNAPL is present?	Text, simple table and graphic	LNAPL volume/ extent tool	LDRM resources and video
How far will LNAPL migrate?	Text and simple graphic	LNAPL additional migration tool and Mahler migration model	HSSM and UTCHEM resources and video
How long will LNAPL persist?	Text, simple graphic and table	LNAPL lifetime calculator	LNAST and REMFuel resources and videos
How will LNAPL risk change over time?	Text and simple tables	LNAPL dissolution calculator	LNAST resources and video
Will LNAPL recovery be effective?	Text and simple graphics	LNAPL transmissivity and Darcy flux calculator	Computer modelling resources
How can one estimate NSZD?	Text and simple graphic	NSZD rate converter, NSZD temperature enhancement calculator	NSZD resources and videos

Conceptual example

The use of the Toolbox can be illustrated by the following conceptual example, in which an LNAPL body is currently being recovered using LNAPL skimming wells. The site owner would like to determine whether the installed LNAPL recovery system is still needed to meet the remediation objectives. There is uncertainty about some fundamental aspects of this LNAPL site, and the conceptual site model (CSM) needs to be updated.

The existing LNAPL CSM (LCSM) has these problematic features:

- There is a large volume of LNAPL in the subsurface, indicated by a calculation whereby the site-wide average thickness of the LNAPL in the monitoring wells was multiplied by the area of the LNAPL body.
- It was assumed that much of this LNAPL was recoverable by the existing LNAPL skimming system, even though LNAPL recovery is much lower than the initial LNAPL recovery rate.
- It was assumed that LNAPL recovery had to continue until no more LNAPL is observed in each of the site monitoring wells (i.e. reaching an apparent LNAPL thickness of zero).
- Although long-term LNAPL monitoring data indicated that the LNAPL body was stable and no longer expanding, a US EPA LNAPL model (HSSM) had been used many years ago and indicated that the LNAPL body was likely to continue to expand for the next 30 years without LNAPL recovery. These old modelling results greatly complicated efforts to retire the existing LNAPL recovery system comprised of LNAPL skimmer wells.
- Based on the scientific knowledge from the mid-1990s, the only process that was removing LNAPL was the dissolution of higher-solubility constituents in the LNAPL; it would take hundreds of years to remove these soluble constituents, and the lower solubility compounds would likely persist forever.

How to update the LCSM using the LNAPL Toolbox

Step 1. The 'How much LNAPL is present?' Tier 1 tab (Figure 2) is used to develop a much more accurate estimate of the specific volume of LNAPL based on soil type and LNAPL apparent thickness. When the specific volume is multiplied by the LNAPL body area, an updated estimate of the LNAPL volume in the subsurface is developed. This new estimate is many times lower than the original estimate because the previous LCSM volume estimation method was based on inaccurate understanding and assumptions.

Figure 2: Excerpt from the 'How much LNAPL is present?' Tier 1 tab How much LNAPL is present? Tier 3 Tier 1 Tier 2 Quick Info Models/Tools Gateway to Complex Tools Introduction: Specific Volume In the past, a common misconception of the vertical distribution of free product at the water table was based on the idea that LNAPL occurs as a distinct lens in which the drainable pore space is completely saturated with LNAPL and that the thickness of LNAPL in a monitoring well accurately represented the thickness of LNAPL in the formation. This was often referred to as the "pancake layer" model for LNAPL, but it does not reflect the important part soil properties play in the relationship between the amount of LNAPL in the formation and the thickness LNAPL in a well (referred to as "apparent thickness"). 0.1 metre 0.3 metre 1 metre Soil Type This much LNAPL is in the formation (m³/m²)

In the table to the right, the amount of LNAPL in the formation for three different apparent LNAPL thicknesses in a monitoring well is described in terms of a "specific volume". The specific volume is the volume of LNAPL in a given location divided by the surface area. This is a calculated value of the actual amount of LNAPL present in an area divided by the area. This would be the thickness of LNAPL that would remain in an LNAPL zone if the soil and water in that area were hypothetically removed.

