

# **Air Control Toolbox (ACT\_v1.0): a machine learning flexible surrogate model to explore mitigation scenarios in air quality forecasts.**

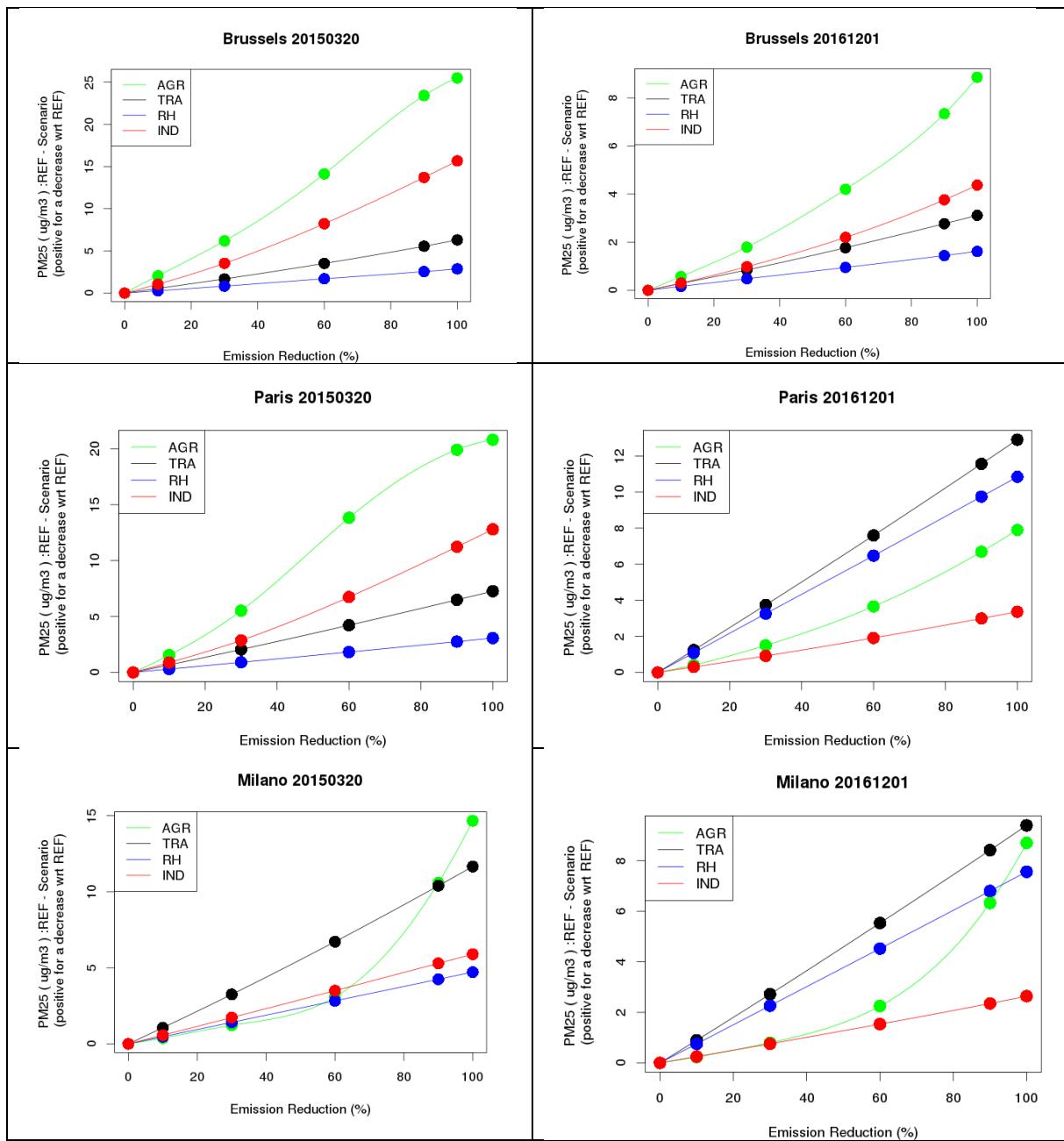
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## **Supplementary Figures**



**Figure S.1 :** Modelled PM<sub>2.5</sub> reduction (y-axis : positive for a decrease with respect to the reference,  $\mu\text{g}/\text{m}^3$ ) for a given reduction in Agriculture (green), Industrial (red), Residential Heating (blue), and Traffic (black) emissions (x-axis: in %) in Brussels, Paris and Milano (top to bottom) and for 20150320 (left) and 20161201 (right).

