

Calculations of annual ethanol fluxes from experimental data

Kirstine et al. (1998) (pasture in Australia)

	Value	Min	Max	Units	Comments
Total VOC flux	1.9			$q(C) m^{-2} y^{-1}$	
Percentage of ethanol		6	21		
Ethanol flux		0.22	0.76	$q(eth) m^{-2} y^{-1}$	mult by 46/24

Fukui and Doskey (1998) (grassland in USA)

	Value	Min	Max	Units	Comments
Mean ethanol flux	206			$\mu q(eth) m^{-2} h^{-1}$	=5760.9/28 (from Table 2)
No.of daylight hours per yr	1500	1000	2000		
Mean ethanol flux		0.21	0.41	$q(eth) m^{-2} y^{-1}$	

Schade & Goldstein (2001) (pine plantation in California) - *Pinus ponderosa*

	Value	Min	Max	Units	Comments
Average daily emission	0.27			$mq(C) m^{-2} h^{-1}$	from Table 3
Length of day	12			hr	from Fig 7
Average daily emission	3.24	2.59	3.89	$mq(C) m^{-2} d^{-1}$	+/- 20% based on Fig 7
Average nightly emission	0.10			$mq(C) m^{-2} h^{-1}$	from Table 3
Length of night	12			hr	
Average nightly emission	1.2	0.96	1.44	$mq(C) m^{-2} d^{-1}$	
Average total emssion	4.44	3.55	5.33	$mq(C) m^{-2} d^{-1}$	(day + night)
No of emitting days per yr	160	140	190	days	
Annual emission flux		0.36	0.74	$q(C) m^{-2} y^{-1}$	
Annual emission flux		0.70	1.42	$q(eth) m^{-2} y^{-1}$	mult by 46/24

Grabmer et al. (2006) (spruce forest in Germany) - *Picea abies*

	Value	Min	Max	Units	Comments
Midday max emission	0.40			$\mu q(C) q(dm)^{-1} h^{-1}$	
Daily integrated emission	2.7	2.16	3.24	$\mu q(C) q(dm)^{-1} d^{-1}$	from Fig 3(b), +/- 20%
Foliage density	900	750	1000	$q m^{-1}$	Guenther et al. (1994) for northwest conifers +
Daily integr.emission flux	2430	1620	3240	$\mu q(C) m^{-2} d^{-1}$	Kellomaki et al. (2001) for Finnish spruce
No of emitting days per yr	120	100	130	days	
Annual emission flux	0.29	0.16	0.42	$q(C) m^{-2} y^{-1}$	
Annual emission flux	0.56	0.31	0.81	$q(eth) m^{-2} y^{-1}$	mult by 46/24

Holzinger et al. (2000) (Holm oak) - Quercus ilex

	Value	Min	Max	Units	Comments
Midday max emission	200	100	275	$\text{nmol m}^{-2} \text{min}^{-1}$	average midday values from Fig 3
Midday max emission	552	276	759	$\mu\text{g(eth) m}^{-2} \text{h}^{-1}$	(x 46*60/1000)
Daily integrated emission	3726	1863	5123	$\mu\text{g(eth) m}^{-2} \text{d}^{-1}$	using integration factor of Grabmer (2.7/0.40)
No of emitting days per yr	150	120	180	days	
Annual emission flux	0.56	0.22	0.92	$\text{g(eth) m}^{-2} \text{y}^{-1}$	

Helmig et al. (1999) (Tulip poplar in Fernbank Forest, Georgia) - Liriodendron tulipifera

	Value	Min	Max	Units	Comments
Midday max emission	0.5			$\mu\text{g(C) g(dm)}^{-1} \text{h}^{-1}$	Table 2 +/- 20%
Daily integrated emission	3.38	2.7	4.1	$\mu\text{g(C) g(dm)}^{-1} \text{d}^{-1}$	using integration factor of Grabmer (2.7/0.40)
Foliage density	670	500	700	g m^{-1}	Guenther et al. (1994) for southeast mixed
Daily integr.emission flux	2261	1350	2835	$\mu\text{g(C) m}^{-2} \text{d}^{-1}$	
No of emitting days per yr	150	120	180	days	
Annual emission flux	0.34	0.16	0.51	$\text{g(C) m}^{-2} \text{y}^{-1}$	
Annual emission flux	0.65	0.31	0.98	$\text{g(eth) m}^{-2} \text{y}^{-1}$	mult by 46/24

