Electronic Supplement to the paper: "Modelling the impact of the introduction of the EURO 6d-TEMP/6d regulation for light-duty vehicles on EU air quality**."**

1.1. Description experimental setup for the establishment of the emission factors.

All vehicles were tested in the VELA laboratories of the STU between 2018 and 2020. Fifteen vehicles were tested in VELA2 and fifteen in VELA8. VELA2 is a chassis dynamometer test cell comprising two roller benches with 48'' diameter (MAHA Haldenwang, Germany), a constant volume sampling system (CVS with a flow rate range of 3 - 30 $m^3 min^{-1}$) with a critical flow Venturi, and a MEXA-7400 gas analyser for the measurement of total hydrocarbons (THC), carbon monoxide (CO), carbon dioxide (CO_2), nitrogen oxides (NO_X), methane (CH_4), non-methane hydrocarbons (NMHC) from Tedlar bags (HORIBA, Japan). VELA 8 is also a two roller bench chassis dynamometer (48'' diameter and inertia range 250-4500 kg from ZÖLLNER GmbH, Bensheim, Germany), a CVS (i60 LD, flow rate range 2 - 20 $m^3 min^{-1}$) with a critical flow Venturi, and AMA160R1 gas analyser benches for the measurement of the same gaseous pollutants (NO_X, CO, THC, CH_4, NMHC and CO_2) from the bags (AVL, Graz, Austria). Both testing facilities are equipped with Fourier Transformed Infrared analysers (FTIR) that allow the measurement of tailpipe emissions ammonia (NH_3).

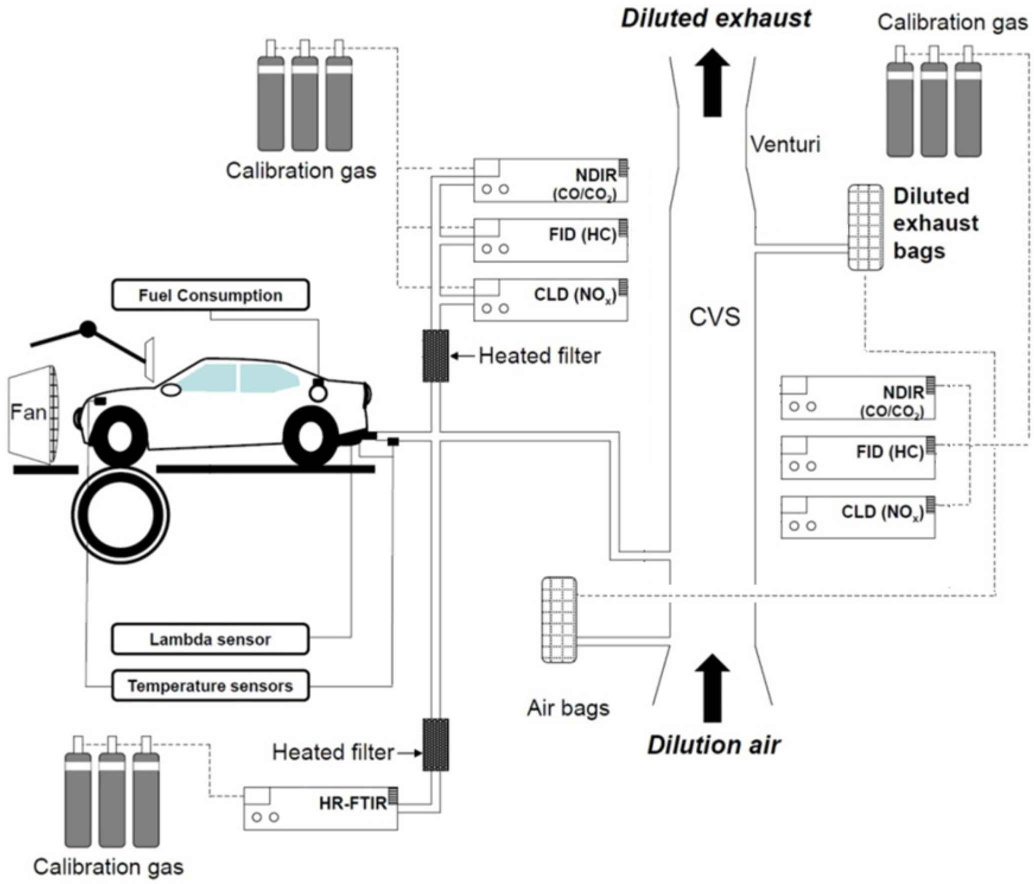


Figure S1. Instrumentation and sampling scheme in VELA laboratory.