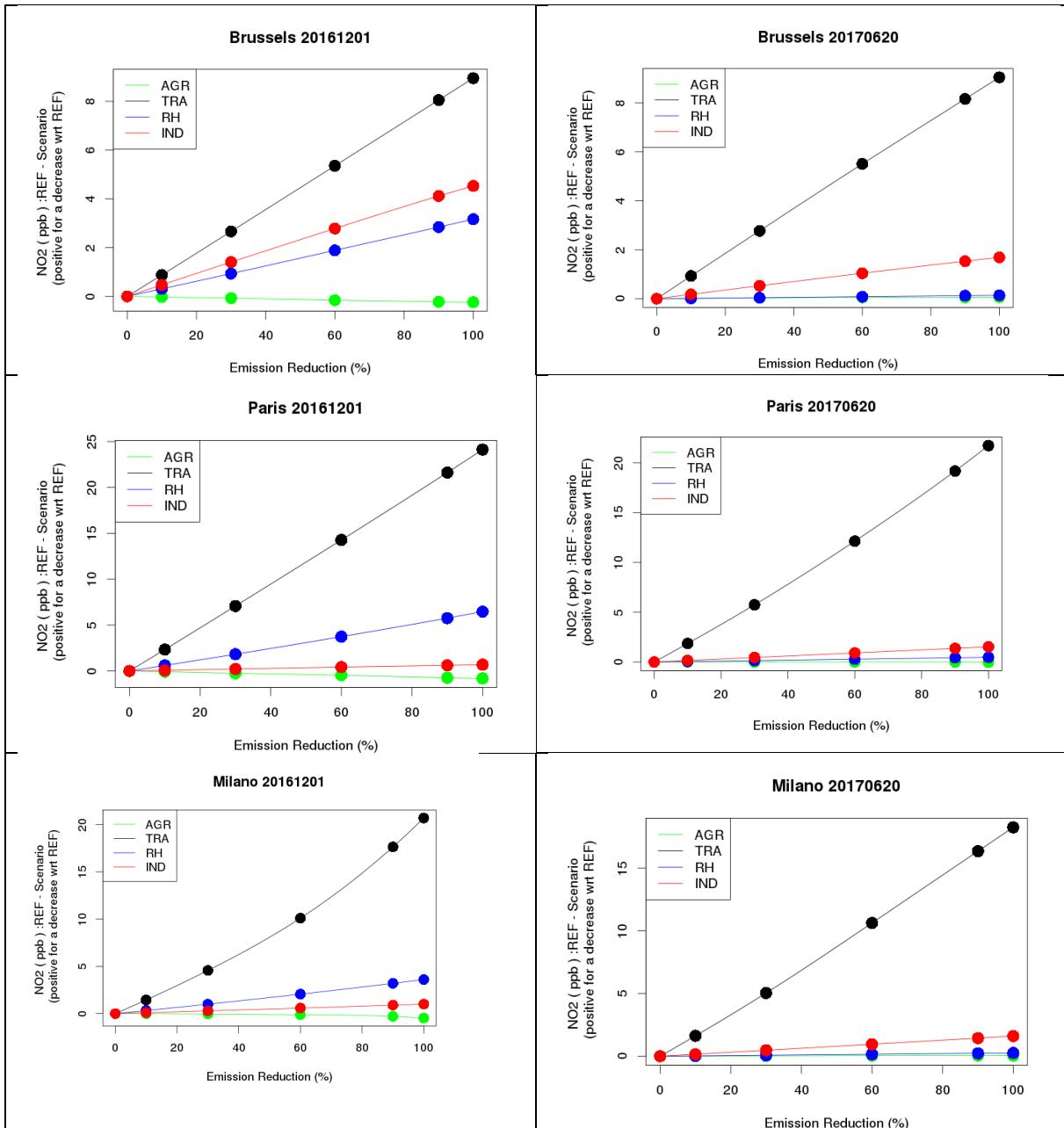
