Supplement of Atmos. Chem. Phys., 15, 2139–2158, 2015
http://www.atmos-chem-phys.net/15/2139/2015/
doi:10.5194/acp-15-2139-2015-supplement

Atmospheric Chemistry and Physics Open Access

Supplement of

Receptor modelling of fine particles in southern England using CMB including comparison with AMS-PMF factors

J. Yin et al.

Correspondence to: R. M. Harrison (r.m.harrison@bham.ac.uk)

Table S1. Listof all organic markers analysed

n-Alkanes	Abbreviation	***Hopanes***	Abbreviation	***PAHs***	Abbreviation
n-Tetracosane	C24	17α(H)-22,29,30-Trisnorhopane	17αTNohop	Benzo[k]fluoranthene	B[k]F
n-Pentacosane	C25	17α(H),21β(H)-Hopane	17αβHop	Benzo[b]fluoranthene	B[b]F
n-Hexacosane	C26	17β(H),21α(H)-30-norhopane	17βαNohop	Benzo[e]pyrene	B[e]P
n-Heptacosane	C27	22S-17α(H),21β(H)-30-Homohopane	22SαβHH	Benzo[a]pyrene	B[a]P
n-Octacosane	C28	22R-17α(H),21β(H)-30-Homohopane	22RαβHH	Perylene	PER
n-Nonacosane	C29	22S-17α(H),21β(H)-30-Bishomohopane	22SαβBHH	Indeno[1,2,3-cd]pyrene	IP
n-Triacontane	C30	22R-17α(H),21β(H)-30-Bishomohopane	22RαβBHH	Dibenz[a,h]anthracene	D[ah]A
n-Hentriacontane	C31	22S-17α(H),21β(H)-30,31,32-trishomohopane	22SαβTHH	Benzo[ghi]perylene	B[ghi]PER
n-Dotriacontane	C32	22R-17α(H),21β(H)-30,31,32-trishomohopane	22RαβTHH	Coronene	COR
n-Tritriacontane	C33	***Fatty acids***		Picene	PIC
n-Tetratriacontane	C34	Tetradecanoic acid/Myristic acid (C14)	MyrA	***Secondary markers***	
n-Pentatriacontane	C35	Pentadecanoic acid/Pentadecylic acid (C15)	PentA	Pinonic acid	PinoA
Sterols		Hexadecanoic acid/Palmitic acid (C16)	PalmA	Pinic acid	PinicA
Levoglucosan	Levo	Octadecanoic acid/Stearic acid (C18)	SteaA	2-methylthreitol	MethT
Cholesterol	Chol	9-octadecenoic acid/Oleic acid (C18:1)	OleiA	2-methylerythritol	MethE
		9,12-octadecadienoic acid/Linoleic acid (C18:2)	LinoA		

Table S2. Precision (%) and method detection limit (MDL)(ng m^{-3}) for the target compounds

n-Alkanes	Precision	MDL	***Hopanes***	Precision	MDL	***PAHs***	Precision	MDL
C24	5.1	0.027	17aTNohop	4.7	0.010	B[b]F	6.2	0.015
C25	4.4	0.041	17abNohop	5.1	0.011	B[k]F	4.3	0.017
C26	7.1	0.055	17baNohop	3.4	0.017	B[e]P	5.3	0.019
C27	5.7	0.026	17abHop	5.5	0.014	B[a]P	4.9	0.014
C28	10.8	0.019	22SabHH	4.3	0.015	PER	5.8	0.010
C29	13.4	0.048	22RabHH	4.4	0.018	IP	8.9	0.008
C30	10.7	0.066	22SabBHH	5.1	0.016	D[ah]A	6.6	0.011
C31	8.1	0.034	22RabBHH	5.7	0.047	PIC	15.0	0.025
C32	8.8	0.044	22SabTHH	5.2	0.014	B[ghi]PER	7.5	0.017
C33	15.9	0.034	22RabTHH	6.3	0.035	COR	3.2	0.016
C34	3.3	0.015	***Fatty acids***					
C35	7.5	0.054	MA	11.9	0.57			
Sterols			PentA	8.8	0.23	***Secondary Markers***		
Levo	15.4	0.23	PA	20.4	2.1	PinoA	15.7	0.37
Chol	5.6	0.024	LOA	6.8	0.097	PinicA	8.1	0.19
			OA	9.2	0.31	MethT	5.9	0.035
			SA	19.2	1.3	MethE	7.4	0.10

Table S3. Dependence of mean mass of PMF factors upon value of fpeak=0

Factor / fPeak value	OOA Mean mass	SFOA1 Mean mass	SFOA2 Mean mass	COA Mean mass	HOA Mean mass
-0.6	0.897374	0.757835	0.882626	1.02376	0.68164
0	0.933063	0.747544	0.857564	0.875335	0.829156
1	0.940803	0.696752	0.776001	0.682512	1.14724

Table S4: Source contribution estimates (SCE) (μg m^{-3}) and standard deviation (S.D.) for fine particulate OC and $PM_{2.5}$at NK and HAR from the CMB model (averaged from daily CMB outputs)

		OC			$PM_{2.5}$			$OC/PM_{2.5}$ or
Source Name		**NK[a]**	**NK[b]**	**HAR[a]**	**NK[a]**	**NK[b]**	**HAR[a]**	**OC/OM CF[c]**
Vegetation	*SCE*	0.069	0.069	0.11	0.21	0.21	0.35	0.324
	S.D.	0.010	0.010	0.015	0.030	0.030	0.048	-
Woodsmoke	*SCE*	0.53	0.53	0.64	0.64	0.64	0.77	0.836
	S.D.	0.11	0.11	0.14	0.14	0.14	0.16	-
Natural Gas	*SCE*	0.046	0.046	0.042	0.054	0.054	0.050	0.849
	S.D.	0.009	0.009	0.007	0.011	0.011	0.008	-
Dust/Soil	*SCE*	0.049	0.049	***0.018***	0.38	0.38	***0.14***	0.131
	S.D.	0.037	0.037	0.015	0.29	0.29	0.11	0.0133
Coal	*SCE*	0.075	0.075	0.041	0.17	0.17	0.094	0.432
	S.D.	0.020	0.020	0.009	0.046	0.046	0.021	0.0834
Food Cooking	*SCE*	0.32	0.32	0.070	0.56	0.56	0.12	0.566
	S.D.	0.055	0.055	0.013	0.10	0.10	0.023	0.030
Total Traffic	*SCE*	0.81	0.81	0.35	1.40	1.40	0.59	0.579
	S.D.	0.39	0.39	0.16	0.88	0.88	0.29	0.051
Biogenic Secondary	*SCE*	-	0.90	-	-	1.63	-	0.556
	S.D.	-	0.17	-	-	0.31	-	-
Other OC/OM	*SCE*	1.62	0.72	1.03	2.92	1.29	1.85	0.556
	S.D.	-	-	-	-	-	-	-
Sea Salt	*SCE*	-	-	-	1.1	1.1	0.82	-
	S.D.	-	-	-	0.020	0.020	0.020	-
Ammonium Sulphate	*SCE*	-	-	-	2.2	2.2	2.1	-
	S.D.	-	-	-	0.028	0.028	0.028	-
Ammonium Nitrate	*SCE*	-	-	-	5.8	5.8	4.1	-
	S.D.	-	-	-	0.072	0.072	0.072	-
Measured $OC/PM_{2.5}$	*Mass*	3.5	3.5	2.3	15.7	15.7	11.0	-

Note: Figures in bold were not statistically different from zero; *a* - Modelled without biogenic secondary source profile; *b* – Modelled with biogenic secondary source profile; *c* – Conversion factor