The driving cycle within the WLTP is the so called World-wide harmonized Light duty Test Cycle (WLTC) which is a 23.2 km long test that was developed from real world driving data and represents average driving characteristics around the world [1]. Two repetitions of the cycle according with the WLTP procedure were performed on each vehicle at an ambient temperature of 23 degree Celsius. All tests were performed using commercial fuels. For each vehicle, the distance-specific emissions were calculated as the arithmetic mean of the two repetitions. The distance-specific emission factors were transformed into fuel-specific emission factors (expressed in kg TJ^{-1}) assuming the energy content of the fuels described in the documentation supporting the Alternative Fuel Infrastructure Directive (https://ec.europa.eu/transport/sites/transport/files/2017-01-fuel-price-comparison.pdf Table 2).

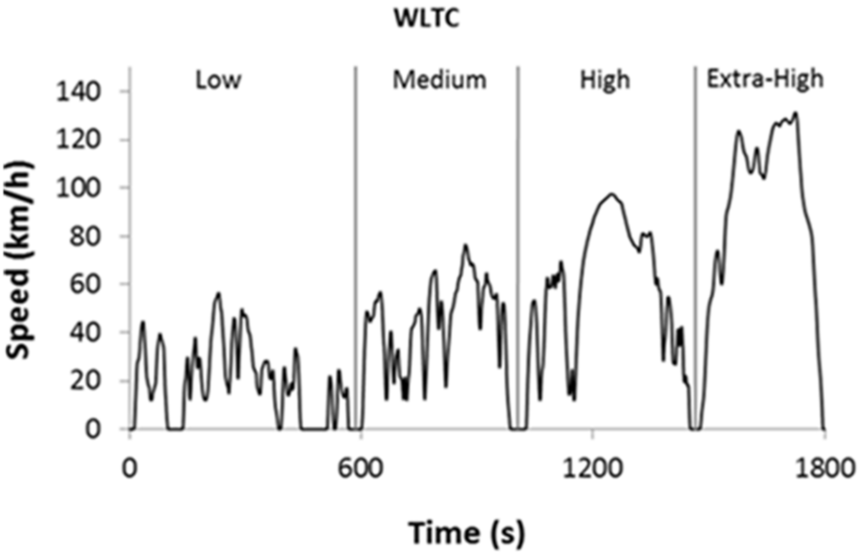


Figure S2. Test cycles speed profile WLTC

The propulsion type of twenty-three of the vehicles was only an internal combustion engine (ICE – also known as pure-ICE vehicles) whereas 7 vehicles had some level of hybridization. In particular, four vehicles were plug-in hybrid vehicles (PHEV), one conventional hybrid, and two micro-hybrids (vehicles in which the electric motor never propels the vehicle by themselves). The performed tests on the PHEV were in charge sustaining operation that is starting with a fully depleted battery and hence running mostly with the ICE, similar to a conventional hybrid. Among the pure-ICE, eight were diesel-fuelled, thirteen gasoline-fuelled, one fuelled with compressed natural gas (CNG) and one fuelled with liquefied petroleum gas (LPG). The tested vehicle fleet covers a range of engine displacement (from 0.875 l to 3 l), fuel injection types, and emission after-treatment technologies.

Powertrain-specific emission factors were then calculated averaging the emission factors of all the vehicles within the same powertrain (ICE Diesel, ICE Gasoline and PHEV Gasoline). The emission factors are for the following species of interest THC, CO, CO_2, NO_X, CH_4, NMHC and NH_3). All gaseous species, with the exception of NH_3, were measured using the regulatory procedure, i.e. a sample of the exhaust is collected in a gas sampling Tedlar bag and analysed immediately after the end of the driving cycle. Ammonia was measured directly from the tailpipe.

Figure S3. Set up and vehicle in the VELA laboratory.

1.2. Emission factors

The fuel-specific emission factors derived from the experimental activity are shown in Table S1 for conventional ICE diesel and gasoline Euro 6d-TEMP/6d vehicles. The emission factors correspond to the complete WLTC cycle and thus represent a combination of urban, rural, and motorway driving.

Nitrogen oxides emissions are slightly lower than 10 kg/TJ for gasoline cars (equivalent to ~20 mg/km) and twice as much for diesel vehicles (~ 35 mg/km). All vehicles met the Euro 6 emission limit under the realistic WLTP test.

Regarding total hydrocarbon emissions, diesel vehicles emit roughly 20% lower than gasoline cars. For three out of the eight diesel vehicles tested, methane emissions (average of 30 mg/km) were significantly above the methane emissions measured in the other five vehicles (average of 2 mg/km) which in turn were similar to the gasoline average (2.5 mg/km). Methane emissions are in line with emission factors reported in the literature [2]. Non-methane hydrocarbons emissions, which can be used as a proxy for volatile organic compounds, were 66% higher in gasoline vehicles than in their diesel counterparts. Most of the hydrocarbon emissions (CH_4, and NMVOC) tend to occur shortly after the first ignition of the ICE. During the cold-start period the engine and after-treatment systems do not operate efficiently resulting in a large production of emissions coming out from the engine that cannot be properly oxidized in the catalysts, hence with relatively high emissions exiting the tailpipe.