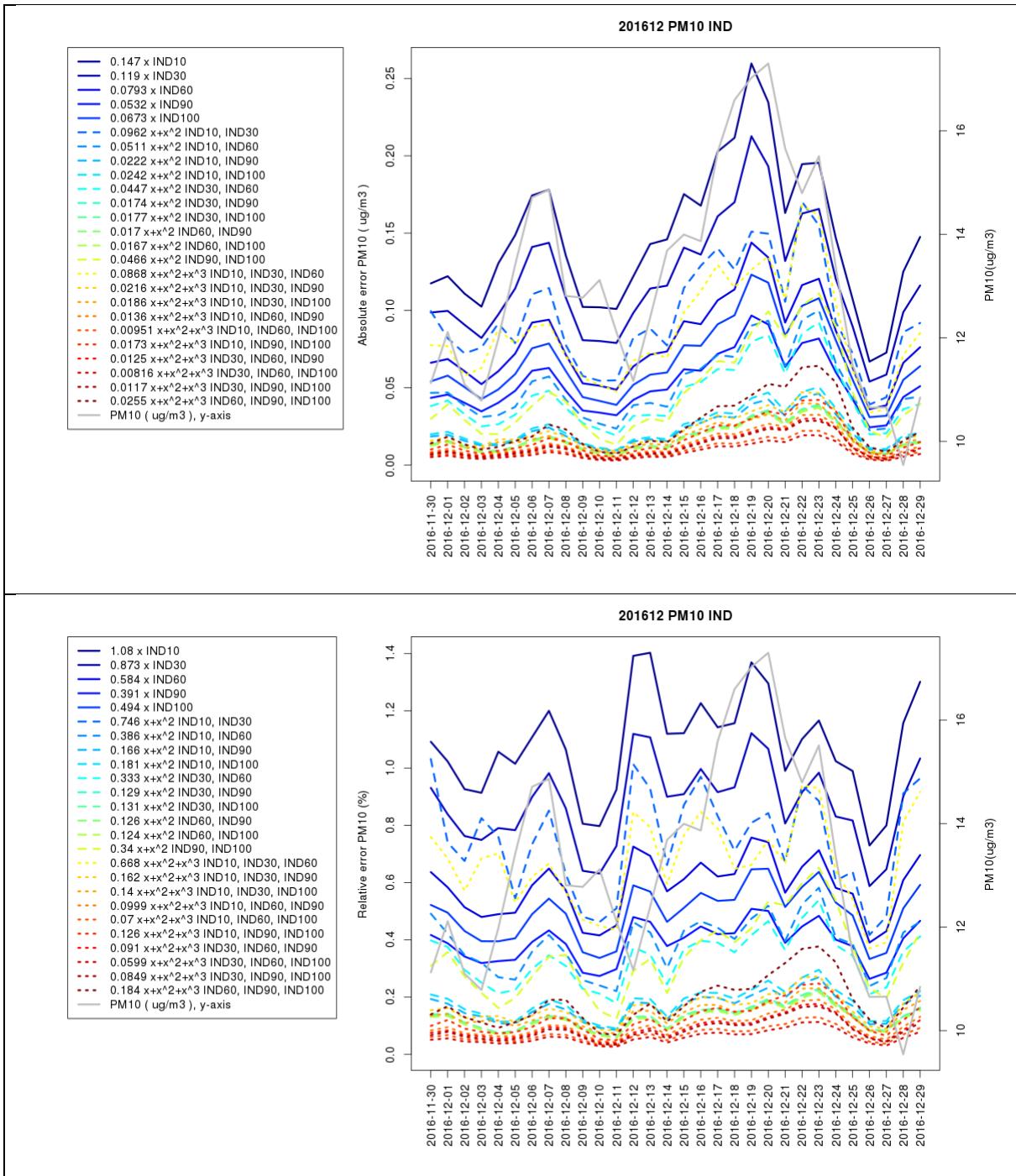


