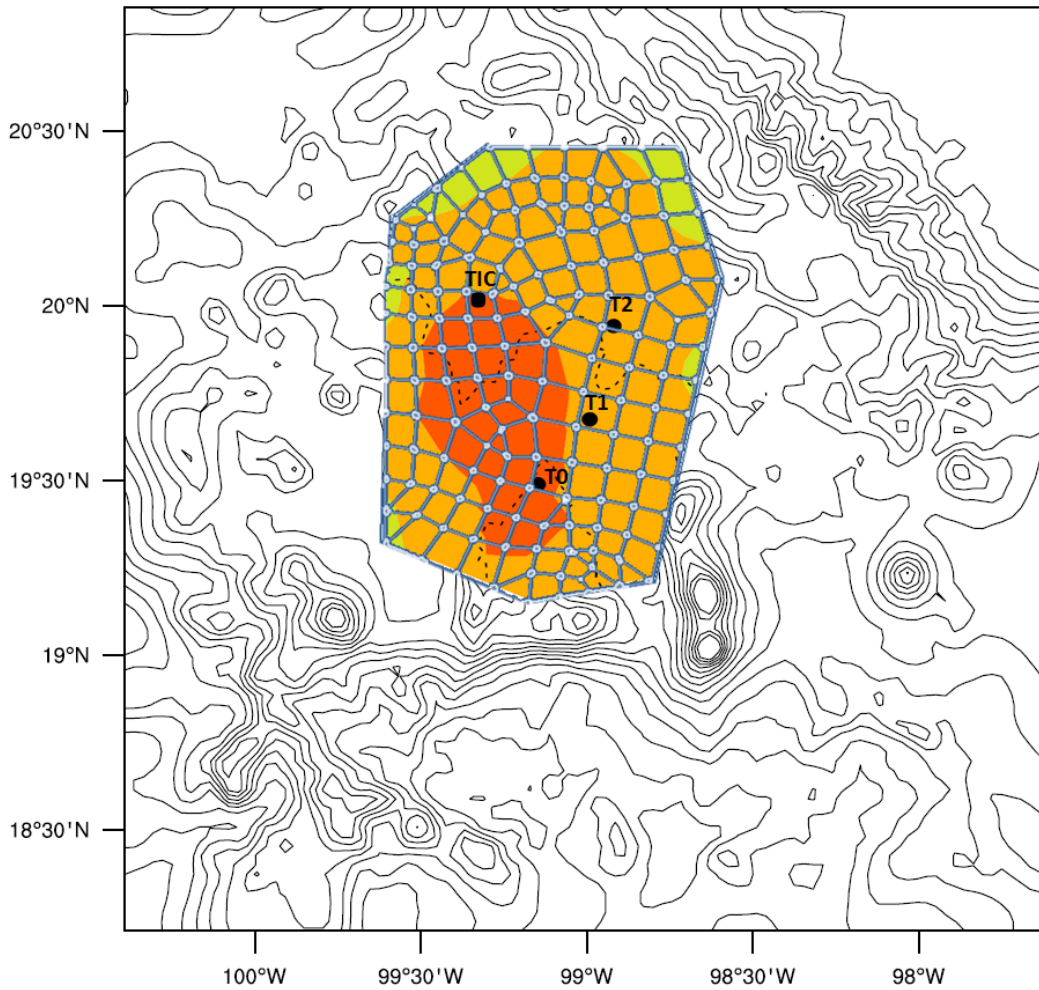


1 **Supplementary Material to Referee's comments**

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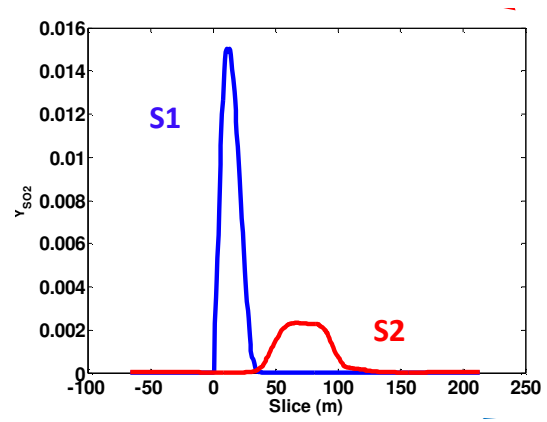
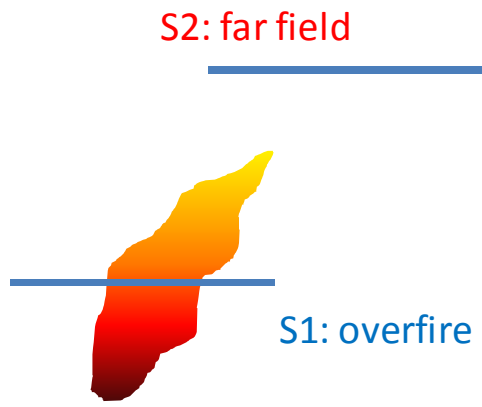


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4 Figure SM1. Region location used in the contribution plot. A set of points within this region is
5 constructed and further interpolated to domain 3 of WRF-Chem. These points were defined
6 for ease of calculation within NCL in order to obtain smooth contours. The pass of the plume
7 in this enclosed region is estimated by counting the number of hours in which a threshold was
8 exceeded in each of these points during the simulation period. Finally a contour plot with the
9 proportion of hours is constructed.