Helmig et al. (1999) (White oak in Fernbank Forest, Georgia) - Quercus alba

	Value	Min	Max	Units	Comments
Midday max emission	0.2			$\mu\text{g(C) g(dm)}^{-1} \text{h}^{-1}$	Table 2 +/- 20%
Daily integrated emission	1.35	1.1	1.62	$\mu\text{g(C) g(dm)}^{-1} \text{d}^{-1}$	using integration factor of Grabmer (2.7/0.40)
Foliage density	670	500	700	g m^{-1}	Guenther et al. (1994) for southeast mixed
Daily integr.emission flux	905	540	1134	$\mu\text{g(C) m}^{-2} \text{d}^{-1}$	
No of emitting days per yr	150	120	180	days	
Annual emission flux	0.14	0.065	0.204	$\text{g(C) m}^{-2} \text{y}^{-1}$	
Annual emission flux	0.26	0.12	0.39	$\text{g(eth) m}^{-2} \text{y}^{-1}$	mult by 46/24

Helmig et al. (1999) (Gambel oak at Temple Ridge, Colorado) - Quercus gambelii

	Value	Min	Max	Units	Comments
Midday max emission	0.4			$\mu\text{g(C) g(dm)}^{-1} \text{h}^{-1}$	Table 4 +/- 20%
Daily integrated emission	2.70	2.2	3.24	$\mu\text{g(C) g(dm)}^{-1} \text{d}^{-1}$	using integration factor of Grabmer (2.7/0.40)
Foliage density	330	200	400	g m^{-1}	Guenther et al. (1994) for oak scrub

Daily integr.emission flux	891	432	1296	$\mu\text{g(C) m}^{-2} \text{d}^{-1}$	
No of emitting days per yr	150	120	180	days	
Annual emission flux	0.13	0.052	0.233	$\text{g(C) m}^{-2} \text{y}^{-1}$	
Annual emission flux	0.26	0.10	0.45	$\text{g(eth) m}^{-2} \text{y}^{-1}$	mult by 46/24

Rottenberger et al. (2008) (mixed rainforest species)

Flooding period = 210 days

	Units	S.martina	L.corym.	T.juruana	P.glomer.	Mean	Comments
Total for the 6-days following flooding	$\mu\text{mol m}^{-2}$	60.9	242.1	678.9	85.5	266.9	from Figure 4 (a-d)
Total for the 6-days following flooding	g(eth) m^{-2}	0.0028	0.0111	0.0312	0.0039	0.0123	*46/1E6
Min. annual emission flux calculated assuming 4 flood events per 210 day season interspersed with background fluxes of $0.1 \mu\text{mol m}^{-2} \text{d}^{-1}$							
Minimum annual emission flux	$\mu\text{mol m}^{-2} \text{y}^{-1}$	262	987	2734	361	1086	
Minimum annual emission flux	$\text{g(eth) m}^{-2} \text{y}^{-1}$	0.012	0.045	0.126	0.017	0.050	
Max. annual emission flux calculated assuming the 6-day cycle of Fig. 4 is repeated throughout the 210 days of the flooding period.							
Maximum annual emission flux	$\mu\text{mol m}^{-2} \text{y}^{-1}$	2131	8474	23763	2993	9340	
Maximum annual emission flux	$\text{g(eth) m}^{-2} \text{y}^{-1}$	0.098	0.390	1.093	0.138	0.430	210 days per year
Daily emission for the 6-day flooding period	$\mu\text{mol m}^{-2} \text{d}^{-1}$	10.1	40.4	113.2	14.3	44.5	