Figure S.2 : Same as Figure S.1 for NO<sub>2</sub> 20161201 and 20170620



**Figure S.3 : Absolute (top,  $\mu\text{g}/\text{m}^3$ ) and relative (bottom, %) error over Western Europe of the univariate surrogate model for the Industry activity sector in December 2016. The colored lines are for individual surrogate models, with the complexity and training scenario provided in the legend, as well as the error averaged over the whole time-period. The grey curve gives the day-to-day variation of PM<sub>10</sub> ( $\mu\text{g}/\text{m}^3$ ) averaged over the region (displayed on the right-hand-side y-axis)**

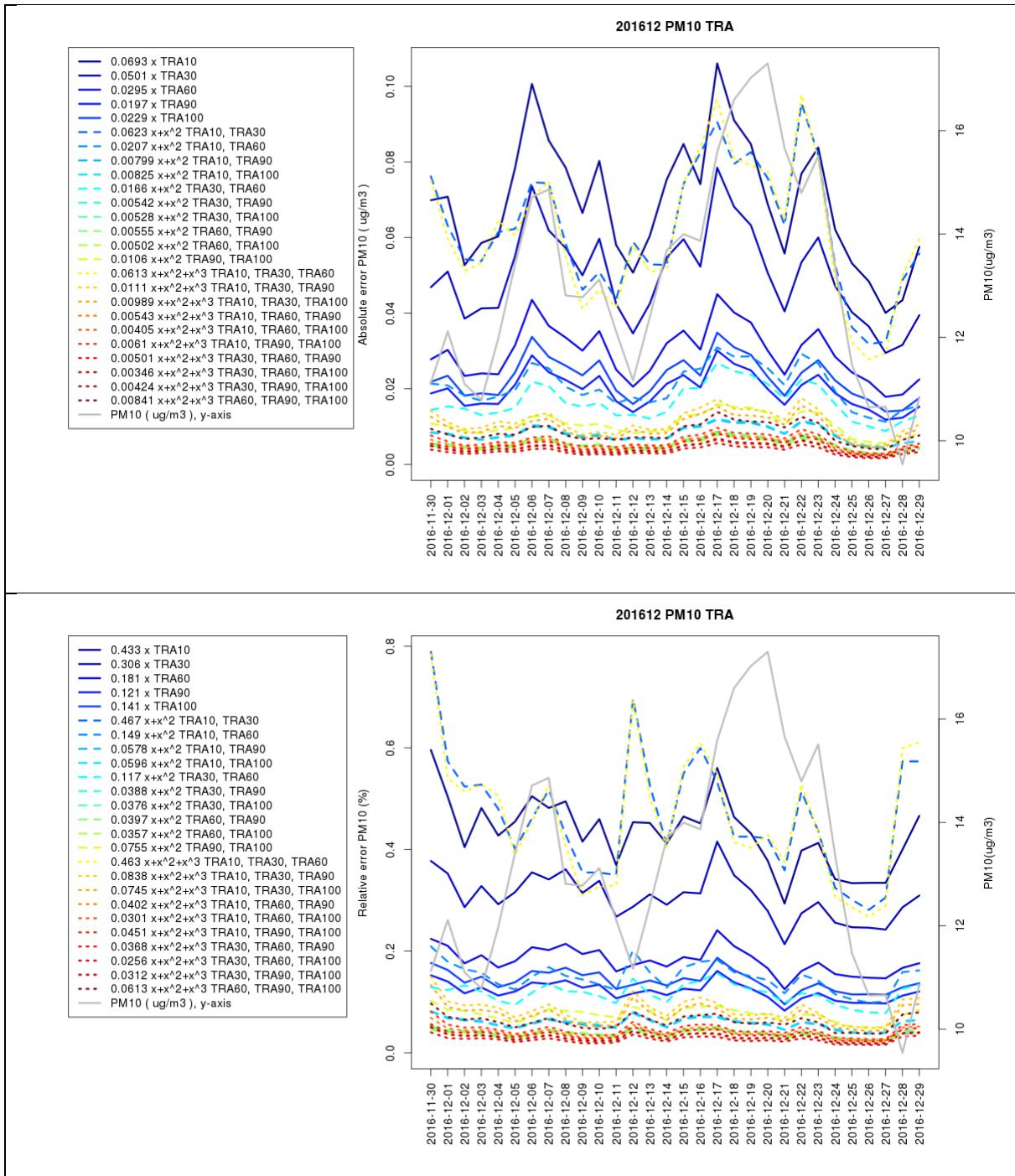


Figure S.4 : Same as Figure S.3 for Traffic

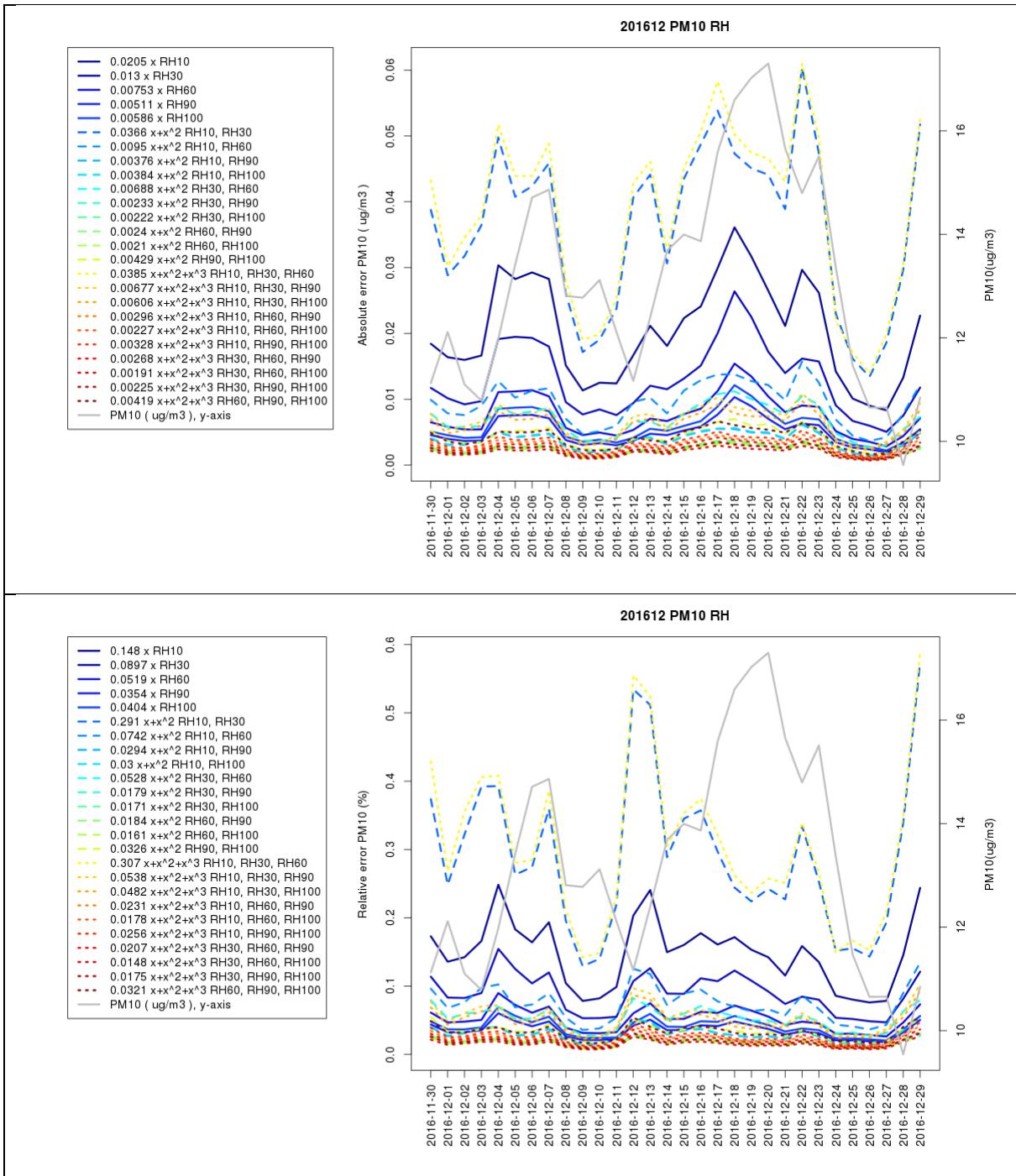
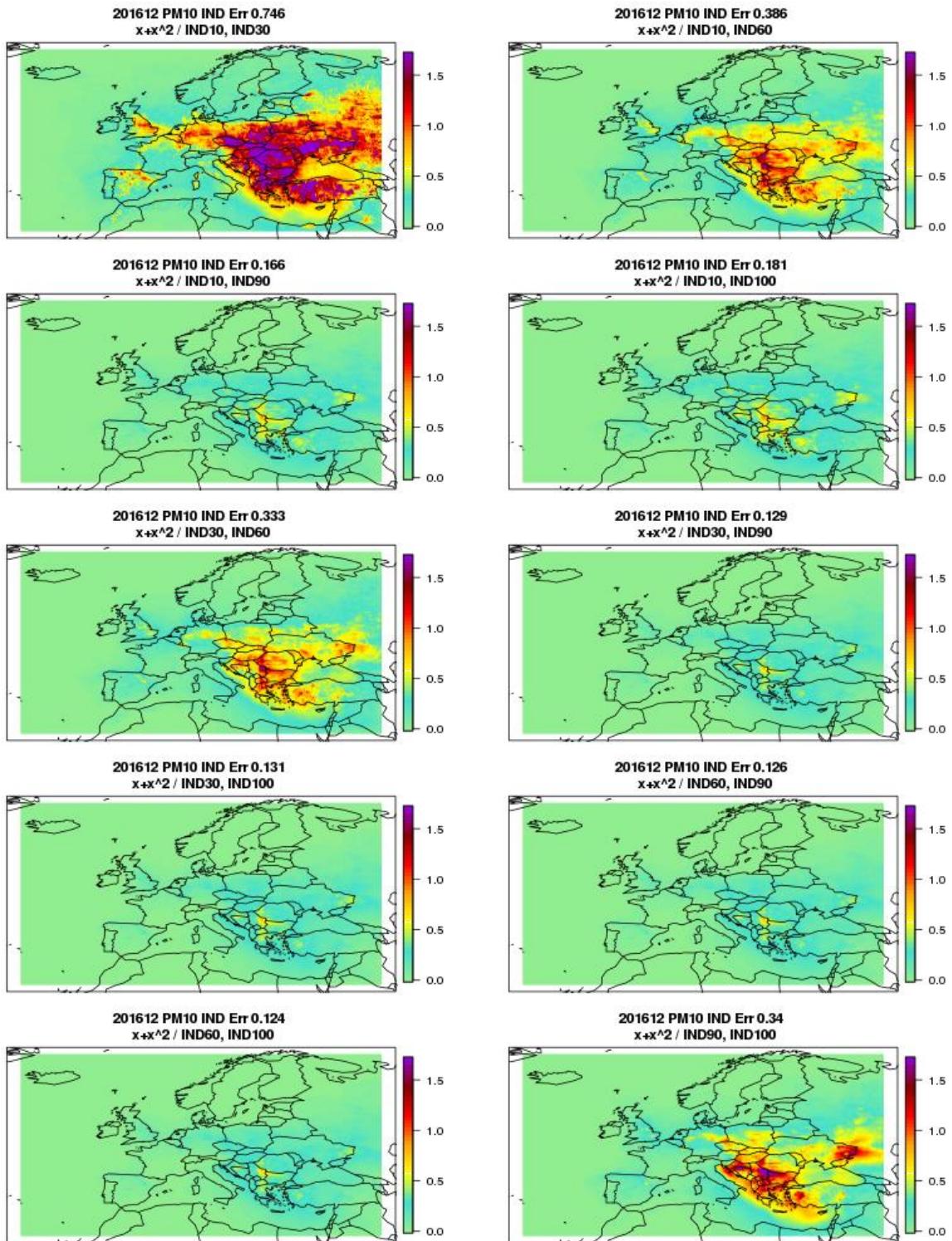