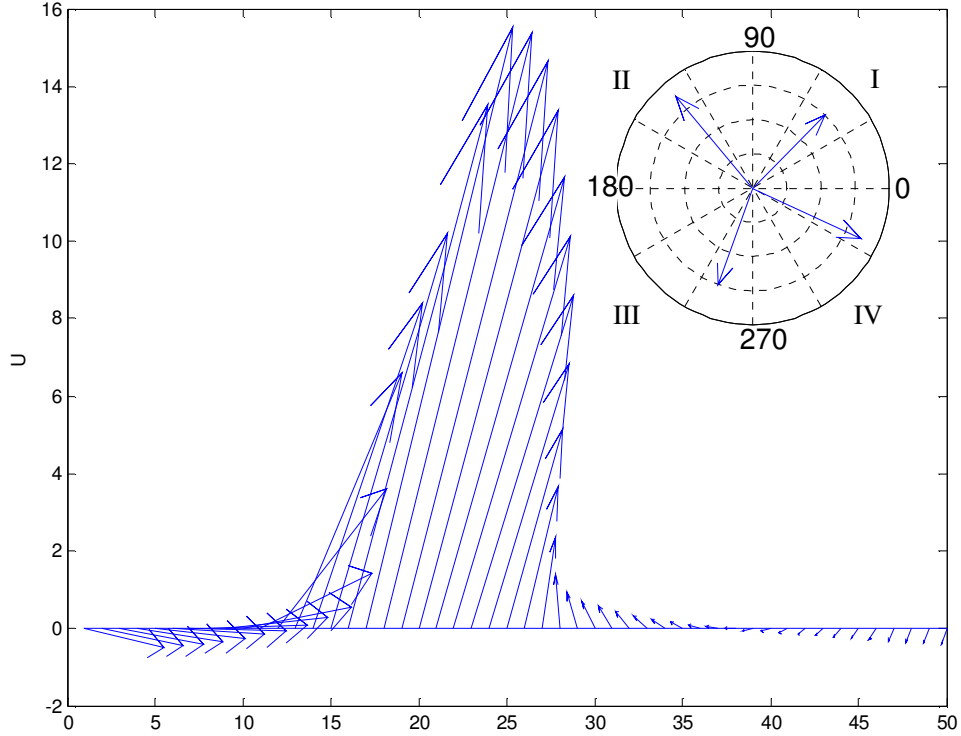
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Figure SM2. Plot showing the SO₂ mass fraction along two slices a) S1 near flame tip; b) 61 m from the flame tip. Given the relative coarse cell size outside the flame region, an artificial spread of the plume can contribute to estimate higher mass flow rates. For this reason, only the data of the concentration profile within two standard deviations were retained for the calculation.



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2 Figure SM3. Velocity vectors along a slice located near the flame tip. Reference line at zero
 3 represents the slice. Vectors below the reference line are considered as inflow into the slice,
 4 whereas outflow is represented by vectors above the reference line. Thus, taking a Cartesian
 5 plane as a reference, inflow corresponds to quadrants III and IV and outflow to quadrants I
 6 and II for each point of the slice. The figure in the upper right corner shows representative
 7 vectors for each quadrant.

