Supporting Information

for

Reactive transport of iomeprol during stream-groundwater interactions

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Analysis of the X-ray contrast media

Table SI1: Measured concentrations [nmol/L] of iomeprol and its transformation products

Sampling Location: Schwarzbach

Time	Iomeprol	TP819	TP805	TP791	TP789	TP775	TP761	TP745	TP731	TP717	TP701	TP687	TP657	TP643	TP629	TP599
16.09.2010	**0.26**	< LOQ	**0.02** **0.08**	**0.02** **0.06**	< LOQ	< LOQ	< LOQ	**0.12** **0.15**	< LOQ	**0.01**	**0.03**	**0.11**	< LOQ	**0.10**	**0.43**	**0.18**
17.09.2010	**0.44**	< LOQ	**0.16** **0.14**	**0.12** **0.12**	< LOQ	< LOQ	< LOQ	**0.31** **0.33**	< LOQ	**0.02**	**0.03**	**0.09**	< LOQ	**0.09**	**0.38**	**0.17**
20.09.2010	**0.13**	< LOQ	**0.11** **0.12**	**0.06**	< LOQ	< LOQ	< LOQ	**1.0** **1.2**	< LOQ	**0.02**	**0.07**	**0.32**	< LOQ	**0.15**	**0.70**	**0.34**
23.09.2010	**0.53**	< LOQ	< LOQ	**0.06**	< LOQ	< LOQ	< LOQ	**0.23**	< LOQ	**0.04**	**0.08**	**0.28**	< LOQ	**0.20**	**0.85**	**0.51**
26.09.2010	**0.29**	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	**0.39**	< LOQ	**0.04**	**0.12**	**0.50**	< LOQ	**0.28**	**1.3**	**0.65**
29.09.2010	**0.50**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.43**	< LOQ	**0.03**	**0.09**	**0.30**	< LOQ	**0.22**	**1.1**	**0.51**
03.10.2010	**0.24**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.24**	< LOQ	**0.02**	**0.05**	**0.24**	< LOQ	**0.15**	**0.81**	**0.31**
06.10.2010	**0.28**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	**0.01**	**0.03**	**0.16**	< LOQ	**0.13**	**0.71**	**0.29**
09.10.2010	**1.2**	< LOQ	< LOQ	**0.11**	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	**0.04**	**0.06**	**0.28**	< LOQ	**0.18**	**1.0**	**0.47**
LOQ	*0.02*	*0.02*	*0.02*	*0.02*	*0.02*	*0.02*	*0.02*	*0.02*	*0.02*	*0.01*	*0.02*	*0.01*	*0.02*	*0.02*	*0.01*	*0.02*

