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Supplement of

Quasi-Newton methods for atmospheric chemistry simulations: implementation in UKCA UM vn10.8

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1. Extended UKCA Box-Model analysis.

The following is a short discussion of the extra model scenarios carried out for the BOX-MODEL analysis: Rural, Marin and Strat. Equivalent figures to Figures 2 and 3 from the main paper are included for each of these scenarios. The Urban scenario proved to be the most challenging to solve, and have the largest errors, so is shown in the main paper. The QN methods proved to be robust and improved solving speed in all scenarios. However, the choice of what was the ideal iteration number to call the QN iterations varied from scenario to scenario. In the Urban scenario, calling the QN iteration after the first NR iteration often increased the number of iterations required to reach a stable solution, so was counter-productive. In the Rural, Marine and Strat runs, calling the QN method on the first iteration is generally effective at reducing the number of NR iterations required. However, given that the Urban cases were generally the most challenging to solve, the risk of calling the QN on the first iteration causing increase instability was considered to be great. In all scenarios, the QN2-3 experiment consistently improved over the CTNL run, so was the setup chosen to be used in the 3D model.

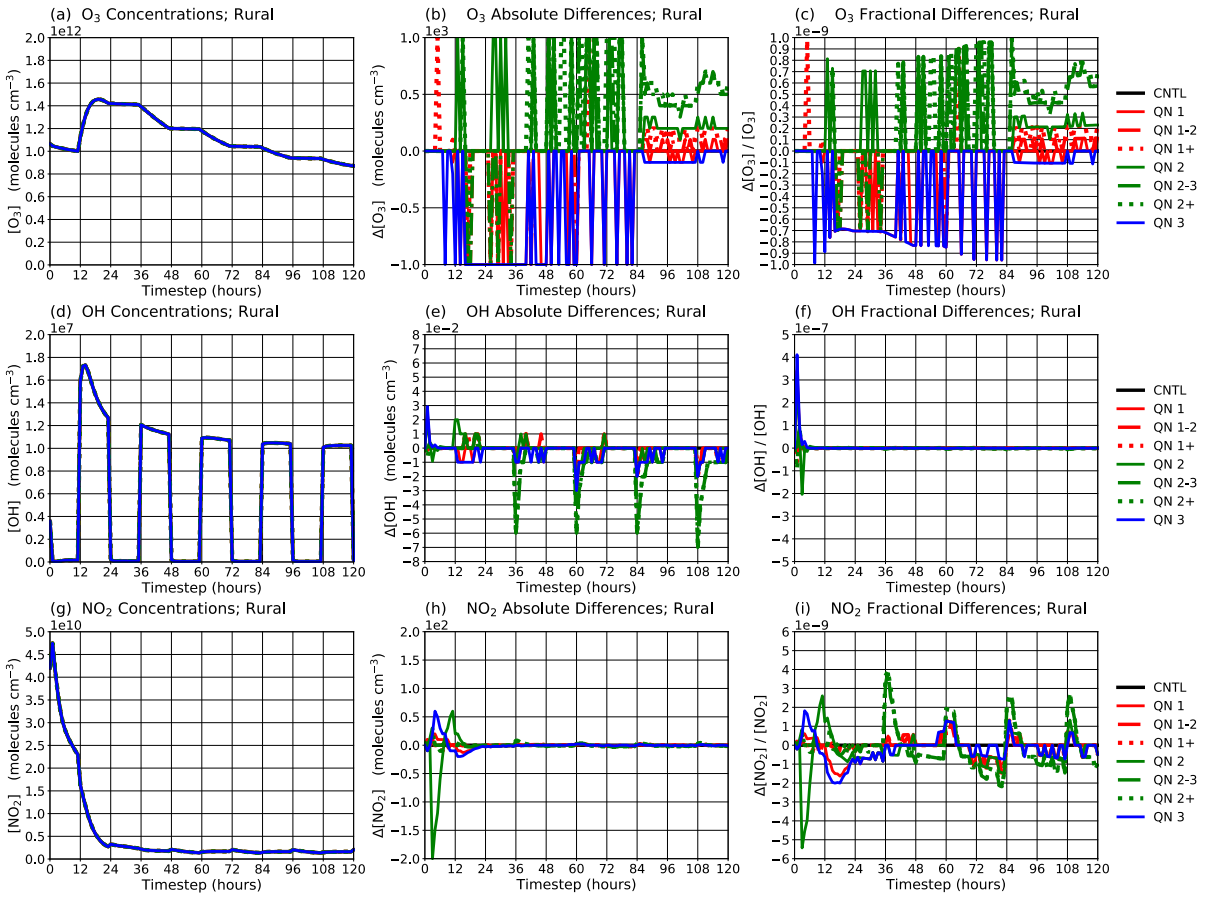

Figure S1. Same as Figure 2 in main paper, but for the Rural scenario

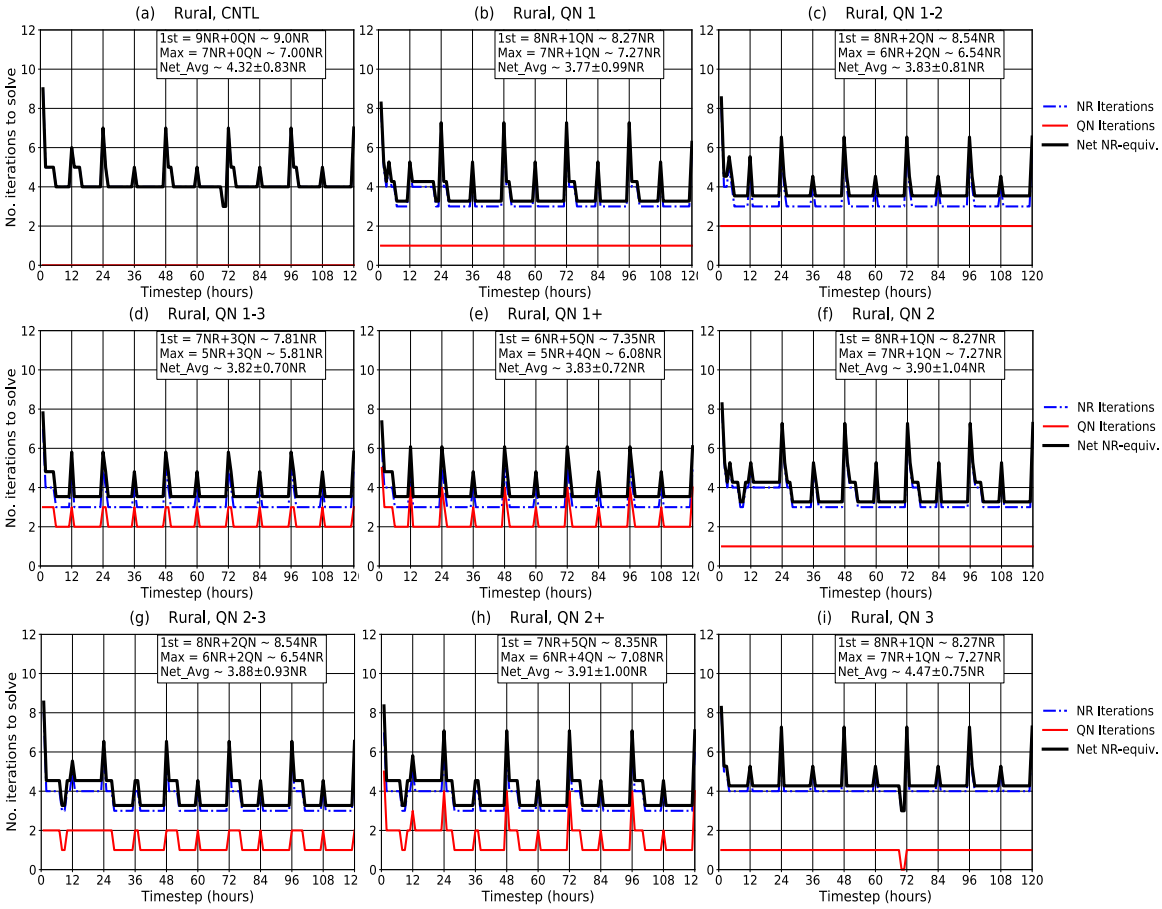

Figure S2. Same as Figure 3 in main paper, but for the Rural scenario

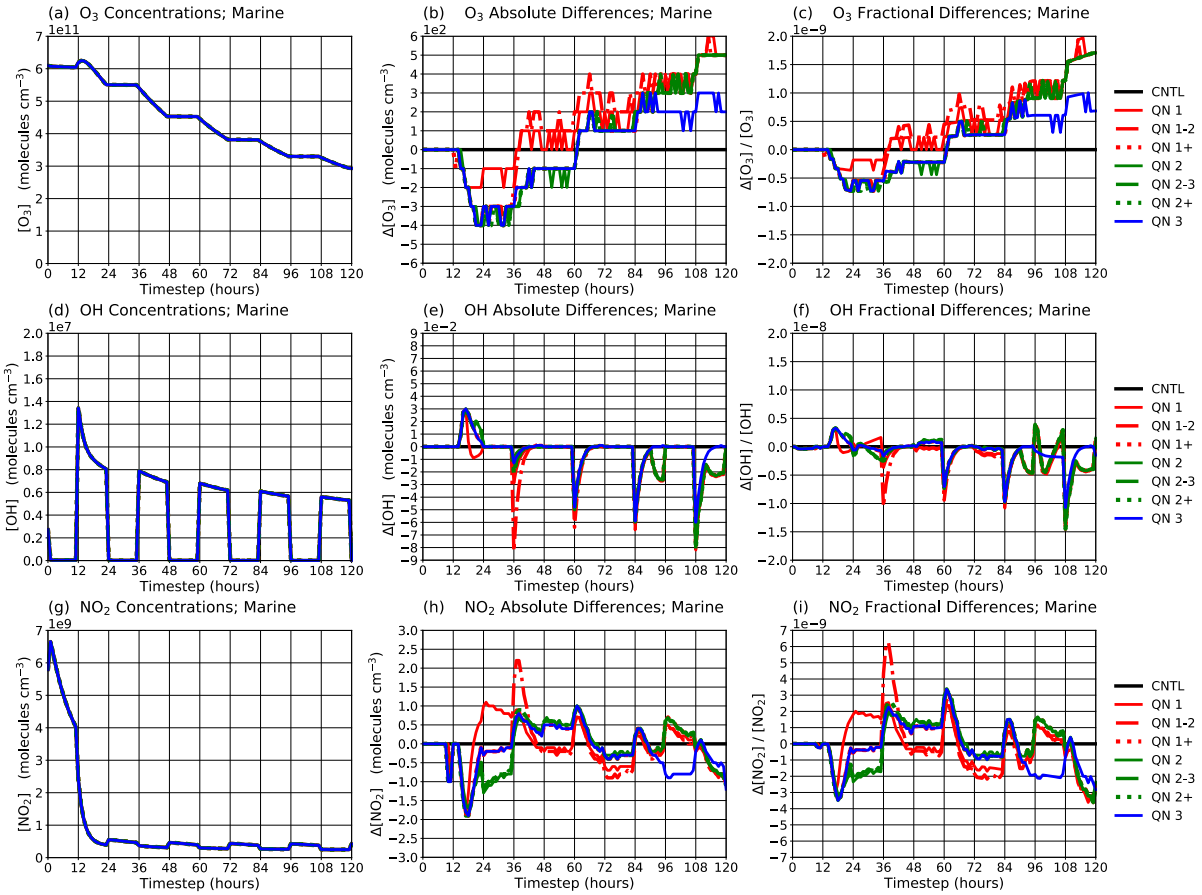

