

## 1D Horizontal Model

First guess:  $c_0^p(x) = c_0(x)(1 + r(x)\alpha)$ ,  $r(x) \in (0, 1)$

Species	$\alpha$
O3	0.3
OH	2.0
NO	2.0
NO2	1.0
NO3	1.0
HO2	1.0
N2O5	2.0
HNO3	0.3
HONO	1.0
HCHO	1.0

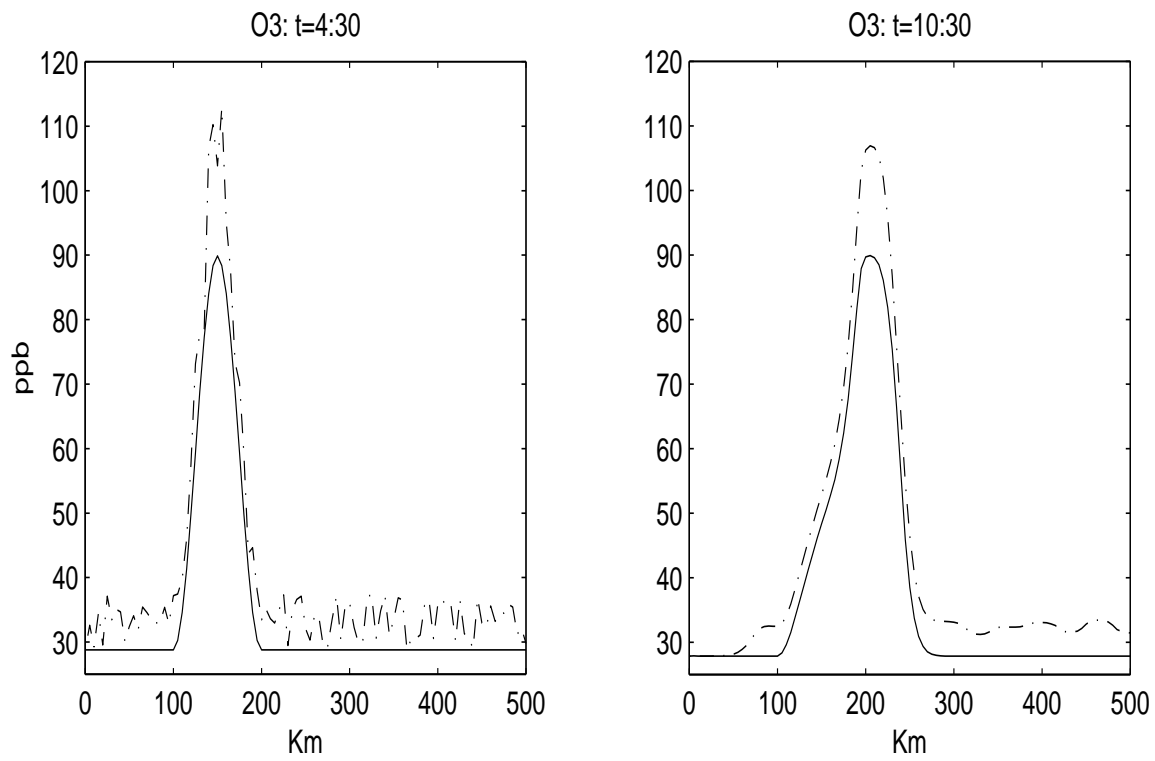


Figure 1: Initial (left) and final (right) distribution of the O<sub>3</sub> concentrations. Reference run with solid line, first guess run with dotted line.