Figure S.5 : Same as Figure S.3 for Residential Heating



**Figure S.6 :** Relative error (%) averaged over the month of December 2016 for the quadratic univariate PM<sub>10</sub> models with respect to the industry activity sector. The sensitivity scenarios used to train the individual models are indicated in the title of each panel, as well as the average error.

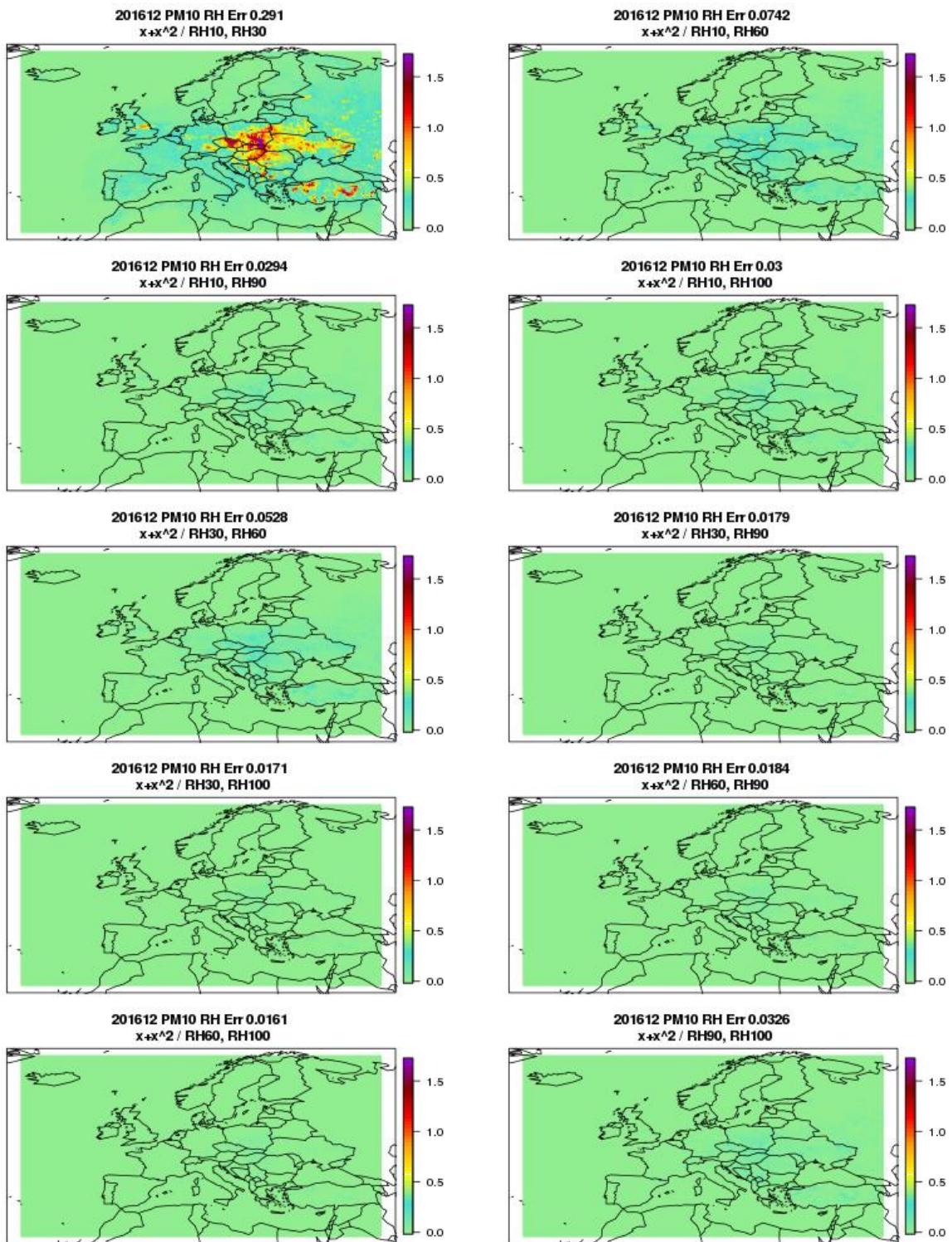


Figure S.7 : Same as Figure S.6 for Residential heating

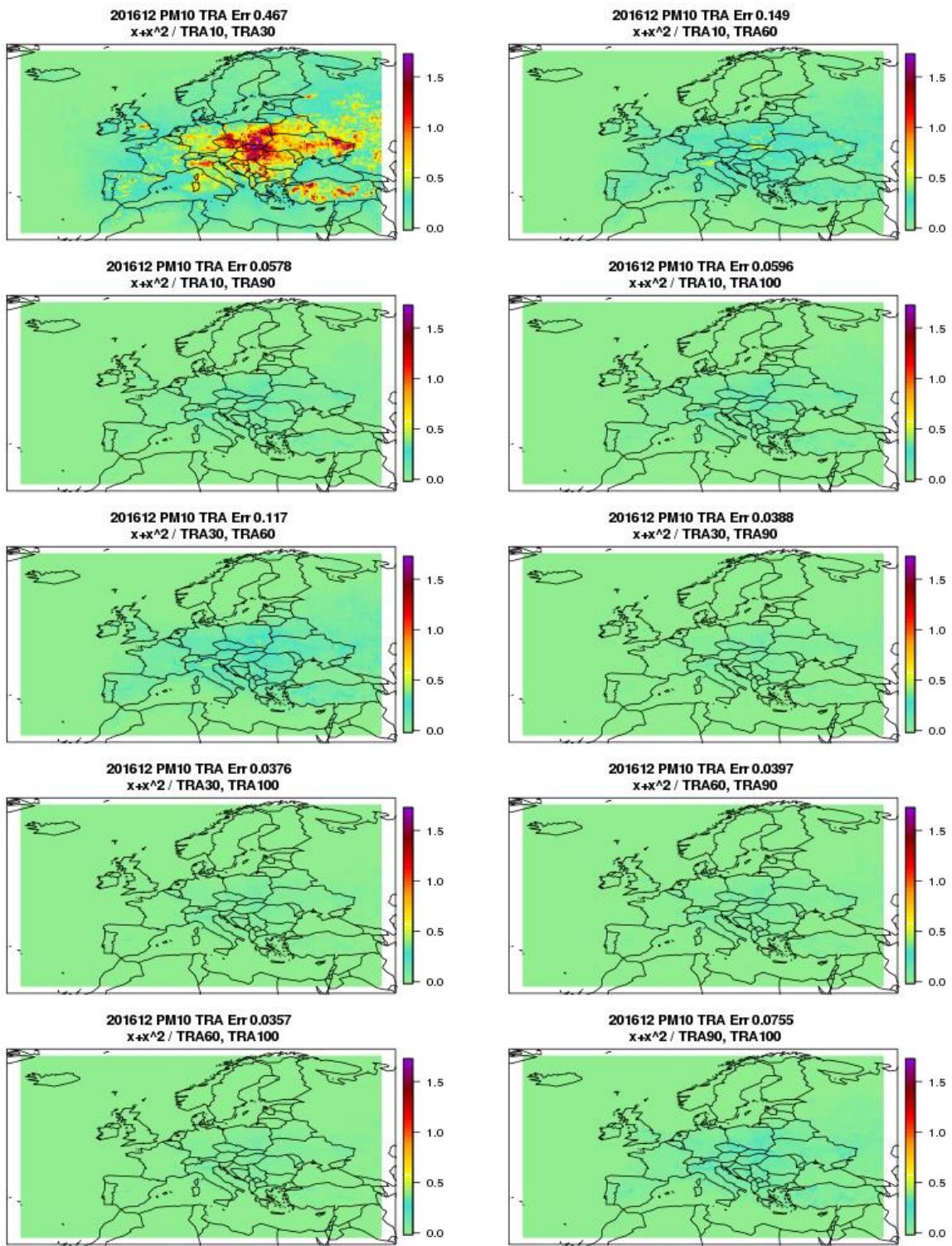


Figure S.8 : Same as Figure S.6 for Traffic

Polynomial	Training	AGR	IND	RH	TRA
x	10	3,933	1,133	0,130	0,339
x	30	3,123	0,894	0,082	0,236
x	60	1,983	0,573	0,047	0,137
x	90	1,310	0,382	<u>0,032</u>	0,092
x	100	1,463	0,471	0,036	0,106
x+x2	10 30	3,540	0,698	0,284	0,407
x+x2	10 60	2,097	0,329	0,066	0,117
x+x2	10 90	0,833	0,137	0,027	0,046
x+x2	10 100	0,856	0,147	0,027	0,047
x+x2	30 60	1,917	0,285	0,055	0,096
x+x2	30 90	0,663	0,104	0,018	0,031
x+x2	30 100	0,646	0,105	0,017	0,030
x+x2	60 90	0,697	0,101	0,017	0,032
x+x2	60 100	<u>0,634</u>	<u>0,099</u>	0,015	<u>0,028</u>
x+x2	90 100	1,563	0,254	0,029	0,058
x+x2+x3	10 30 60	3,437	0,634	0,315	0,428
x+x2+x3	10 30 90	0,867	0,140	0,054	0,076
x+x2+x3	10 30 100	0,736	0,122	0,049	0,068
x+x2+x3	10 60 90	0,596	0,081	0,022	0,034
x+x2+x3	10 60 100	0,407	0,057	0,017	0,026
x+x2+x3	10 90 100	0,739	0,099	0,024	0,038
x+x2+x3	30 60 90	0,560	0,074	0,020	0,032
x+x2+x3	30 60 100	0,360	0,049	0,015	0,022
x+x2+x3	30 90 100	0,514	0,068	0,017	0,027
x+x2+x3	60 90 100	1,150	0,143	0,029	0,051

Table S.1 : Relative error (%) of the PM10 univariate polynomial surrogate models averaged over Western Europe for three air pollution episodes (201503, 201612, 201701) for various polynomial structures, and various set of Chimere simulations used in the training. A color shading is applied to highlight the worst (red) and best (green) performances.