Carbon monoxide emissions are low for both diesel and gasoline Euro 6d-TEMP/6d vehicles over the WLTP, largely fulfilling the Euro 6 limits. However, gasoline vehicles emit 90% more CO than diesels. CO emissions from gasoline cars tend to concentrate during the cold start as well as during harsh accelerations when the mixture of air and fuel in the combustion chamber is richer in fuel.

Ammonia emissions of gasoline vehicles ranged from 4 to 20 mg/km with an average of 9 mg/km that corresponds to 4.7 kg/TJ. In gasoline cars, NH_3 is formed in the catalyst during rich operation after the catalyst light-off. For diesel vehicles instead, the measured NH_3 was slightly above 0 mg/km for all vehicles except one for which emissions were ~28 mg/km resulting in an average of 3.2 kg/TJ. NH_3 from modern diesel vehicles tend to occur as a by-product of the SCR catalysts that uses urea to reduce NO_X emissions. A growing number of diesel vehicles are now equipped with an ammonia oxidation catalyst downstream of the SCR to avoid NH_3 emissions, however as there is no Euro 6 limit for NH_3. The use of this ad-hoc catalyst is optional and certain vehicle manufacturers do not equip their vehicles with it. The NH_3 emissions reported here are close to those reported in the literature for other Euro 6 and Euro 5 vehicles [3,4].

Table S1. Emission Factors for Road Traffic in Edgar.

Sector/fuel/type	Substance	implied EF (kg/TJ)
TRO.ROA.DIE.LD+PC	NH3	0.550284988
TRO.ROA.DIE.LD+PC	NMVOC	10.58041207
TRO.ROA.DIE.LD+PC	NOx	256.1300959
TRO.ROA.MOG.LD+PC	NOx	67.45130685
TRO.ROA.MOG.LD+PC	NH3	22.49487648
TRO.ROA.MOG.LD+PC	NMVOC	65.60918433

LD= light duty, PC=passenger cars, DIE=diesel, MOG=motor gasoline

Table S2. Average fuel-specific emission factors of diesel and gasoline Euro 6d-TEMP/Euro 6d vehicles over WLTP.

	THC [kg/TJ]	CO [kg/TJ]	NOx [kg/TJ]	CH4 [kg/TJ]	NMHC [kg/TJ]	NH3 [kg/TJ]
Diesel	10.3	15.3	18.6	7.1	3.7	3.2
Gasoline	12.6	208.1	9.4	1.3	11.4	4.7

1.3. Additional information of the scenarios

It has been shown, that the entry into force of the RDE further reduced the emissions of vehicles on most driving situations as compared to Euro 6b (pre-RDE vehicles), even if the emission limits for both standards are the same. Particularly, for diesel Euro 6b vehicles, real life NO_x emissions tend to exceed by a factor of 6-7 the laboratory emission limit of 80 mg/km whereas gasoline direct injection vehicles emitted 40% above the particulate limit applicable in the laboratory test [5]. Euro 6d-TEMP and Euro 6d diesel vehicles comply well with the Euro 6 limit of NO_x on the road and gasoline vehicles emit 1 to 2 orders of magnitude lower PN emissions on the road than Euro 6b GDIs. These changes in emissions behaviour are related to improved engine calibration strategies as well as emission after-treatment technologies, namely urea-based catalysts in diesel vehicles and gasoline particulate filters in GDIs [6].

Comparison of modelled concentrations, relative difference between Reference Case and Scenario 1.