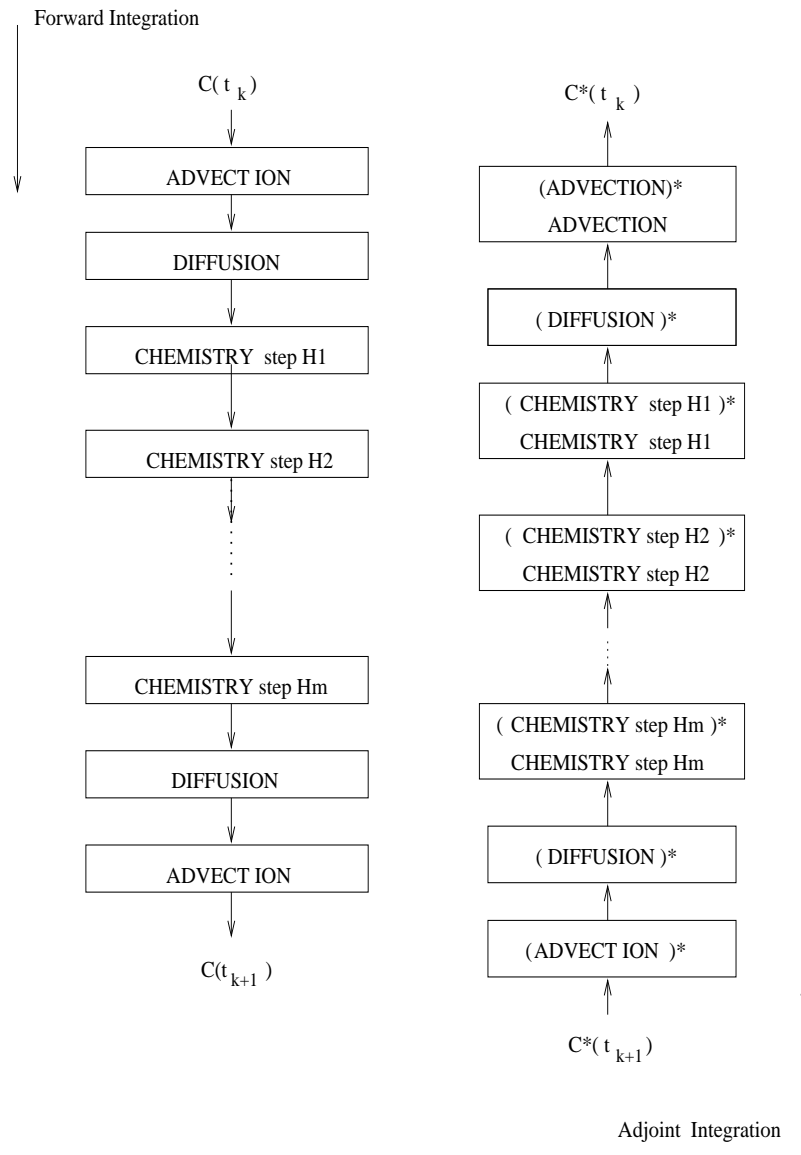


Figure 2: One step of operator splitting: concentrations are stored after each step during the forward integration and reloaded during the backward integration. Intermediate results inside a step need to be recomputed. At least 2-level checkpointing required for full model.

