Impact of enhanced ozone deposition and halogen chemistry on model performance

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1. Introduction

Studies have suggested that enhanced ozone (O_3) deposition over sea-water and halogen chemistry are important atmospheric processes (Chang et al., 2004 and Read et al., 2008). However, these processes are currently not accounted for in most air quality models. Here, we examine the impacts of these processes on O_3 using the hemispheric the Community Multiscale Air Quality (CMAQ) model.

2.1 Model configuration

Feature	Description	Reference
Domain	Northern hemisphere	Mathur et al., 2011
Horizontal grid size	108-km x 108-km	
Vertical layers	44 layers (1000-50 mb)	
Simulation period	May-August, 2006	
Meteorological model	WRFv3.3	Skamarock et al., 2008
Anthropogenic emissions	Emissions Database for Global Atmospheric Research	edgar.jrc.ec.europa.eu
Biogenic emissions	Global Emissions InitiAtive	www.geiacenter.org
Boundary conditions	Static profile	
Initial conditions	Previous model results	
Model simulations		
Case A	CB05TUCl	Whitten et al., 2010
Case B	Case A + halogen chemistry	
Case C	Case B + enhanced O_3 deposition	

2.2 Halogen chemistry and emissions

Feature	Description	Reference
Bromine chemistry	37 chemical reactions	Yang et al., 2005
Iodine chemistry	50 chemical reactions	Saiz-Lopez et al., 2014
Halogen emissions		
Halocarbons	Based on chlorophyll	Yarwood, et al., 2012 Ordonez et al., 2012
Br_2	Based on sea-salt emissions	Yang et al., 2006
HOI and I_2	Based on SST, wind speed, O_3	McDonald et al., 2014

2.3 Enhanced O_3 deposition over sea-water

Feature	Description	Reference
Deposition velocity	$v_d = \frac{1}{R_a + R_b + R_s}$	
Current R_s	$R_s = \frac{\left(S_c / P_r \right)^{2/3}}{H_{eff} d_3 u_*}$	
Revised R_s	$\frac{1}{1.75 \frac{(d_3 u_*)}{\left(S_c / P_r \right)^{2/3}} + heff\,(2.0e5 * C_I * Diff_{H_2O})^{0.5}}$	Chang et al., 2004
Sea-water iodide (C_I)	Based on sea-surface temperature	Carpenter et al., 2014

3.1 BRO and IO

- Predicted monthly-mean daytime surface BrO values over marine environments are generally <1.0 pptv while predicted IO values are >1.0 pptv (Figure 1).
- Ship-based measured BrO values are <3.0-3.6 pptv and IO ~3.5 pptv while satellite based measured IO values are ~2.4-3.3 pptv (Saiz-Lopez et al., 2012). Predicted daytime BrO values are generally lower than observations while predicted IO values tend to be closer to the observed data.