See the soil texture triangle to the bottom right to convert soil data in terms of % Sand, % Silt, and % Clay to the USDA soil classification system shown in the specific volume table to the right.

Silty Clay 0.000041 0.00039 0.0045 0.00020 0.0028 0.040 Silt oam 0.00034 0.0058 0.084 Sand 0.0025 0.059 0.32

able developed for Concawe Toolbox 2020 using LNAPL tool developed l de Blanc, P. and S. K. Farhat, 2018. 25th IPEC: International Petroleum

See more soil types

The Concawe LNAPL Toolbox

Step 2. Step 1 indicated that more detailed information would be beneficial, hence two models are evaluated: the mid-level complexity Tier 2 model in the Concawe Toolbox (Figure 3); and a more complex model called the LNAPL Distribution and Recovery Model (LDRM, API) that is explained in the Tier 3 text and videos. Based on this information, the Tier 2 model is selected, site data is compiled and entered into the input data spreadsheet, and the model is run. The 'How much LNAPL is present?' Tier 2 model provides a more refined estimate of the total LNAPL present in the subsurface, as well as additional information, namely the amount of LNAPL that is potentially mobile and the amount of LNAPL that is permanently trapped as residual LNAPL.

Figure 3: Excerpt from 'How much LNAPL is present?' Tier 2 tab

How much LNAPL is pr	esent?							
Tier 1 Tier 2 Qulck Info Models/Tools Gateway	Tier 3 to Complex Tools							
Multi-Site LNAPL Volume and Externation What the Model Does	ent Model Inputs:	Choose Input File Browse No file selected	Map Interpolation	Map Interpolation Model Output Select Parameter to View:				
This too calculates several key LNAPL values, including sy and transmissivity, at multiple lacations for multiple layer are used to calculate a total subsurface LNAPL volume. B the user, estimated LNAPL velocities are also calculated. T depicted graphically.	eiche volume, recoverable volume, co differing all pipes. These values seed on LNAPL gradients specified by The distribution of calculated values is from Input Fil Will reset all input	Les Laport Model Results and Input Tables	Save Map					

Step 3. The 'How much LNAPL is present?' Tier 2 model (Figure 3) is used to develop a map of the LNAPL transmissivity based on site-specific LNAPL properties, site-specific soil characteristics, and site-specific layering/stratigraphy. With this map, guidance from the US Interstate Technology and Regulatory Council (ITRC) is consulted, which suggests that:

- If the LNAPL transmissivity is less than 0.0093 m²/day, hydraulic recovery of LNAPL is unlikely to be
 efficient, sustainable or cost-effective.
- If the LNAPL transmissivity is greater than 0.074 m²/day, hydraulic recovery of LNAPL is likely to be
 effective.

Surprisingly, only one of the LNAPL skimming wells exceeds the 0.0093 m²/day threshold, indicating that the rest of the skimming wells are not providing any significant environmental benefit. The simple 'Will LNAPL recovery be effective?' Tier 1 tab (Figure 4 on page 61) also shows similar results, increasing confidence that LNAPL recovery should be terminated at all but one of the existing LNAPL skimmer wells.

The Concawe LNAPL Toolbox



Figure 4: Excerpt from the 'Will LNAPL recovery be effective?' Tier 1 tab

Step 4. The 'How far will LNAPL migrate?' Tier 1 tab (Figure 5) indicates that NSZD is a key factor in stopping the continued migration of LNAPL bodies, and the 'How far will LNAPL migrate?' Tier 2 tab (Figure 6 on page 62) indicates that LNAPL models that do not consider NSZD are likely to overestimate LNAPL migration because of this. The site consultants and site owners determine that more NSZD information would be key to updating the LCSM but do not have a strong background in NSZD. Therefore, they consult the three Tiers in the 'How can one estimate NSZD?' tab in the Toolbox.

