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Passive-tracer modelling at super-resolution with Weather Research and Forecasting – Advanced Research WRF (WRF-ARW) to assess mass-balance schemes

Sepehr Fathi et al.

Correspondence to: Sepehr Fathi (sepehr.fathi@ec.gc.ca) and Mark Gordon (mgordon@yorku.ca)

Table S1. Discrete integral expressions of Eqs. (3), (4), (5), (B1) and (B2) to be substituted in Eq. (6). Constants Δx, Δy and Δs are equal to model grid resolution in the horizontal, 50 m. t is the time index; i, j and k are the 3D-space indices and s is the path index around the control volume (box). Model wind fields were linearly interpolated onto mass grid-points for the discrete integral calculations. Throughout, the second-order central finite-difference scheme was used to numerically solve the time derivatives ($\Delta/\Delta t$) with the residual error of order $O(\Delta t^2)$, where Δt is equal to the 1 sec model output time-step.

Term		Discrete Numerical Integration
S^t_{C}	$=$	$\Delta x \Delta y \sum_{i,j,k}^{n_x,n_y,n_z} \frac{\Delta \chi^t_{\mathrm{C},ijk}}{\Delta t} \Delta z_k$
$F^t_{\mathrm{C,H}}$	$=$	$\Delta s \sum_{s,k}^{n_s,n_z} \chi^t_{\mathrm{C},sk} U^t_{\perp,sk} \Delta z_k$
$F^t_{\mathrm{C,HT}}$	$=$	$-K_h\, \Delta s \sum_{s,k}^{n_s,n_z} \frac{\Delta \chi^t_{\mathrm{C},ijk}}{\Delta x_\perp} \Delta z_k$
$F^t_{\mathrm{C,V}}$	$=$	$\Delta x \Delta y \sum_{i,j}^{n_x,n_y} \chi^{t,\mathrm{top}}_{\mathrm{C},ij} W^{t,\mathrm{top}}_{ij}$
$F^t_{\mathrm{C,VT}}$	$=$	$-K_v\, \Delta x \Delta y \sum_{i,j}^{n_x,n_y} \frac{\Delta \chi^t_{\mathrm{C},ijk}}{\Delta z_\perp}$

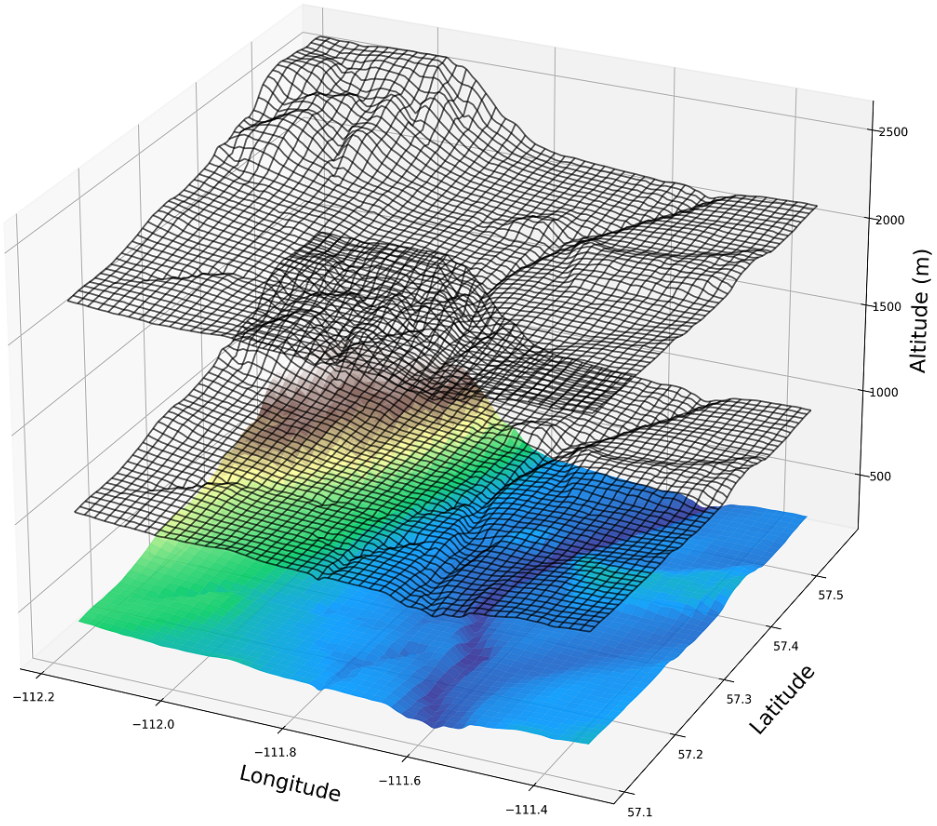

Figure S1. Topography of the modelling region for domain d05 (finest domain) is shown, lower elevations such as the Athabasca river valley are shown in dark blue and higher elevations are shown with colours green and brown. Our WRF model simulations use terrain-following model layers to ensure continuity in the modelling layers and proper treatment of the interaction between the atmospheric flow and the topography. Two model layers at levels 42 and 55 are also shown (mesh).