Calculation of Annual Ethanol Loss by OH Oxidation in the Troposphere

Ethanol Loss in the Continental Boundary Layer through OH oxidation

Cell	Units	1	3	5	7	
Latitude		90N-30N	30N - 0	0 - 30S	30S-90S	
Pressure	mbar	1000-900	1000-900	1000-900	1000-900	
Ocean fraction		0.505	0.721	0.783	0.821	Duxbury and Duxbury (1984)
Land Fraction		0.495	0.279	0.217	0.179	
Air mass in CBL	kg	6.36E+16	3.58E+16	2.79E+16	2.30E+16	
Moles of air in CBL	moles	2.19E+18	1.24E+18	9.62E+17	7.94E+17	
[OH] in CBL	molec. cm ⁻³	1.10E+06	1.10E+06	1.10E+06	1.10E+06	Galbally and Kirstine (2002)
[OH] _{max} in CBL		1.40E+06	1.40E+06	1.60E+06	1.60E+06	
Temperature	K	282	288	288	282	mean = 285 (Seinfeld and Pandis 2006)
k _{OH} (ethanol)	cm ³ molec ⁻¹ s ⁻¹	3.18E-12	3.20E-12	3.20E-12	3.18E-12	
k _{OH} (ethanol) _{max}		3.93E-12	3.95E-12	3.95E-12	3.93E-12	
Ethanol loss coefficient	s ⁻¹	3.50E-06	3.52E-06	3.52E-06	3.50E-06	
Ethanol conc. in CBL	mol mol ⁻¹	1.00E-09	1.00E-09	1.00E-09	1.00E-09	Estimated from observations
Ethanol mass (CBL)	moles	2.19E+09	1.24E+09	9.62E+08	7.94E+08	
Ethanol loss in CBL	mol s ⁻¹	7.68E+03	4.36E+03	3.39E+03	2.78E+03	Total loss= 1.82E+04 mol s ⁻¹
Ethanol loss in CBL	Tg y ⁻¹	11.2	6.3	4.9	4.0	26.5 Tg y ⁻¹
NH ethanol loss	Tg y ⁻¹	17.5				
SH ethanol loss	Tg y ⁻¹	9.0				

Ethanol Loss in the Marine Boundary Layer through OH oxidation

Cell	Units	1	3	5	7	
Latitude		90N-30N	30N - 0	0 - 30S	30S-90S	
Pressure	mbar	1000-900	1000-900	1000-900	1000-900	
Ocean fraction		0.505	0.721	0.783	0.821	Duxbury and Duxbury (1984)

Air mass in MBL	kg	6.48E+16	9.26E+16	1.01E+17	1.05E+17	
Moles of air in MBL	moles	2.24E+18	3.20E+18	3.47E+18	3.64E+18	
[OH] in MBL	radicals cm ⁻³	5.79E+05	1.29E+06	1.53E+06	5.47E+05	Prinn et al. (2001) for 1000-500 mbar
[OH] _{min} in MBL		4.49E+05	9.97E+05	1.21E+06	4.33E+05	
[OH] _{max} in MBL		7.03E+05	1.56E+06	1.85E+06	6.59E+05	
Temperature	K	282	288	288	282	mean = 285
kOH(ethanol)	cm ³ mol ⁻¹ s ⁻¹	3.18E-12	3.20E-12	3.20E-12	3.18E-12	Jiménez et al. (2003)
kOH(ethanol) _(max)		3.93E-12	3.95E-12	3.95E-12	3.93E-12	
Loss rate	s ⁻¹	1.84E-06	4.12E-06	4.90E-06	1.74E-06	
Loss rate _(max)		2.76E-06	6.17E-06	7.29E-06	2.59E-06	
Ethanol conc in MBL	mol mol ⁻¹	1.50E-10	1.50E-10	7.50E-11	7.50E-11	(Singh et al. 1995, 2004)
Ethanol conc in MBL	nmol mol ⁻¹	0.150	0.150	0.075	0.075	