Figure 5: Excerpt from the 'How far will the LNAPL migrate?' Tier 1 tab





Figure 6: Excerpt from the 'How far will the LNAPL migrate?' Tier 2 tab



Step 5. Based on the discussion of NSZD in the 'How far will LNAPL migrate?' Tier 1 tab (Figure 5), the 'How can one estimate NSZD? Tier 1 tab (Figure 7) is consulted and quickly shows that almost all LNAPL bodies are naturally attenuating at 10 or 100 times the rate assumed in the existing LCSM. The new LCSM indicated that, typically, when NSZD is measured at a site, the rates are in the thousands to tens of thousands of litres of LNAPL being biodegraded by NSZD per hectare per year. The 'How can one estimate NSZD?' Tier 3 tab (Figure 8 on page 63) provides links and videos on methods to measure NSZD at an LNAPL site, and the site consultants can then begin to evaluate whether the literature NSZD values shown in the Concawe LNAPL Toolbox are sufficient to update to the new LCSM, or whether site-specific measurements are needed.

Figure 7: Excerpt from the 'How can one estimate NSZD?' Tier 1 tab



Figure 8: Excerpt from the 'How can one estimate NSZD?' Tier 3 tab

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wo videos were developed for the NSZD article								Flows 1 1
Carbon Traps NSZD								Ker VOCs CH, CO, Q
Thermal Monitoring NS2D								Figure 2. Conceptual model of NSZD processes, gos f
What NSZD Rates are Seen a	at Hydrocarbon Sites?							erences shown in Table 1 and Figures 1 and 3. For the LNAPL smear zone and the capillary fringe are lifty shown in the processes depicted in the convertin
e following table from Garg et al. (2017) summ	marizes measured NSZD rates at various hydrocarbon sites in the	U.S. The middle 50% of	the NSZD rates range from 3	700 – 2,800 gallons per acre per	year.			Too an on the part of the part
		E	kamples of Site-Wid	de Average NSZD Rate	Measurements at Field Sites			
					Site Wide NSZD Rate (Gallon	/Acre/Year)		
	NSZD Study			Number of Sites	All Sites	Middle 50%	Reference	
Refir	inery terminal sites			6	2100-7700	2400-3700	McCoy 2012	
1975	79 crude oil spill			1	1600		Sihota et al. 2011	
Seas	isonal range				310-1100		Sihota et al. 2016	
Refi	inery/terminal sites			2	1100-1700	1250-1550	Workgroup, L.A LANPL 2015	
Fuel	el/diesel/gasoline			5	300-3100	1050-2700	Piontek et al. 2014	
Dive	erse petroleum sites			11	300-5600	600-800	Palaia 2016	
All g	studies			25	300-7700	700-2800		
Satu	urated zone electron acceptor biodegradation capacity			9	0.4-53	1.7-19	This paper (see Appendix S1)	
Note	es: Middle 50% column shows the 25th and 75th percentile val	ues. To demonstrate the	e significance of methanoge	enesis, NSZD rates calculated fr	om the biodegradation capacity of electror	acceptors in the saturate	zone, ignoring methanogenesis, are shown in	the last row.
			SUMM	ARY OF NSZD RATES	ROM 31 SITES			
	Fuel Type	Fuel Carbon Range	Number of Distinct Sites	Total No. of Measuremen	nts Range of NSZD Rates Measured (I	/ha/yr) Median NSZD	Rate (L/ha/yr)	
	Natural Gas Liquid*	C3-C6	5	1661	1,590 - 54,800	4,1	100	
	Mixed	-	6	855	1,760 - 57,060	4,4	100	
	Crude Oil	C8-C44	2	77	2,250 - 24,000	7	100	
	Gasoline	C5-C12	4	144	2 800 - 41 500	93	00	
	Diesel and let Fuel	C9-C24	12	134	650 - 99 400	12	250	
	Fuel-Grade Ethanol	C2H60	2	134	123,200 - 152,500	12,	.000	
	Total		31	3054		fedian: 8,3	50	

Step 6. Using mid-range NSZD rates from the Tier 1 NSZD estimation tab, the 'How far will LNAPL migrate?' Tier 2 tab (Figure 6) is consulted and the Kirkman Additional LNAPL Migration Model built into the Toolbox (Figure 6) is then applied using existing site data. This shows that the existing LNAPL body is not likely to expand to any significant degree even if the LNAPL skimmer wells were shut down. This provides additional support to the assumption that most of the LNAPL skimmer wells had done their job and are ready to be retired.