8 The expression:

$$\rho Y_j(\vec{u} \cdot \vec{n})|_{\nabla_{ps}}$$

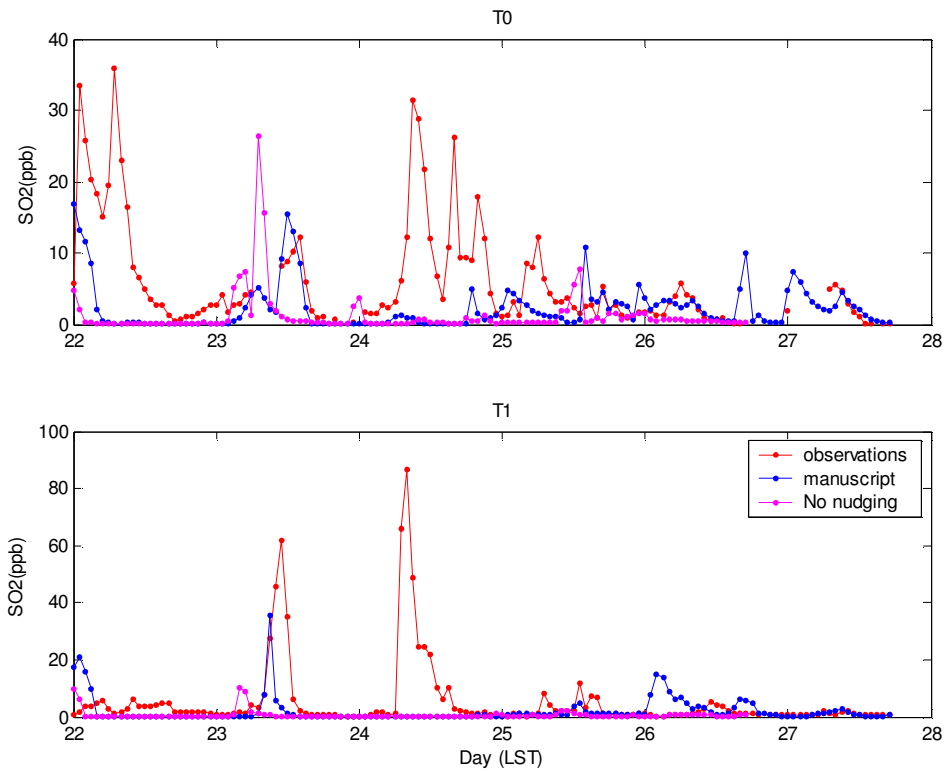
9 is evaluated at each point, ps , of the j th species profile that are within two standard
 10 deviations. The result is further integrated to obtain the mass flow.

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2 Figure SM4. SO₂ time series at T0 and T1 with the set-up as in the manuscript. It compares
 3 the results of applying nudging as in the set-up of the manuscript, versus the case without
 4 nudging. The timing and concentration of the peak on 23 March is better reproduced when
 5 applying nudging as in the manuscript.

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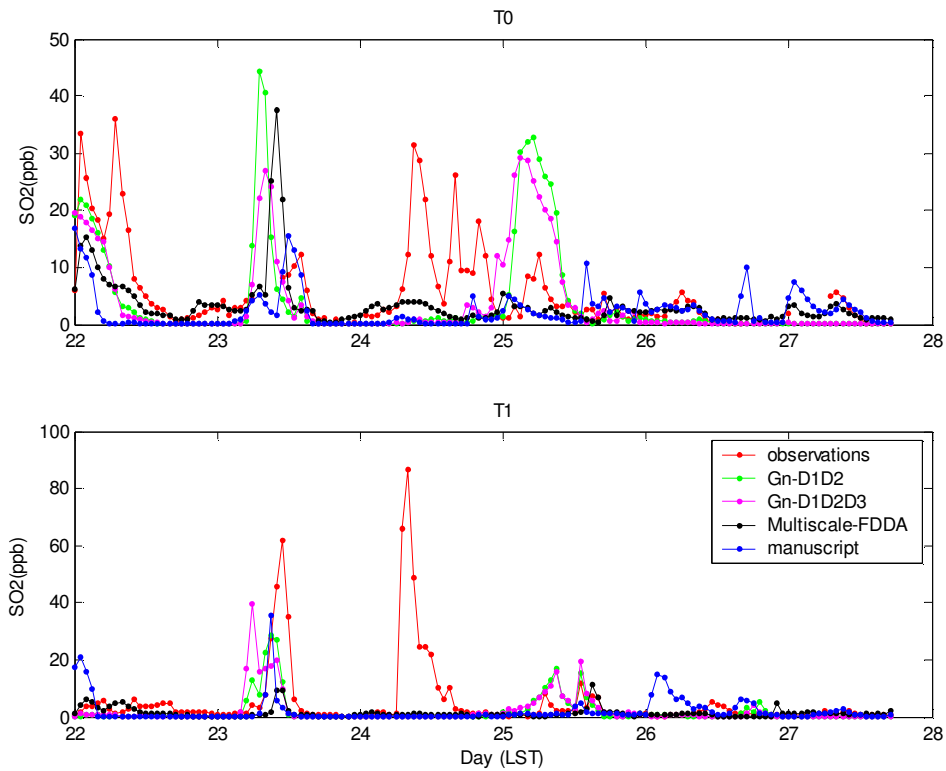
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2 Figure SM5. SO₂ time series at T0 and T1 with nudging in all the simulation period. All of
 3 these cases apply Objective Analysis to reanalyze meteorology. When applying only grid
 4 nudging, either in domain 1 and 2 (Gn-D1D2), or in all domains (Gn-D1D2D3), there is a
 5 significant concentration overprediction on 23 March and on 25 March with respect to
 6 observations. In addition, the timing of the peak occurs earlier on 23 March. Although not
 7 shown, similar overpredictions were present when applying observation nudging only. In
 8 contrast, Multiscale-FDDA showed the best performance statistics. This reflected in a sharp
 9 decrease of concentration on March 25 compared with the aforementioned cases. However,
 10 the first results of the manuscript are similar to the results of Multiscale-FDDA.