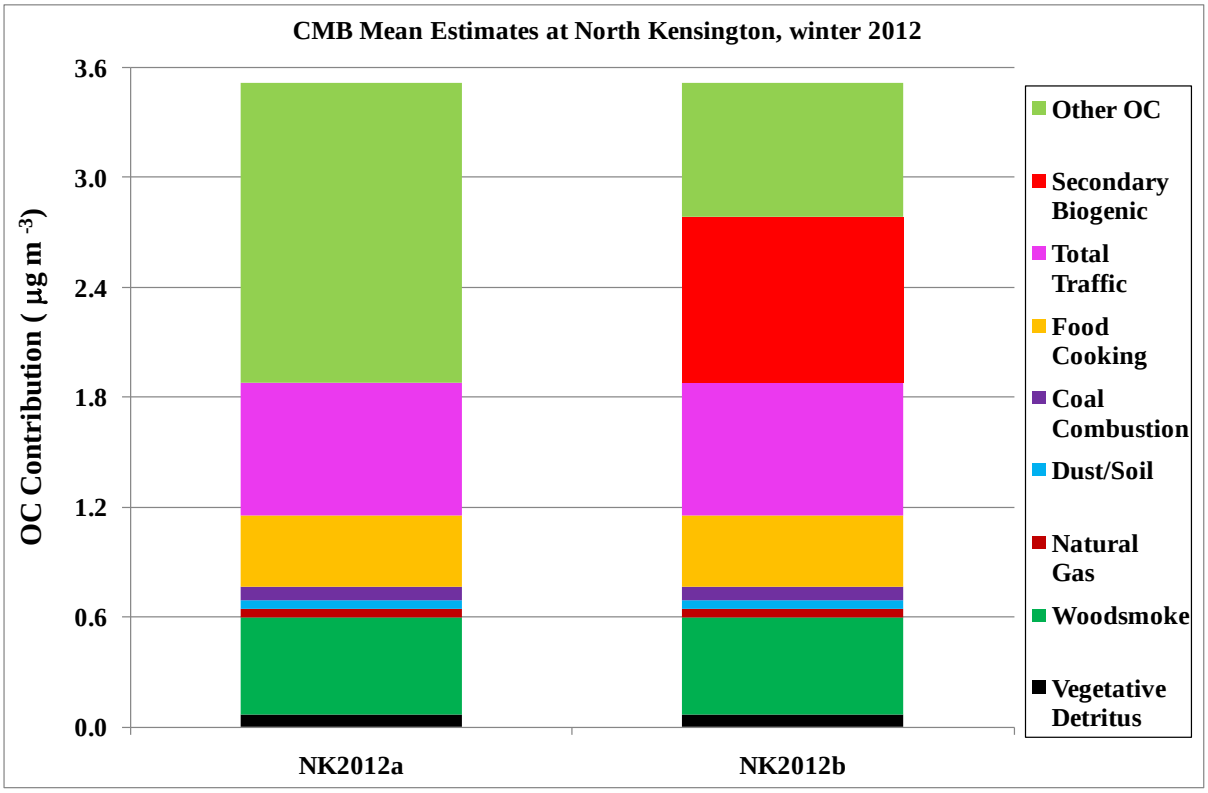
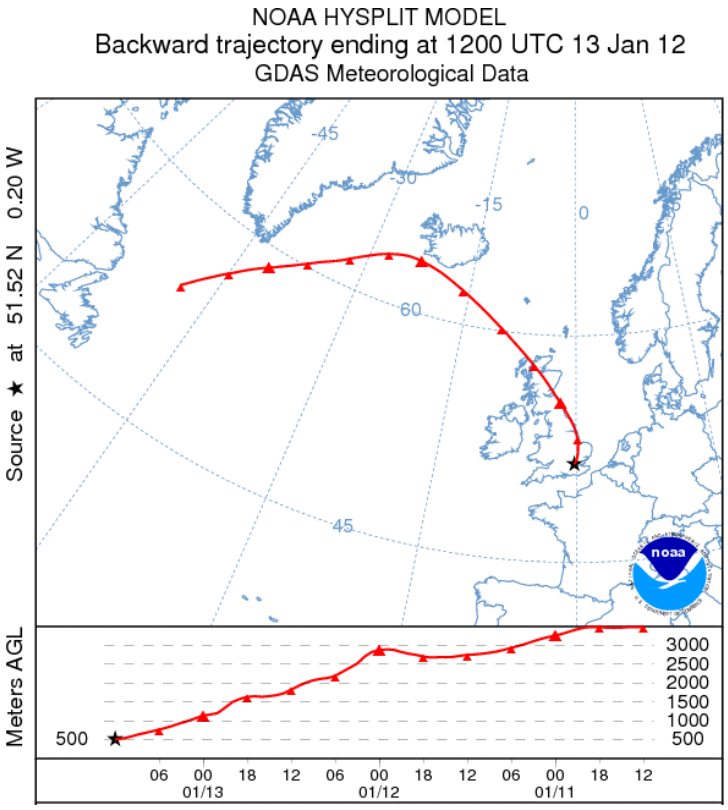
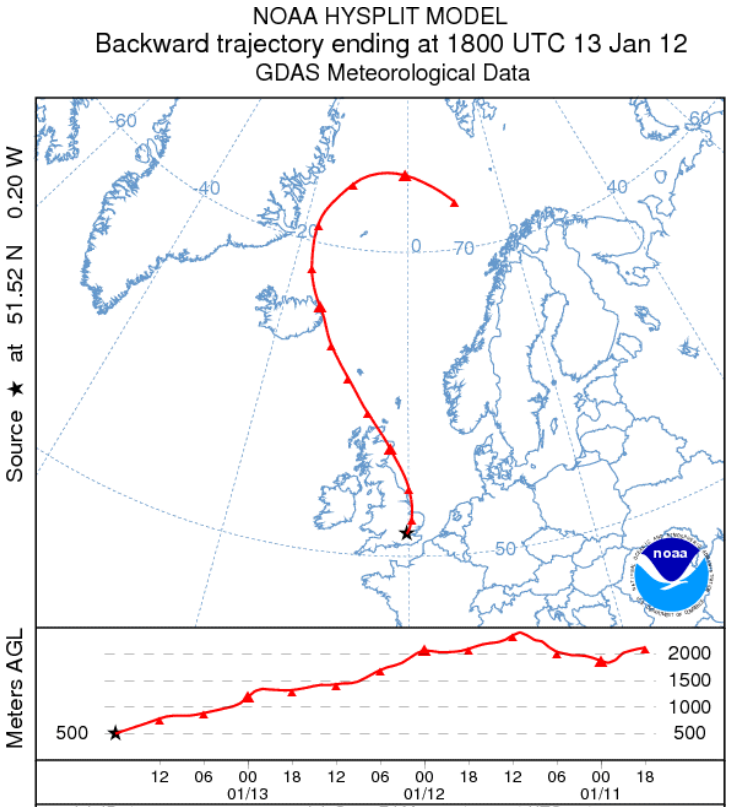
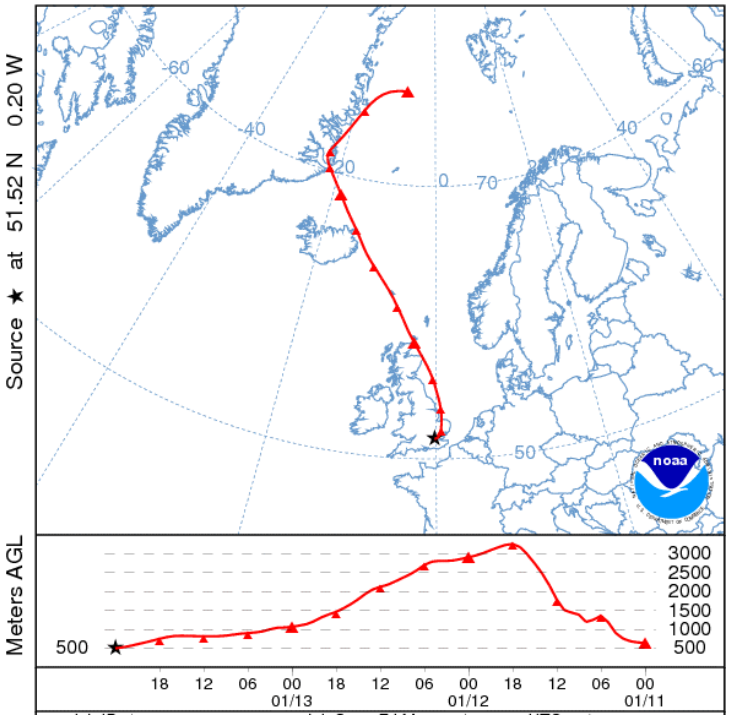


Figure S1: Mean OC source contribution estimates with (b) and without (a) secondary biogenic component at NK