Sampling Location: GWM 0

Time	Depth	Iomeprol	TP819	TP805	TP791	TP789	TP775	TP761	TP745	TP731	TP717	TP701	TP687	TP657	TP643	TP629	TP599
14.09.2010	top	**0.08**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.02**	< LOQ	< LOQ	**0.05**	**0.15**	< LOQ	**0.29**	**0.17**	**0.26**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.02**	**0.06**	**0.28**	< LOQ	**0.19**	**0.16**	**0.19**
17.09.2010	top	**0.07**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.17**	< LOQ	**0.07**	**0.19**	**0.52**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.09**	**0.24**	**0.29**
20.09.2010	top	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.14**	< LOQ	**0.24**	**0.16**	**0.22**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	**0.11**	< LOQ	**0.21**	**0.15**	**0.22**
23.09.2010	top	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.03**	**0.19**	< LOQ	**0.18**	**0.13**	**0.21**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.25**	< LOQ	< LOQ	**0.07**	**0.47**	< LOQ	**0.21**	**0.13**	**0.20**
26.09.2010	top	**0.07**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.25**	< LOQ	**0.08**	**0.23**	**0.44**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.44**	< LOQ	**0.08**	**0.22**	**0.49**
29.09.2010	top	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	**0.23**	< LOQ	**0.23**	**0.14**	**0.21**
		0.04	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.14**	< LOQ	**0.16**	**0.13**	**0.19**
03.10.2010	top	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	< LOQ	< LOQ	**0.17**	< LOQ	**0.19**	**0.12**	**0.21**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.18**	< LOQ	< LOQ	**0.07**	**0.37**	< LOQ	**0.17**	**0.11**	**0.20**
06.10.2010	top	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	< LOQ	**0.05**	**0.25**	< LOQ	**0.16**	**0.11**	**0.16**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	< LOQ	**0.04**	**0.20**	< LOQ	**0.17**	**0.12**	**0.15**
09.10.2010	top	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	< LOQ	< LOQ	**0.28**	< LOQ	**0.12**	**0.13**	**0.12**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	**0.19**	< LOQ	**0.09**	**0.10**	**0.11**
14.09.2010	middle	**0.07**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.11**	**0.26**	**0.32**
		0.08	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	**0.31**	< LOQ	**0.10**	**0.24**	**0.38**
17.09.2010	middle	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	**0.07**	**0.24**	**0.53**
		0.07	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	**0.10**	**0.28**	**0.50**
20.09.2010	middle	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	**0.19**	< LOQ	**0.21**	**0.15**	**0.22**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	**0.19**	< LOQ	**0.21**	**0.13**	**0.24**
23.09.2010	middle	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	< LOQ	**0.04**	**0.28**	< LOQ	**0.20**	**0.14**	**0.20**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.20**	< LOQ	< LOQ	**0.06**	**0.41**	< LOQ	**0.17**	**0.10**	**0.19**
26.09.2010	middle	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	0.03	< LOQ	**0.38**	< LOQ	**0.08**	**0.18**	**0.39**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.07**	**0.18**	**0.40**
29.09.2010	middle	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	< LOQ	**0.03**	**0.20**	< LOQ	**0.16**	**0.12**	**0.18**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	**0.17**	< LOQ	**0.19**	**0.14**	**0.20**
03.10.2010	middle	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	**0.17**	**0.10**	**0.19**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	< LOQ	**0.06**	**0.31**	< LOQ	**0.15**	**0.11**	**0.16**
06.10.2010	middle	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	< LOQ	**0.05**	**0.28**	< LOQ	**0.13**	**0.08**	**0.18**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.14**	**0.11**	**0.16**
09.10.2010	middle	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	< LOQ	**0.02**	**0.20**	< LOQ	**0.11**	**0.11**	**0.10**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.10**	**0.09**	**0.11**
14.09.2010	bottom	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.16**	< LOQ	< LOQ	< LOQ	**0.36**	< LOQ	**0.12**	**0.17**	**0.26**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	**0.19**	< LOQ	**0.11**	**0.17**	**0.27**
17.09.2010	bottom	**0.07**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.20**	< LOQ	**0.09**	**0.24**	**0.41**
		0.07	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.10**	**0.23**	**0.56**
20.09.2010	bottom	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	< LOQ	**0.06**	**0.23**	< LOQ	**0.17**	**0.11**	**0.21**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	< LOQ	**0.04**	**0.22**	< LOQ	**0.16**	**0.10**	**0.19**
23.09.2010	bottom	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	< LOQ	**0.06**	**0.32**	< LOQ	**0.15**	**0.12**	**0.18**
		0.04	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	**0.03**	**0.17**	< LOQ	**0.13**	**0.11**	**0.19**
26.09.2010	bottom	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	0.04	< LOQ	**0.55**	< LOQ	**0.08**	**0.18**	**0.28**
29.09.2010	bottom	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	< LOQ	**0.05**	**0.32**	< LOQ	**0.17**	**0.12**	**0.22**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	< LOQ	**0.05**	**0.31**	< LOQ	**0.18**	**0.11**	**0.18**
03.10.2010	bottom	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	< LOQ	**0.04**	**0.22**	< LOQ	**0.13**	**0.10**	**0.14**
		< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	**0.15**	**0.10**	**0.17**
06.10.2010	bottom	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	**0.16**	< LOQ	**0.11**	**0.10**	**0.16**
		0.02	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.13**	**0.10**	**0.16**
09.10.2010	bottom	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.09**	**0.09**	**0.08**
		0.02	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.08**	**0.09**	**0.09**
LOQ		*0.02*	*0.02*	*0.02*	*0.02*	*0.01*	*0.02*	*0.02*	*0.02*	*0.01*	*0.02*	*0.01*	*0.01*	*0.01*	*0.02*	*0.002*	*0.01*