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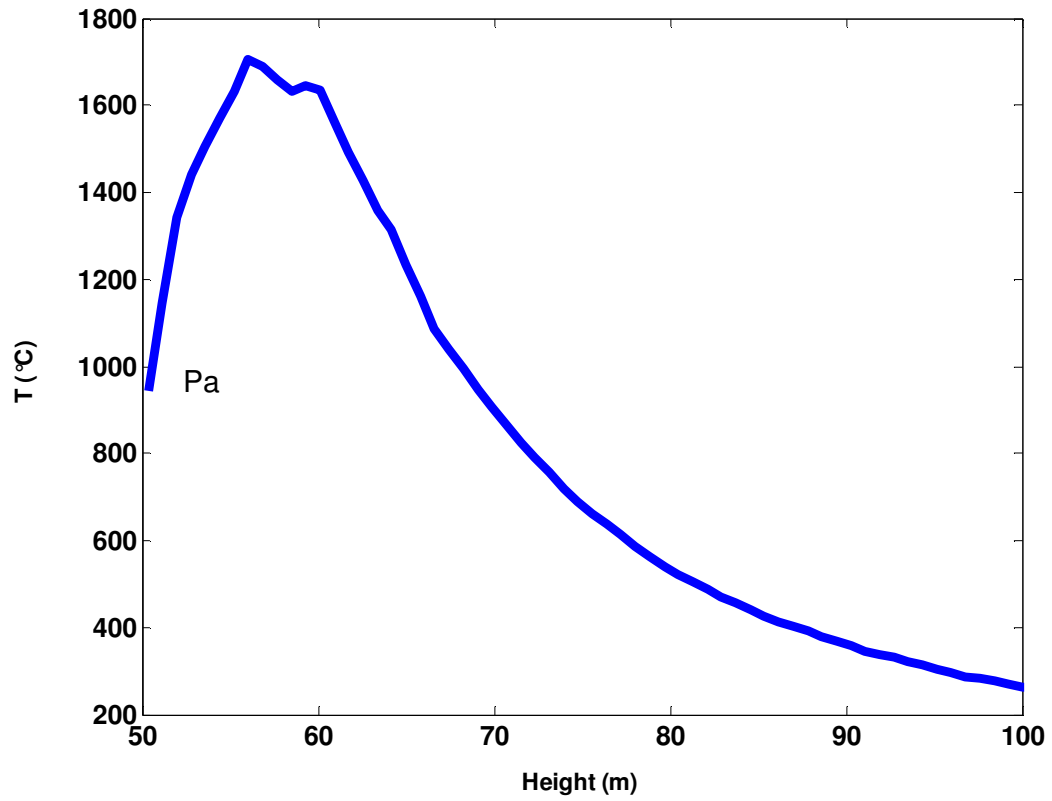
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2 Figure SM6. Vertical profile of maximum temperature along the plume centerline. Pa: top of
3 the flare stack.

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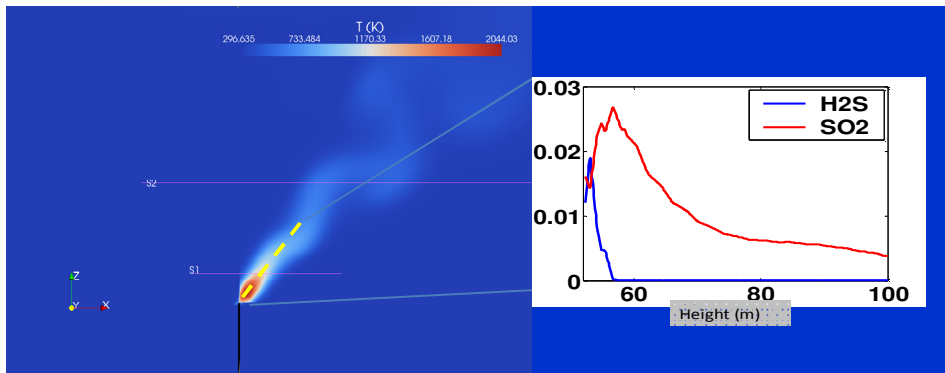
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4 Figure SM7. Vertical profiles of H2S and SO2 mass fraction concentration along the plume.
5 S1 and S2 are the over fire and far field slices. Dashed yellow line represents the plume center
6 line.