Using the newly-developed space-time extremely randomized trees (STET) model, this study is aimed at estimating the 1-km-resolution PM$_{2.5}$ surface concentrations across China. Besides meteorology, land surface conditions and population, a space term and a time term representing the spatial autocorrelation and temporal variation of PM$_{2.5}$, respectively are also included to derive the PM$_{2.5}$-AOD relationship. Overall this manuscript is well written, and potentially improves our understanding regarding how to retrieve the PM$_{2.5}$ concentrations from AOD products and other auxiliary data. However, before I recommend this manuscript to be published, the authors should carefully address and clarify my several comments.

General comments:

1. The relationship between (surface layer) PM$_{2.5}$ and AOD might largely depend on the compositions (including aerosol water, as Reddington et al. (2019) indicated that aerosol water uptake and hygroscopic growth would also impact the AOD), vertical profile and size distribution of PM$_{2.5}$. Thus I find that some results in Figure 2 are confusing, and needs further analysis and clarification: 1) In Section 3.2, it is unclear how the importance scores of all selected independent variables and spatiotemporal information to PM$_{2.5}$ estimates for the STET model are calculated. 2) Why RH turns out to be a much less important parameter, and it has an importance score that is only slightly higher than those negligible parameters do. RH is an important factor determining the aerosol compositions and water uptake, and recent air quality studies (e.g., Sun et al., 2014; Zheng et al., 2015) showed that high RH conditions facilitate rapid production of secondary PM. 3) Furthermore, the parameter of precipitation could significantly impact the removal of PM, but is negligible in the STET model. Both RH and precipitation are associated with cloud, and what is the uncertainty for the predicted PM$_{2.5}$-AOD relationship caused by the treatment of AOD data on cloudy dates?

2. The authors declared that STET model exhibited a strong predictive power and could be used to predict the historical PM$_{2.5}$ records in the Abstract Section (in Line 39). This conclusion could be inappropriate as the authors only tested the year of 2017. Emissions were not expected to change greatly between 2017 and 2018. Actually I doubt the applicability for the STET model. The space and time terms seem confusing to me, and the former term is represented by the geographical difference between two pixels, while the latter term is represented by the difference for a given pixel on different days in a year. I think they might be "residual terms" to implicitly resolve the "unknown parts" unexplained by other independent parameters. I mean, the authors need more independent parameters that could explicitly explain the PM$_{2.5}$ compositions, vertical profile and size distribution. Why not emissions for different precursors (e.g., SO$_2$, NO$_x$ and VOCs) as well as fine size dust are included as independent parameters?

3. Equation 1 is confusing. The authors mean:

$$\tau_T = k_1 \tau_{A, original} + b_1 \quad \text{and} \quad \tau_A = k_2 \tau_{T, original} + b_2$$

What is the R$^2$ for each linear regression? Are these two linear regressions consistent with each other? Why not to average the Terra and Aqua data directly?

4. The description for the STET method in Section 3 is not readily to understand. Please add clarification (better to include a schematic) so that ACP readers with less experiences in machine learning could generally understand the fundamentals of the STET method.

5. In Figure 7, what is surprising is that I see a good positive correlation pattern between R and RMSE. Generally a good model performance is associated with a high R and a low RMSE against
observations. Please check and clarify.

Specific comments:
1. Line 48, the "evenly dispersed" is confusing, and is conflict with the "PM$_{2.5}$ shows great spatial and temporal heterogeneities" in Line 80.
2. Line 175, better replace "differences" by variation.
3. Line 227, typos: Figure 2 or Figure 3?
4. Line 247, what is definition for MAE and MRE?
5. Figure 9, typos: the year is 2018 or 2017? Also please add the season labels for each plot.