NO_2

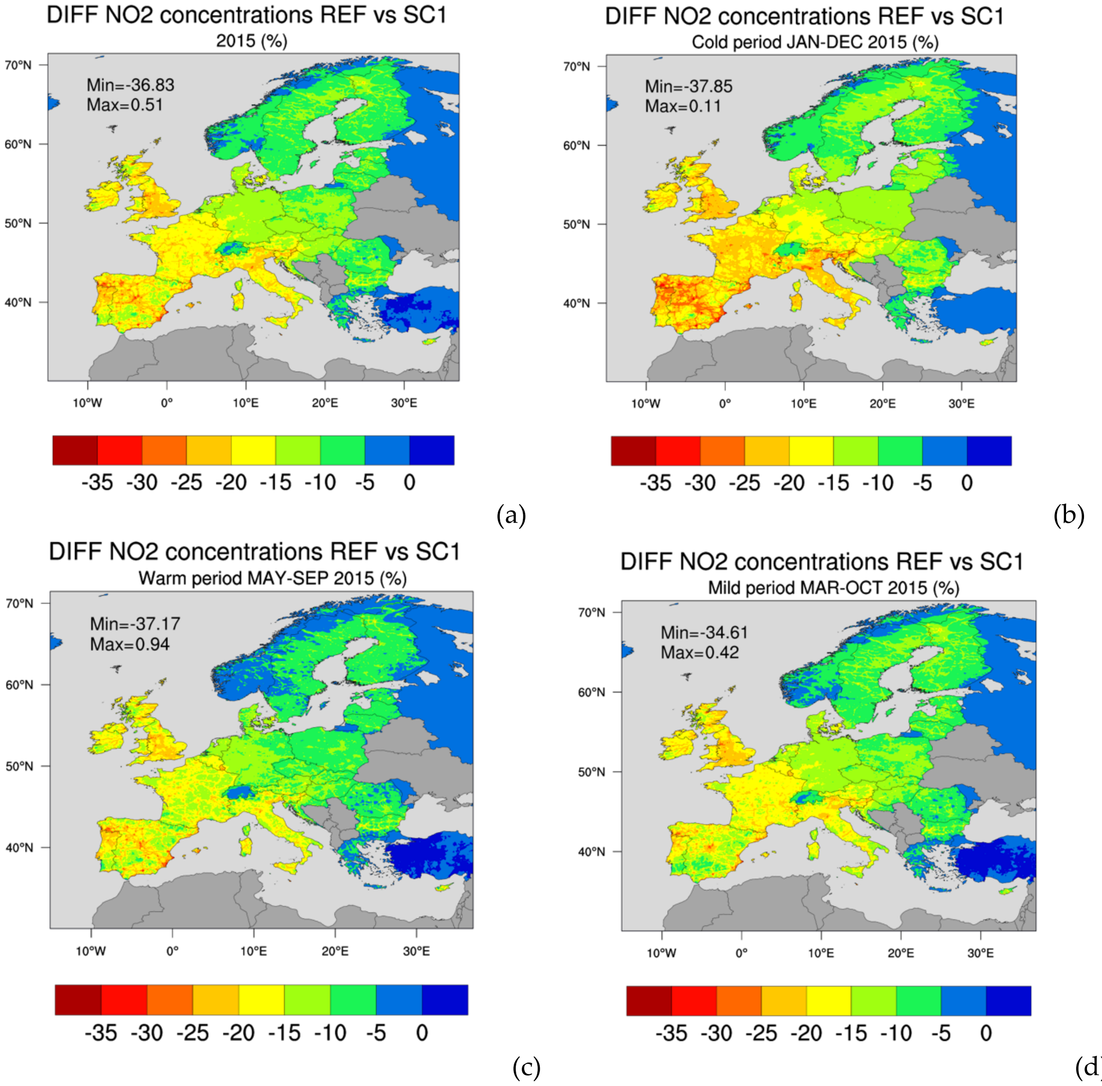


Figure S4. Calculated yearly relative mean differences (%) between Reference Case and Scenario 1 for NO2 (a). Together with the differences in averaged concentrations between the two simulations for three main periods, i.e. (b) a cold/winter period (November till February), (c) warm/summer period (May till September), and (d) mild/transition period (March, April and October).