Figure S3. Same as Figure 2 in main paper, but for the Marine scenario

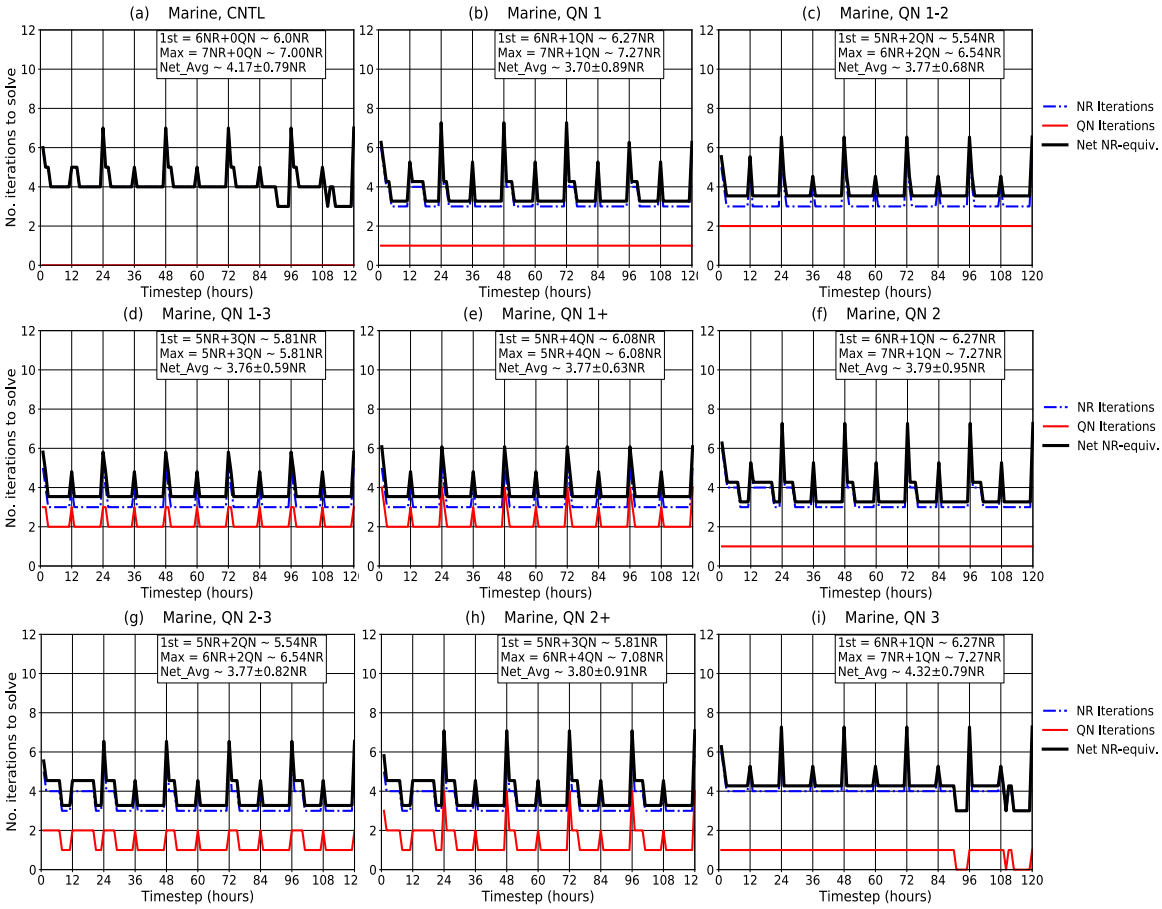

Figure S4. Same as Figure 3 in main paper, but for the Marine scenario

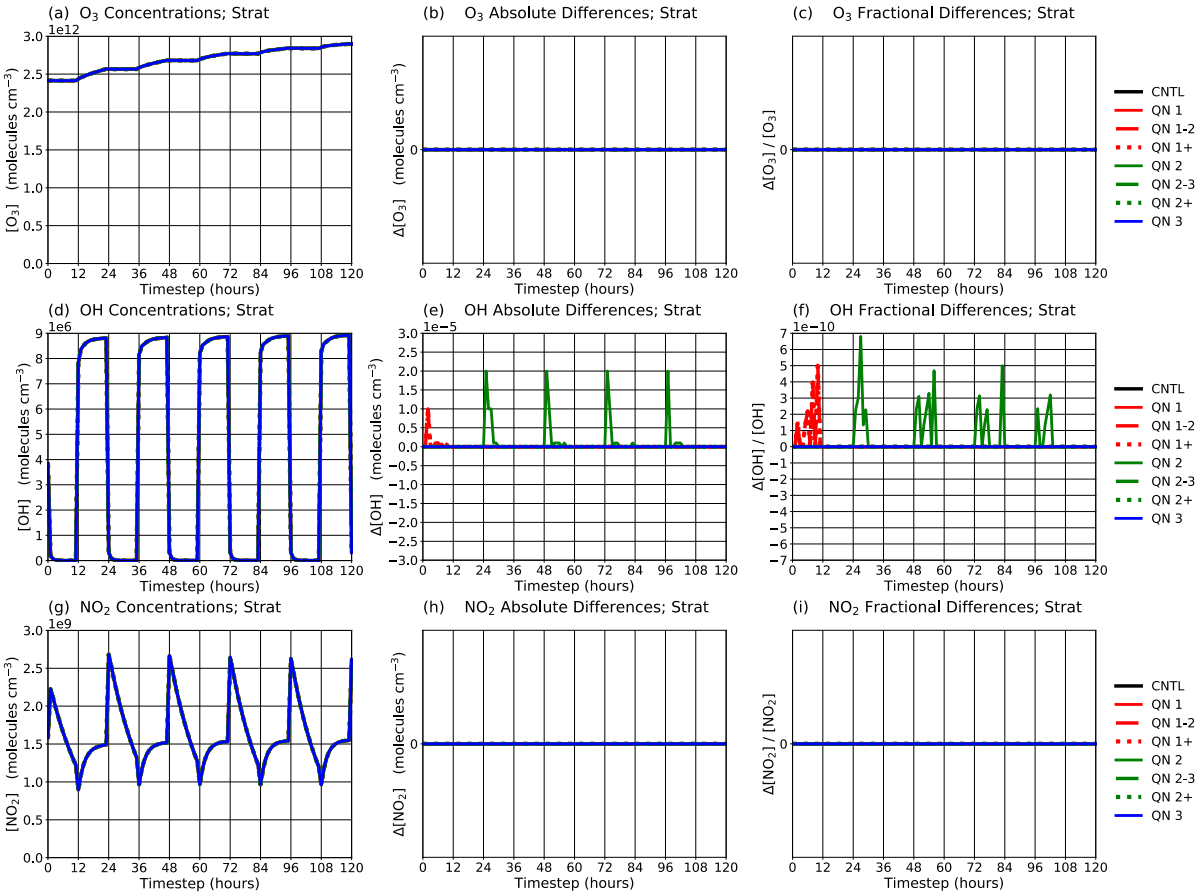

Figure S5. Same as Figure 2 in main paper, but for the Strat scenario

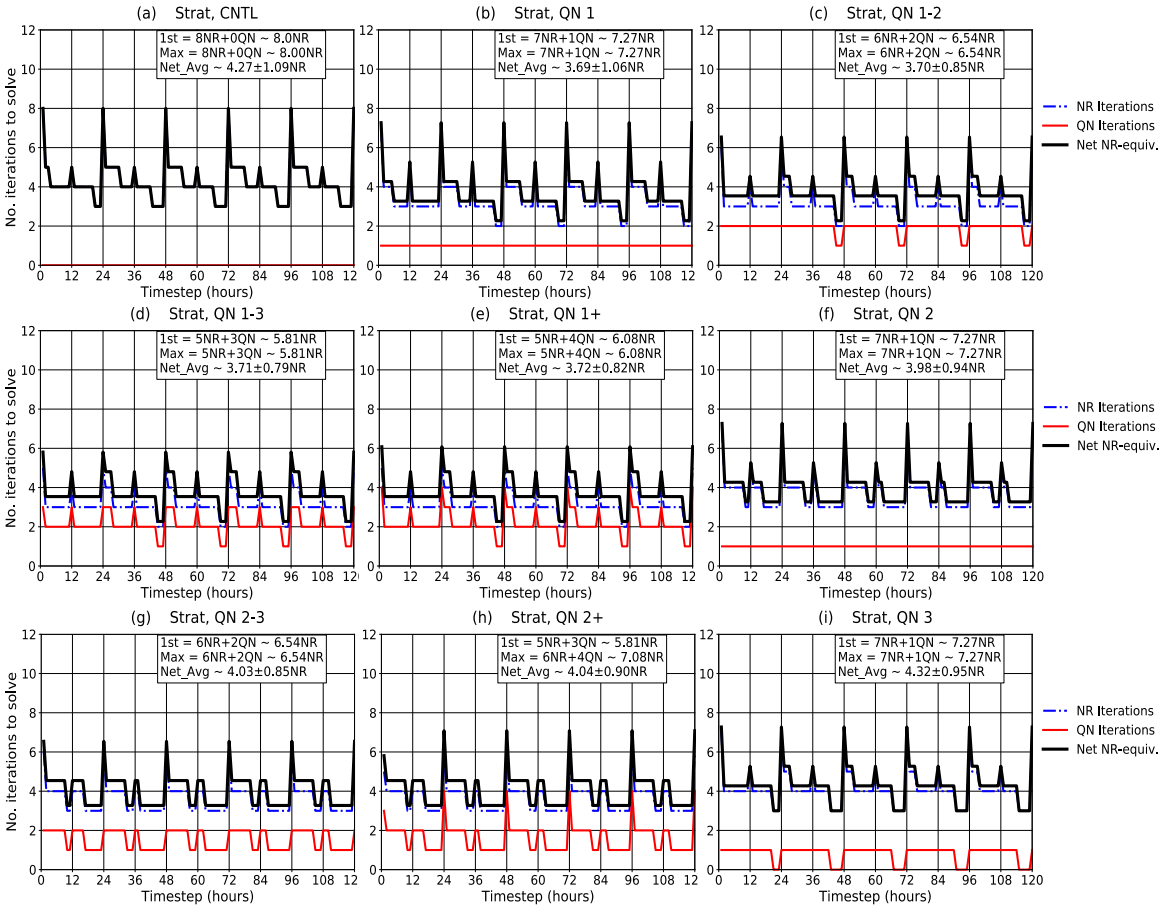

Figure S6. Same as Figure 3 in main paper, but for the Strat scenario

2. ADDITIONAL UM-UKCA PLOTS and ANALYSIS

a) QN Performance over 20-year run

The following plot gives a neat visual of the performance of the QN method for the 20-year run on 432 cores.

