The scientific premise of the paper - to use measured NMOC profiles to predict the underlying burned fuel - is interesting and worth publishing (although from a modeling perspective, perhaps the inverse would be more useful). However, the paper is so poorly written and organized it is difficult to discern what algorithm the authors have developed, and it would surely not be reproducible by a reader. I recommend to reconsider this paper after major revisions.

The authors do not report what NMOC compounds make up their training and testing datasets. At some point, they do mention that there are 93 to select from. They should be listed and described. The authors write about generating a synthetic dataset, but no information was given on how this data was generated. The laboratory burn dataset used included a broad variety of biomass fuels, but in the end only a handful of fuels were considered, and no explanation was given, which calls into question the extent of the applicability of the algorithm.