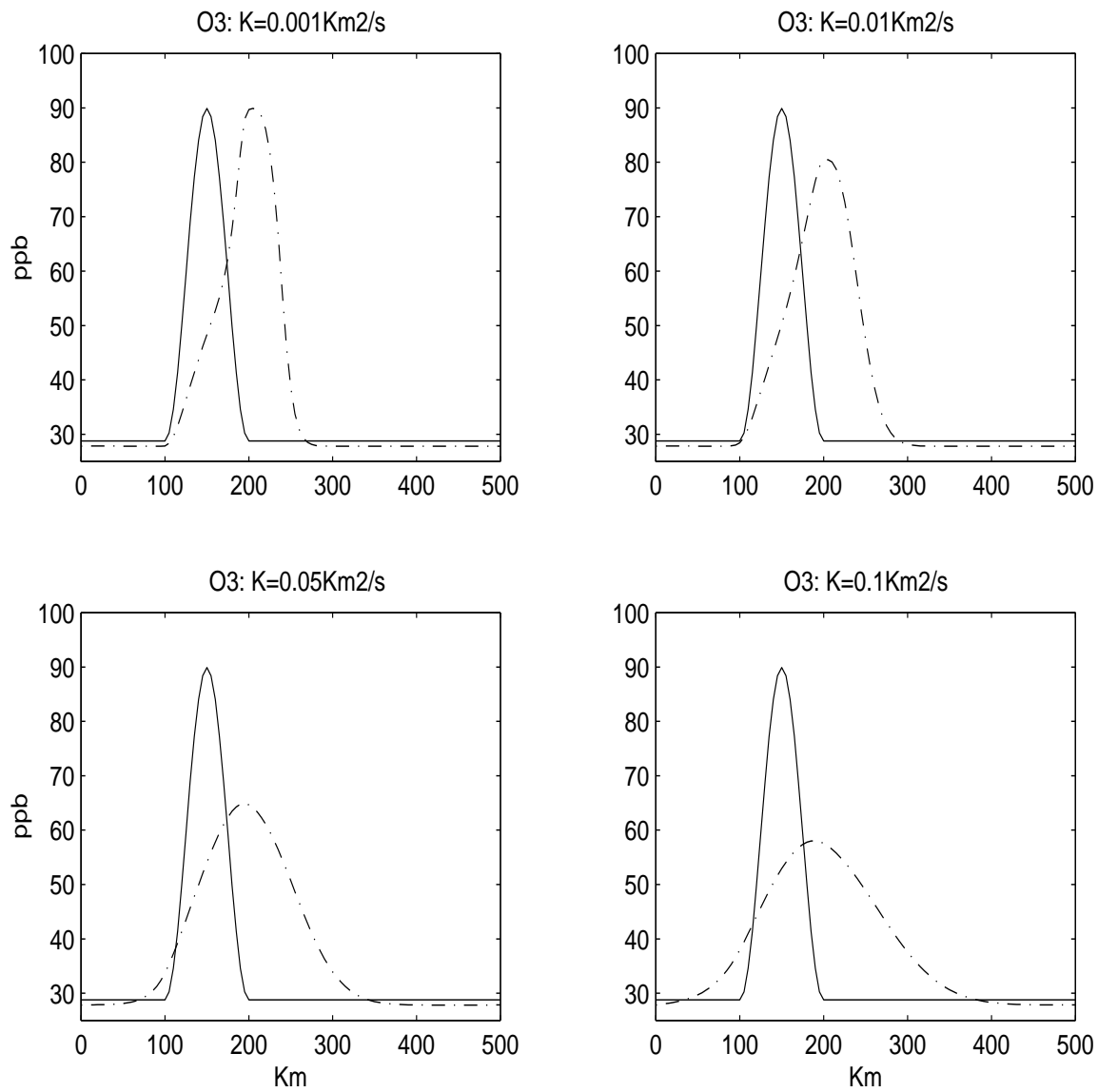


Figure 3: In order to check the stability of the W-method, the diffusion coefficient  $K$  is increased by a factor of 10, 50, 100;  $u=10\text{Km/h}$ , constant

## Performance of the optimization:

### Operator Splitting:

Run	No. iter.	$\sim$ time/iter (sec)	$\sim t(\mathcal{F} + \nabla\mathcal{F}) / t(\mathcal{F})$	$\mathcal{F}_{opt} / \mathcal{F}_{init}$
1.	43	7.5	3.8	9.9e-5
2.	23	7.9	3.8	9.8e-5
3.	16	7.8	3.8	9.1e-5

### W-Method:

Run	No. iter.	$\sim$ time/iter (sec)	$\sim t(\mathcal{F} + \nabla\mathcal{F}) / t(\mathcal{F})$	$\mathcal{F}_{opt} / \mathcal{F}_{init}$
1.	44	2.4	2.8	9.75e-5
2.	27	2.4	2.8	9.70e-5
3.	18	2.6	2.8	8.66e-5

Measurements are provided only for *O3* and *NO2* as follows:

- In Run 1 every 15 min. at all grid points
- In Run 2 every 15 min., 10 grid points apart (every 50 Km)
- In Run 3 every hour, 10 grid points apart.

## Qualitative Analysis

Species	$\alpha$	$\mathcal{F}_{init}^i$	$\mathcal{F}_{opt}^i / \mathcal{F}_{init}^i$		
			Run 1	Run 2	Run 3
O	0.0	32.0	9.7e-5	6.2e-3	7.1e-3
O3	0.3	27.5	1.6e-4	2.2e-3	3.1e-3
OH	2.0	25.7	1.0e-2	4.7e-2	5.2e-2
NO	2.0	68.1	1.7e-3	1.0e-1	1.2e-1
NO2	1.0	114	9.3e-5	7.6e-2	8.6e-2
NO3	1.0	200	7.0e-3	3.3e-2	3.6e-2
HO2	1.0	8.92	4.9e-1	6.4e-1	6.4e-1
N2O5	2.0	609	3.1e-3	5.1e-2	6.0e-2
HNO3	0.3	46.9	4.7e-1	5.0e-1	5.0e-1
HONO	1.0	147	2.6e-1	3.0e-1	3.1e-1
HCHO	1.0	104	6.4e-1	8.8e-1	9.0e-1