Polynomial	Training	AGR	IND	RH	TRA
x	10	0,083	0,500	0,002	0,738
x	30	0,070	0,390	0,001	0,571
x	60	0,053	0,241	0,001	0,347
x	90	0,037	0,159	0,001	0,229
x	100	0,045	0,191	0,001	0,273
x+x2	10 30	0,115	0,184	0,002	0,263
x+x2	10 60	0,077	0,104	0,001	0,141
x+x2	10 90	0,034	0,040	0,000	0,053
x+x2	10 100	0,036	0,043	0,000	0,057
x+x2	30 60	0,072	0,090	0,000	0,122
x+x2	30 90	0,028	0,030	0,000	0,039
x+x2	30 100	0,028	0,030	0,000	0,039
x+x2	60 90	0,029	0,030	0,000	0,039
x+x2	60 100	0,028	<u>0,029</u>	0,000	<u>0,038</u>
x+x2	90 100	0,078	0,068	0,000	0,083
x+x2+x3	10 30 60	0,114	0,125	0,002	0,179
x+x2+x3	10 30 90	0,035	0,029	0,000	0,038
x+x2+x3	10 30 100	0,029	0,025	0,000	0,033
x+x2+x3	10 60 90	0,027	0,018	0,000	0,022
x+x2+x3	10 60 100	0,018	0,012	0,000	0,016
x+x2+x3	10 90 100	0,034	0,022	0,000	0,027
x+x2+x3	30 60 90	0,025	0,016	0,000	0,020
x+x2+x3	30 60 100	0,016	0,011	0,000	0,014
x+x2+x3	30 90 100	0,024	0,015	0,000	0,018
x+x2+x3	60 90 100	0,054	0,032	0,000	0,039

Table S.2 : Same as Table S.1 for ozone daily maximum for the month of 201706.

AI	AR	IR	TA	TI	TR	model
0,355	0,102	0,051	0,244	0,069	0,039	1
0,355	0,102	0,051	0,244	0,069	0,039	2
0,878	0,286	0,158	0,651	0,271	0,090	3
1,025	0,289	0,147	0,704	0,283	0,091	4

Table S.3 : Relative error (%) of the PM<sub>10</sub> univariate polynomial surrogate models averaged over Western Europe for three air pollution episodes (201503, 201612, 201701) when including or excluding interaction terms. A color shading is applied to highlight the worst (red) and best (green) performances

AI	AR	IR	TA	TI	TR	model
0,011	0,001	0,003	0,008	0,032	0,005	1
0,011	0,001	0,003	0,008	0,032	0,005	2
0,017	0,001	0,012	0,022	0,317	0,019	3
0,020	0,002	0,011	0,019	0,312	0,018	4

Table S.4 : Same as Table S.3 for ozone daily maximum for the month of 201706.

