Supplementary Material

Multiscale Applications of Two Online-Coupled Meteorology-Chemistry Models during Recent Field Campaigns in Australia, Part II: Comparison of WRF/Chem and WRF/Chem-ROMS and Impacts of Air-Sea Interactions and Boundary Conditions

Yang Zhang¹, Kai Wang¹, Chinmay Jena¹, Clare Paton-Walsh², Élise-Andrée Guérette², Steven Utembe³, Jeremy David Silver³, and Melita Keywood⁴

- ¹ Department of Marine, Earth and Atmospheric Sciences, North Carolina State University, Raleigh, NC 27695, USA; <u>kwang@ncsu.edu (K.W.); cjena@ncsu.edu (C.J.)</u>
- ² Centre for Atmospheric Chemistry, University of Wollongong, Wollongong NSW 2500, Australia; <u>clarem@uow.edu.au</u> (C. P.-W.); <u>eag873@uowmail.edu.au</u> (E.-A. G)
- ³ School of Earth Sciences, University of Melbourne, Melbourne, Victoria VIC 3052, Australia; <u>sutembe@unimelb.edu.au (S. U.); jeremy.silver@unimelb.edu.au (J.D.S.)</u>
- ⁴ Climate Science Centre, The Commonwealth Scientific and Industrial Research Organisation, Oceans and Atmosphere, Aspendale VIC 3195, Australia; <u>Melita.Keywood@csiro.au</u> (M.K.)
- * Correspondence: e-mail: <u>yzhang9@ncsu.edu</u>; Tel.: +01-919-515-9688 (Y.Z.)



Figure S1. Observed and simulated LHF over southeastern Australia (d02). Two sets of simulations results at 3-km are compared: one from WRF/Chem-NCSU and one from WRF/Chem-ROMS.



Figure S2. Observed and simulated SHF over southeastern Australia (d02). Two sets of simulations results at 3-km are compared: one from WRF/Chem-NCSU and one from WRF/Chem-ROMS.



Figure S3. Absolute differences in simulated radiative variables between WRF/Chem-ROMS and WRF/Chem-NCSU over the Greater Sydney (d04).



Figure S4. Observed and simulated temporal profiles of precipitation at selected sites over the Greater Sydney at 3-km (d04) during SPS2 and MUMBA. Two sets of simulations results at 3-km are compared: one from WRF/Chem-NCSU and one from WRF/Chem-ROMS.



Figure S5. Differences in simulated gases between WRF/Chem-ROMS and WRF/Chem-NCSU over the Greater Sydney (d04).



Figure S6. Observed and simulated column mass abundances of gases and AOD without and with adjustment of boundary conditions over the Greater Sydney (d04) for SPS2. The simulation results are from WRF/Chem-NCSU.



Figure S7. Observed and simulated surface concentrations of CO at selected sites during SPS1 (left) and SPS2 (right). Two sets of simulations results from WRF/Chem-NCSU at 3-km are compared: one using CO boundary conditions derived from CESM simulations (Base) and one using CO boundary conditions constrained by satellite data (Final).

Variable	Boundary	SPS1	SPS2	MUMBA
PM _{2.5} ^a	South	1.25482	0.814832	1.322459
	North	4.077799	1.0 ^b	5.575185
	East	1.0 ^b	0.772541	1.146297
	West	1.14355	0.763121	1.530221
СО	South	1.373572	1.360706	1.364776
	North	1.0 ^b	1.0 ^b	1.0 ^b
	East	1.088019	1.239348	1.134917
	West	1.205903	1.294666	1.306423
O ₃	South	1.4636	1.279148	2.5456
	North	1.0 ^b	1.312874	1.517
	East	1.02929	1.159937	1.3747
	West	1.135327	1.015153	1.2137
NO ₂	South	1.0 ^b	1.0 ^b	1.0 ^b
	North	0.595348	0.685131	0.757906
	East	0.49336	0.731152	0.663425
	West	0.621125	0.775164	0.797313
НСНО	South	1.389166	1.0 ^b	1.636667
	North	1.52647	1.255414	1.500742
	East	1.318888	1.529815	1.194535
	West	1.197265	2.193148	1.352154

Table S1. The adjustment factors used for the satellite-constrained BCONs for the AUS simulations.

^aThe factors were applied for all the major PM species in the model.

^bThe value of 1.0 indicates no adjustment was applied because of poor quality of satellite data at the boundary. CO: carbon monoxide; O₃: ozone; NO₂: nitrogen dioxide; HCHO: formaldehyde; SPS1 and SPS2: Sydney Particle Study Stages 1 and 2; MUMBA: the Measurements of Urban, Marine and Biogenic Air.