The Concawe LNAPL Toolbox

Step 7. The potential longevity of the LNAPL is then evaluated to update the existing LCSM. After reviewing the 'How long will LNAPL persist?' Tier 1 tab (Figure 9), the simple Tier 2 LNAPL lifetime model is applied by entering the volume of LNAPL from Step 2, the area of the LNAPL body, and mid-range NSZD rates from the Tier 1 NSZD estimation tab (Figure 7). Two different LNAPL volume versus time graphs are obtained. One method assumes a constant NSZD rate into the future and suggests that the LNAPL would all be removed by the year 2030. The second method assumes that NSZD rates decline over time and suggests that 90% of the LNAPL present now would be gone by the year 2050. Overall, this wide range of LNAPL longevity estimates inform the new LCSM that estimates of LNAPL longevity decades into the future have significant uncertainty, but agree that LNAPL is being removed over time.

Figure 9: Excerpt from the 'How long will the LNAPL persist?' Tier 1 tab



Step 8. Because of the uncertainty in the LNAPL longevity estimates, the site consultants and site owners become interested in estimates of how the hypothetical ingestion risk associated with LNAPL dissolution products might change over time (there is no ongoing risk at this site as no exposure pathways were complete). The 'How will LNAPL risk change over time?' Tier 2 model (Figure 10 on page 65) is run initially to obtain a forecast of the benzene concentration over time. Later, a more sophisticated LNAPL model is run, described in the 'How will LNAPL risk change over time?' Tier 3 tab, called Remediation Evaluation Model for Fuel hydrocarbons (REMFuel; US EPA); this model is run based on the comments included in the Concawe Tier 3 description of REMFuel and the information given in the video link provided in the Tier 3 tab (Figure 11 on page 65). This modelling effort shows that the risk associated with the hypothetical ingestion pathway over time reduces faster than the likely LNAPL removal rate.

Figure 10: Excerpt from the 'How will LNAPL risk change over time?' Tier 2 tab

	Hydraulic Conductivity (cm/s)	LINAPLCC	instruents chemis	uy mputs.	Malandarum Jaka (a (mal)	Calubility (as (1)	Descinded on B
What the Model Does	3000		LNAPL Constituents	volume traction	Molecular weight (g/mol)	Solubility (mg/L)	Density (g/cm-)
his model calculates the theoretical concentration of dissolved hydrocarbons in groundwater downgradient of an UNAPL source over me due to dissolution processes. The model produces a graph of dissolved constituent (such as 8,T,E, X and MTBE) in groundwater	Hadrandia Readiant (m/m)	1	benzene	0.05	78.1	1770	0.87
ver time in units of mg/L as an LNAPL source is depleted of these soluble constituents.	0.005	2	toluene	0.1	92.1	530	0.74
low the Model Works	Width of LNAPL Lens (m)	3	other	0.85	100	10	0.78
known volume of LNAPL is released to the subsurface. The LNAPL is comprised of several components whose volume fractions and	30	4					
insities are known. The unidentified fraction of the LNAPL is a mixed petroleum product with unknown components, but with a rown average molecular weight and density.	Average Thickness of LNAPL Lens (m)	5	an Marine a				
te LNAPL establishes a lens in the groundwater with a known width and average thickness. Groundwater flows through the LNAPL	0.5	Showing 1 to 5 on Add up to 5 con	of 5 entries stituents. Double click to edit				
ns and dissolves the LNAPL constituents, reducing the remaining volume of LNAPL and changing its composition as the more soluble impounds dissolve out of the LNAPL. Equilibrium between the water and LNAPL within the lens is assumed, so that the	Time Step (days)	Click Calculate Ba	itten				
incentration of constituents downgradient of the LNAPL are equal to the effective solubility of the LNAPL constituents. Effective Jubility is the solubility of a pure phase component times its mole fraction in the LNAPL.	0.005						
e key strengths of the model are:	LNAPL Body Volume (Liters)						
The model is simple and easy to understand. Because of its simplicity, the model can be modified by users if needed.	3000						
leakness of the model are:	Length of Simulation (years)						
 Equilibrium is unlikely to be completely achieved at actual sites, so the model over-estimates downgradient aqueous phase concentrations. 	0.1						
 The explicit solution scheme can become inaccurate or unstable if the time step is too large. 	Click Colculate to Update Plot						
ev Assumptions							
y assumptions of the model are as follows:	Calculate						
The groundwater concentration is directly downgradient of the LNAPL body before any attenuation or mixing occurs.							
Volume is conserved upon fluid mixing. The concentration of a constituent in the aqueous phase in equilibrium with the LNAPL is the constituent's mole fraction in the INAPI time the constituent's use phase and billing	Note: If the colculated solution appears to be unstable try reducing the model time step.						
Water exiting the UNAPL lens is saturated with each UNAPL constituent; i.e., there is perfect mixing between groundwater and INAPL constituents in the INAPL lens.		Y-Axis I	.og Scale				
LNAPL does not impede groundwater flow.							
 Fluid densities and solubilities do not change significantly with temperature. 							

