

## Supplementary Material

### **GPU-HADVPPM4HIP V1.0: higher model accuracy on China's domestically GPU-like accelerator using heterogeneous compute interface for portability (HIP) technology to accelerate the piecewise parabolic method (PPM) in an air quality model (CAMx V6.10)**

**Kai Cao<sup>1</sup>, Qizhong Wu<sup>1,5</sup>, Lingling Wang<sup>2</sup>, Hengliang Guo<sup>3</sup>, Nan Wang<sup>2</sup>, Huaqiong Cheng<sup>1,5</sup>, Xiao Tang<sup>4</sup>, Lina Liu<sup>3</sup>, Dongqing Li<sup>1</sup>, Hao Wu<sup>3</sup>, and Lanning Wang<sup>1,5</sup>**

<sup>1</sup>College of Global Change and Earth System Science, Faculty of Geographical Science, Beijing Normal University, Beijing 100875, China

<sup>2</sup>Henan Ecological Environmental Monitoring Centre and Safety Center, Henan Key Laboratory of Environmental Monitoring Technology, Zhengzhou 450008, China

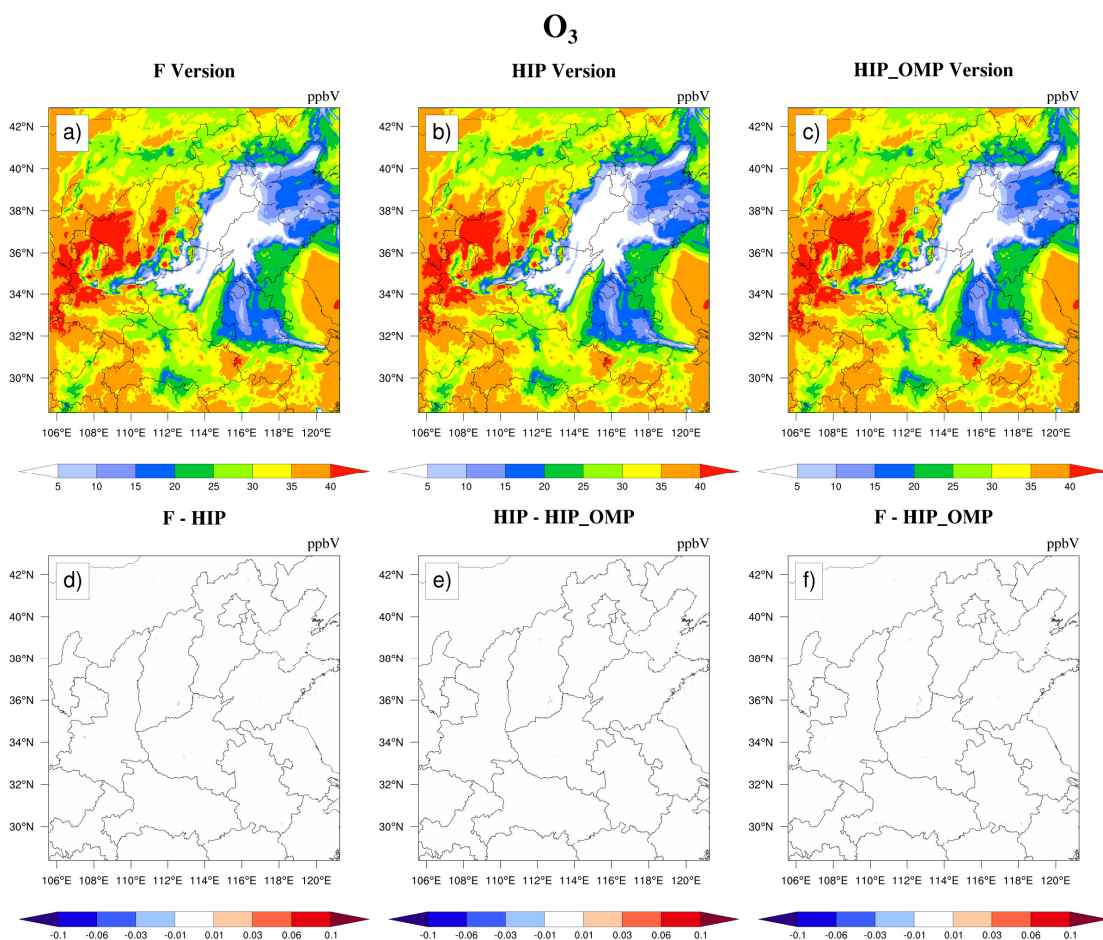
<sup>3</sup>National Supercomputing Center in Zhengzhou, Zhengzhou, 450001, China