Assuming NH and SH have same ethanol concentration

Latitude		90N-30N	30N - 0	0 - 30S	30S-90S	
Ethanol conc in MBL	mol mol ⁻¹	1.50E-10	1.50E-10	1.50E-10	1.50E-10	(Singh et al. 1995, 2004)
Ethanol loss in MBL	Tg y ⁻¹	0.90	2.87	3.71	1.38	
NH ethanol loss	Tg y ⁻¹	3.77				
SH ethanol loss	Tg y ⁻¹	5.09				
Total ethanol loss	Tg y ⁻¹	8.87				

Assuming ethanol concentration in SH is half that in the NH

Latitude		90N-30N	30N - 0	0 - 30S	30S-90S	
Ethanol conc in MBL	mol mol ⁻¹	1.50E-10	1.50E-10	7.50E-11	7.50E-11	
Ethanol loss in MBL	Tg y ⁻¹	0.90	2.87	1.86	0.69	
NH ethanol loss	Tg y ⁻¹	3.77				
SH ethanol loss	Tg y ⁻¹	2.55				

Total ethanol loss Tg y⁻¹ 6.32

Assuming ethanol concentration in SH is 0.2 that in the NH

Latitude		90N-30N	30N - 0	0 - 30S	30S-90S
Ethanol conc in MBL	mol mol ⁻¹	1.50E-10	1.50E-10	3.00E-11	3.00E-11
Ethanol loss in MBL	Tg y ⁻¹	0.90	2.87	0.74	0.28
NH ethanol loss	Tg y ⁻¹	3.77			
SH ethanol loss	Tg y ⁻¹	1.02			
Total ethanol loss	Tg y ⁻¹	4.79			

Ethanol Loss in the Free Troposphere through OH oxidation

<u>Cell</u>	Units	1	2	3	4	5	6	7	8
Latitude		90N-30N	90N-30N	30N - 0	30N - 0	0 - 30S	0 - 30S	30S-90S	30S-90S
Pressure	mbar	900-500	500-200	900-500	500-200	900-500	500-200	900-500	500-200
Ocean fraction		0.505	0.505	0.721	0.721	0.783	0.783	0.821	0.821
Tropospheric air mass	kg	6.42E+17	3.85E+17	6.42E+17	3.85E+17	6.42E+17	3.85E+17	6.42E+17	3.85E+17
Air mass in FT	kg	5.14E+17	3.85E+17	5.14E+17	3.85E+17	5.14E+17	3.85E+17	5.14E+17	3.85E+17
Moles of air in FT	moles	1.77E+19	1.33E+19	1.77E+19	1.33E+19	1.77E+19	1.33E+19	1.77E+19	1.33E+19
[OH] in FT	radicals cm ⁻³	5.79E+05	5.20E+05	1.29E+06	1.13E+06	1.53E+06	1.32E+06	5.47E+05	5.72E+05
[OH] _{min} in FT		4.49E+05	4.03E+05	9.97E+05	8.77E+05	1.21E+06	1.05E+06	4.33E+05	4.52E+05
[OH] _{max} in FT		7.03E+05	6.31E+05	1.56E+06	1.38E+06	1.85E+06	1.59E+06	6.59E+05	6.89E+05
Temperature	K	261	230	276	242	276	242	261	230
kOH(ethanol)	cm ³ mol ⁻¹ s ⁻¹	3.11E-12	2.97E-12	3.16E-12	3.03E-12	3.16E-12	3.03E-12	3.11E-12	2.97E-12
kOH(ethanol) _(max)		3.85E-12	3.72E-12	3.91E-12	3.77E-12	3.91E-12	3.77E-12	3.85E-12	3.72E-12
Loss rate	s ⁻¹	1.80E-06	1.54E-06	4.07E-06	3.42E-06	4.84E-06	4.00E-06	1.70E-06	1.70E-06
Loss rate _(max)		2.71E-06	2.35E-06	6.11E-06	5.19E-06	7.22E-06	6.02E-06	2.54E-06	2.56E-06