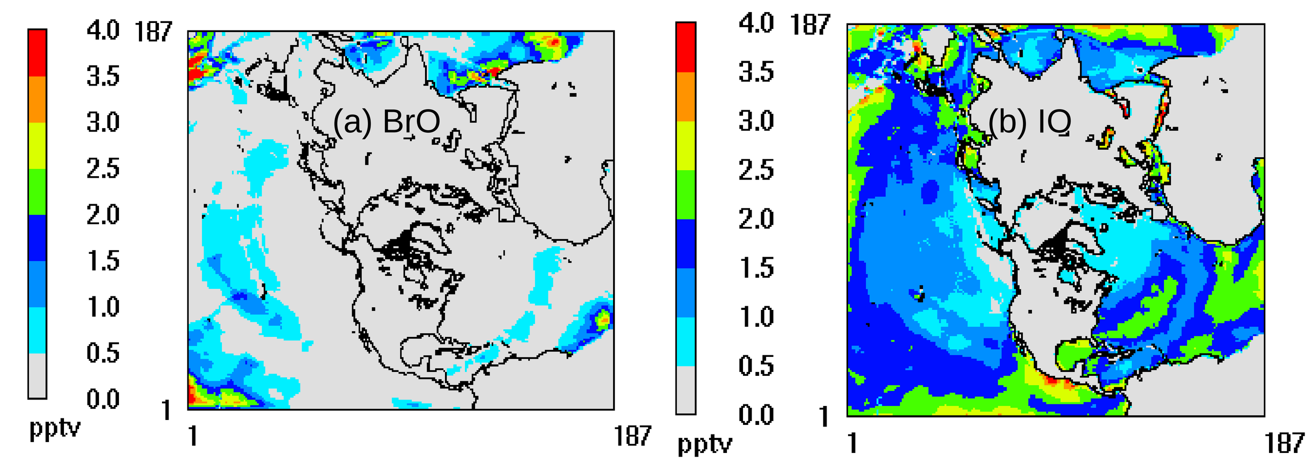

Figure 1: Predicted monthly-mean (August) daytime surface (a) BrO (b) IO

3.2 Impact on surface-level O_3

- Halogen chemistry reduces monthly-mean surface O_3 by 4.0-6.0 ppbv over large areas of marine environments while enhanced deposition reduces O_3 by 1.0-2.0 ppbv (Figure 2). Overall, the halogen chemistry reduces O_3 by 3.0 ppbv averaged over the entire domain while the enhanced deposition reduces O_3 by 0.6 ppbv.
- The odd oxygen destruction rate (Saiz-Lopez, et al., 2014) (averaged over all layers in marine environment) due to the halogen chemistry is 0.4 ppbv/day. The majority of the loss was triggered by the iodine chemistry.

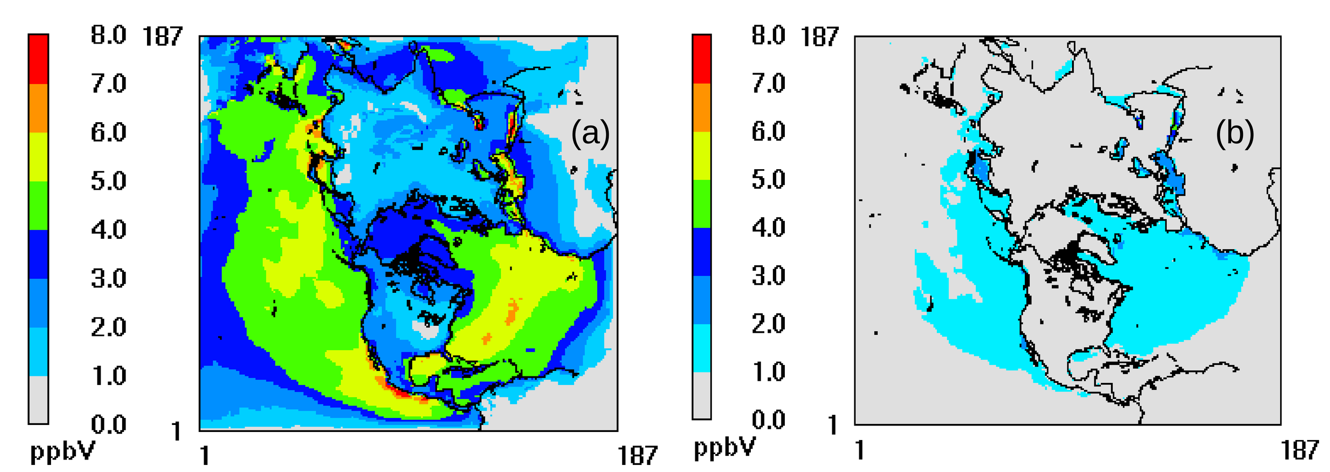

Figure 2: (a) Predicted changes (Case A – Case B) in monthly-mean (August) surface O_3 concentrations due to halogen chemistry (b) predicted changes (Case B – Case C) in monthly-mean O_3 concentrations due to enhanced deposition

3.3 Comparison with observed O_3

- Model predictions with these processes improve the comparison with observed O_3 data at remote locations (Table 1 and Figure 3).
- Mean bias for Case A = 8.6 ppbv, Case B = 4.8 ppbv, and Case C = 3.9 ppbv.