Figure 11: Excerpt from the 'How will LNAPL risk change over time?' Tier 3 tab

How wi	II LNAPL	risk change over	time?
Tier 1 Quick Info	Tier 2 Models/Tools	Tler 3 Gateway to Complex Tools	
The risk posed by provided in Tier	the toxic components and shows how the di	of an LNAPL plume is a function of the cost of the cos	stre page. Statistients' concentration in groundwater in contact with the LNAPL. A multi-component LNAPL dissolution model based on the LNAPL constituent mole fraction and Raoult's law (Mayer and Hassanizadeh, 2005) is elisted violamentation of an LNAPL body chance over time.
A more sophistic	ated computer tool, AP	I's LNAST model, also shows the change i I LNAPL, are also reviewed below.	n dissolved phase LNAPL concentrations over time (Huntley and Beckett, 2002). It is summarized below. Finally, two other key LNAPL attenuation studies, a LNAPL mass balance developed by Ng et al. (2014) and a
Overview	of API's LNAI	PL Dissolution and Trans	sport Screening Tool (LNAST)
Predics L Calculate Shows res Simulates Combines Combines Accounts Zones of I God tool Powerful Key outpu Does not LINAST car Video A short video to I	NAPL distribution, diss downgradient dissoliv ults both with and with the smear zone and the multi-phase transport. for relative permeability hUAPL staruration h for estimating how low loss to see if LNAPL res is concentration of di account for Natural Soc het remediation occur be downloaded here.	Judion, and volatilization over time. edynase concertation through time. Jout hydraulic recovery of LNAPL. ed owngadient dissolved plume. dissoluton, and solute transport. y effects caused by LNAPL. ave much less groundwater flow through ga ni LNAPL-generated plume will genis overy reduces the longevity of the source solved constituents in the plume vs. tim ree Zone Depletion (NSZD). shortly after the LNAPL release. You can I can be found here.	them, extending the longevity of these zones. and plume. a an observation well. not release LNAPL many years ago and then start the remediation now a few decades later. The REMFuel model will do this, see Tier 3 of "How long will LNAPL persist?" portion of the Concawe LNAPL Toolbox.
			Quick Tour of LNAST Interfaces
			Input
			Link to LNAPL Dissolution and Transport Screening Tool

The Concawe LNAPL Toolbox

Step 9. The Toolbox helps site owners and consultants update the existing, incorrect LCSM, and greatly strengthens the case for:

- retiring most of the old, inefficient LNAPL skimming wells at the site because of low LNAPL recoverability and the expectation of little or no LNAPL expansion in the future;
- a better understanding that further significant LNAPL migration was unlikely and that benzene concentrations were expected to go down over time;
- using NSZD as the LNAPL management technology in the future; and
- continued long-term groundwater monitoring to ensure that the long-term removal of the LNAPL body by NSZD remains on-track.