Ethanol conc in FT	mol mol ⁻¹	5.00E-11
Ethanol conc in FT	nmol mol ⁻¹	0.050

Singh et al. (1995), (2004) at altitude of 5-10 km (540 - 260 mbar)

Assuming NH and SH have same ethanol concentration

Latitude		90N-30N	90N-30N	30N - 0	30N - 0	0 - 30S	0 - 30S	30S-90S	30S-90S
Pressure	mbar	900-500	500-200	900-500	500-200	900-500	500-200	900-500	500-200
Ethanol conc in FT	mol mol ⁻¹	5.00E-11	5.00E-11	5.00E-11	5.00E-11	5.00E-11	5.00E-11	5.00E-11	5.00E-11
Ethanol loss in FT	Tg y ⁻¹	2.32	1.49	5.25	3.31	6.24	3.87	2.19	1.64
NH ethanol loss	Tg y ⁻¹	12.37							
SH ethanol loss	Tg y ⁻¹	13.95							
Total ethanol loss	Tg y ⁻¹	26.32							

Assuming ethanol concentration in SH is half that in the NH

Latitude		90N-30N	90N-30N	30N - 0	30N - 0	0 - 30S	0 - 30S	30S-90S	30S-90S
Pressure	mbar	900-500	500-200	900-500	500-200	900-500	500-200	900-500	500-200
Ethanol conc in FT	mol mol ⁻¹	5.00E-11	5.00E-11	5.00E-11	5.00E-11	2.50E-11	2.50E-11	2.50E-11	2.50E-11
Ethanol loss in FT	Tg y ⁻¹	2.32	1.49	5.25	3.31	3.12	1.93	1.10	0.82
NH ethanol loss	Tg y ⁻¹	12.37							
SH ethanol loss	Tg y ⁻¹	6.97							
Total ethanol loss	Tg y ⁻¹	19.34							

Assuming ethanol concentration in SH is 0.2 that in the NH

Latitude		90N-30N	90N-30N	30N - 0	30N - 0	0 - 30S	0 - 30S	30S-90S	30S-90S
Pressure	mbar	900-500	500-200	900-500	500-200	900-500	500-200	900-500	500-200
Ethanol conc in FT	mol mol ⁻¹	5.00E-11	5.00E-11	5.00E-11	5.00E-11	1.00E-11	1.00E-11	1.00E-11	1.00E-11
Ethanol loss in FT	Tg y ⁻¹	2.32	1.49	5.25	3.31	1.25	0.77	0.44	0.33
NH ethanol loss	Tg y ⁻¹	12.37							
SH ethanol loss	Tg y ⁻¹	2.79							
Total ethanol loss	Tg y ⁻¹	15.16							

Ethanol Loss by OH Oxidation in Clouds

		NH	SH	
Mass of cloudwater	g	3.80E+16	4.22E+16	
Volume of cloudwater	L	3.80E+13	4.22E+13	
Mean cloud temperature	K	276	276	Lelieveld & Crutzen (1991)
Pressure at cloud height	atm	0.8	0.8	
Henry's Law constant	mol L ⁻¹ atm ⁻¹	968.7	968.7	
k _{OH_aq} (ethanol)	L mol ⁻¹ s ⁻¹	1.29E+09	1.29E+09	Ervens et al. (2003)
[OH _{aq}]	mol L ⁻¹	7.0E-14	7.0E-14	Leriche et al. (2000) and Herrmann et al. (2000)
Ethanol loss coefficient	s ⁻¹	9.05E-05	9.05E-05	
Ethanol loss rate	mol s ⁻¹	133.43	147.89	H*Ca*P*V*(k _{OH} *[OH])
Ethanol loss rate	Tg y ⁻¹	0.19	0.22	total = 0.41
Ethanol conc in clouds	mol L ⁻¹	3.87E-08	3.87E-08	
				TOTAL
<u>Total ethanol loss by OH</u>	Tg y ⁻¹	33.83	18.70	52.53