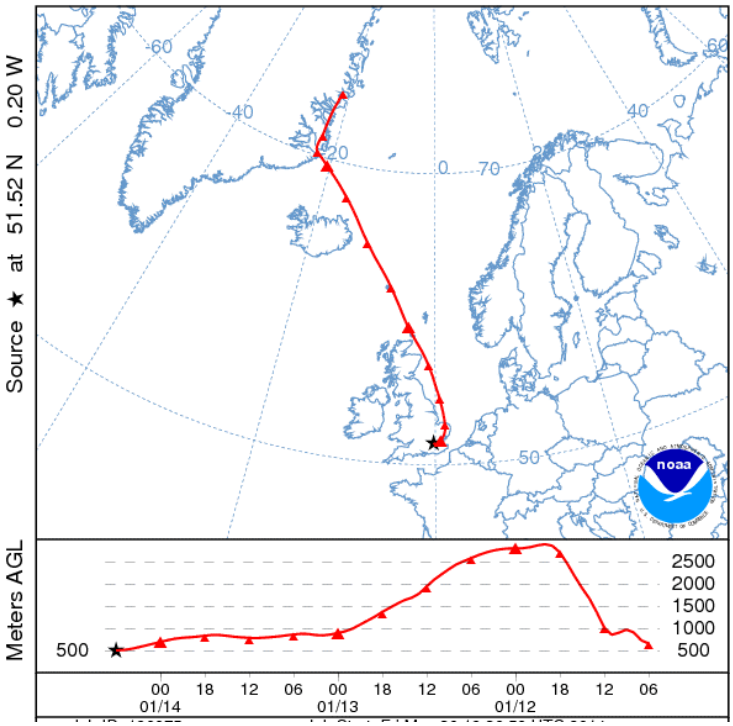

NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 13 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
3000
2500
2000
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
01/13 01/12 01/11

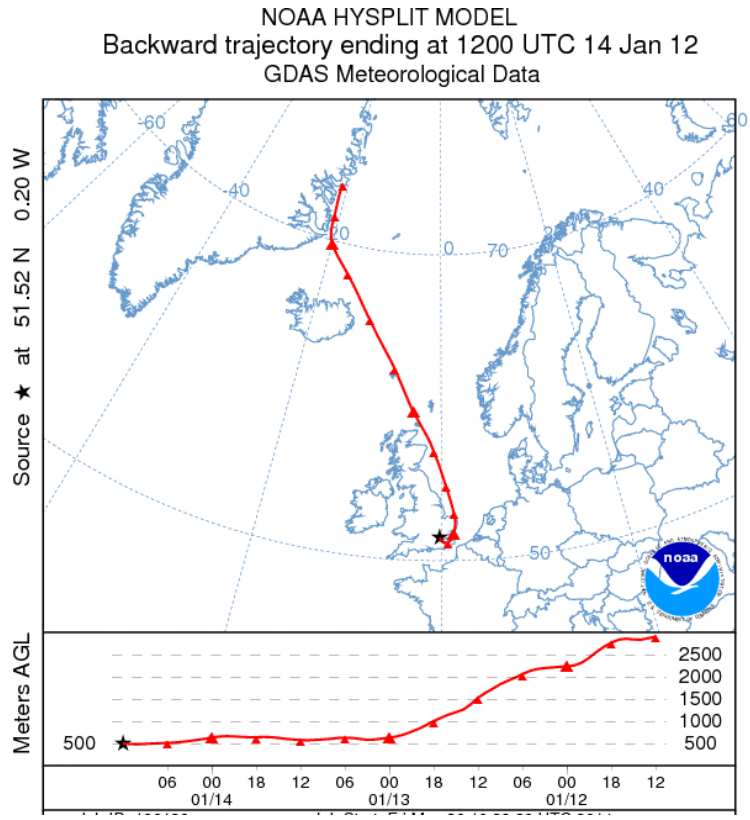

NOAA HYSPLIT MODEL
Backward trajectory ending at 1800 UTC 13 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
2000
1500
1000
500
500
12 06 00 18 12 06 00 18 12 06 00 18
01/13 01/12 01/11

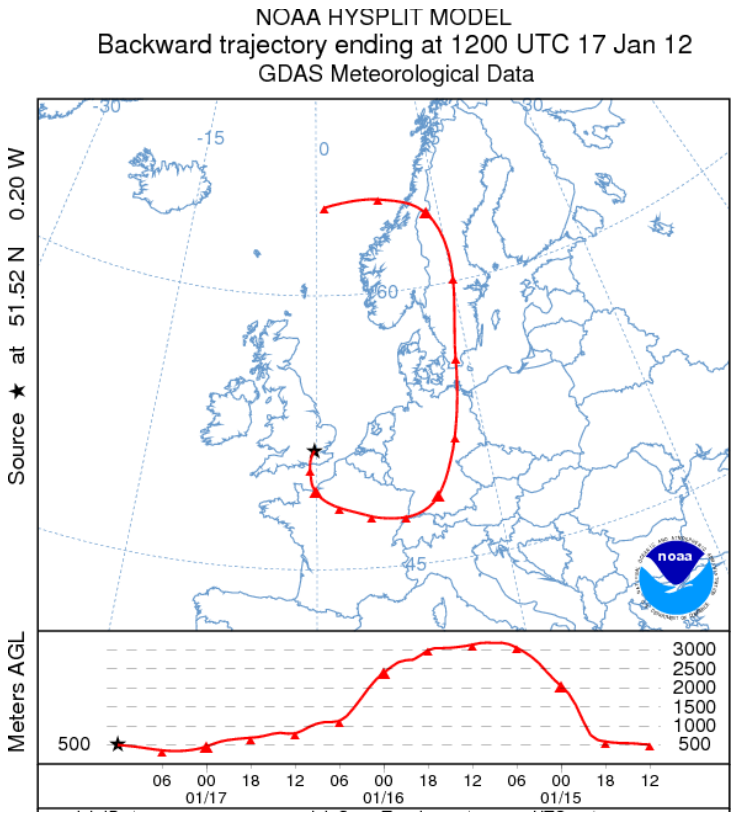
NOAA HYSPLIT MODEL
Backward trajectory ending at 0000 UTC 14 Jan 12
GDAS Meteorological Data

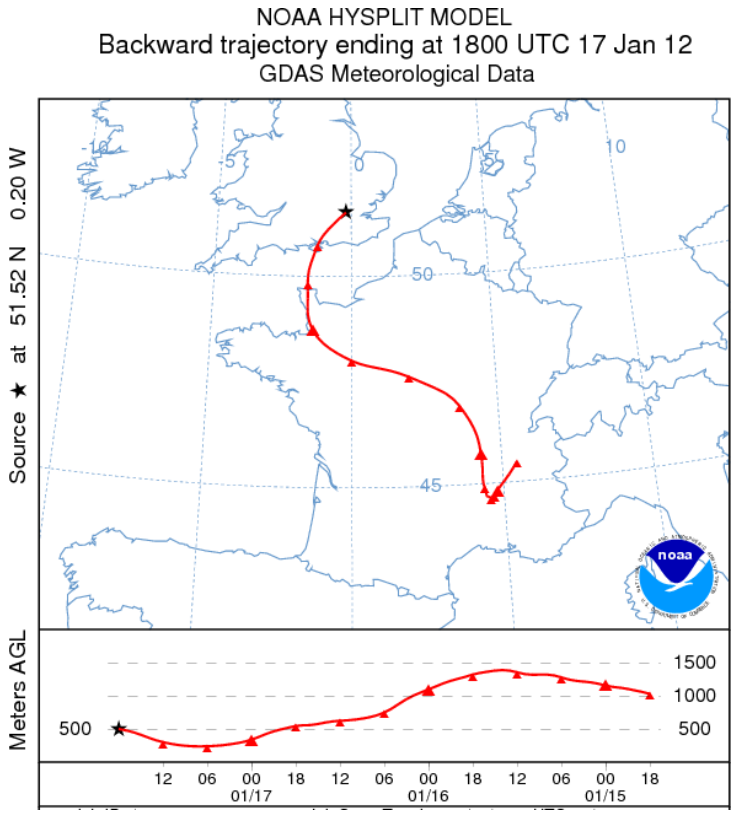


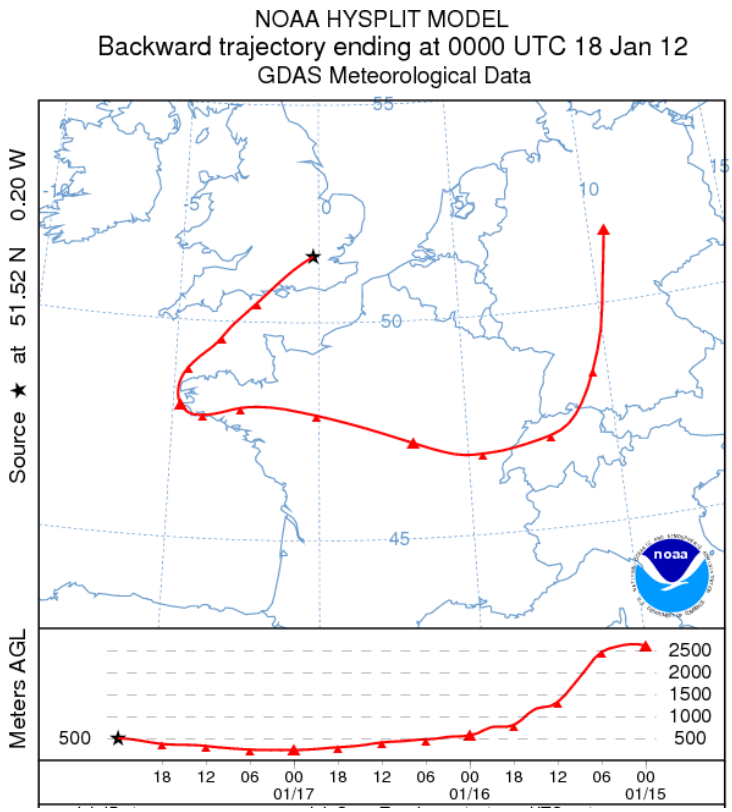
NOAA HYSPLIT MODEL
Backward trajectory ending at 0600 UTC 14 Jan 12
GDAS Meteorological Data