37 Sampling Location: GWM 2a top (depth equals m below groundwater surface)

Time	Depth	Iomeprol	TP819	TP805	TP791	TP789	TP775	TP761	TP745	TP731	TP717	TP701	TP687	TP657	TP643	TP629	TP599
14.09.2010	2.0-2.5	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.02**	**0.11**	**0.15**	< LOQ	**2.2**	**1.3**	**2.3**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	**0.12**	< LOQ	**2.1**	**1.4**	**2.5**
14.09.2010	2.5-3.0	**0.10**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	**0.12**	< LOQ	**1.6**	**1.2**	**1.7**
		0.10	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	**0.15**	< LOQ	**2.1**	**1.6**	**1.6**
14.09.2010	3.0-3.5	**0.60**	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.08**	< LOQ	**0.08**	< LOQ	**0.27**	**0.71**	**0.31**
		0.55	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.08**	< LOQ	**0.13**	< LOQ	**0.25**	**0.62**	**0.29**
14.09.2010	3.75-4.25	**0.13**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.10**	< LOQ	**1.4**	**1.3**	**1.4**
		0.17	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.10**	< LOQ	**1.7**	**2.0**	**1.1**
14.09.2010	5.0-5.5	**0.16**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.02**	< LOQ	**0.17**	< LOQ	**0.98**	**1.6**	**0.88**
		0.17	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.02**	< LOQ	**0.15**	< LOQ	**0.89**	**1.2**	**0.95**
17.09.2010	0.25	**0.18**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.12**	< LOQ	**0.65**	**1.0**	**0.62**
		0.16	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.03**	< LOQ	**0.15**	< LOQ	**0.58**	**0.87**	**0.63**
20.09.2010	0.25	**0.15**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.16**	< LOQ	**0.30**	**1.2**	**0.22**
23.09.2010	0.25	**0.09**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.02**	< LOQ	**0.26**	< LOQ	**0.19**	**1.1**	**0.21**
		0.10	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.24**	< LOQ	**0.06**	**0.05**	**0.55**	< LOQ	**0.18**	**0.89**	**0.21**
26.09.2010	0.25	**0.10**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.18**	< LOQ	**0.05**	**0.05**	**0.56**	< LOQ	**0.19**	**0.83**	**0.21**
		0.12	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.28**	< LOQ	**0.10**	**0.07**	**0.60**	< LOQ	**0.23**	**0.81**	**0.22**
29.09.2010	0.25	**0.07**	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	**0.13**	**0.10**	**0.44**	< LOQ	**0.50**	**1.4**	**0.43**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.06**	**0.06**	**0.24**	< LOQ	**0.43**	**1.0**	**0.42**
03.10.2010	0.25	**0.08**	< LOQ	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	**0.10**	**0.07**	**0.24**	< LOQ	**0.68**	**1.2**	**0.60**
		0.08	< LOQ	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	**0.11**	**0.06**	**0.21**	< LOQ	**0.56**	**1.2**	**0.53**
06.10.2010	0.25	**0.09**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.04**	< LOQ	**0.25**	< LOQ	**0.20**	**1.1**	**0.20**
		0.09	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.06**	< LOQ	**0.34**	< LOQ	**0.22**	**1.3**	**0.21**
09.10.2010	0.25	**0.11**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.22**	< LOQ	**0.08**	**0.04**	**0.60**	< LOQ	**0.17**	**1.0**	**0.18**
		0.09	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.04**	**0.03**	**0.30**	< LOQ	**0.15**	**0.92**	**0.16**
17.09.2010	0.75	**0.20**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.14**	< LOQ	**0.60**	**1.3**	**0.55**
		0.19	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.14**	< LOQ	**0.52**	**1.2**	**0.47**
20.09.2010	0.75	**0.16**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.04**	< LOQ	**0.24**	< LOQ	**0.32**	**1.2**	**0.26**
		0.16	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	**0.31**	< LOQ	**0.27**	**1.2**	**0.26**
23.09.2010	0.75	**0.13**	< LOQ	**0.01**	< LOQ	< LOQ	< LOQ	< LOQ	**0.31**	< LOQ	**0.13**	**0.06**	**0.64**	< LOQ	**0.19**	**0.96**	**0.20**
		0.16	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.15**	< LOQ	**0.09**	**0.05**	**0.46**	< LOQ	**0.26**	**1.4**	**0.24**
26.09.2010	0.75	**0.12**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.09**	**0.05**	**0.61**	< LOQ	**0.23**	**1.4**	**0.24**
		0.13	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.19**	< LOQ	**0.08**	< LOQ	**0.46**	< LOQ	**0.27**	**1.4**	**0.22**
29.09.2010	0.75	**0.09**	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	**0.19**	< LOQ	**0.24**	**0.10**	**0.56**	< LOQ	**0.34**	**1.2**	**0.28**
		0.10	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	**0.12**	< LOQ	**0.46**	**1.6**	**0.33**
03.10.2010	0.75	**0.09**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.11**	< LOQ	**0.45**	**1.1**	**0.45**
		0.10	< LOQ	**0.01**	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.10**	< LOQ	**0.21**	< LOQ	**0.49**	**1.3**	**0.45**
06.10.2010	0.75	**0.10**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	**0.05**	< LOQ	**0.35**	< LOQ	**0.22**	**1.3**	**0.21**
		0.10	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.14**	< LOQ	**0.09**	< LOQ	**0.38**	< LOQ	**0.20**	**1.1**	**0.19**
09.10.2010	0.75	**0.11**	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.29**	< LOQ	**0.14**	**0.05**	**0.76**	< LOQ	**0.17**	**1.1**	**0.16**
		0.09	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.08**	< LOQ	**0.36**	< LOQ	**0.14**	**0.88**	**0.14**
17.09.2010	1.25	**0.41**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.06**	< LOQ	**0.30**	**1.0**	**0.26**
20.09.2010	1.25	**0.20**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.15**	< LOQ	**0.24**	**1.1**	**0.22**
		0.19	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.04**	< LOQ	**0.24**	< LOQ	**0.17**	**1.1**	**0.18**
23.09.2010	1.25	**0.18**	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	**0.08**	< LOQ	**0.17**	**0.74**	**0.15**
		0.18	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.11**	< LOQ	**0.11**	< LOQ	**0.16**	**0.82**	**0.17**
26.09.2010	1.25	**0.17**	< LOQ	**0.09**	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.19**	< LOQ	**0.27**	< LOQ	**0.09**	**0.68**	**0.15**
		0.15	< LOQ	**0.11**	< LOQ	< LOQ	< LOQ	< LOQ	**0.14**	< LOQ	**0.24**	< LOQ	**0.31**	< LOQ	**0.11**	**0.66**	**0.14**
29.09.2010	1.25	**0.14**	< LOQ	**0.08**	< LOQ	< LOQ	< LOQ	< LOQ	**0.17**	< LOQ	**0.22**	**0.04**	**0.40**	< LOQ	**0.18**	**0.93**	**0.21**
		0.12	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.18**	< LOQ	**0.32**	< LOQ	**0.18**	**0.79**	**0.19**
03.10.2010	1.25	**0.10**	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.14**	< LOQ	**0.32**	< LOQ	**0.26**	**0.93**	**0.31**
		0.09	< LOQ	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	**0.16**	< LOQ	**0.15**	**0.04**	**0.38**	< LOQ	**0.26**	**0.89**	**0.29**
06.10.2010	1.25	**0.11**	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.15**	< LOQ	**0.13**	< LOQ	**0.14**	**0.92**	**0.13**
		0.10	< LOQ	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	**0.23**	< LOQ	**0.22**	< LOQ	**0.15**	**0.77**	**0.12**
09.10.2010	1.25	**0.10**	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.08**	< LOQ	**0.25**	< LOQ	**0.13**	**0.76**	**0.14**
		0.10	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	**0.08**	< LOQ	**0.28**	< LOQ	**0.13**	**0.92**	**0.13**