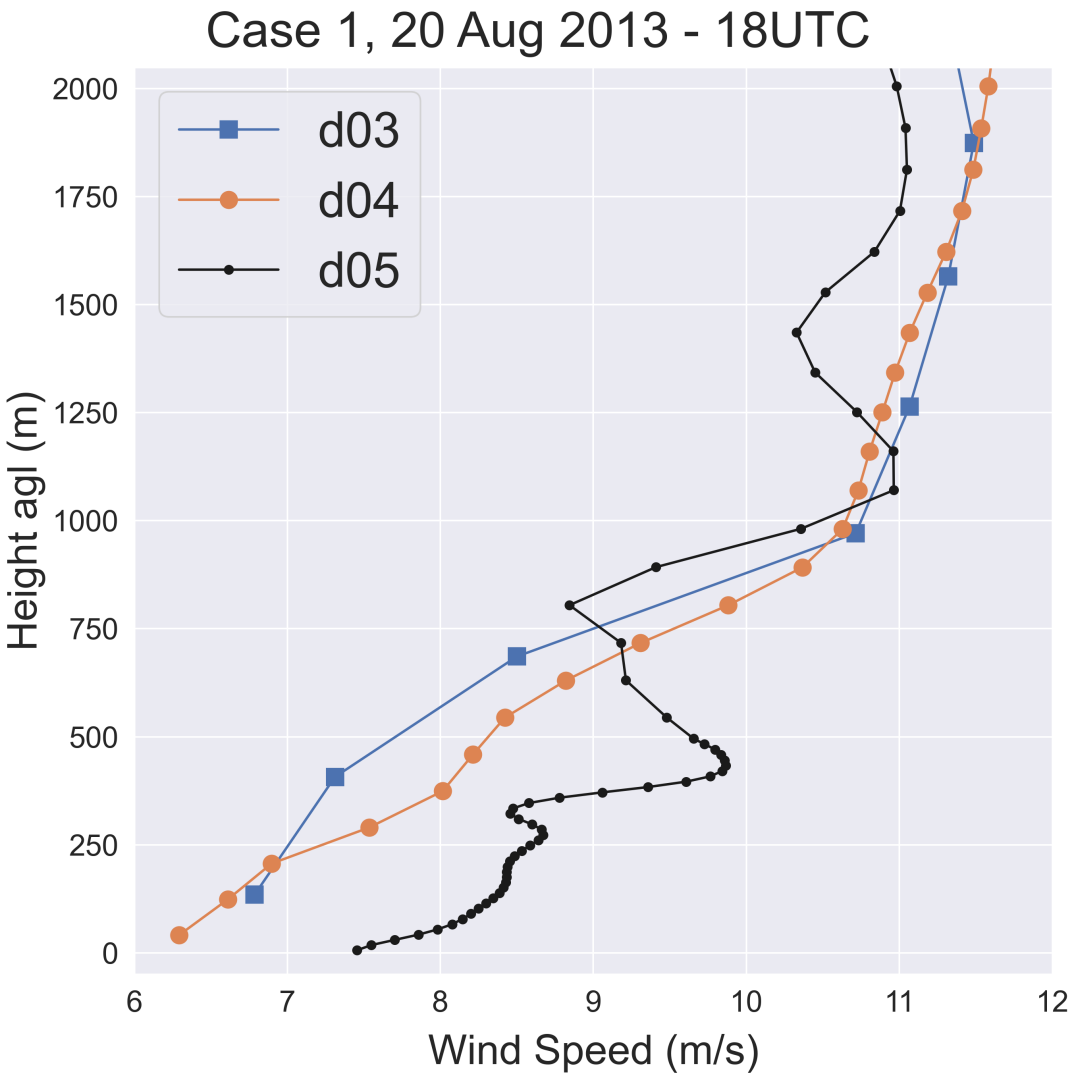

Figure S2. Wind vertical profiles from domains d03, d04 and d05 compared at the location of the main CNRL stack for case 1 on 20 Aug 2013 at 18 UTC.