O3

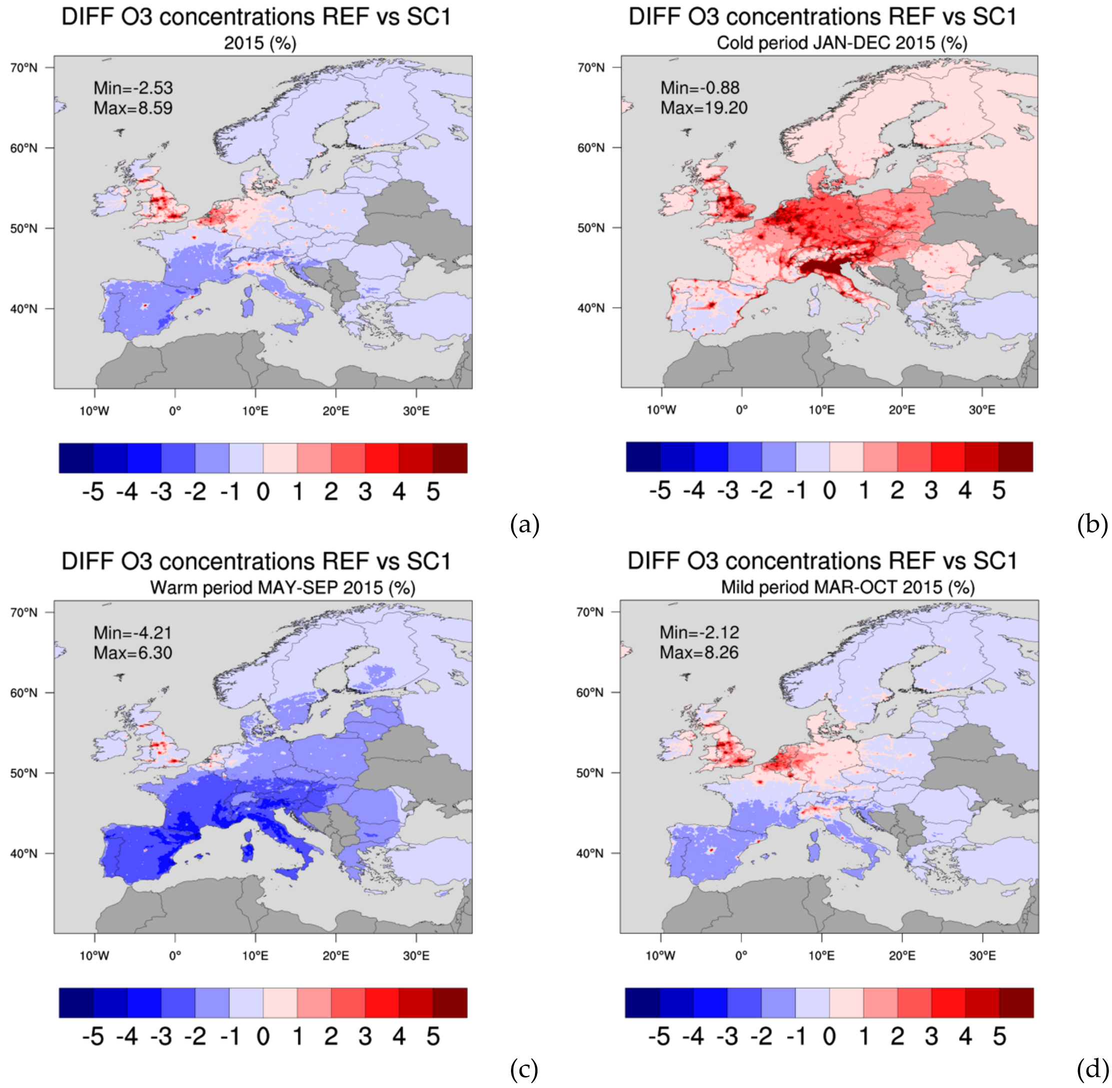


Figure S5. Same as Figure S4, but for O3.

PM25

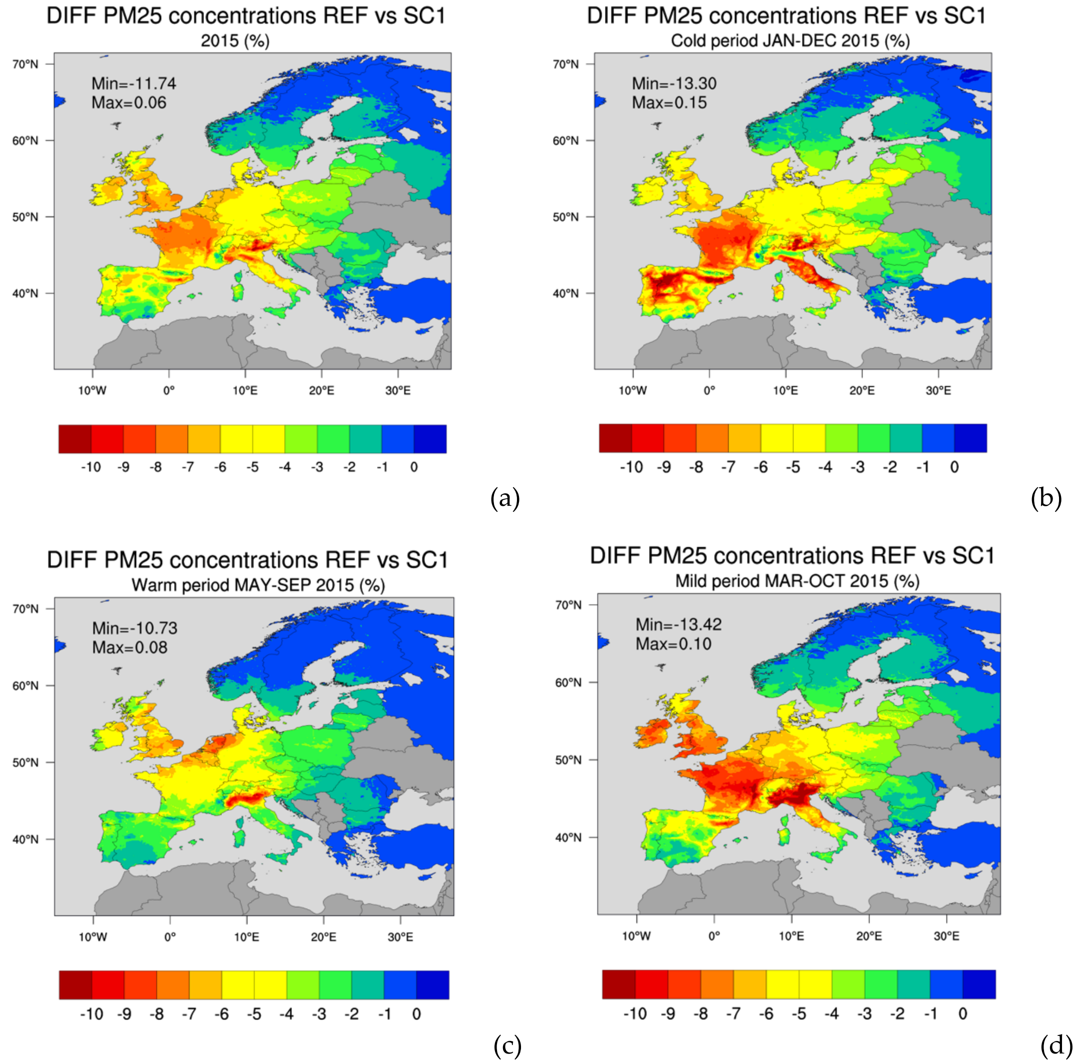
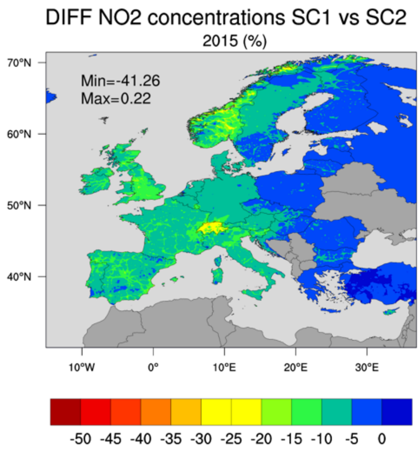