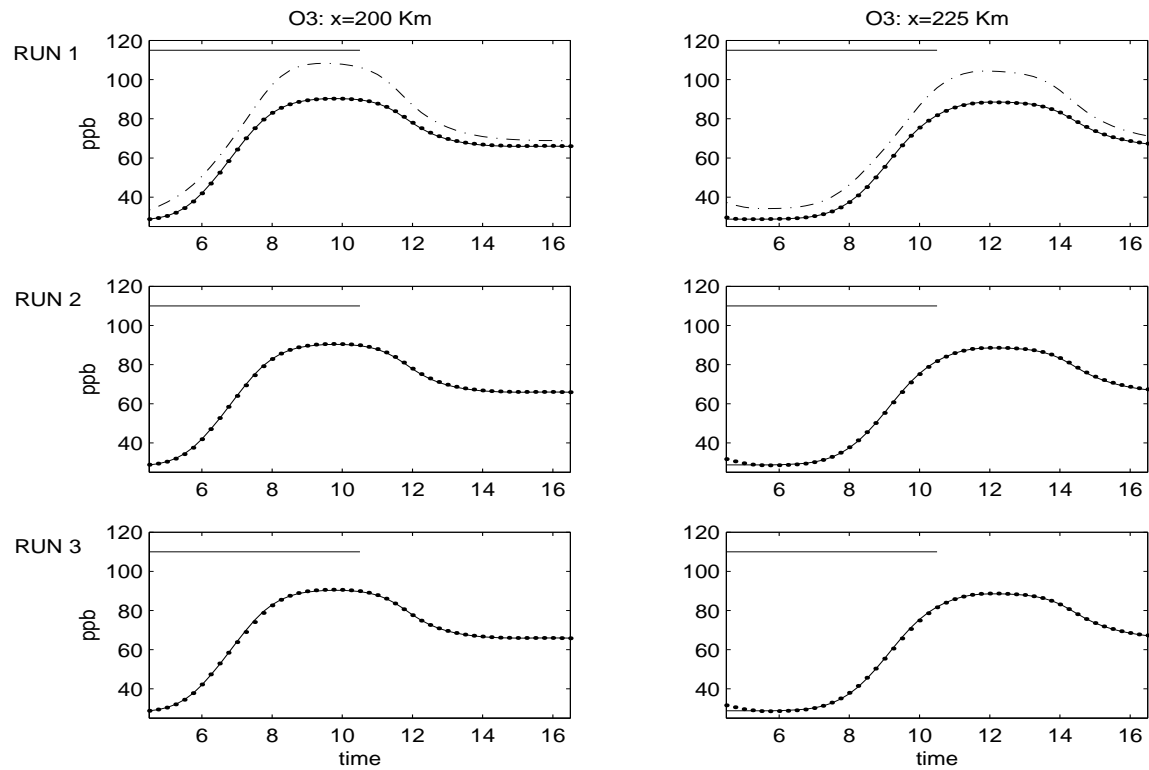


Figure 4: O3 at 200Km and 225Km. Assimilation takes place from 4:30 to 10:30. Reference run with solid line, initial guess run with dotted line, assimilation run with solid dots.