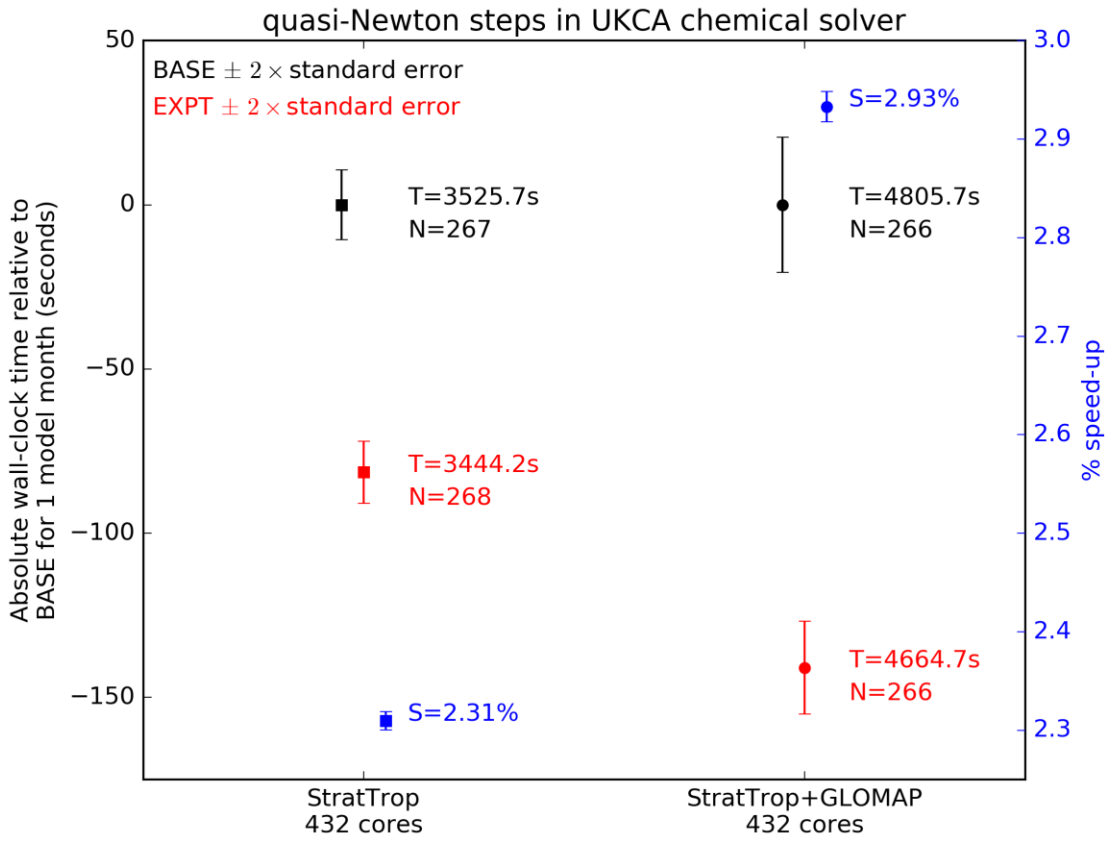

Figure S7. UM speed up for the StratTrop and StratTrop-GLOMAP modes with CNTL and QN implemented runs

b) Time Dependence of Differences Between Simulations and Bias

For the results to be reliable not only we need to show high accuracy (small difference) as demonstrated in the article but also that the differences between the modified and original simulations do not grow and stay bounded in time.

The first set of three plots (S8-S10) below show, for the OH, normalised absolute mean difference (NMAD), normalised root mean square difference (NRMSD) and normalised mean bias (NMB). The second set of three plots show the same quantities for the Ozone.

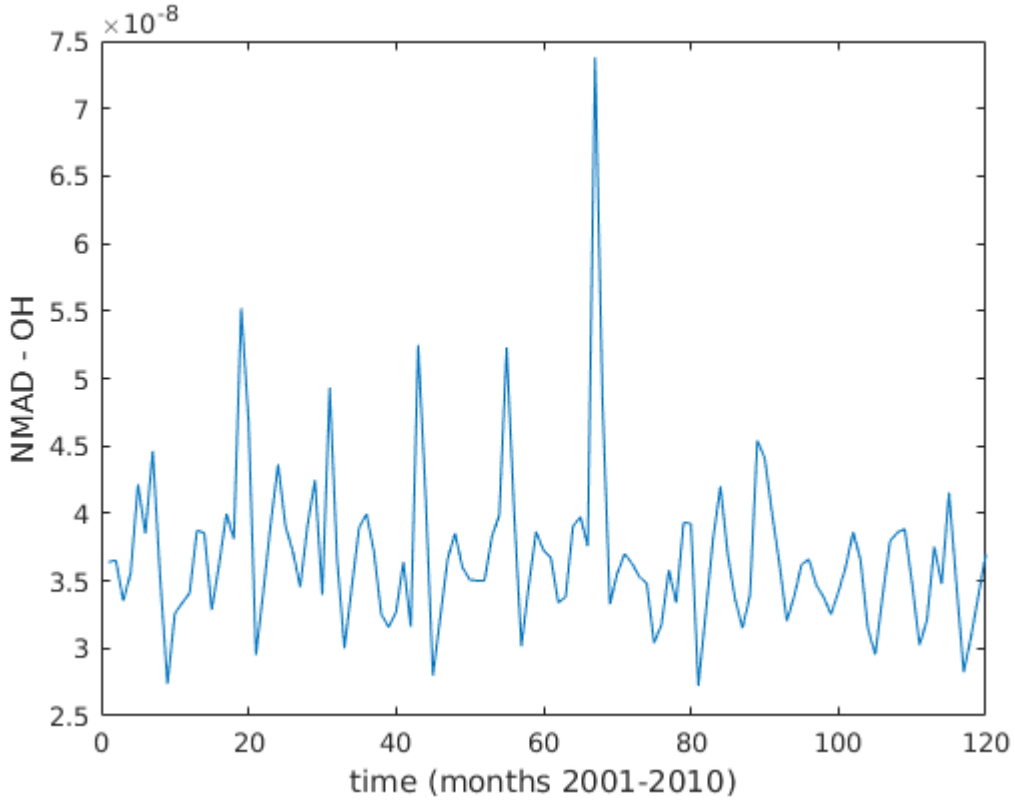

Figure S8. NMAD *for monthly averaged OH concentration for the StratTrop Run (Years 2001-2010).*

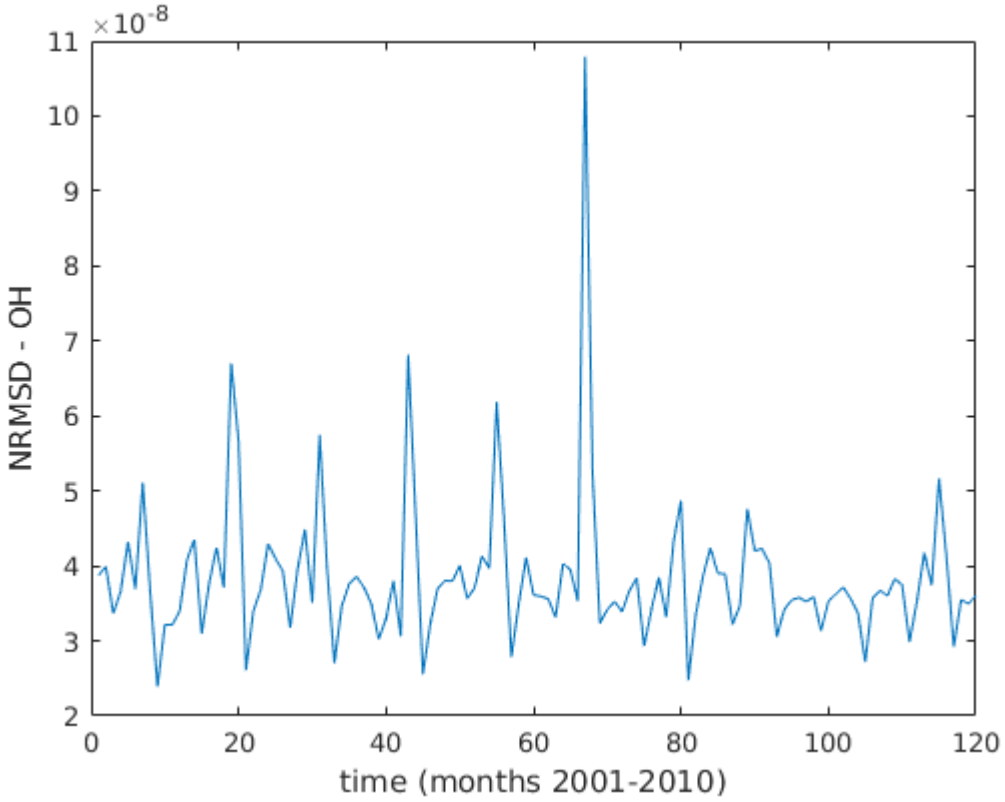

Figure S9. NRMSD for monthly averaged OH concentration for the StratTrop Run (Years 2001-2010).

