**ABSTRACT**

 A theoretical study on the reaction mechanism of methyl salicylate (MeSA), a green leaf volatile organic compound with OH radical and ozone, has been carried out using density functional theory methods using B3LYP, M06-2X and MPW1K functional with 6-311++G(d,p) basis set. The atmospheric degradation pathways of MeSA with OH radical are studied under two different pathways, viz. H-atom abstraction and electrophilic addition of OH radical. The hydrogen abstraction from –OH group is found to be the dominant reaction channel with small barrier height. Likewise, the electrophilic addition of OH radicals at the para position of MeSA is found to be favourable rather than the ortho and meta positions because of the small barrier height. However, the reaction of MeSA with respect to the addition of O3 is initiated only through the cycloaddition to the C¼C bond, resulting in primary ozonide. The Arrhenius plot for most of the addition reaction shows positive temperature dependence, while for the abstraction reaction, it exhibits negative temperature dependence over the temperature range of 278–350 K. The calculated theoretical rate constants are in good agreement with available experimental data. Overall, the addition of both OH radical and ozone possesses ability to degrade MeSA, but slower when compared with the Cl radical.