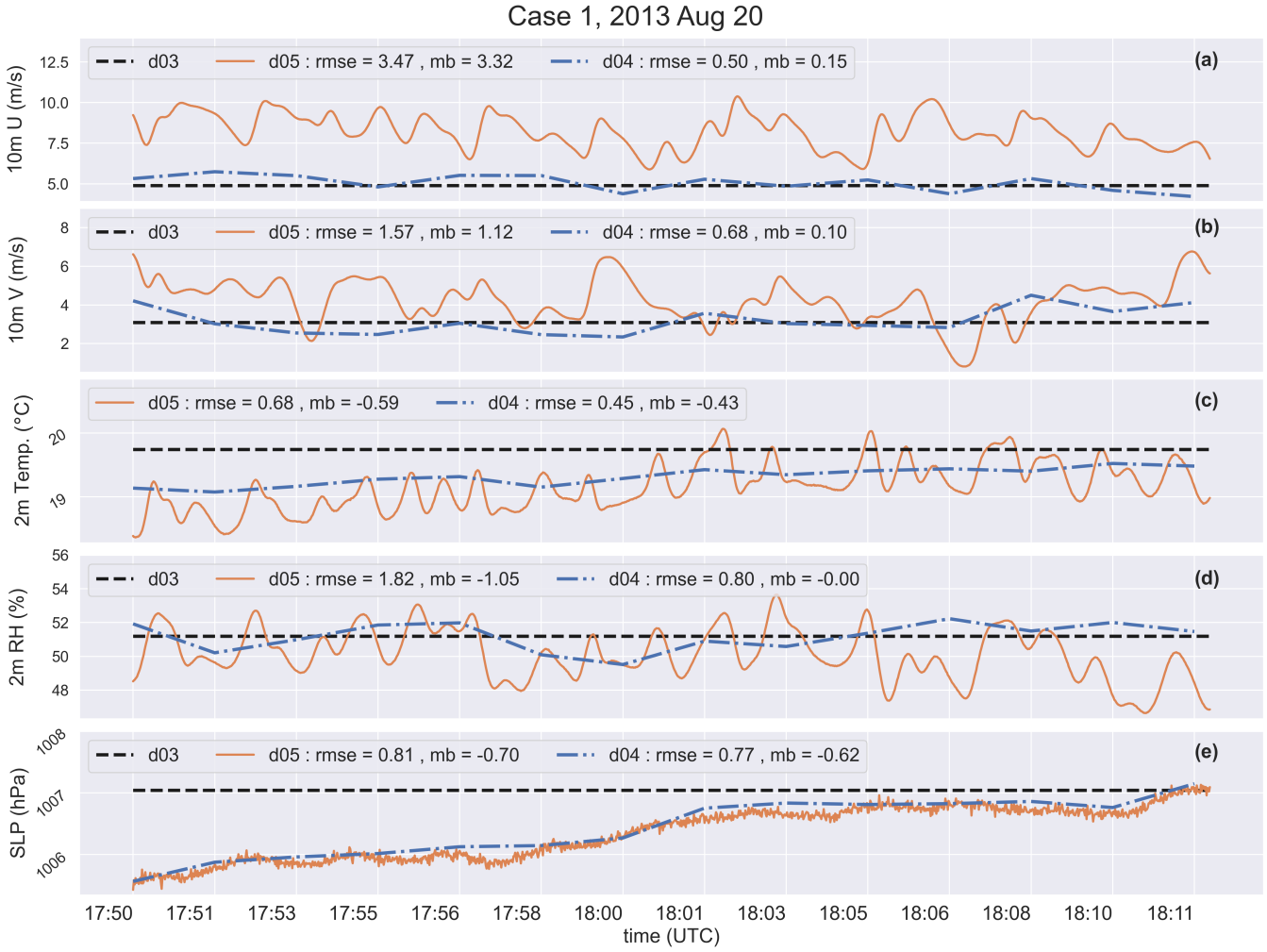

Figure S3. Model output meteorological fields from the two fine resolution domains d04 and d05 were evaluated against domain d03 output for the location of CNRL facility in terms of root mean square error (rmse) and mean bias (me). Time series are shown for wind speed at 10 m agl (a, b), temperature at 2 m agl (c), relative humidity at 2 m agl (d), and seal level pressure (e).