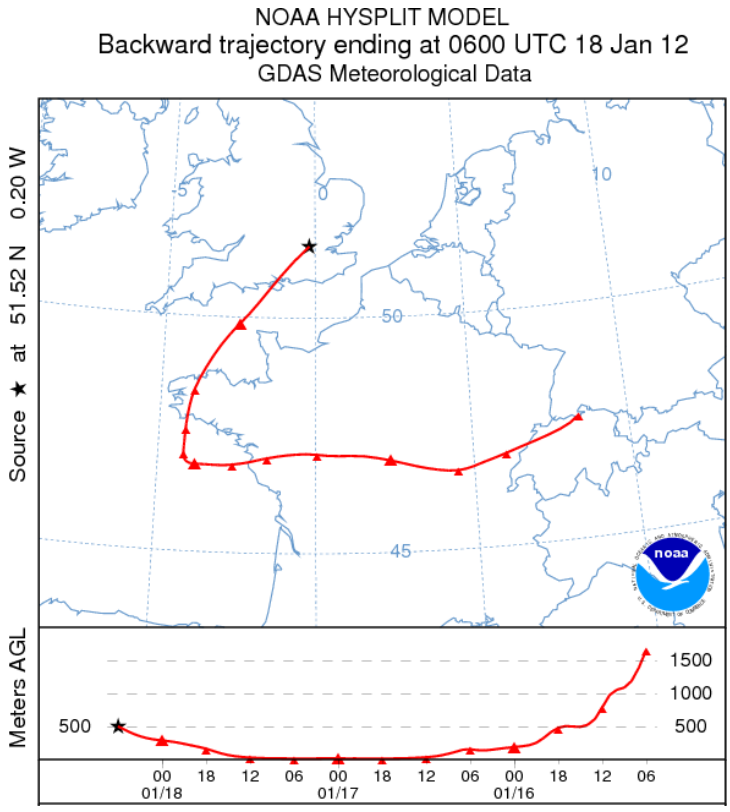


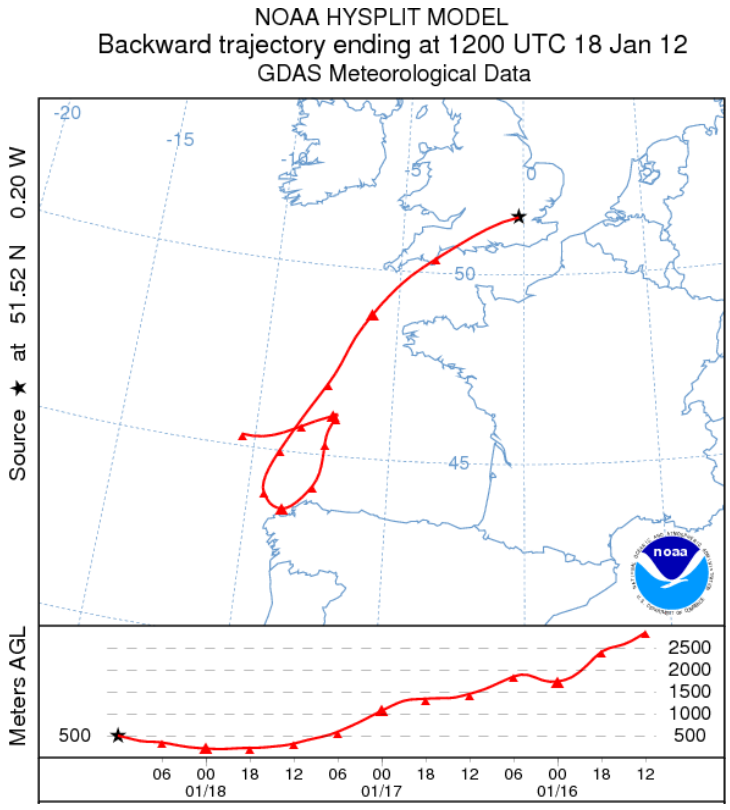

NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 14 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
2500
2000
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
01/14 01/13 01/12

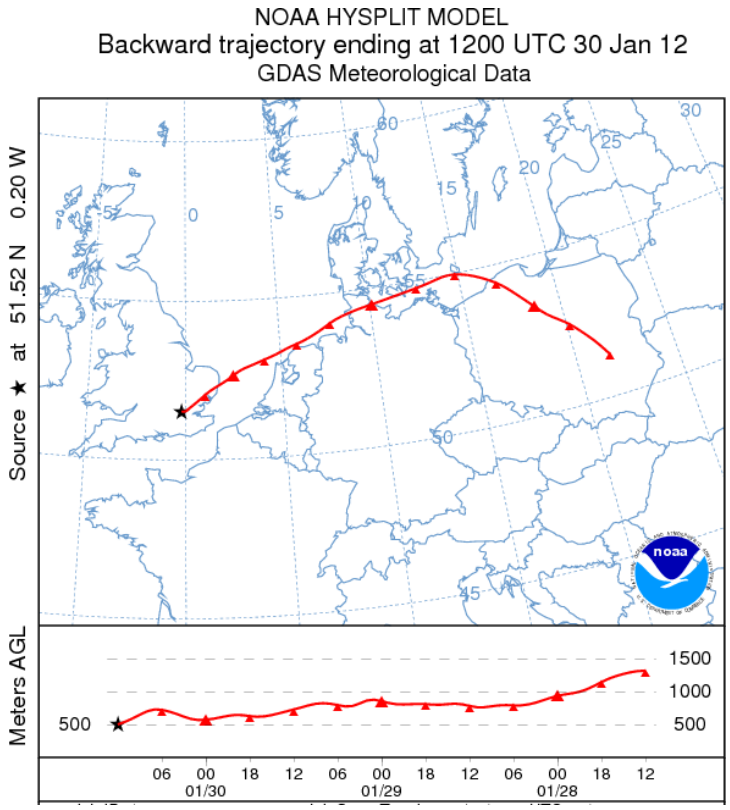

NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 17 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
3000
2500
2000
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
01/17 01/16 01/15

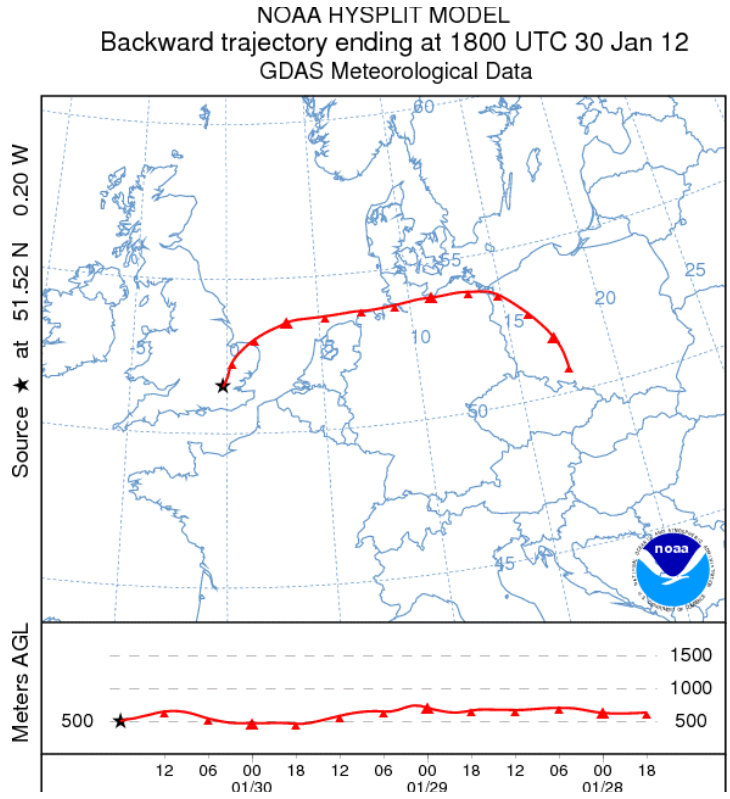

NOAA HYSPLIT MODEL
Backward trajectory ending at 1800 UTC 17 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
12 06 00 18 12 06 00 18 12 06 00 18
01/17 01/16 01/15