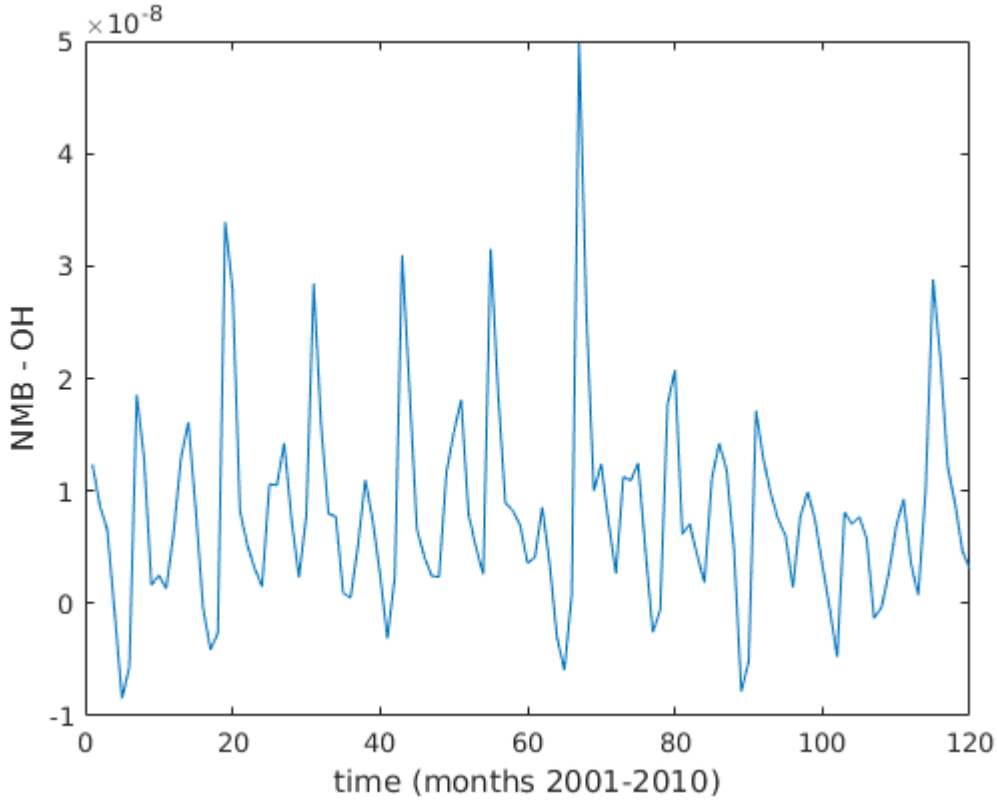

Figure S10. NMB for monthly averaged OH concentration for the StratTrop Run (Years 2001-2010).

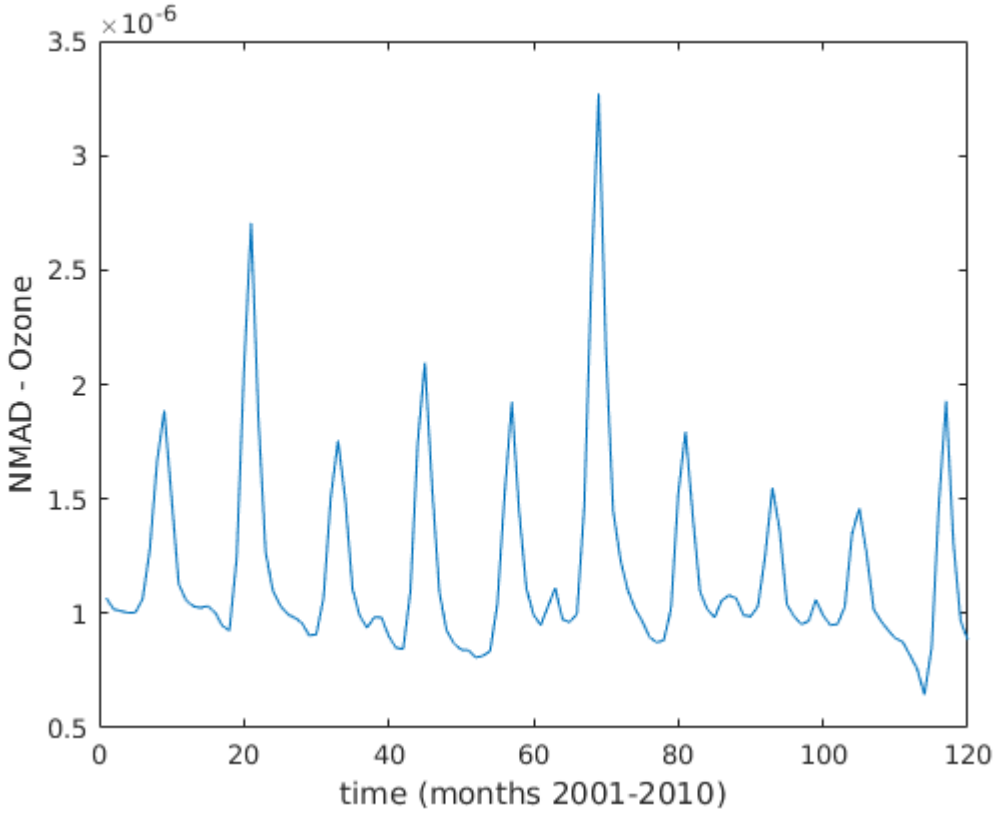

Figure S11. NMAD of monthly averaged Ozone concentration for the StratTrop Run (Years 2001-2010).