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Sampling Location: GWM 2a middle and bottom

Time	Depth	Iomeprol	TP819	TP805	TP791	TP789	TP775	TP761	TP745	TP731	TP717	TP701	TP687	TP657	TP643	TP629	TP599
17.09.2010	middle	**0.24**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.02**	< LOQ	**0.07**	< LOQ	**0.18**	< LOQ	**0.47**	**1.2**	**0.47**
		0.22	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.07**	< LOQ	**0.21**	< LOQ	**0.54**	**1.4**	**0.47**
20.09.2010	middle	**0.21**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.02**	< LOQ	**0.20**	< LOQ	**0.20**	**1.3**	**0.16**
		0.18	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.02**	< LOQ	**0.23**	< LOQ	**0.18**	**1.1**	**0.23**
23.09.2010	middle	**0.15**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.04**	< LOQ	**0.15**	< LOQ	**0.18**	**0.91**	**0.19**
		0.14	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	**0.22**	< LOQ	**0.09**	< LOQ	**0.34**	< LOQ	**0.15**	**0.74**	**0.18**
26.09.2010	middle	**0.12**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.15**	< LOQ	**0.23**	**1.2**	**0.24**
		0.12	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.23**	< LOQ	**0.12**	< LOQ	**0.54**	< LOQ	**0.21**	**1.1**	**0.22**
29.09.2010	middle	**0.10**	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.15**	< LOQ	**0.16**	**0.04**	**0.40**	< LOQ	**0.24**	**0.95**	**0.21**
				0.02							**0.13**	**0.05**				**1.2**	
03.10.2010	middle	**0.13**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.10**	< LOQ	**0.18**	**0.95**	**0.22**
		0.13	< LOQ	**0.13**	< LOQ	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	**0.27**	< LOQ	**0.29**	< LOQ	**0.20**	**0.84**	**0.24**
06.10.2010	middle	**0.08**	< LOQ	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.12**	< LOQ	**0.16**	< LOQ	**0.10**	**0.63**	**0.12**
		0.09	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.08**	< LOQ	**0.13**	**0.77**	**0.13**
09.10.2010	middle	**0.10**	< LOQ	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.10**	< LOQ	**0.19**	< LOQ	**0.09**	**0.63**	**0.11**
		0.10	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.08**	< LOQ	**0.19**	< LOQ	**0.10**	**0.63**	**0.12**
17.09.2010	bottom	**0.14**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	< LOQ	< LOQ	**0.25**	< LOQ	**0.56**	**1.4**	**0.54**
		0.16	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	**0.03**	< LOQ	**0.25**	< LOQ	**0.55**	**1.4**	**0.52**
20.09.2010	bottom	**0.16**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.02**	< LOQ	**0.19**	< LOQ	**0.23**	**1.2**	**0.22**
		0.15	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.03**	< LOQ	**0.30**	< LOQ	**0.23**	**1.1**	**0.24**
23.09.2010	bottom	**0.13**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.46**	< LOQ	**0.06**	**0.09**	**0.87**	< LOQ	**0.20**	**0.84**	**0.27**
		0.15	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.03**	**0.04**	**0.33**	< LOQ	**0.20**	**1.1**	**0.25**
26.09.2010	bottom	**0.10**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.33**	< LOQ	**0.04**	**0.07**	**0.70**	< LOQ	**0.17**	**0.99**	**0.20**
		0.09	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.27**	< LOQ	**0.06**	**0.08**	**0.82**	< LOQ	**0.26**	**1.5**	**0.24**
29.09.2010	bottom	**0.09**	< LOQ	**0.01**	< LOQ	< LOQ	< LOQ	< LOQ	**0.13**	< LOQ	**0.11**	**0.04**	**0.44**	< LOQ	**0.19**	**1.0**	**0.24**
		0.11	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	**0.22**	< LOQ	**0.12**	**0.07**	**0.56**	< LOQ	**0.25**	**1.1**	**0.27**
03.10.2010	bottom	**0.08**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.15**	< LOQ	**0.06**	**0.07**	**0.36**	< LOQ	**0.22**	**0.97**	**0.21**
		0.10	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.26**	< LOQ	**0.07**	**0.05**	**0.60**	< LOQ	**0.20**	**0.93**	**0.23**
06.10.2010	bottom	**0.09**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.23**	< LOQ	**0.04**	**0.05**	**0.63**	< LOQ	**0.23**	**1.2**	**0.23**
		0.11	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.04**	< LOQ	**0.03**	**0.03**	**0.37**	< LOQ	**0.25**	**1.4**	**0.24**
09.10.2010	bottom	**0.07**	< LOQ	**0.01**	< LOQ	< LOQ	< LOQ	< LOQ	**0.24**	< LOQ	**0.03**	**0.04**	**0.43**	< LOQ	**0.14**	**0.75**	**0.17**
		0.07	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.02**	< LOQ	**0.32**	< LOQ	**0.16**	**0.89**	**0.19**
LOQ		*0.01*	*0.01*	*0.01*	*0.01*	*0.02*	*0.05*	*0.01*	*0.02*	*0.02*	*0.02*	*0.02*	***0.01***	*0.01*	*0.01*	*0.01*	*0.01*