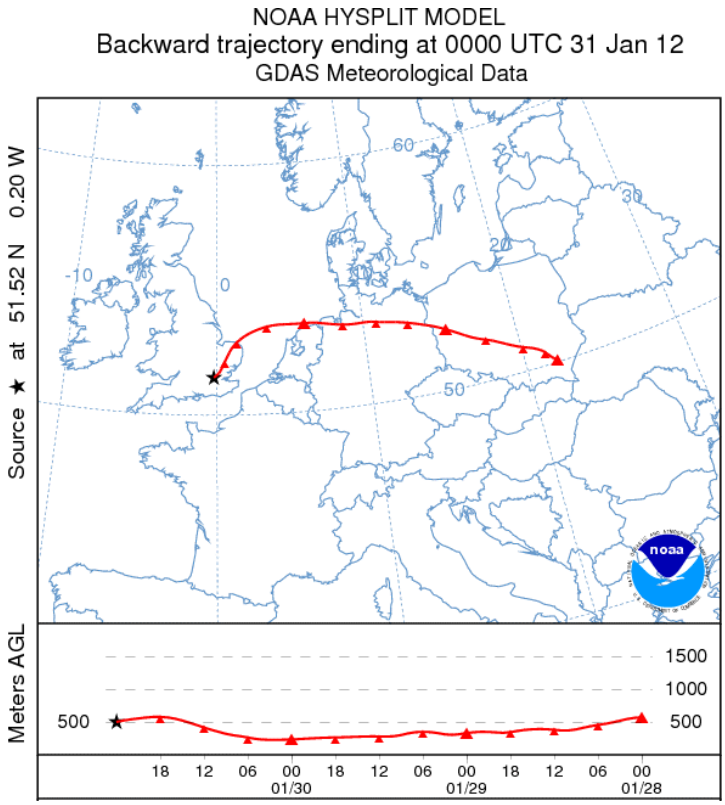

NOAA HYSPLIT MODEL
Backward trajectory ending at 0000 UTC 18 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
2500
2000
1500
1000
500
500
18 12 06 00 18 12 06 00 18 12 06 00
01/17 01/16 01/15

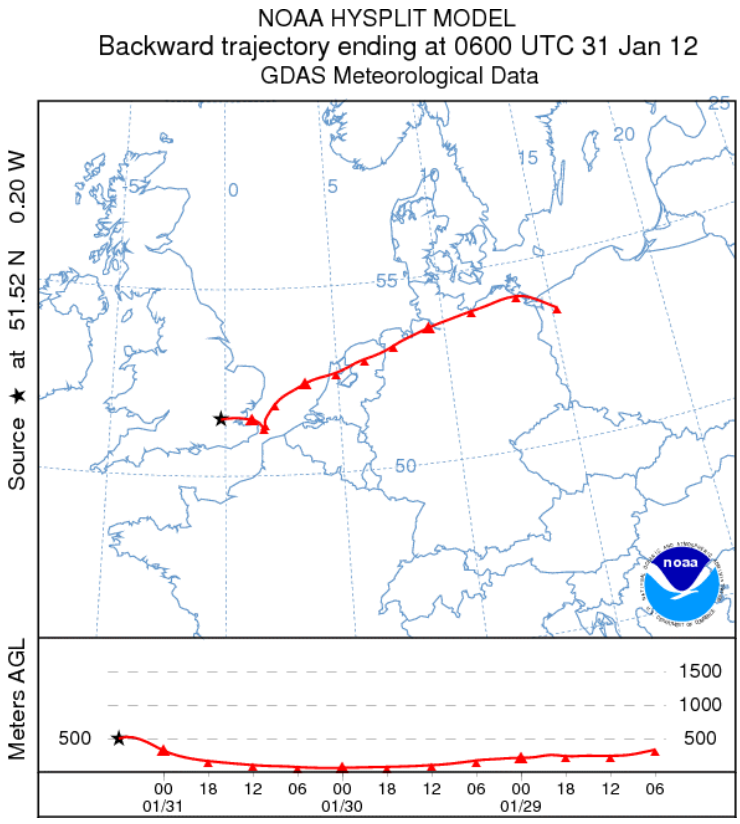

NOAA HYSPLIT MODEL
Backward trajectory ending at 0600 UTC 18 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
00 18 12 06 00 18 12 06 00 18 12 06
01/18 01/17 01/16


NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 18 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
2500
2000
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
01/18 01/17 01/16

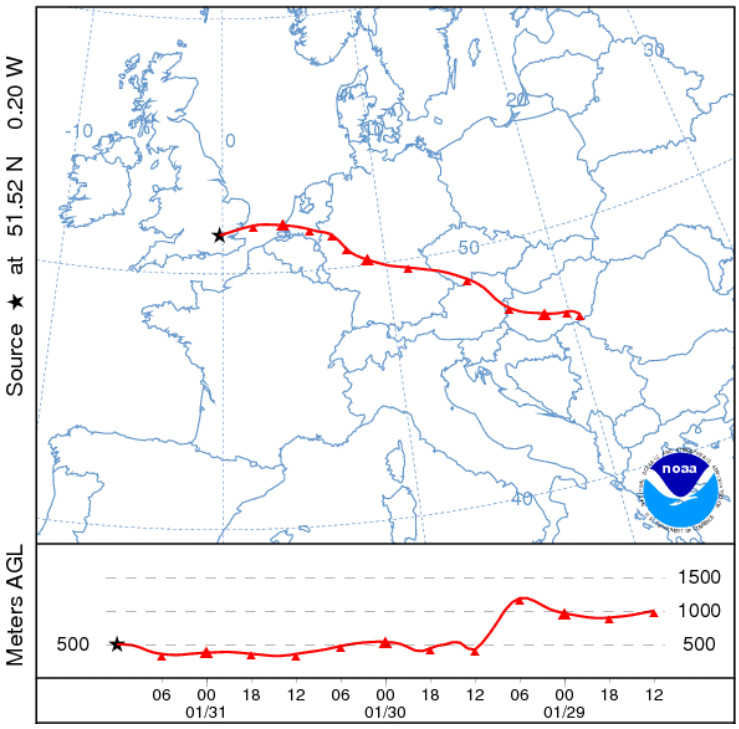

NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 30 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
01/30 01/29 01/28


NOAA HYSPLIT MODEL
Backward trajectory ending at 1800 UTC 30 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
12 06 00 18 12 06 00 18 12 06 00 18
01/30 01/29 01/28

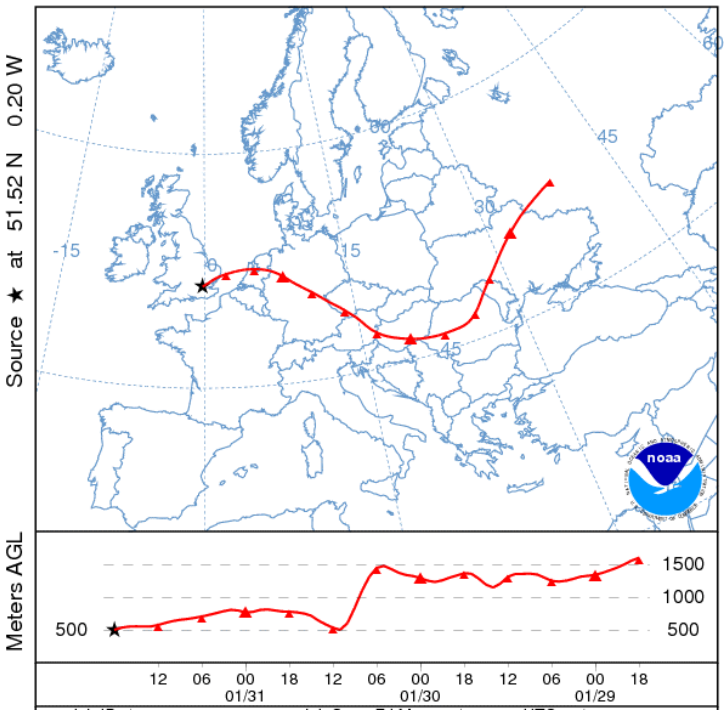

NOAA HYSPLIT MODEL
Backward trajectory ending at 0000 UTC 31 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
18 12 06 00 18 12 06 00 18 12 06 00
01/30 01/29 01/28