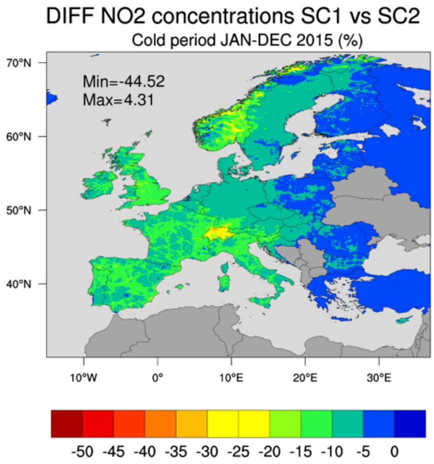
Figure S6. Same as Figure S4, but for PM25.

Comparison of modelled concentrations, relative difference between Scenario 1 and Scenario 2

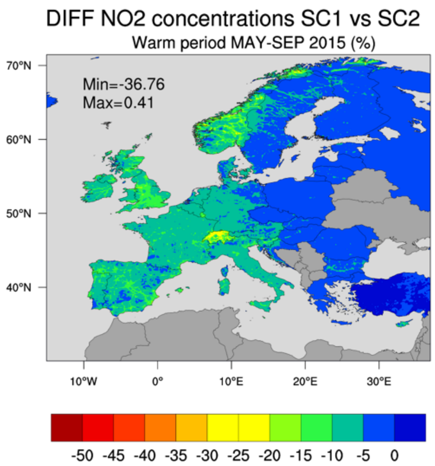
NO2



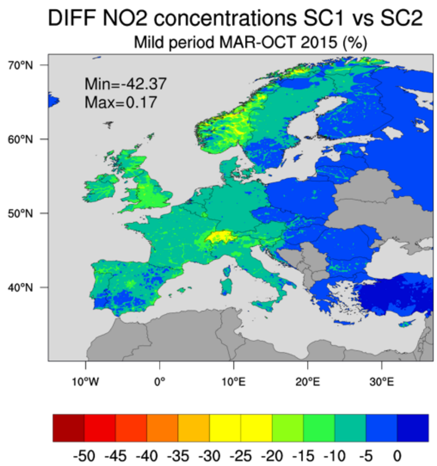
(a)



(b)



(c)



(d)

Figure S7. Calculated yearly mean relative differences (%) between Scenario 1 and Scenario 2 for NO2 (a). Together with the differences in averaged concentrations between the two simulations for three main periods, i.e. (b) a cold/winter period (November till February), (c) warm/summer period (May till September), and (d) mild/transition period (March, April and October).