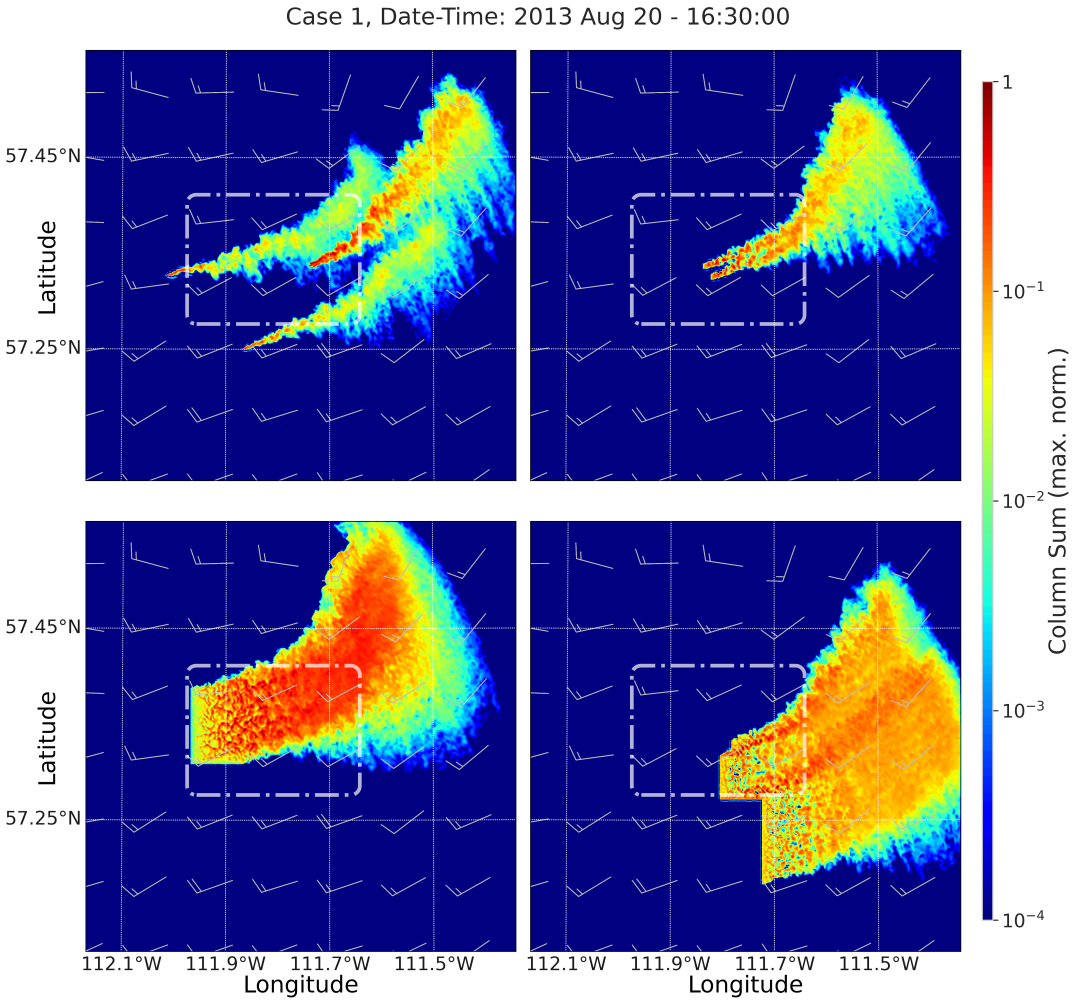

Figure S4. Case 1: top view of the 50 m resolution modelling domain with tracer plumes from our eleven emission scenarios at 16:30UT on 20 August 2013. Tracer plumes are dispersed and advected well beyond the boundaries of the CNRL facility, shown with the dashed curve (same as the small box in Fig. 6). 10-m wind data is shown with wind barbs over the entire domain (flag: half 5 knots, full 10 knots). The data shown is the tracer column total normalized to the maximum value for each panel. (top left) point/stack sources CNRL0-4, CNRLs and CNRLw. (top right) surface/area sources MINE1 and MINE2. (bottom left) the large area (surface) sources POND. (bottom right) the multi-segment line (surface) source HWY. Refer to Table 2 for source specifications.