Table 1: A comparison of model and observed O_3 at remote surface locations (ppbv)

Location	Observed mean	Predictions Case A	Predictions Case B	Predictions Case C
Trinadad Head, CA	25.9	32.8	29.6	28.8
Ragged Pt., Barb.	18.2	25.1	20.9	20.2
Tudor Hill, Bermuda	27.2	37.3	32.2	31.1
Hilo, HI	14.2	29.0	24.7	23.9
Barrow, AK	23.1	31.2	28.2	27.7
Sable Island	38.4	46.6	42.5	41.0
Houston, TX	41.4	46.3	43.5	43.2
Average	**26.9**	**35.5**	**31.7**	**30.8**

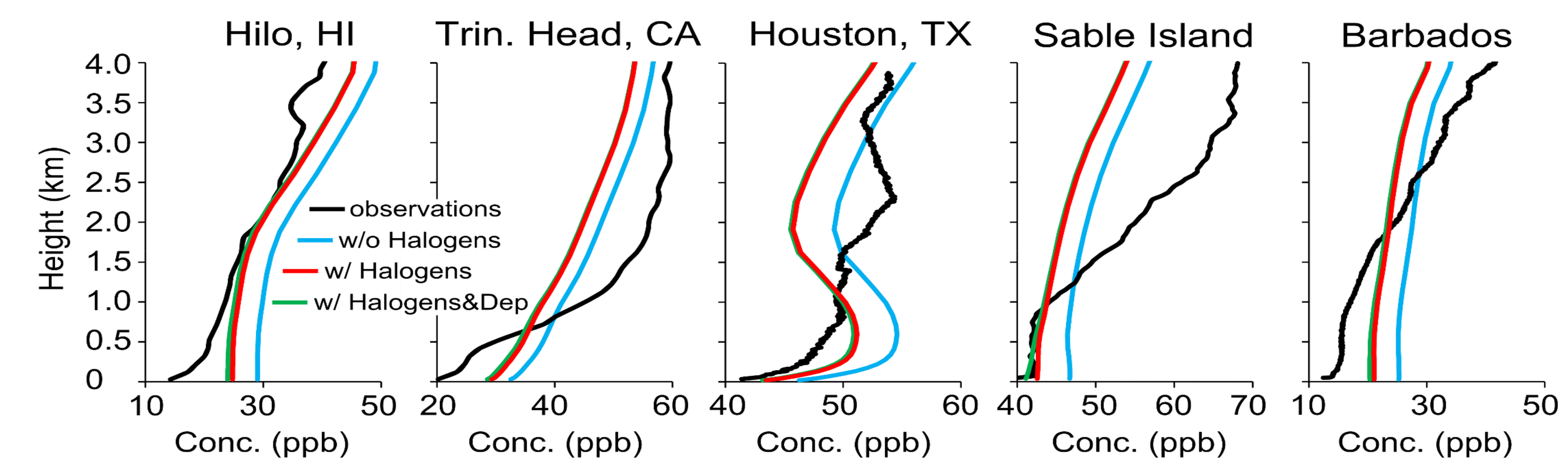

Figure 3: A comparison of predicted O_3 concentrations with ozonesonde data

4. Summary

- Both the enhanced deposition and halogen chemistry reduce O_3 concentrations over marine environments. The halogen chemistry reduces more O_3 than the enhanced deposition.
- Model without these processes over-predicts O_3 while the inclusion of these processes improve model performance over marine environments.
- Enhanced deposition and halogen chemistry are important processes and need to be incorporated into air quality models.

5. References

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