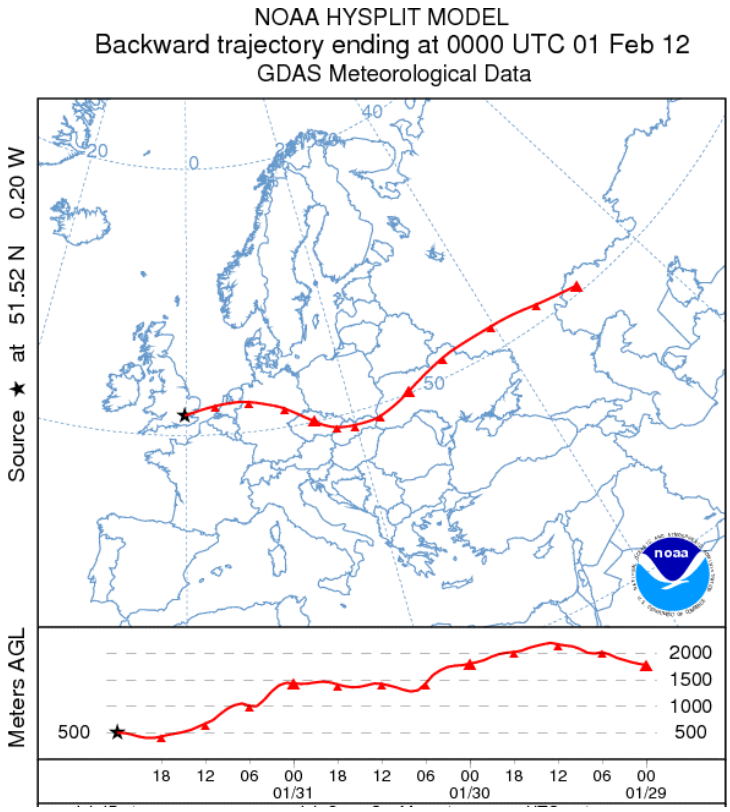

NOAA HYSPLIT MODEL
Backward trajectory ending at 0600 UTC 31 Jan 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
00 18 12 06 00 18 12 06 00 18 12 06
01/31 01/30 01/29

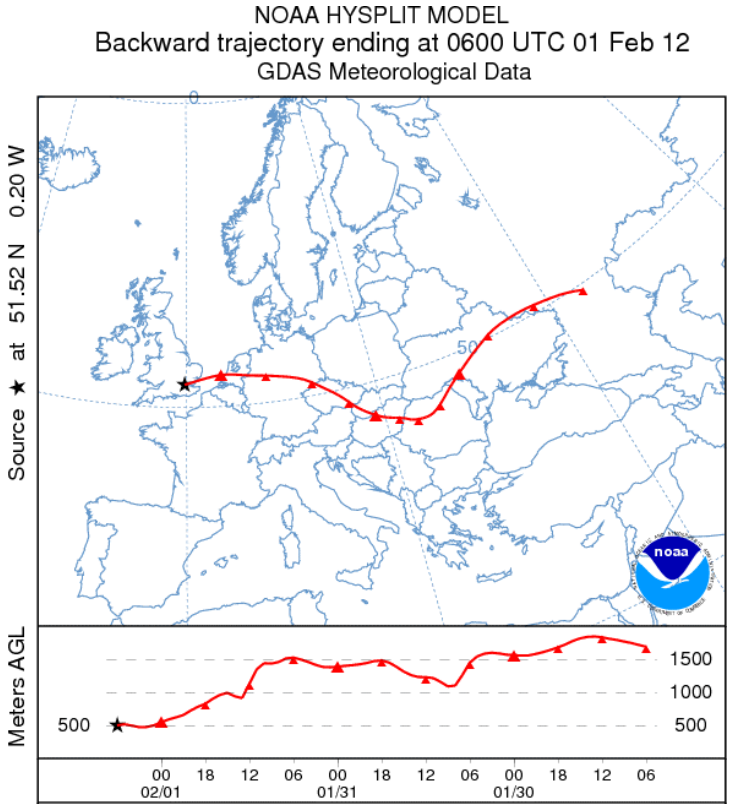
NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 31 Jan 12
GDAS Meteorological Data

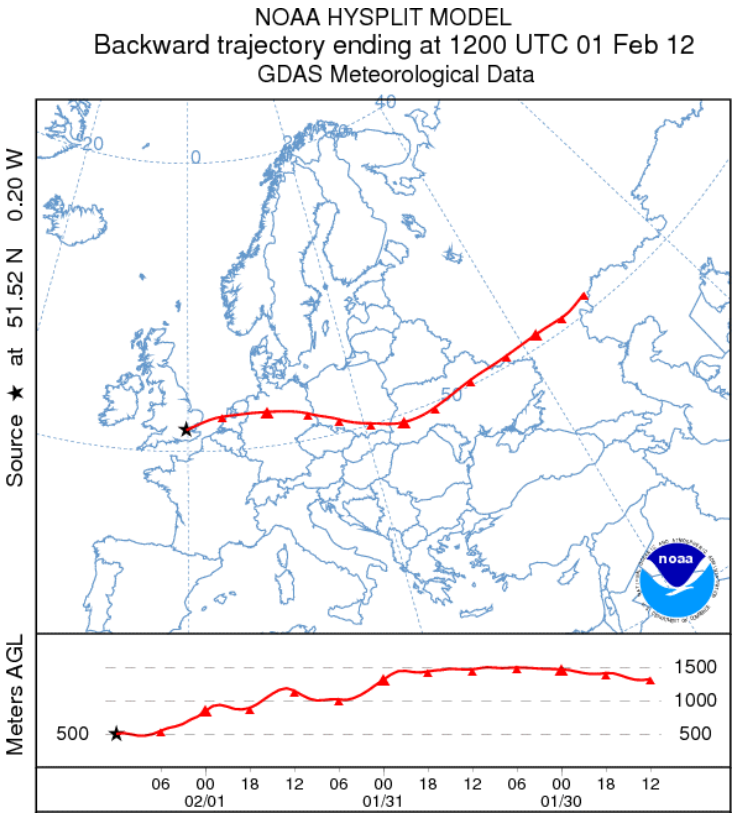


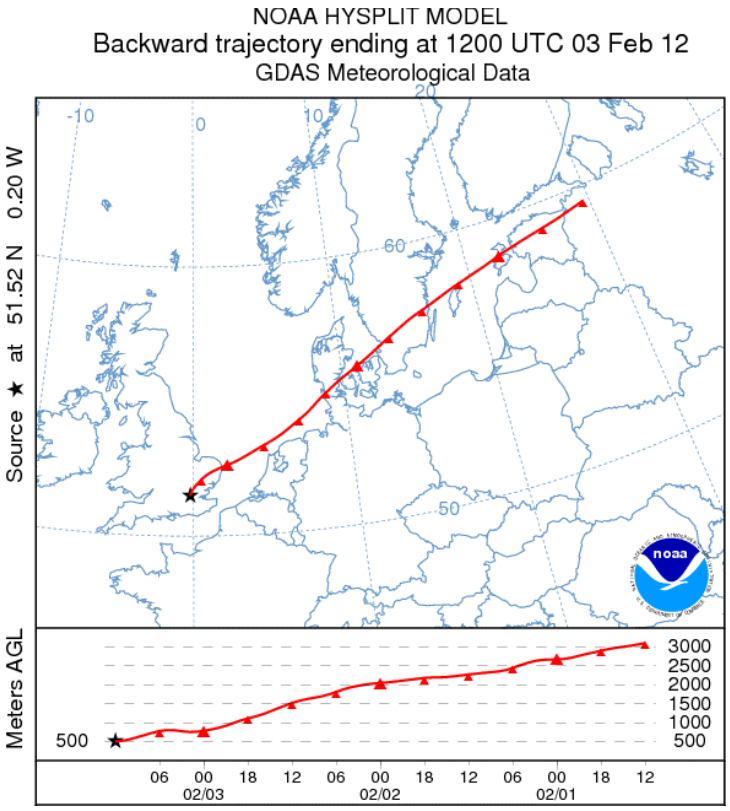
NOAA HYSPLIT MODEL
Backward trajectory ending at 1800 UTC 31 Jan 12
GDAS Meteorological Data