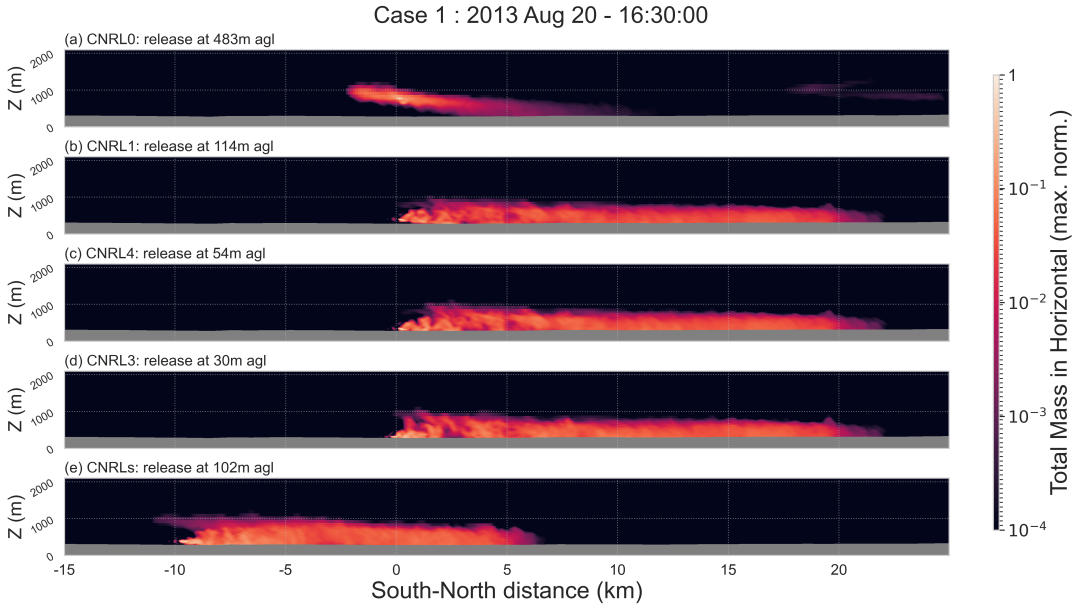

Figure S5. Domain d05 south-north vertical cross-section for case 1 on 20 August 2013. Vertical cross-section of tracer plumes from stack/point emission sources are shown with release heights indicated for each source. Data shown is the tracer amount summed in the horizontal level and normalized to the maximum value for each source. The origin for south-north distance in km is at domain centre.

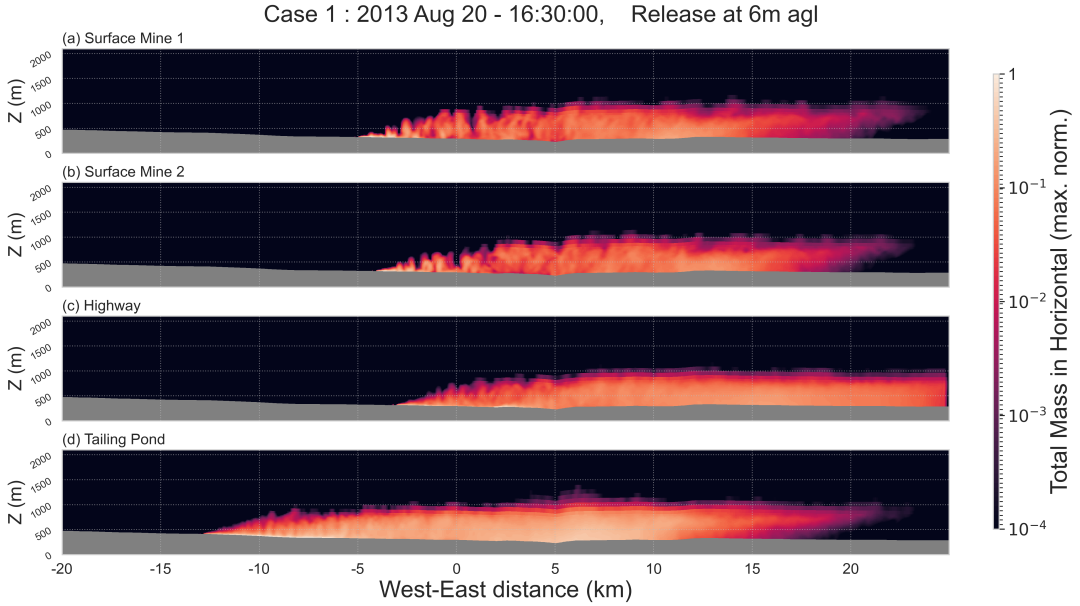

Figure S6. Domain d05 west-east vertical cross-section for case 1 on 20 August 2013. Vertical cross-section of tracer plumes from surface emission sources (area, line) are shown. Release height above ground is 6 m agl for all sources. Data shown is the tracer amount summed in the horizontal level and normalized to the maximum value for each source. The origin for west-east distance in km is at domain centre.

