## Accepted Manuscript

Photochemical ozone creation potentials for volatile organic compounds: Rationalization and estimation

M.E. Jenkin, R.G. Derwent, T.J. Wallington

PII: S1352-2310(17)30325-4

DOI: 10.1016/j.atmosenv.2017.05.024

Reference: AEA 15333

To appear in: Atmospheric Environment

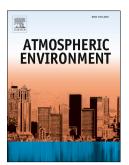
Received Date: 31 January 2017

Revised Date: 3 April 2017

Accepted Date: 16 May 2017

Please cite this article as: Jenkin, M.E., Derwent, R.G., Wallington, T.J., Photochemical ozone creation potentials for volatile organic compounds: Rationalization and estimation, *Atmospheric Environment* (2017), doi: 10.1016/j.atmosenv.2017.05.024.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



## ACCEPTED MANUSCRIPT

1	Photochemical ozone creation potentials for volatile organic compounds:
2	rationalization and estimation
3	
4	M. E. Jenkin <sup>a,b,*</sup> , R. G. Derwent <sup>c</sup> and T. J. Wallington <sup>d</sup>
5	
6	<sup>a</sup> Atmospheric Chemistry Services, Okehampton, Devon, EX20 4QB, UK;
7	<sup>b</sup> School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK;
8	<sup>c</sup> rdscientific, Newbury, Berkshire, RG14 6LH, UK;
9	<sup>d</sup> Research and Advanced Engineering, Ford Motor Company, SRL-3083, PO Box 2053,
10	Dearborn, Michigan 48121-2053, USA.
11	
12	* Corresponding author. E-mail address: atmos.chem@btinternet.com (M. E. Jenkin)
13	
14	
15	Abstract
16	The Photochemical Ozone Creation Potential (POCP) scale quantifies the relative abilities of volatile
17	organic compounds (VOCs) to produce ground level ozone. POCP values are usually calculated using
18 19	atmospheric boundary layer models containing detailed representations of atmospheric VOC degradation chemistry. The sensitivity of POCP values to variation of a number of kinetic and
20	mechanistic parameters has been investigated here. It is shown that POCP values for VOCs can be
21	rationalized in terms of their molecular structure and OH reactivity. As a result, a simple method has
22	been developed and optimized that allows POCP values for north-west European and USA urban
23	reference conditions to be estimated for alkanes, alkenes, aromatic hydrocarbons, and several
24	oxygenated VOC classes without the requirement to construct a detailed chemical mechanism or
25	run an atmospheric model. The procedure for determining the estimated POCP value (POCP <sub>E</sub> ) is
26	described, and the results are presented and discussed.
27	
28	

Keywords: VOC oxidation; Tropospheric chemistry; POCP; Ozone formation potential; Secondarypollutants; Impact assessment.

Download English Version:

## https://daneshyari.com/en/article/5753194

Download Persian Version:

https://daneshyari.com/article/5753194

Daneshyari.com