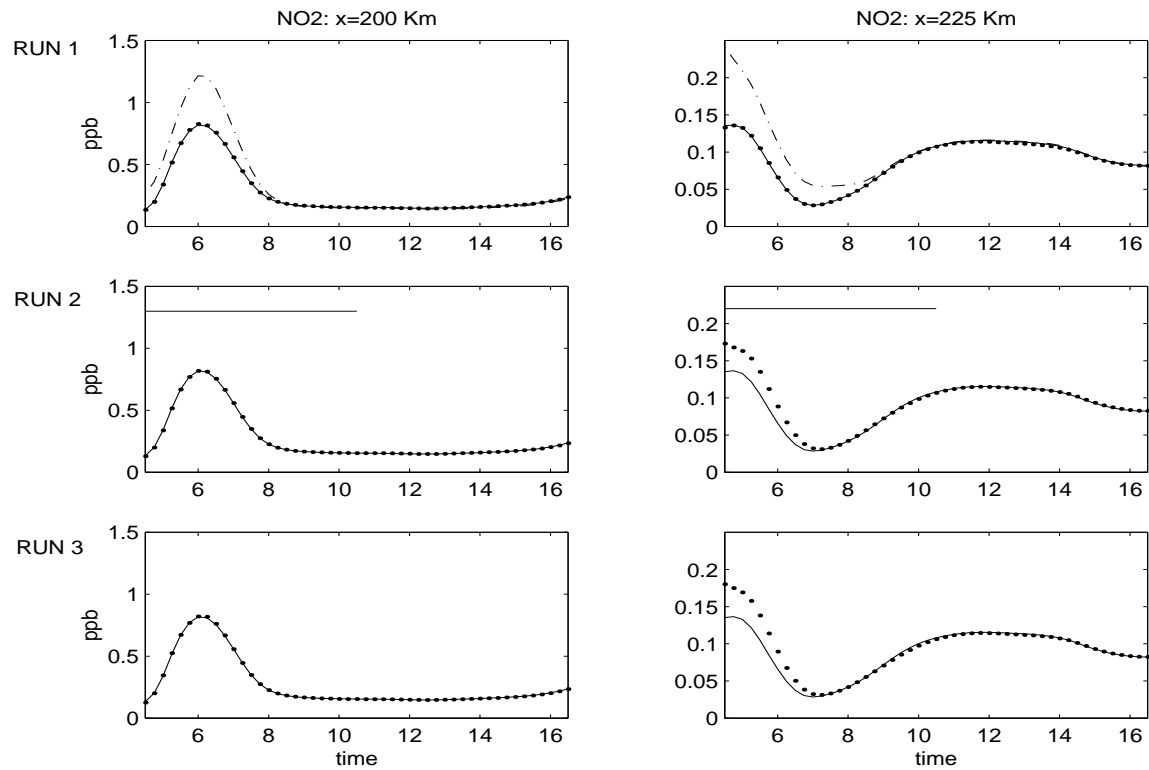


Figure 5: NO<sub>2</sub> at 200Km and 225Km. Assimilation takes place from 4:30 to 10:30. Reference run with solid line, initial guess run with dotted line, assimilation run with solid dots.

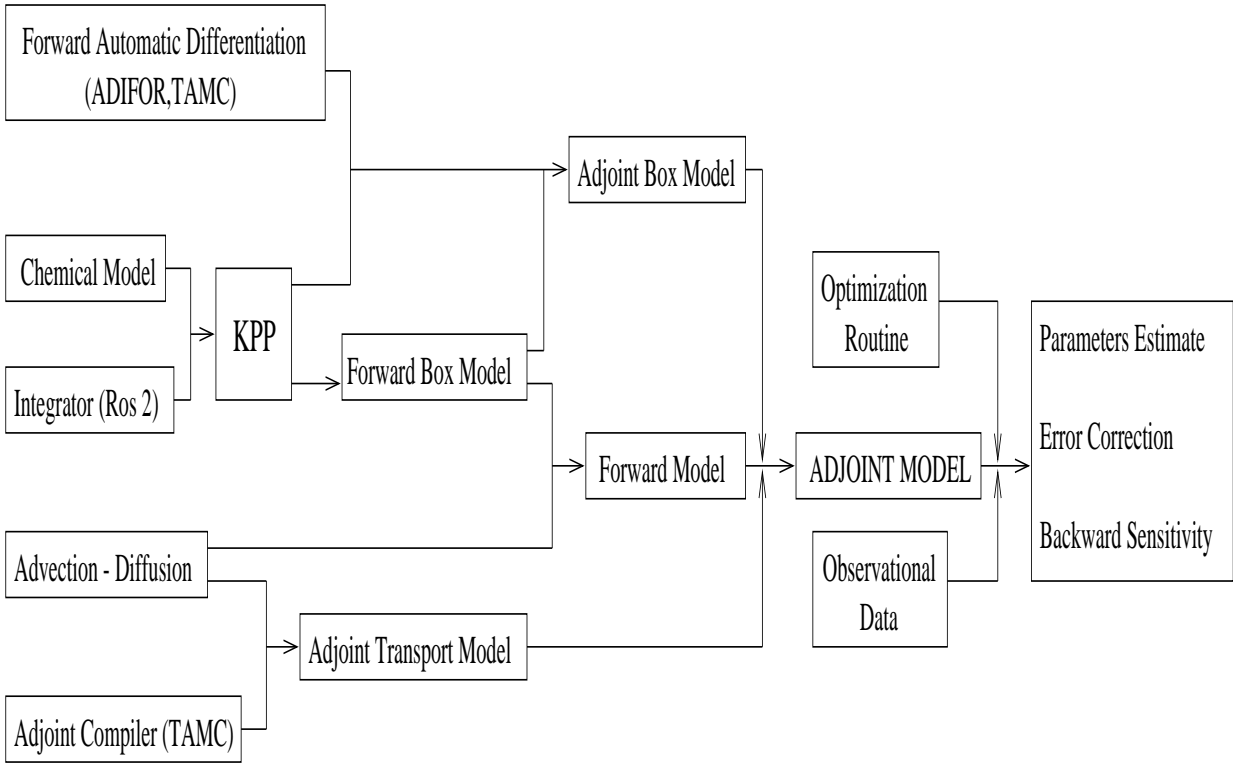


Figure 6: Implementation of the adjoint of a general transport-chemistry model in the KPP context applied to the 4D-var data assimilation.