Sampling Location: GWM 2c

Time	Depth	lomeprol	TP819	TP805	TP791	TP789	TP775	TP761	TP745	TP731	TP717	TP701	TP687	TP657	TP643	TP629	TP599
17.09.2010	top	**0.05**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.15**	**0.23**	**0.17**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.02**	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	**0.15**	**0.22**	**0.19**
20.09.2010	top	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.10**	**0.24**	**0.13**
		0.07	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	< LOQ	**0.12**	< LOQ	**0.07**	**0.23**	**0.16**
23.09.2010	top	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.03**	**0.13**	< LOQ	**0.13**	**0.10**	**0.15**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.12**	< LOQ	**0.15**	**0.13**	**0.19**
26.09.2010	top	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.37**	< LOQ	**0.01**	**0.10**	**0.33**	< LOQ	**0.14**	**0.12**	**0.18**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.16**	< LOQ	< LOQ	**0.07**	**0.25**	< LOQ	**0.13**	**0.13**	**0.16**
29.09.2010	top	**0.06**	< LOQ	**0.81**	< LOQ	< LOQ	< LOQ	< LOQ	**0.23**	< LOQ	< LOQ	**0.06**	**0.25**	< LOQ	**0.13**	**0.14**	**0.19**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.12**	< LOQ	**0.17**	**0.21**	**0.19**
03.10.2010	top	**0.13**	< LOQ	**0.80**	< LOQ	< LOQ	< LOQ	< LOQ	**0.18**	< LOQ	< LOQ	**0.06**	**0.23**	< LOQ	**0.16**	**0.26**	**0.20**
		0.12	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.09**	< LOQ	**0.16**	**0.25**	**0.20**
06.10.2010	top	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	< LOQ	**0.04**	**0.18**	< LOQ	**0.13**	**0.14**	**0.16**
		0.04	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.29**	< LOQ	**0.01**	**0.07**	**0.27**	< LOQ	**0.13**	**0.16**	**0.15**
09.10.2010	top	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.14**	< LOQ	**0.01**	**0.05**	**0.14**	< LOQ	**0.08**	**0.08**	**0.11**
		0.04	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.02**	**0.07**	< LOQ	**0.11**	**0.12**	**0.12**
17.09.2010	middle	**0.06**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	< LOQ	**0.04**	**0.13**	< LOQ	**0.12**	**0.24**	**0.14**
		0.07	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	**0.01**	**0.04**	**0.17**	< LOQ	**0.12**	**0.24**	**0.18**
20.09.2010	middle	**0.08**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.15**	< LOQ	**0.04**	**0.31**	**0.21**
		0.07	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	**0.03**	**0.29**	**0.20**
23.10.2010	middle	**0.07**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	**0.01**	**0.04**	**0.15**	< LOQ	**0.13**	**0.12**	**0.15**
		0.06	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	< LOQ	**0.04**	**0.15**	< LOQ	**0.13**	**0.13**	**0.17**
26.10.2010	middle	**0.07**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.10**	< LOQ	**0.13**	**0.19**	**0.15**
		0.05	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	**0.04**	**0.15**	< LOQ	**0.10**	**0.15**	**0.13**
29.09.2010	middle																
03.10.2010	middle	**0.09**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.10**	< LOQ	**0.01**	< LOQ	**0.19**	< LOQ	**0.12**	**0.22**	**0.15**
		0.09	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	**0.03**	**0.03**	**0.15**	< LOQ	**0.09**	**0.18**	**0.13**
06.10.2010	middle	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.11**	< LOQ	< LOQ	**0.05**	**0.15**	< LOQ	**0.09**	**0.11**	**0.13**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	< LOQ	**0.03**	**0.17**	< LOQ	**0.11**	**0.12**	**0.13**
09.10.2010	middle	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.06**	< LOQ	**0.01**	**0.03**	**0.12**	< LOQ	**0.09**	**0.09**	**0.12**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.17**	< LOQ	**0.01**	**0.05**	**0.22**	< LOQ	**0.08**	**0.11**	**0.10**
17.09.2010	bottom	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.14**	< LOQ	< LOQ	**0.08**	**0.25**	< LOQ	**0.29**	**0.19**	**0.39**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.21**	< LOQ	**0.01**	**0.10**	**0.25**	< LOQ	**0.30**	**0.16**	**0.41**
20.09.2010	bottom	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.03**	**0.11**	< LOQ	**0.14**	**0.09**	**0.20**
		0.04	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.11**	< LOQ	**0.17**	**0.11**	**0.16**
23.09.2010	bottom	**0.04**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.05**	< LOQ	< LOQ	**0.05**	**0.13**	< LOQ	**0.16**	**0.07**	**0.21**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.03**	< LOQ	< LOQ	**0.04**	**0.13**	< LOQ	**0.16**	**0.07**	**0.19**
26.10.2010	bottom	**0.03**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.14**	< LOQ	< LOQ	< LOQ	**0.24**	< LOQ	**0.13**	**0.11**	**0.22**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.17**	< LOQ	**0.07**	**0.16**	**0.29**
29.10.2010	bottom	**0.01**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.07**	< LOQ	< LOQ	**0.09**	**0.19**	< LOQ	**0.31**	**0.08**	**0.39**
		0.02	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	**0.01**	**0.09**	**0.20**	< LOQ	**0.30**	**0.07**	**0.33**
03.10.2010	bottom	**0.02**	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.94**	< LOQ	**0.02**	**0.16**	**0.47**	< LOQ	**0.21**	**0.09**	**0.32**
		0.03	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.09**	< LOQ	**0.01**	**0.07**	**0.19**	< LOQ	**0.29**	**0.10**	**0.30**
06.10.2010	bottom	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.57**	< LOQ	**0.01**	**0.16**	**0.47**	< LOQ	**0.26**	**0.04**	**0.36**
		0.01	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.08**	< LOQ	< LOQ	**0.08**	**0.25**	< LOQ	**0.30**	**0.04**	**0.42**
09.10.2010	bottom	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.42**	< LOQ	**0.01**	**0.13**	**0.46**	< LOQ	**0.29**	**0.07**	**0.36**
		0.01	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	**0.39**	< LOQ	< LOQ	**0.10**	**0.35**	< LOQ	**0.24**	**0.06**	**0.32**
LOQ		*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	0.01	0.01	*0.02*	*0.02*	*0.01*	*0.02*	*0.01*	*0.01*	*0.02*	*0.01*	*0.01*