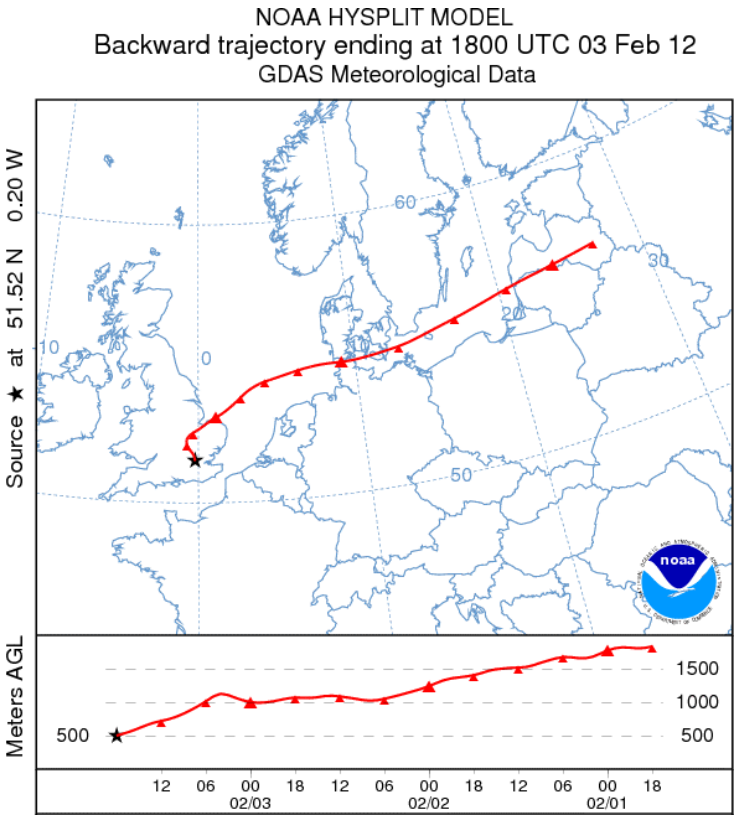


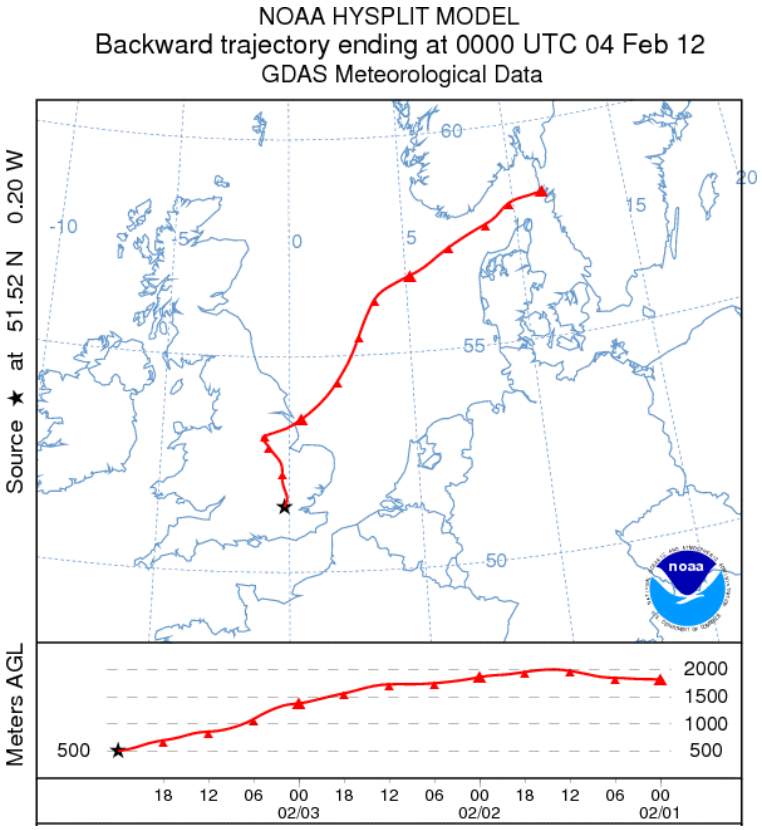

NOAA HYSPLIT MODEL
Backward trajectory ending at 0000 UTC 01 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
2000
1500
1000
500
500
18 12 06 00 18 12 06 00 18 12 06 00
01/31
01/30
01/29

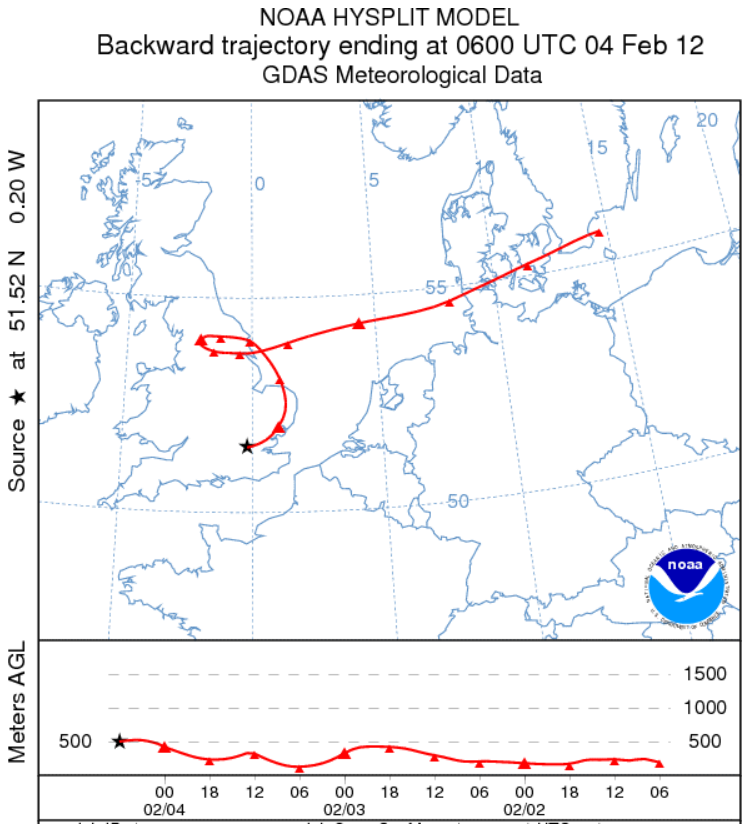

NOAA HYSPLIT MODEL
Backward trajectory ending at 0600 UTC 01 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
00 18 12 06 00 18 12 06 00 18 12 06
02/01
01/31
01/30

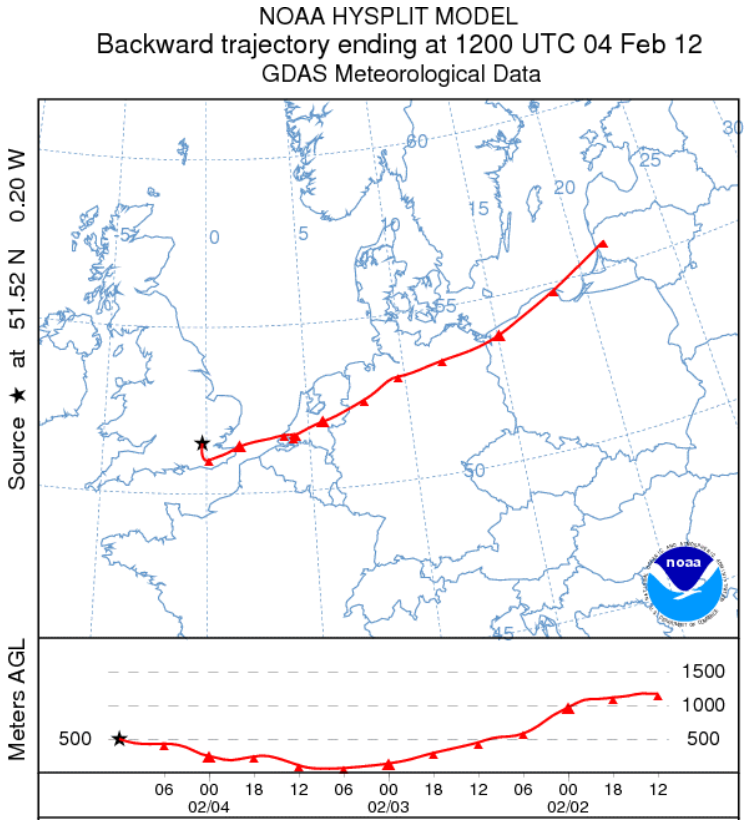

NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 01 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
02/01 01/31 01/30