AI	AR	IR	TA	TI	TR	model
1,003	0,941	0,128	0,535	0,067	0,057	1
0,638	0,558	0,072	0,614	0,074	0,028	2
0,884	0,781	0,095	0,519	0,060	0,031	3
0,996	0,832	0,127	0,353	0,128	0,054	4

Table S.5 : Relative error (%) of the PM<sub>10</sub> univariate polynomial surrogate models averaged over Western Europe for three air pollution episodes (201503, 201612, 201701) when using different interaction sensitivity scenarios. A color shading is applied to highlight the worst (red) and best (green) performances

AI	AR	IR	TA	TI	TR	Model
0,047	0,037	0,045	0,065	0,049	0,060	1
0,040	0,022	0,026	0,048	0,034	0,034	2
0,047	0,030	0,036	0,062	0,037	0,047	3
0,037	0,031	0,034	0,048	0,153	0,043	4

Table S.6 : Same as Table S.5 for O<sub>3</sub>max

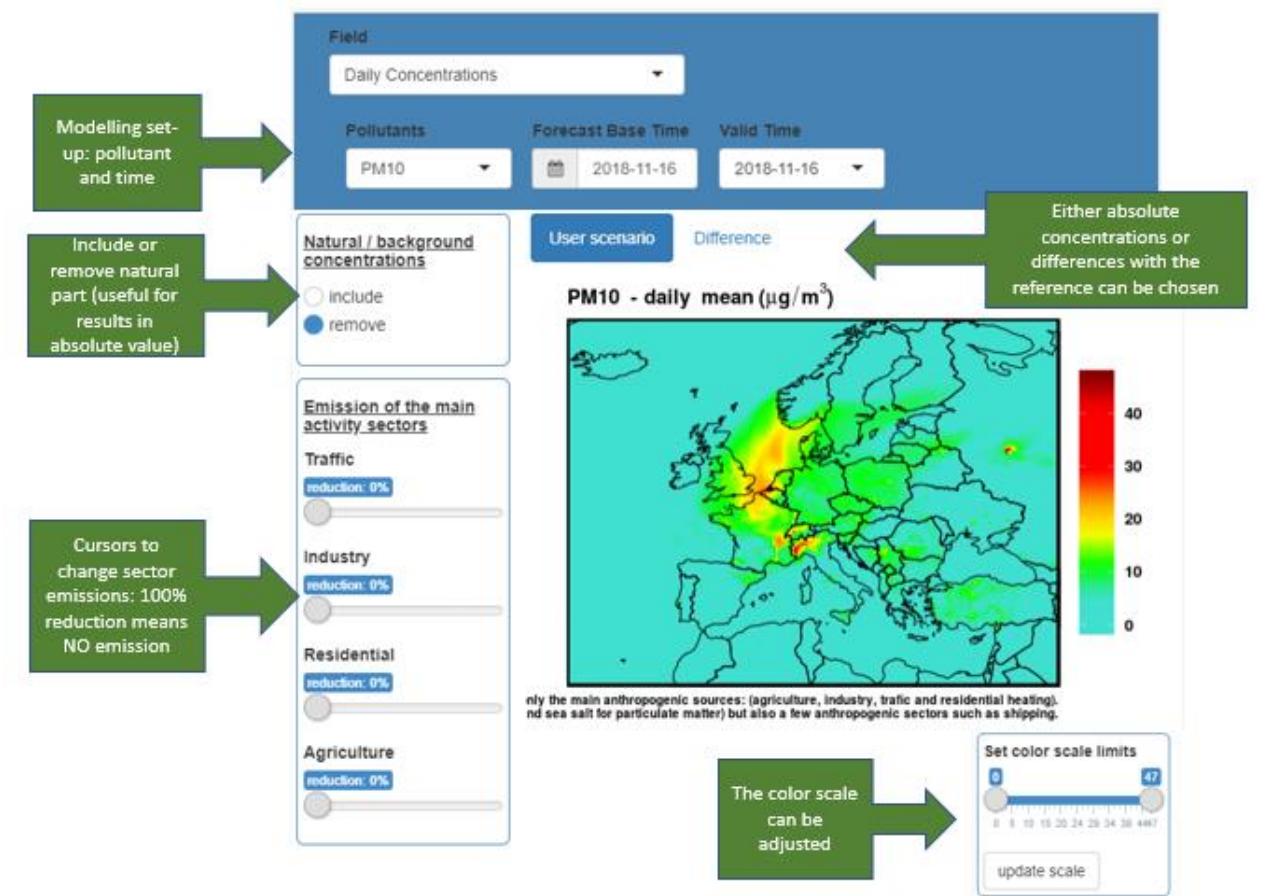


Figure S.9: Screenshot of the ACT web interface, [https://policy.atmosphere.copernicus.eu/CAMS\\_ACT.php](https://policy.atmosphere.copernicus.eu/CAMS_ACT.php).