O3

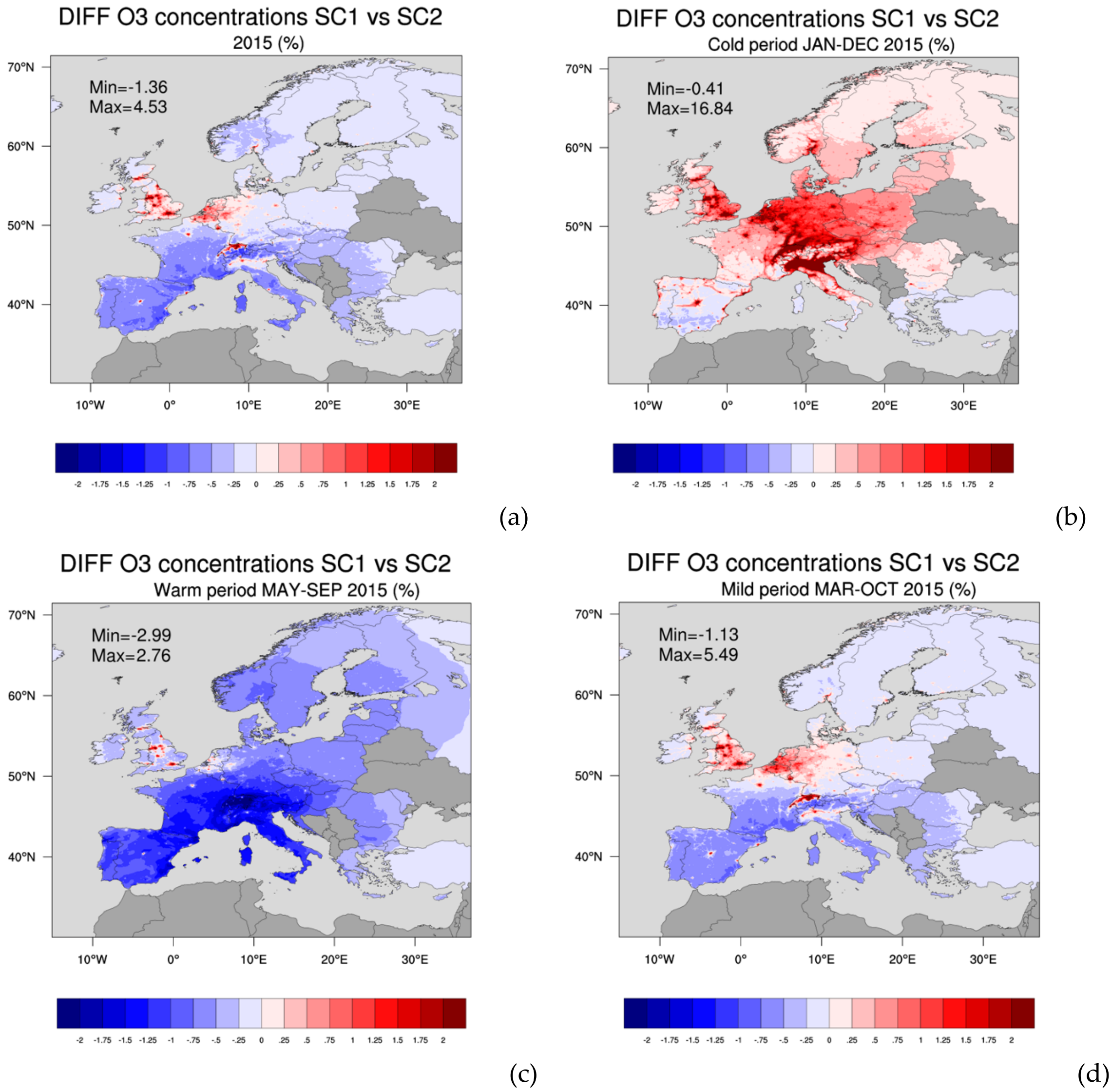


Figure S8. Same as Figure S7, but for O3.