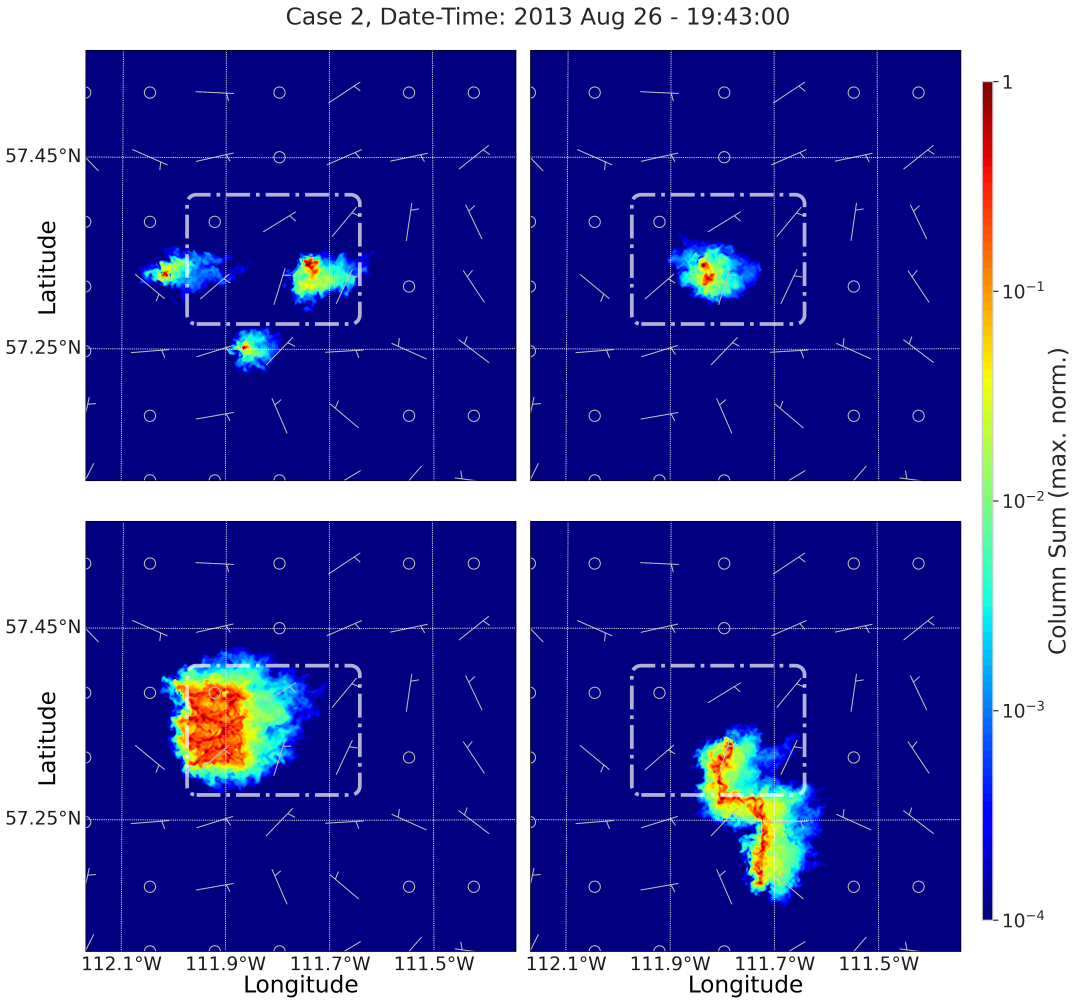

Figure S7. Case 2: top view of the 50 m resolution modelling domain with tracer plumes from our eleven emission scenarios at 19:43UT on 26 August 2013. 10-m wind data is shown with wind barbs over the entire domain (flag: half 5 knots, full 10 knots). The data shown is the tracer column total normalized to the maximum value for each panel. (top left) point/stack sources CNRL0-4, CNRLs and CNRLw. (top right) surface/area sources MINE1 and MINE2. (bottom left) the large area (surface) sources POND. (bottom right) the multi-segment line (surface) source HWY. For this case tracer plumes were not advected considerably, due to low and spatially variable winds. Refer to Table 2 for source specifications.