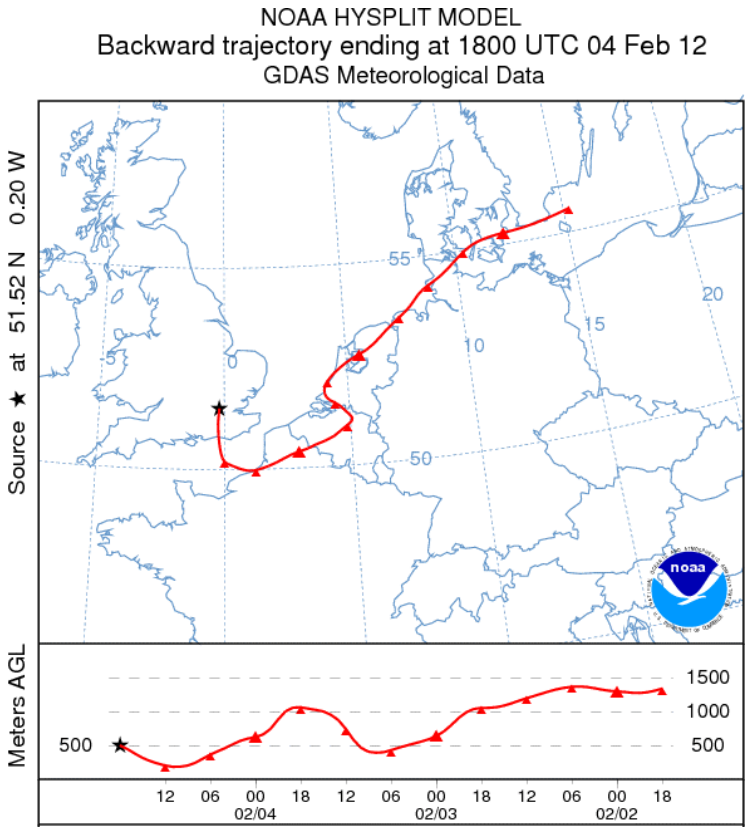

NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 03 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
3000
2500
2000
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
02/03 02/02 02/01

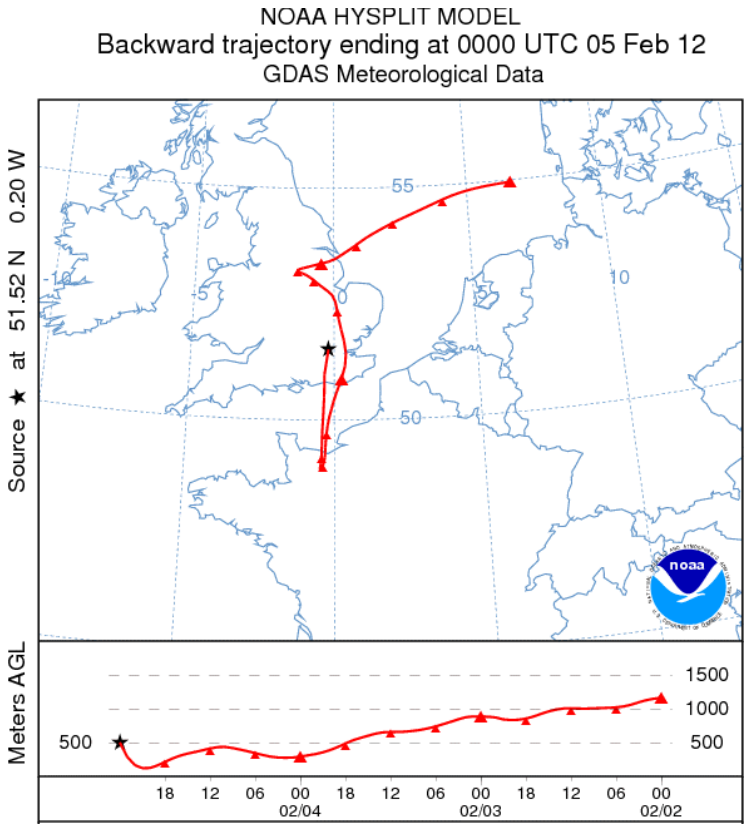

NOAA HYSPLIT MODEL
Backward trajectory ending at 1800 UTC 03 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
12 06 00 18 12 06 00 18 12 06 00 18
02/03 02/02 02/01


NOAA HYSPLIT MODEL
Backward trajectory ending at 0000 UTC 04 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
2000
1500
1000
500
500
18 12 06 00 18 12 06 00 18 12 06 00
02/03 02/02 02/01


NOAA HYSPLIT MODEL
Backward trajectory ending at 0600 UTC 04 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
00 18 12 06 00 18 12 06 00 18 12 06
02/04
02/03
02/02


NOAA HYSPLIT MODEL
Backward trajectory ending at 1200 UTC 04 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
06 00 18 12 06 00 18 12 06 00 18 12
02/04
02/03
02/02


NOAA HYSPLIT MODEL
Backward trajectory ending at 1800 UTC 04 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
12 06 00 18 12 06 00 18 12 06 00 18
02/04 02/03 02/02


NOAA HYSPLIT MODEL
Backward trajectory ending at 0000 UTC 05 Feb 12
GDAS Meteorological Data
Source ★ at 51.52 N 0.20 W
Meters AGL
1500
1000
500
500
18 12 06 00 18 12 06 00 18 12 06 00
02/04 02/03 02/02

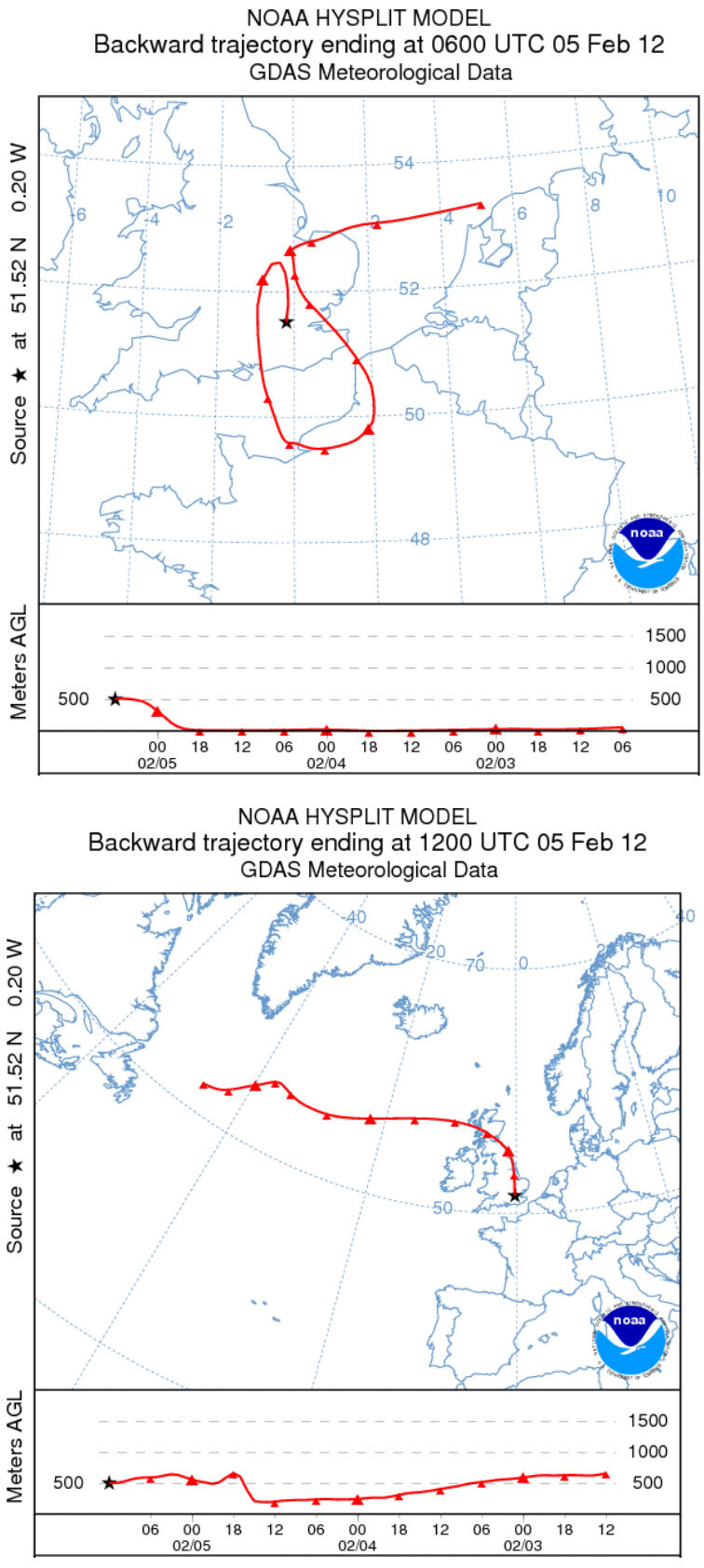


Figure S2. Air mass back trajectories at NK for starting dates of January 13th, 17th, 30th, 31st and February 3rd, 4th.