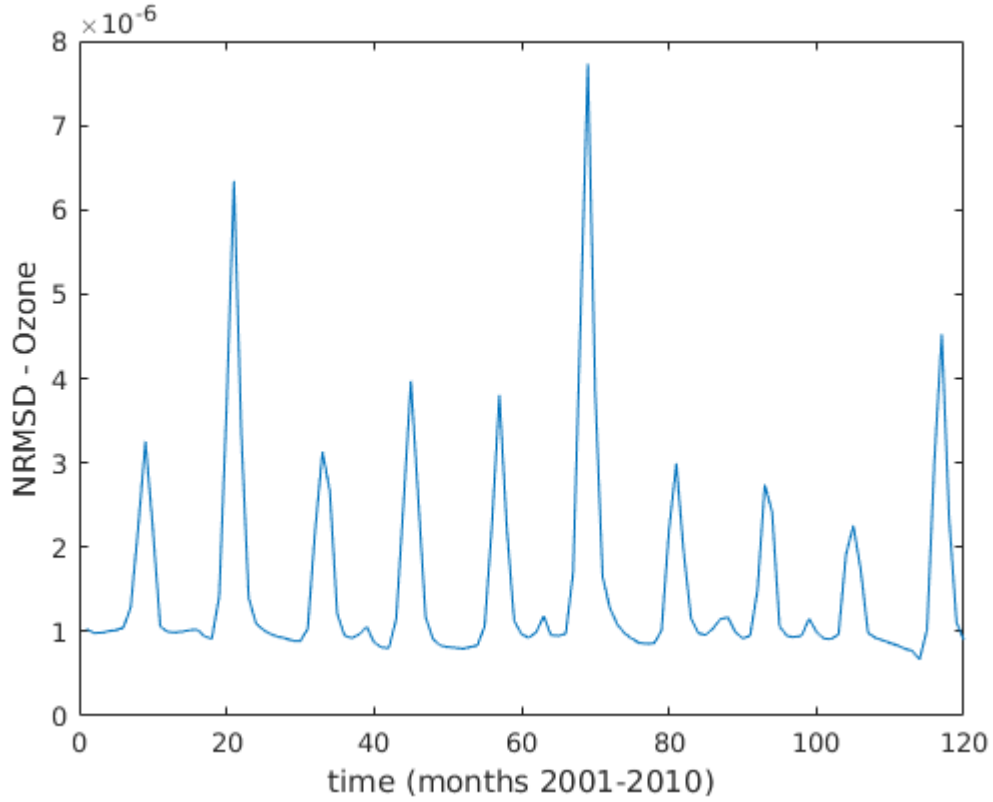

Figure S12. NRMSD of monthly averaged Ozone concentration for the StratTrop Run (Years 2001-2010).

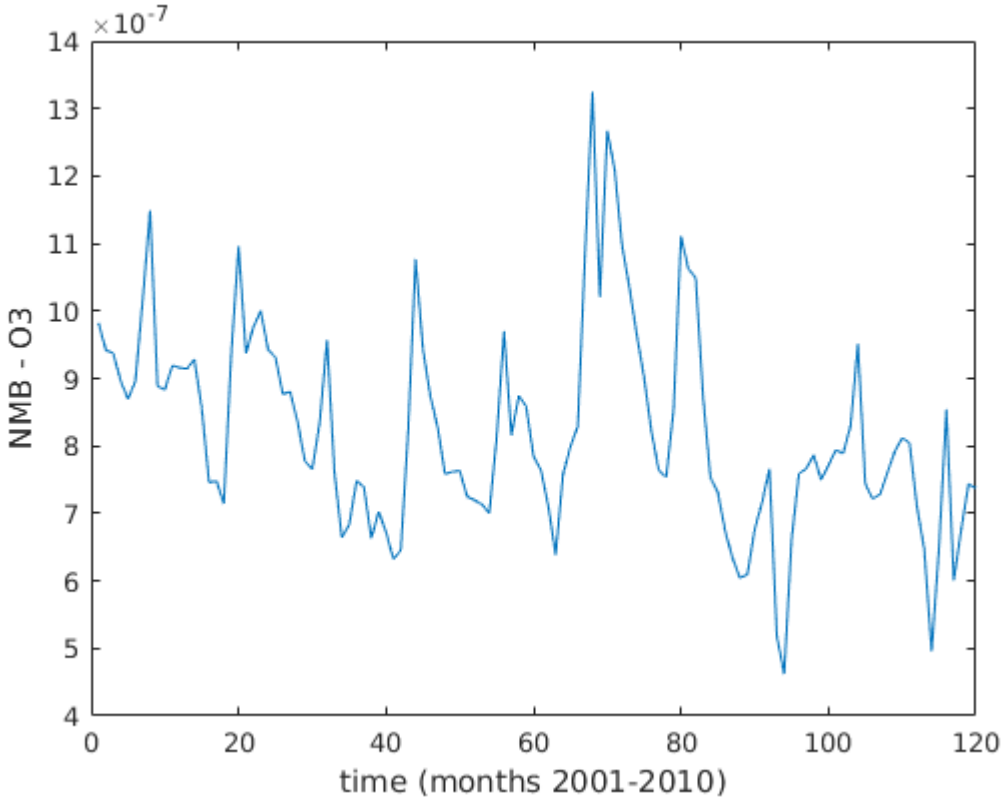

Figure S13. NMB of monthly averaged Ozone concentration for the StratTrop Run (Years 2001-2010).

c) NMAD, NRMSD and NMB Values for all Species

Below, we give a full table of NMAD, NRMSD and NMB values of all species for the UM-UKCA global model.