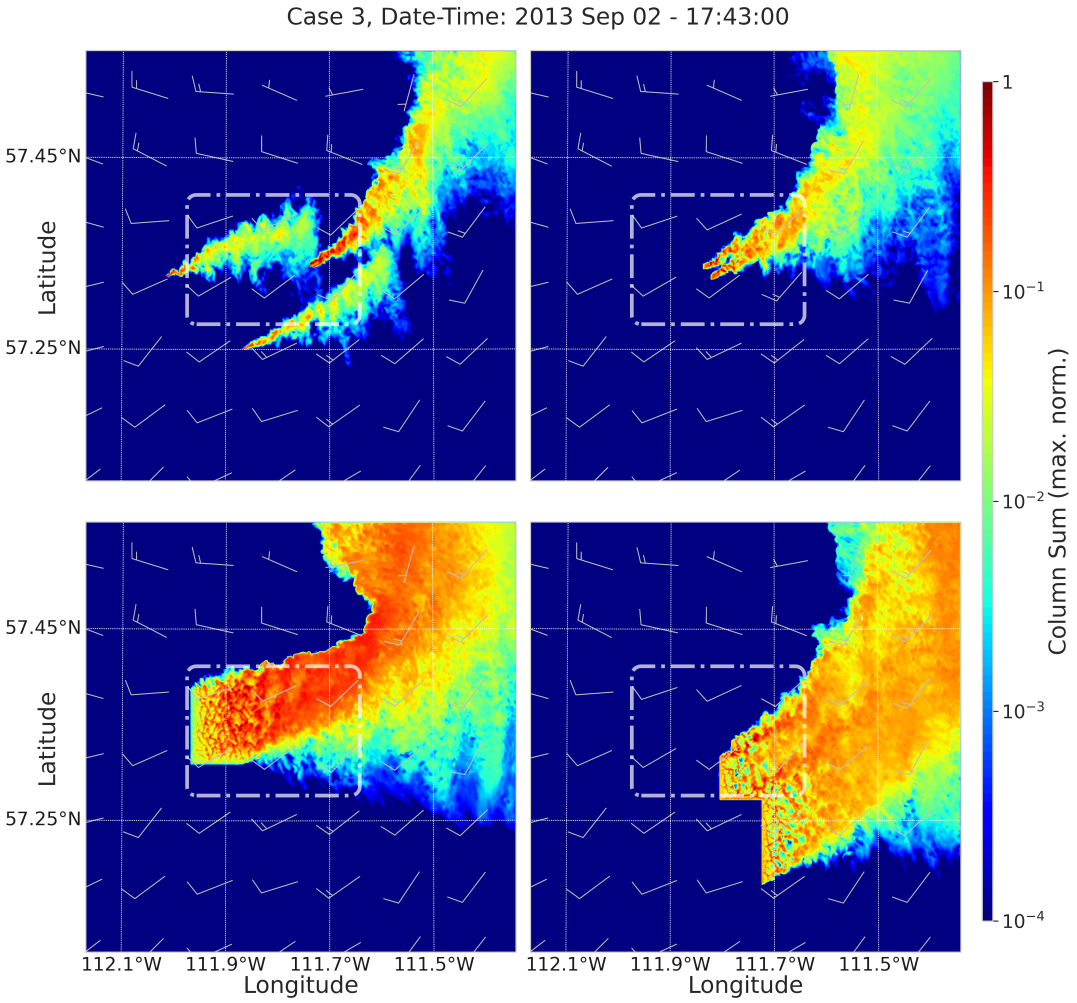

Figure S8. Case 3: top view of the 50 m resolution modelling domain with tracer plumes from our eleven emission scenarios at 17:43UT on 2 September 2013. Tracer plumes are dispersed and advected well beyond the boundaries of the CNRL facility (dashed curve) as in case 1. Wind data at 10 m agl is shown with wind barbs over the entire domain (flag: half 5 knots, full 10 knots). The data shown is the tracer column total normalized to the maximum value for each panel. (top left) point/stack sources CNRL0-4, CNRLs and CNRLw. (top right) surface/area sources MINE1 and MINE2. (bottom left) the large area (surface) sources POND. (bottom right) the multi-segment line (surface) source HWY. Refer to Table 2 for source specifications.

