

## Evaluation and improvements of two community models in simulating dry deposition velocities for peroxyacetyl nitrate (PAN) over a coniferous forest

Zhiyong Wu,<sup>1</sup> Xuemei Wang,<sup>1</sup> Andrew A. Turnipseed,<sup>2</sup> Fei Chen,<sup>2</sup> Leiming Zhang,<sup>3</sup> Alex B. Guenther,<sup>2</sup> Thomas Karl,<sup>2</sup> L. G. Huey,<sup>4</sup> Dev Niyogi,<sup>5</sup> Beicheng Xia,<sup>1</sup> and Kiran Alapaty<sup>6</sup>

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[1] Dry deposition velocities ( $V_d$ ) for peroxyacetyl nitrate (PAN) calculated using two community dry deposition models with different treatments of both stomatal and nonstomatal uptakes were evaluated using measurements of PAN eddy covariance fluxes over a Loblolly pine forest in July 2003. The observed daytime maximum of  $V_d(\text{PAN})$  was  $\sim 1.0 \text{ cm s}^{-1}$  on average, while the estimates by the WRF-Chem dry deposition module (WDDM) and the Noah land surface model coupled with a photosynthesis-based Gas Exchange Model (Noah-GEM) were only  $0.2 \text{ cm s}^{-1}$  and  $0.6 \text{ cm s}^{-1}$ , respectively. The observations also showed considerable PAN deposition at night with typical  $V_d$  values of  $0.2\text{--}0.6 \text{ cm s}^{-1}$ , while the estimated values from both models were less than  $0.1 \text{ cm s}^{-1}$ . Noah-GEM modeled more realistic stomatal resistance ( $R_s$ ) than WDDM, as compared with observations of water vapor exchange fluxes. The poor performance of WDDM for stomatal uptake is mainly due to its lack of dependence on leaf area index. Thermal decomposition was found to be relatively unimportant for measured PAN fluxes as shown by the lack of a relationship between measured total surface conductance and temperature. Thus, a large part of the underprediction in  $V_d$  from both models should be caused by the underestimation of nonstomatal uptake, in particular, the cuticle uptake. Sensitivity tests on both stomatal and nonstomatal resistances terms were conducted and some recommendations were provided.

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### 1. Introduction

[2] Peroxyacetyl nitrate (PAN,  $\text{CH}_3\text{C}(\text{O})\text{OONO}_2$ ) is an abundant secondary pollutant of photochemical oxidation, which is produced in the atmosphere by reactions 1 and 2f:



The reverse reaction (R2r) represents the thermal decomposition of PAN, a process highly sensitive to temperature. The reaction of the peroxyacetyl radical (PA,  $\text{CH}_3\text{C}(\text{O})\text{OO}$ ) with NO is the primary removal mechanism of PAN from the atmosphere:



Other chemical decay mechanisms for PAN, including oxidation by hydroxyl radical (OH) and photolysis, are relatively slow and negligible relative to thermal decomposition in the lower troposphere [Singh, 1987; Talukdar *et al.*, 1995].

[3] PAN acts as an important reservoir of reactive nitrogen and plays an important role in photochemical reactions. PAN is thought to contribute significantly to the global transport and distribution of reactive nitrogen as it can be transported over long distances in the free troposphere where low temperatures prevent its thermal decomposition, and it can return to the warmer, lower troposphere in remote areas where  $\text{NO}_2$  is released from the thermal decomposition reaction and contributes to ozone formation [Singh and Hanst, 1981; Cox and Roffey, 1977; Moxim *et al.*, 1996].

<sup>1</sup>School of Environmental Science and Engineering, Sun Yat-sen University, Guangzhou, China.

<sup>2</sup>National Center for Atmospheric Research, Boulder, Colorado, USA.

<sup>3</sup>Air Quality Research Division, Science and Technology Branch, Environment Canada, Toronto, Ontario, Canada.

<sup>4</sup>School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, Georgia, USA.

<sup>5</sup>Purdue University, West Lafayette, Indiana, USA.

<sup>6</sup>Atmospheric Modeling and Analysis Division, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, USA.