Conclusions and outreach

The Concawe LNAPL Toolbox is a wide-ranging but easy-to-use web-based toolbox capable of delivering key LNAPL knowledge to the LNAPL remediation community, to help LNAPL scientists and engineers better understand how to manage LNAPL at their sites.

The Toolbox is designed to be freely accessed on the web via an internet browser (https://lnapltoolbox.concawe.eu/lnapl_toolbox) or by downloading the Toolbox code for use on a personal computer (https://github.com/concawe/LNAPL-Toolbox-). The Toolbox User Manual is also published on the Concawe website (Concawe Report 5/22, https://www.concawe.eu/wp-content/uploads/Rpt_22-5.pdf).

The Toolbox was launched in April 2022. As part of a promotional campaign, two targeted webinars were organised in May 2022. After the webinars, a pre-recording of the LNAPL Toolbox presentation was made freely available (see https://www.youtube.com/watch?v=LBkT887vjzY). Further to the webinars, the Toolbox was presented at RemTech Europe in September 2022, at the RemTEC & Emerging Contaminants Summit in October 2022, and as a dedicated webinar given under the umbrella of NICOLA in December 2022.

References

A full list of references is provided in Strasert, B., C. Newell, P. de Blanc, P. Kulkarni, K. Whitehead, B. Sackmann, and H. Podzorski (2021), *User Manual for Concawe LNAPL Toolbox*. Concawe Report 5/22, Concawe, Brussels, Belgium, Version 1 (https://www.concawe.eu/wp-content/uploads/Rpt_22-5.pdf) and within the LNAPL toolbox itself (https://inapltoolbox.concawe.eu/inapl_toolbox/).

Abbreviations and terms

AAQ	Ambient Air Quality	EMEP	European Monitoring and Evaluation
API	American Petroleum Institute	5.46	Programme
Apparent	Observed monitoring well LNAPL thickness.	EMS	Energy Management Strategy
LNAPL thickness	l erms that others have used to describe the observed monitoring well	EU	
	thickness are 'apparent thickness' and	EU-27	The 27 countries of the European Union
100	observed thickness .	FC	Fuel Consumption
AQG	Air Quality Guidelines	FEMG	Concawe's Fuels and Emissions Management Group
AS	Arsenic	GAINS	Greenhouse gas and Air pollution
ARTEMIS	Assessment and Reliability of Transport Emissions Models and Inventory Systems		INteractions and Synergies
ASTM	American Society for Testing and Materials	GHG	Greenhouse Gas
B7	Diesel fuel blend containing up to	HC	Total Hydrocarbons
	7% biodiesel	HEV	Hybrid Electric Vehicle
BaP	Benzo(a)pyrene	HSSM	US EPA's Hydrocarbon Spill Screening Model
BEV	Battery Electric Vehicle		for modelling LINAPL migration
B.I.A.	Biodiversity Impact Assessment	HVAC	Heating, Ventilation and Air Conditioning
BVI	Biodiversity Value Increment	HVO	Hydrotreated Vegetable Oil
C ₆ H ₆	Benzene	ICCT	International Council on Clean Transportation
CAO2	The Second Clean Air Outlook (published by the European Commission in 2021)	ICE	Internal Combustion Engine
Cd		IFPEN	IFP Energy nouvelles
CD		IIASA	International Institute of Applied Systems
CDF			Analysis
СН	Methane	IT	Interim Target
	Current Legislation	ITRC	Interstate Technology and Regulatory Council, A United States coalition of
CO			environmental regulators, site owners,
CO.			academics, and consultants working to reduce barriers to the use of innovative air.
CO.e			water, waste, and remediation environmental
CS	Charge Sustaining		technologies and processes.
CSM	Concentual Site Model	LCA	Life-Cycle Assessment
DoF		LCSM	LNAPL Conceptual Site Model
E10	Petroleum fuel blend containing un to	LDRM	LNAPL Distribution and Recovery Model. The API LDRM simulates the performance of
210	10% ethanol		proven hydraulic technologies for recovering
E20	Petroleum fuel blend containing up to 20% ethanol		groundwater.
EC	Electricity Consumption	LNAPL	Light Non-Aqueous Phase Liquids. These are lighter-than-water separate phase liquids,
ECMS	Equivalent Consumption Minimisation Strategy		such as crude oil, gasoline, diesel fuel, etc. that can migrate into the subsurface and
EEA	European Environment Agency		Sometimes referred to as 'product' or, if found in wells, 'free product'.