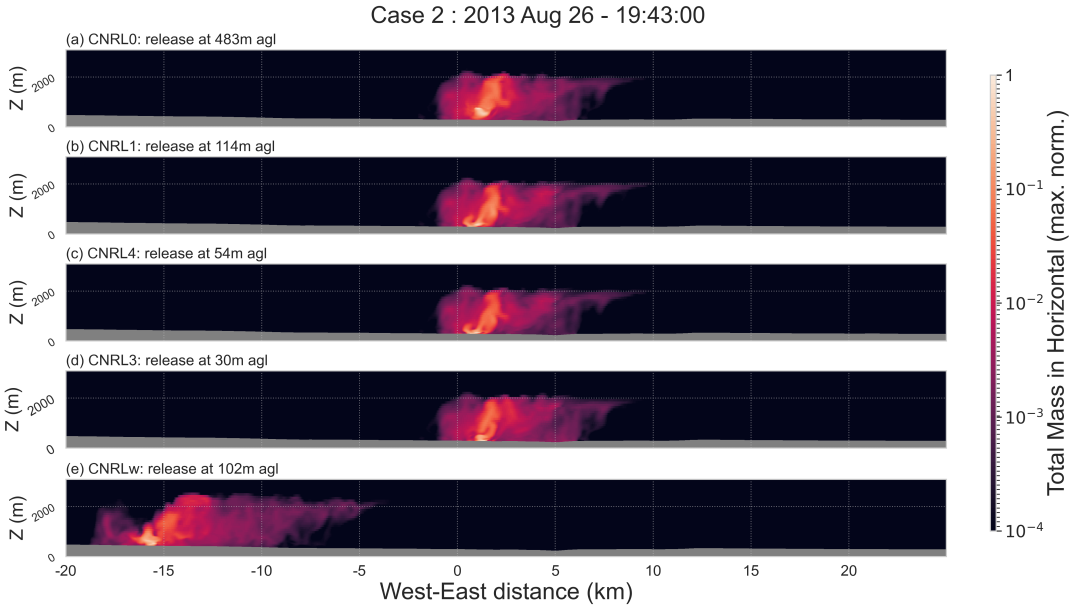

Figure S9. Domain d05 west-east vertical cross-section for case 2 on 26 August 2013. Vertical cross-section of tracer plumes from stack/point emission sources are shown with release heights indicated for each source. Data shown is the tracer amount summed in the horizontal level and normalized to the maximum value for each source. The origin for south-north distance in km is at domain centre.

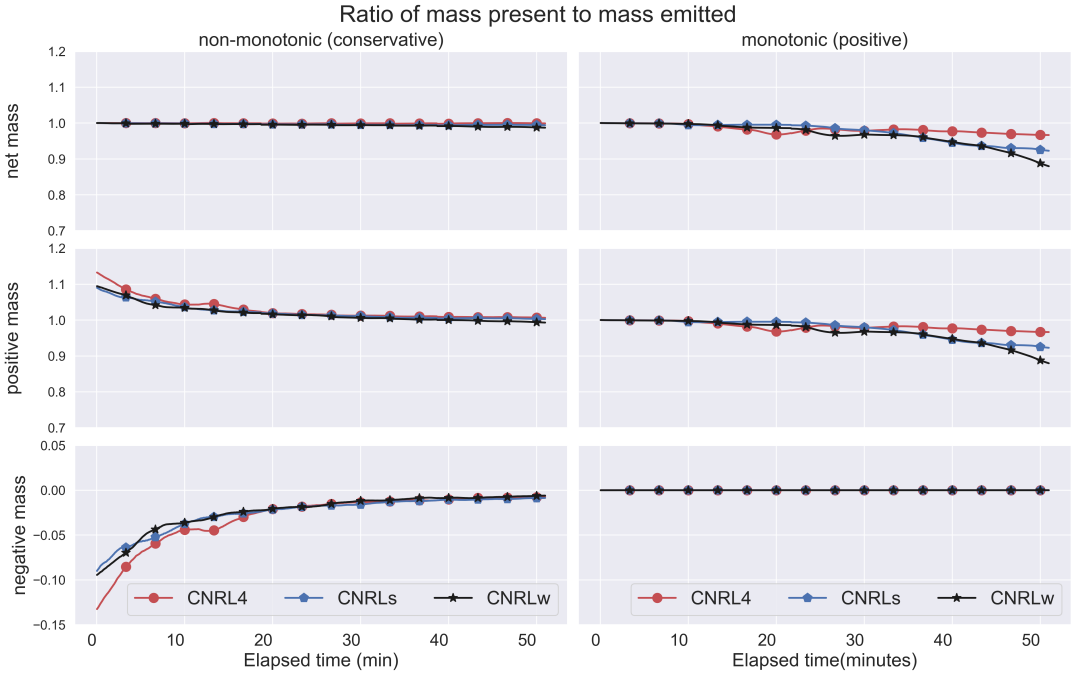

Figure S10. Comparison of WRF-ARW default non-monotonic diffusion scheme (left column) with the monotonic-positive diffusion scheme (right column), as the ratio of mass present in the modelling domain to mass emitted.