Species	**NMAD (*E-3) After 120 months**	**NMAD (*E-3) After 240 months**	**NRMSD (*E-3) After 120 months**	**NRMSD (*E-3) After 240 months**	**NMB (*E-3) After 120 months**	**NMB (*E-3) After 240 months**
O3	0.0011	0.00088	0.0010	0.00090	0.00098	0.00074
NO	0.0441	0.0340	0.0066	0.0077	-0.0032	-0.0020
NO3	0.0027	0.0040	0.0074	0.0170	-0.0011	-0.0021
N2O5	0.0045	0.0027	0.0052	0.0074	-0.0037	-0.0016
HO2NO2	0.0053	0.0059	0.0079	0.0086	-0.0013	-0.0015
HNO3	0.0066	0.0058	0.0074	0.0116	-0.0046	-0.0025
H2O2	0.0150	0.0172	0.0332	0.0423	-0.0135	-0.0158
CH4	0.0003	0.0003	0.0004	0.0004	0.0003	0.0003
CO	0.0024	0.0025	0.0019	0.0020	0.0017	0.0017
HCHO	0.0089	0.0101	0.0276	0.0343	-0.0033	-0.0050
CH3OOH	0.0089	0.0105	0.0180	0.0220	-0.0049	-0.0064
HONO	0.0206	0.0204	0.1723	0.2035	0.0017	0.0040
C2H6	0.0118	0.0137	0.0098	0.0129	0.0118	0.0136
C2H5OOH	0.0156	0.1939	0.0186	0.0279	0.0085	0.0111
CH3CHO	0.0098	0.0012	0.0010	0.0013	0.0056	0.0067
PAN	0.0115	0.0153	0.0319	0.0530	-0.0011	-0.0006
C3H8	0.0092	0.0127	0.0071	0.0140	0.0089	0.0123
n-C3H7OOH	0.0140	0.0225	0.0189	0.0412	0.0103	0.0180
i-C3H7OOH	0.0152	0.0237	0.0198	0.0412	0.0103	0.0180
C2H5CHO	0.0093	0.0134	0.0408	0.0373	0.0072	0.0101
C2H6CO	0.00933	0.01099	0.00783	0.00959	0.00926	0.01086
CH3COCH2OOH	0.01394	0.01660	0.01950	0.02661	0.00301	0.00494
PPAN	0.01001	0.01193	0.03702	0.06292	-0.00931	-0.01031

CH3ONO2	0.01053	0.01355	0.01481	0.01974	-0.00932	-0.01286
C5H8	0.02416	0.02421	0.02180	0.02464	0.01083	0.01182
ISOOH	0.02798	0.02933	0.03170	0.03713	0.01167	0.01110
ISON	0.03209	0.04159	0.06750	0.10933	0.00375	0.01014
MACR	0.02345	0.02557	0.02783	0.03507	0.01884	0.01998
MACROOH	0.04468	0.05189	0.05149	0.07872	0.02563	0.03051
MPAN	0.03073	0.03666	0.04900	0.06991	-0.00697	-0.00842
HACET	0.02630	0.03193	0.03694	0.05458	-0.00538	-0.00461
MGLY	0.14927	0.18045	0.41070	0.63219	-0.14196	-0.17186
NALD	0.04737	0.06276	0.10608	0.17306	0.02292	0.04034
HCOOH	0.01836	0.02537	0.02768	0.04264	-0.00854	-0.00811
CH3CO3H	0.02581	0.03148	0.03700	0.05843	0.01038	0.01493
CH3CO2H	0.02374	0.02903	0.03652	0.05757	-0.00118	0.00231
MVKOOH	0.02997	0.03284	0.05591	0.06614	0.00713	0.00526
Cl	0.00069	0.00035	0.00090	0.00036	-0.00069	-0.00020
ClO	0.00245	0.00247	0.00738	0.00731	0.00015	0.00064
Cl2O2	0.09651	0.05123	0.28837	0.05308	0.00543	0.02153
OClO	0.01277	0.01082	0.01654	0.01336	0.00894	0.00849
Br	0.00051	0.00056	0.00048	0.00065	-0.00029	-0.00023
BrCl	0.01104	0.00941	0.01503	0.01262	0.00771	0.00731
BrONO2	0.00471	0.00439	0.00757	0.00754	-0.00234	-0.00186
N2O	0.00004	0.00003	0.00008	0.00005	0.00004	0.00003
HOCl	0.00639	0.00587	0.01665	0.01657	0.00087	0.00045
HBr	0.008348	0.00908	0.01627	0.015961	-0.00754	-0.0083
HOBr	0.006061	0.00595	0.011883	0.012055	0.00258	0.00168
ClONO2	0.001965	0.00217	0.00272	0.0031523	-8E-05	0.00043
CFCl3	4.35E-05	3.9E-05	8.4E-05	7.53E-05	4.3E-05	3.8E-05
CF2Cl2	3.54E-05	2.7E-05	7E-05	5.03E-05	3.3E-05	2.5E-05
CH3Br	0.00044	0.00047	0.00052	0.00055	0.00044	0.00047
N	0.000798	0.00403	0.0006	0.004242	-0.00077	-0.0027
O(3P)	2.66E-05	1.3E-05	4.6E-05	3.19E-05	-1.9E-05	-5E-06
ORGNIT	0.056804	0.06181	0.08377	0.107436	0.03981	0.04092

H	8.77E-06	5.4E-06	2.7E-05	1.99E-05	8.8E-06	2.2E-06
OH	3.64E-05	3.7E-05	3.9E-05	3.6E-05	1.2E-05	3E-06
HO2	0.001041	0.00108	0.00109	0.001262	0.0003	0.00023
CH3OO	0.00291	0.00492	0.00214	0.003857	0.0025	0.00375
C2H5OO	0.056128	0.0569	0.16649	0.16476	0.04521	0.04526
CH3CO3	0.051005	0.05548	0.21106	0.274743	-0.02183	-0.0224
n-C3H7OO	0.076912	0.08898	0.2034	0.272403	0.07119	0.08267
i-C3H7OO	0.070862	0.08225	0.19265	0.258701	0.06177	0.07211
C2H5CO3	0.032232	0.04066	0.11543	0.191884	-0.01635	-0.0173
CH3COCH2OO	0.043401	0.04446	0.11144	0.119976	0.01727	0.0185
CH3OH	0.005674	0.00593	0.007	0.009182	-0.00167	-0.003
HCl	0.000445	0.00049	0.00135	0.001333	-8.3E-05	-0.0001
BrO	0.001422	0.00155	0.00471	0.004844	-0.00062	-0.0006
NO2	0.004671	0.00346	0.00718	0.012697	-0.00346	-0.002
O(1D)	2.69E-05	1.8E-05	3.2E-05	2.43E-05	1.2E-05	1.1E-05