Reply on RC1
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., https://doi.org/10.5194/gmd-2020-432-AC3, 2021

Dear Reviewer:

The Authors would like to thank you for the meticulous but encouraging comments on the MS. Please find our response to your comments below, with reference to your original text in italics. In the meantime, all typographical errors outlined in minor comments 1 - 14 have been corrected in the MS.

Comment: My main objection is that despite the interesting quantification of the discrepancies between stationary and non-stationary simulations, the study does not show the full potential of the transient setup – the transition between nocturnal and daytime boundary layer and vice versa. In particular, the morning hours would be very interesting with regard to chemistry and boundary layer processes (onset of boundary-layer growth and photochemistry, emission peak) and exposure research. How does urbanChemFoam capture this transition?

Response: For the nocturnal and daytime transition, a neutral boundary layer is assumed under the idealized setup in this study, although urbanChemFoam itself is capable of modelling effects of thermal stratification through advection and natural convection.

Where (natural) convective effects are to be considered in an infinitely long channel such as a street canyon, for instance, by having the corresponding surfaces maintained at different temperatures, convective cells form in the lengthwise direction of the channel, with characteristic length strongly dependent on the canyon aspect ratio and Rayleigh number. This classical observation has been thoroughly discussed analytically and numerically in Davies-Jones (1970; J Fluid Mech 44/4:695-704) at NCAR, and is termed by the author as the “finite rolls”. In other words, with the exception of a strictly two-dimensional numerical arrangement, the presence of natural convection will render the resulting flow field three-dimensional.

Further, substituting the infinitely long canyon geometry with a periodic finite length canyon, as featured in this study, will result in deviations from this “finite rolls” arrangement. This point has also been asserted by Davies-Jones (1970), and is confirmed, at least empirically, by the authors’ early model runs for the idealized street
canyon with convective effects. Hence, under the present idealized street canyon arrangement, not only will the effective two-dimensionality be inapplicable through natural convection, a high degree of grid dependency will also be introduced due to the finite canyon length.

However, it is in the Authors’ plan to apply urbanChemFoam on a fully three-dimensional geometry in the future, such as a city block. In this sense, convective effects will be requisite. It is also expected that the ensuing examination / discussion of the nocturnal-to-daytime transition and vice versa will be appreciatively more applicable and interesting.

**Comment:** In addition, radiation effects of buildings, which are interesting on the scale considered, are not included in this study. This could at least be discussed in the form of a possible outlook.

**Response:** The conclusion of the MS has been amended to indicate the possibility of introducing radiative heating in the future.

**Minor Comment 15:** Figs. 3, 5, 8-10: Maybe better include the legend in the figures.

**Response:** After contemplation and experimentation, the authors have decided against including the key directly on the figure panels to maintain legibility of the contents in the figures in question.

**Minor Comment 16:** Fig. 12: Do the background conditions apply to these results? Some concentrations appear lower than the boundary conditions (cf. Figs. 6 and 12). Suggestion: indicate sun rise/set or night times by grey shadings in the panels.

**Response:** The diurnal profiles of background concentrations have been introduced above the street canyon as non-stationary (time-varying) boundary conditions. The concentrations presented in Figure 12, sampled at various points inside the canyon, are a result of this. Due to mixing and chemical reactions with ground level NO and NO₂ emissions, it is expected that the local pollutant concentrations deviate from background levels. The UTC times for sunrise and sunset, defined at the solar zenith transitioning the 90° mark, have been introduced in the MS.

Sincerely yours,

The Authors.