

Geosci. Model Dev. Discuss., referee comment RC2
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Comment on gmd-2020-433

Anonymous Referee #2

Referee comment on "Air Control Toolbox (ACT_v1.0): a machine learning flexible surrogate model to explore mitigation scenarios in air quality forecasts" by Augustin Colette et al., Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2020-433-RC2>, 2021

This paper addresses an important topic, is interesting and well written. The authors develop a surrogate model for a full CTM to investigate ambient pollution changes in response to sectoral emission reductions. Currently the application is limited to episodes and uniform emission changes over Europe which, as also remarked by the other anonymous referee, limits the practical applicability for policy analysis, but the authors also emphasize that they are planning to extend the tool in this direction. It will be interesting to follow this development.

I have a few comments which should be addressed, but these are mostly clarifications and should not require major changes before publication.

General comments

1. I confess I am not an expert for machine learning but I was wondering whether the title is really appropriate. The toolbox as described in this paper uses a parametric regression (first and second order with interaction terms) to approximate the behaviour of a full CTM, and while I think the methodology is sound, I'm not sure if this can be really termed machine learning.
2. I struggled a bit to understand how the regression is set up. When looking at Eq 1, one could get the impression that everything is known, and the equation can simply be solved with a unique solution in each grid cell for the parameters alpha, beta, gamma (if $C_{i,j}$ and ϵ are scalar values averaged for the time period of interest) and no regression is needed if the right number of training scenarios is used (2 for a linear fit, 3 for quadratic etc). Is this what is done, or is there a regression involved in the sense of solving an overdetermined equation system and estimating optimal alpha, beta, gammas? Also, should Eq 1 not have a sectoral dimension index in alpha, beta, gamma and epsilons?
3. Besides the limitation that emission reductions which can be explored with this tool are

uniform across Europe, also they are specified as reduction of emissions by sector since the coefficients are expressed by sector and not by pollutant, meaning that all pollutants emitted from this sector are reduced proportionally. In practice, emission control policies may reduce different pollutants from the same SNAP sector to a different extent, which cannot be simulated with the current setup. It would be good to mention this somewhere.

Detailed comments

P 5, L 6: The number of training simulations should be constrained by more fundamental principles than the availability of computing time?

P 7 – I would emphasise a bit more the complete reverse response for TRA reductions wrt O3 avg vs peaks. In this context it would be good to mention what is assumed regarding NO/NOx ratio in industrial vs traffic emissions, this may play a role here.

P10 L 22: I am confused what is actually calculated and shown here. Maybe I'm too long after my last statistics class but I don't exactly understand why a confidence interval is calculated here (for what estimated quantity?) and where the formula comes from. Wouldn't it be more useful to show just the 95th or 97.5th percentile of this error distribution?

Section 3.4: Is the final model setup that the authors arrive at in Section 3.4 stable or is this re-evaluated for new time periods in the operational tool?

Section 4.2.2: The conclusion that the December episode is mainly driven by agricultural emissions is rather unexpected, I would have expected a higher contribution from residential heating. How well does the CHIMERE model in this configuration perform in reproducing the measured concentrations of these episodes? The authors note that the emission inventory used may underestimate residential sector emissions, which is an important caveat to highlight when drawing conclusions for wintertime episodes.

Technical corrections

- P 6, L 5. "Emissions": emission changes / reductions
- P9 L21 performance (singular)
- P10 L12: in order to reduce the number of performances in this sentence, I suggest to replace the middle one with 'done'
- Fig 3: The legend is messy and the line colors are not distinguishable. I suggest to change the figure layout. For example, unify to one table with scenario numbers like in Fig 4.
- Fig 4: color scales are exhausted for some of the figures
- P13 L19 – "We are left already" -> We are still left

- Figure 7 caption: raw -> row
- P14 L13 – is tested with / against
- Figure 11 caption: 2015903 ?
- Figure 12 top right - caption unclear
- P16 L 10: NO_x from industry and heating
- P16 L18: in Western Europe