PM25

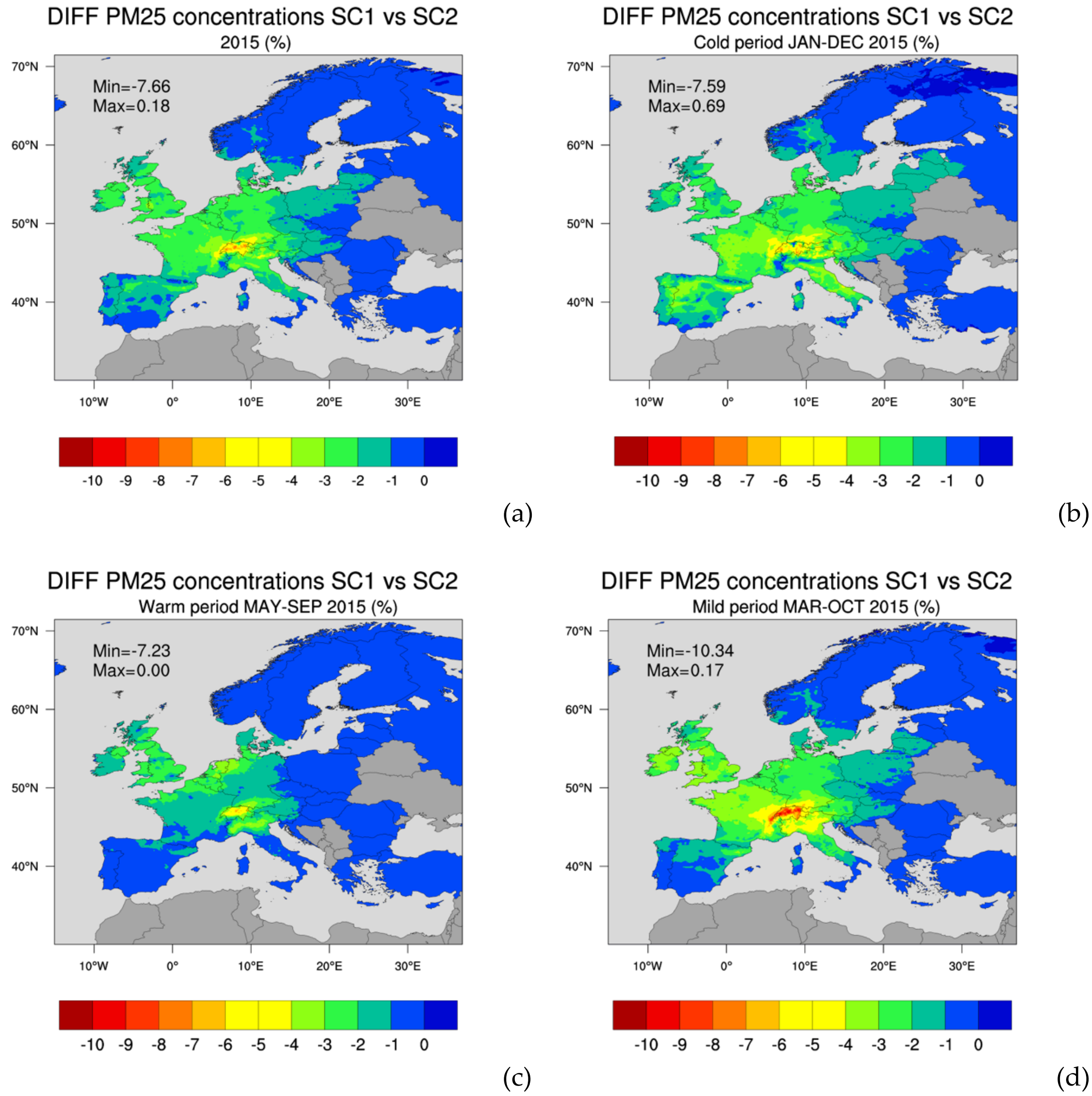


Figure S9. Same as Figure S7, but for PM25.

References

1. Tutuianu, M.; Bonnel, P.; Ciuffo, B.; Haniu, T.; Ichikawa, N.; Marotta, A.; Pavlovic, J.; Steven, H. Development of the World-wide harmonized Light duty Test Cycle (WLTC) and a possible pathway for its introduction in the European legislation. *Transp. Res. Part D Transp. Environ.* **2015**, *40*, 61–75. ISSN 1361-9209. https://doi.org/10.1016/j.trd.2015.07.011.
2. Clairotte, M.; Suarez-Bertoa, R.; Zardini, A.A.; Giechaskiel, B.; Pavlovic, J.; Valverde, V.; Ciuffo, B.; Astorga, C. Exhaust emission factors of greenhouse gases (GHGs) from European road vehicles. *Environ. Sci. Eur.* **2020**, *32*, 125. https://doi.org/10.1186/s12302-020-00407-5.
3. Suarez-Bertoa, R.; Mendoza-Villafuerte, P.; Riccobono, F.; Vojtisek, M.; Pechout, M.; Perujo, A.; Astorga, C. On-road measurement of NH3 emissions from gasoline and Diesel passenger cars during real world driving conditions. *Atmos. Environ.* **2017**, *166*, 488–497. 1352-2310, https://doi.org/10.1016/j.atmosenv.2017.07.056
4. O'Driscoll, R.; ApSimon, H.M.; Oxley, T.; Molden, N.; Stettler, M.E.J.; Thiyagarajah, A. A Portable Emissions Measurement System (PEMS) study of NO_x and primary NO_2 emissions from Euro 6 diesel passenger cars and comparison with COPERT emission factors. *Atmos. Environ.* **2016**, *145*, 81–91. https://doi.org/10.1016/j.atmosenv.2016.09.021.
5. Valverde, V.; Mora, B.A.; Clairotte, M.; Pavlovic, J.; Suarez-Bertoa, R.; Giechaskiel, B.; Astorga-LLorens, C.; Fontaras, G. Emission Factors Derived from 13 Euro 6b Light-Duty Vehicles Based on Laboratory and On-Road Measurements. *Atmosphere* **2019**, *10*, 243. https://doi.org/10.3390/atmos10050243.

6. Valverde, V.; Giechaskiel, B. Assessment of Gaseous and Particulate Emissions of a Euro 6d-Temp Diesel Vehicle Driven > 1300 km Including Six Diesel Particulate Filter Regenerations. *Atmosphere* **2020**, *11*, 645. https://doi.org/10.3390/atmos11060645.
7. Suarez-Bertoa, R.; Zardini, A.A.; Astorga, C. Ammonia exhaust emissions from spark ignition vehicles over the New European Driving Cycle. *Atmos. Environ.* **2014**, *97*, 43–53. https://doi.org/10.1016/j.atmosenv.2014.07.050.