Table SI2: Ambient groundwater composition used in the simulations.

Component	*Ambient groundwater and recharge [mol/L]*
Na	1.92×10^{-3}
Cl	8.51×10^{-3}
K	2.10×10^{-3}
Ca	3.94×10^{-3}
Mg	8.84×10^{-4}
DO	1.25×10^{-3}
NO_3^-	2.29×10^{-3}
NO_2^-	0
N_2	0
SO_4^{2-}	5.33×10^{-4}
S^{2-}	0
Fe(II)	0
Fe(III)	3.78×10^{-3}
Mn	0
CH_4	0
DOC	4.00×10^{-4}
SOC,h	0.67 (stream bed sediment)
SOC,l	0.49 (aquifer)
pH	6.71
pe	13.52
Iomeprol	4.24×10^{-11}
TPs (Phase I)	0.00
TPs (Phase II)	7.23×10^{-10}

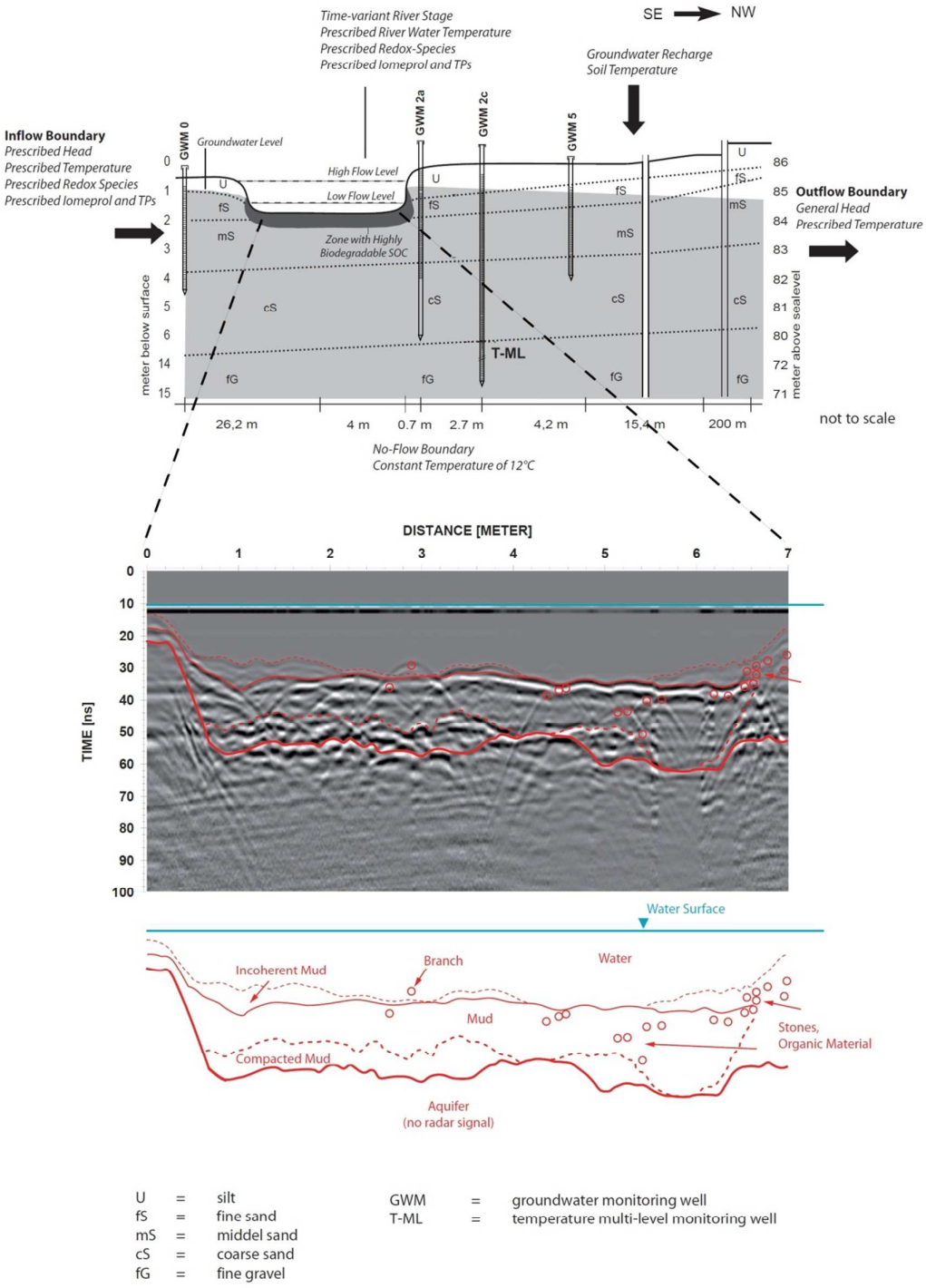


Figure SI1: Investigated 2D transect, hydrostratigraphic layer, monitoring locations, hydraulic and transport boundary conditions (adapted from Engelhardt et al., 2013) used in the numerical model and analyzed ground-penetrating radargram through the stream bed sediments.

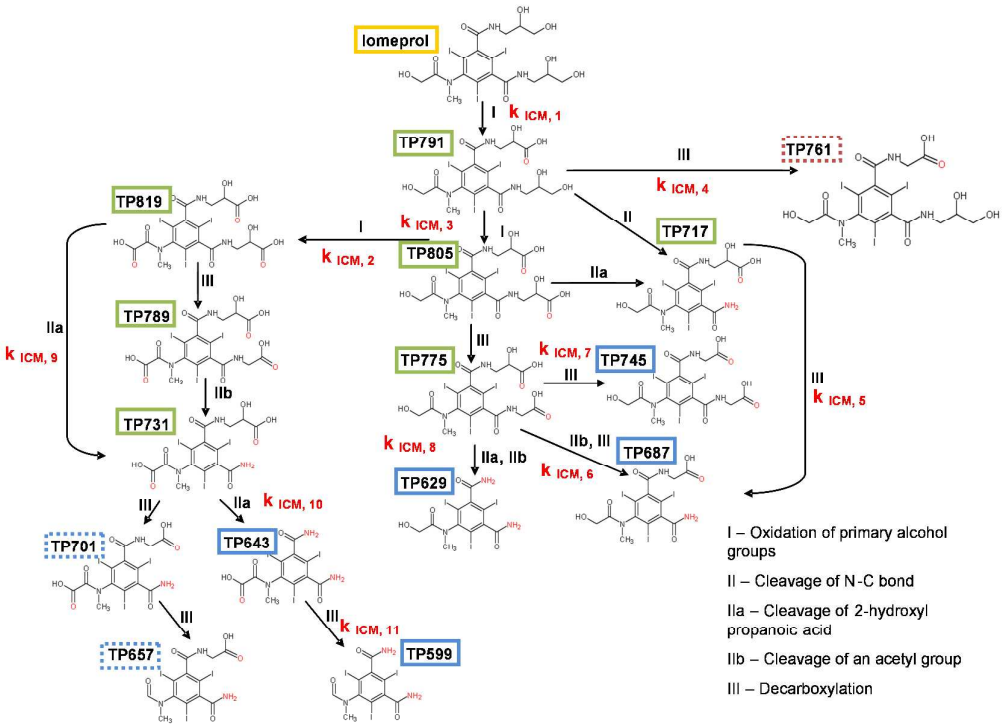
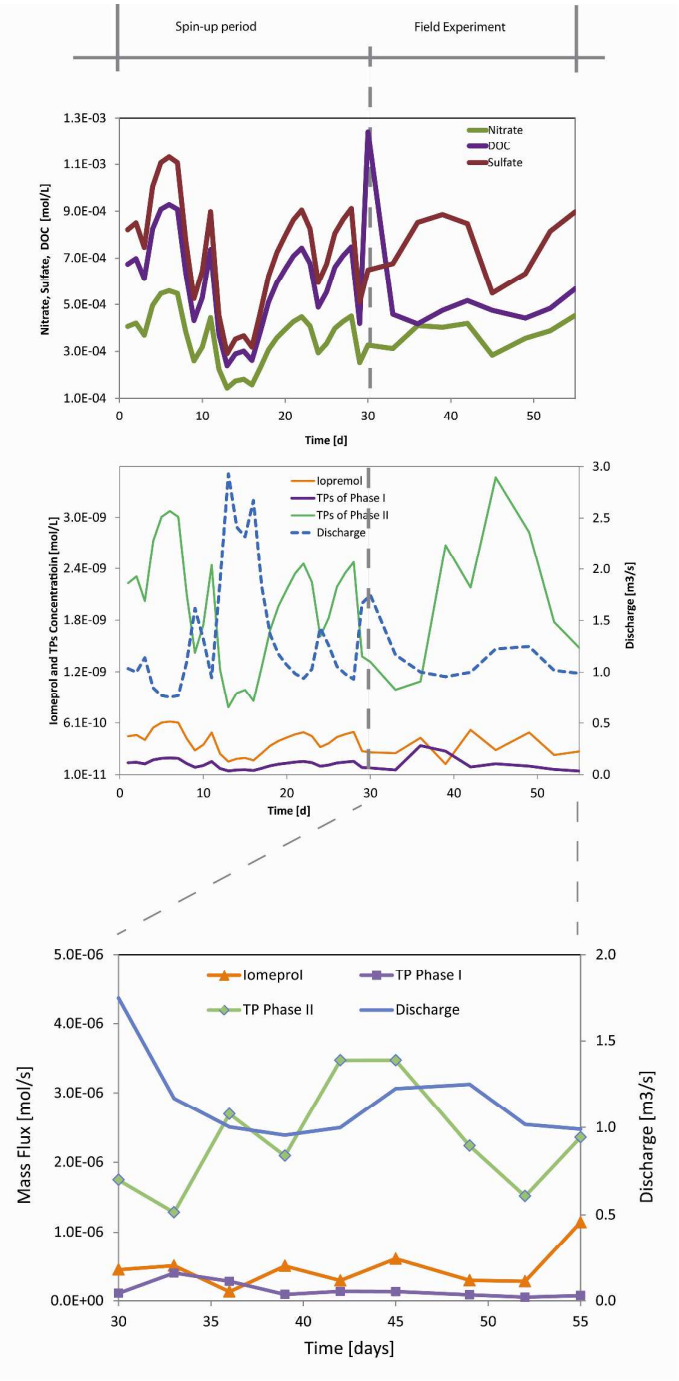