Abbreviations and terms

(continued)

LNAST	LNAPL dissolution And transport Screening Tool — an API model that consists of a suite of calculation tools, information about LNAPL, and LNAPL parameter databases.	REMFuel	Remediation Evaluation Model for Fuel hydrocarbons—a source remediation/ attenuation and plume migration model for LNAPL sites distributed by the US EPA.
	fate at the water table.	Residual LNAPL	LNAPL that represents discontinuous globules of LNAPL within the pore network
MT	Megatonne		and is immobile under prevailing conditions. It can be thought of as 'individual blobs of
Mtoe	Million tonnes of oil equivalent		LNAPL in individual pores' in a gravel, sand or
MTFR	Maximum Technically Feasible Reduction		silt. This concept is complex, with several
N ₂ O	Nitrous Oxide		apply this value, and five methods to
NEC	National Emissions reduction Commitments (EU Directive 2016/2284)	Residual	determine a value for residual saturation. The LNAPL saturation level below which
NH ₃	Ammonia	saturation	naturally occurring capillary forces prevent
Ni	Nickel		immobile.
NICOLA	Network for Industrially Contaminated Land	RIL	Reduced Impact Logging
	in Africa	SO ₂	Sulphur Dioxide
NO2	Nitrogen Dioxide	SoC	State of Charge
NO _x	Nitrogen Oxides	Specific	In a given area, the volume of the actual
NSZD	removal of LNAPL from the subsurface by naturally occurring physical, chemical and biological processes.	volume	would be the thickness of LNAPL that would remain in an LNAPL zone if the soil and water in that area were hypothetically removed.
NUTS 3	Small regions for specific diagnoses as	STF-20	Concawe's Gasoline Special Task Force
	defined in the EU's Nomenclature des Unités Territoriales Statistiques (Nomenclature of	STF-25	Concawe's Diesel Special Task Force
	territorial units for statistics) 2021 classification.	ттw	Tank To Wheels
O ₃	Ozone	UF	Utility Factor
P2	Hybrid configuration where the electric	UK	United Kingdom
	motor is integrated between the internal combustion engine and the transmission	UNECE	United Nations Economic Commission for Europe
Pb	Lead	US EPA	United States Environmental Protection
PDF	Potentially Disappeared Fraction of species		Agency
PHEV	Plug-in Hybrid Electric Vehicle	USDA	United States Department of Agriculture
РМ	Particulate Matter	UTCHEM	University of Texas chemical flood simulator, a 3-D finite-difference numerical model that
PM _{2.5}	Particulate Matter with an aerodynamic diameter of less than or equal to 2.5 µm		can be used to simulate LNAPL migration and dissolution.
PM ₁₀	Particulate Matter with an aerodynamic	VKT	Vehicle Kilometres Travelled
	diameter of less than or equal to 10 µm	VOC	Volatile Organic Compound
PN	Particulate Number	WHO	World Health Organization
PNx	Particulate Number with a diameter greater than x nm	WLTC	Worldwide harmonized Light-duty Test Cycle
R&D	Research and Development	WLTP	Worldwide harmonised Light vehicles Test Procedure
RDE	Real Driving Emissions	WTT	Well To Tank
RED	Renewable Energy Directive	wтw	Well To Wheels

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