<sup>4</sup>State Key Laboratory of Atmospheric Boundary Layer Physics and Atmospheric Chemistry, Institute of Atmospheric Physics, Chinese Academy of Science, Beijing 100029, China

<sup>5</sup>Joint Center for Earth System Modeling and High Performance Computing, Beijing Normal University, Beijing, 100875, China

**Correspondence to:** Qizhong Wu ([wqizhong@bnu.edu.cn](mailto:wqizhong@bnu.edu.cn)); Lingling Wang([928216422@qq.com](mailto:928216422@qq.com)); Lanning Wang ([wangln@bnu.edu.cn](mailto:wangln@bnu.edu.cn))

**Figure S1.** O<sub>3</sub> concentrations outputted by CAMx model for Fortran (F), HIP C(HIP), and HIP C with OpenMP (HIP\_OMP) versions. Panels (a) is from Fortran version. Panels (b) is from HIP C version. Panels (c) is from HIP C with OpenMP version. Panels (d) is the output concentration differences of Fortran and HIP C versions. Panels (e) is the output concentration differences of HIP C and HIP C with OpenMP versions. Panels (f) is the output concentration differences of Fortran and HIP C with OpenMP versions.



**Table S1.** The physical and chemical numerical methods selected during CAMx model simulation.

| Process                                         | Numerical Methods                                                           |
|-------------------------------------------------|-----------------------------------------------------------------------------|
| Horizontal advection                            | PPM (Colella and Woodward, 1984)                                            |
| Vertical diffusion                              | K-theory 1 <sup>st</sup> order closure                                      |
| Aqueous-phase oxidation                         | Regional Acid Deposition Model<br>(RADM-AQ, (Chang et al., 1987))           |
| Inorganic aerosol<br>thermodynamic partitioning | ISORROPIA (Nenes et al., 1999)                                              |
| Gas-Phase Chemistry                             | Carbon Bond 2005 (Yarwood et al., 2005)<br>EBI solver (Hertel et al., 1993) |

---

|                |                                                                                      |
|----------------|--------------------------------------------------------------------------------------|
| Dry deposition | Resistance model for gases (Zhang et al., 2003)<br>and aerosols (Zhang et al., 2001) |
| Wet deposition | Scavenging model for gases<br>and aerosols (Seinfeld et al., 1998)                   |

---

## Reference

- Chang, J. S., Brost, R. A., Isaksen, I. S. A., Madronich, S., Middleton, P., Stockwell, W. R., and Walcek, C. J.: A three-dimensional Eulerian acid deposition model: Physical concepts and formulation, *Journal of Geophysical Research: Atmospheres*, 92, 14681-14700, <https://doi.org/10.1029/JD092iD12p14681>, 1987.
- Colella, P. and Woodward, P. R.: The Piecewise Parabolic Method (PPM) for gas-dynamical simulations, *Journal of Computational Physics*, 54, 174-201, [https://doi.org/10.1016/0021-9991\(84\)90143-8](https://doi.org/10.1016/0021-9991(84)90143-8), 1984.
- Hertel, O., Berkowicz, R., Christensen, J., and Hov, Ø.: Test of two numerical schemes for use in atmospheric transport-chemistry models, *Atmospheric Environment. Part A. General Topics*, 27, 2591-2611, [https://doi.org/10.1016/0960-1686\(93\)90032-T](https://doi.org/10.1016/0960-1686(93)90032-T), 1993.
- Nenes, A., Pandis, S. N., and Pilinis, C.: Continued development and testing of a new thermodynamic aerosol module for urban and regional air quality models, *Atmospheric Environment*, 33, 1553-1560, [https://doi.org/10.1016/S1352-2310\(98\)00352-5](https://doi.org/10.1016/S1352-2310(98)00352-5), 1999.
- Seinfeld, J. H., Pandis, S. N., and Noone, K. J. J. P. T.: *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, 51, 88-90, 1998.
- Yarwood, G., Rao, S., Yocke, M., and Whitten, G.: Updates to the carbon bond chemical mechanism: CB05 final report to the US EPA, RT-0400675, 2005.
- Zhang, L., Brook, J. R., and Vet, R.: A revised parameterization for gaseous dry deposition in air-quality models, *Atmos. Chem. Phys.*, 3, 2067-2082, [10.5194/acp-3-2067-2003](https://doi.org/10.5194/acp-3-2067-2003), 2003.
- Zhang, L., Gong, S., Padro, J., and Barrie, L.: A size-segregated particle dry deposition scheme for an atmospheric aerosol module, *Atmospheric Environment*, 35, 549-560, [https://doi.org/10.1016/S1352-2310\(00\)00326-5](https://doi.org/10.1016/S1352-2310(00)00326-5), 2001.