Figure SI2: Simulated transformation steps ($k_{ICM1,...11}$) based on the proposed microbial transformation of iomeprol under aerobic conditions at lab scale (modified after Kormos et al., 2010). TPs of phase I are marked in green, TPs of phase II in blue. TPs that were not detected in the groundwater and stream are marked in dashed lines.



59

60 **Figure SI3: Reconstruction of the geochemical composition, concentration of iomeprol**
61 **and its TPs during the spin-up period (zero to 29 days), measured**
62 **concentration of the geochemical species, measured concentration and mass**
63 **flux of iomeprol and its TPs during the field experiment (30 to 55 days), and**
64 **measured discharge.**

65

Non-reactive Transport Model

The conservative multi-species transport model was set up by a joined inversion of water, temperature transport and solute transport of the artificial sweetener acesulfame.

Conceptual Model. The five aquifer zones (from top to bottom: silt, fine sand, middle sand, coarse sand, and fine gravel) were discretized by a grid of 243 rows into 31 layers with a thickness of 0.2 m in the zone of water table fluctuations that is increasing successively with depth (Figure SI1). The horizontal grid spacing was 0.5 m.

Initial parameter values were based on the interpretation of pumping test (hydraulic conductivity, storage, porosity) or calculated from literature data (thermal conductivity, specific heat capacity, diffusion, thermal distribution coefficient, bulk density, dispersion) and then optimized during the automated inversion process using PEST (Doherty, 2010).

Flow Simulations. For the description of the hydraulic pattern the SE inflow boundary was defined as transient prescribed hydraulic head derived from measured time series in GWM0 (Figure SI1). The NW boundary equals a general head boundary. Groundwater recharge was applied to the uppermost active model layer calculated from measured precipitation. A prescribed head boundary condition was applied to the cells representing the stream bottom with the defined elevations corresponding to the measured stream stages (Figure SI1). The study period was a highly transient period during which the Schwarzbach regularly alternated between losing and gaining conditions. The start of the investigated period was characterized by stream-losing conditions and included a flush flood between day 12 and 18 with a switch to stream-gaining conditions between days 18 and 29. After day 30, a second losing period prevailed for ~6 days, followed by a third gaining-dominated period between day 44 and 50.

The gaining period was interrupted by many short losing events that lasted for only a few hours. The calibrated numerical flow model reproduced observed hydraulic heads measured at S3 and GWM2 and their dynamic changes generally very well.

Conservative Temperature and Solute Transport Model. Temperature transport was simulated on the base of the a priori computed transient flow-field. Along the SE inflow boundary variable temperatures were defined from daily measured groundwater temperature data. At the model bottom a constant temperature of 12°C prevailed. Recharge temperature was given by soil temperatures measured at 10 cm depth. The surface water temperature was assigned as prescribed temperature boundary to the stream cells according to the measured stream water temperature. For the conservative transport simulation of the artificial sweetener acesulfame a constant concentration was prescribed at the SE (upstream) model boundary. A similar value was used for the initial concentration. The value is an average of all acesulfame data collected. This accounts for the background concentration of acesulfame that prevails already within the environment. For the spin-up period between August 15th and September 14th, 2010, were no acesulfame data were available, time-variant acesulfame concentrations were reconstructed. For the remaining period the acesulfame concentration was assigned to stream cells as measured. This model was constructed for calibrating a reliable conservative transport model using hydraulic, temperature, and acesulfame data sets as constraints to estimate all hydraulic and conservative transport parameter.

Doherty, J. 2010. PEST - Model-Independent Parameter Estimation. User's Manual, 5th ed.; Watermark Numerical Computing: Brisbane, Australia.