

Geosci. Model Dev. Discuss., author comment AC4
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Reply on RC2

Edward C. Chan and Timothy M. Butler

Author comment on "urbanChemFoam 1.0: large-eddy simulation of non-stationary chemical transport of traffic emissions in an idealized street canyon" by Edward C. Chan and Timothy M. Butler, Geosci. Model Dev. Discuss.,
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Dear Reviewer:

Thank you very much for the positive comments. To address your remaining concerns, please find our responses following references to your original text below.

Comment: *Line 259 – 260: Authors mention that "both the fine and coarse mesh results are in excellent agreement". Can you please provide quantitative data to support this sentence?*

Response: The Authors have amended the statement in question, to indicate that the agreement between the model results and the LDA measurements for the time-averaged horizontal velocity are inferred from Figure 3.

Comment: *Along the manuscript concentrations are provided in ppb, while for regulatory purposes in Europe we work in micro grams per cubic meter. Do you have any specific reason for working in ppb?*

Response: In the Authors' part, the decision to use molar based concentration – that is, ppb and related units – are largely based on existing regional modelling studies conducted as presented in the MS references (e.g., Kuik et al, 2016,2017; von Schneidemesser et al, 2017, etc.). However, using ppb, species concentrations are expressed in a way that is independent from molecular mass as well as local thermodynamic state. Therefore, comparison between model results can be done in a standardized fashion, under different ambient and emission conditions, as well as across different mixture constituents.

As a point of interest, species concentrations in OpenFOAM, as well as other open source and commercial computational fluid dynamics (CFD) modelling frameworks, are calculated in terms of mass mixing ratios, that is, the ratio between the mass of the individual species and the mass of the mixture, as indicated in Equation (4) in the MS. Thus conversions to other concentration units relevant for air quality modelling and regulation purposes, such as ppb and micrograms per cubic meter, are necessary and are introduced as a post-processing step.

Comment: *Regarding the differences between the simulations in stationary versus transient conditions, do you have any thoughts about which one is the most suited/*

accurate? Can you highlight the potential advantages and disadvantages of both conditions?

Response: The Reviewer has pointed out one of the major objectives of the study: The comparison between model runs under stationary conditions and non-stationary (transient) conditions. While it is unreasonable to expect stationary model results be applicable over a period of changing ambient conditions, the commonly accepted opinion is that stationary model results would be representative for the point of time at which the ambient conditions are predicated. The development outlined in the present study enabled the examination between stationary and non-stationary model runs.

Two observations can be made from this comparison. First, to the extent of the meteorological conditions considered in this study, there is little change in the in-canyon flow field between stationary and non-stationary runs. This is not surprising, considering that the shear layer in the roof region attenuates the dynamics inside the canyon from those above the buildings. Accordingly, the in-canyon wind should be less sensitive to the temporal variations in the freestream flow. On the other hand, significant changes can be observed in pollutant concentrations under stationary and non-stationary treatment. As such, temporal variations in emissions and background conditions, which are not considered in stationary runs, are significant and cannot be neglected.

Returning to the Reviewer's question concerning suitability and benefits of each approach, in light of the above observations, where wind and flow distributions are of primary concerns, stationary model runs would likely suffice. On the other hand, if the focus of the study is on pollutant transport and transformation, temporal variations of background concentrations and emissions will have an appreciable influence on model concentrations. As such, a non-stationary approach should be considered.

Comment: *The background concentrations are the total concentrations measured at the urban background stations. Is that right?*

Response: This is correct. The background concentrations presented in Figure 6(C) of the MS are obtained by taking the arithmetic mean over two urban background stations closest to the Silbersteinstraße urban traffic station, where the observation takes place.

Sincerely yours,

The Authors.