Supporting Information

Geochemistry of inorganic nitrogen in waters released from coal-bed natural gas production wells in the Powder River Basin, Wyoming

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Supporting Information.

Table 1A. Selected water constituents for CBNG production water discharge samples collected for this study in 2004.

Location	Date Collected	Lat[a] DD	Long[a] DD	pH	Temp ºC	Specific cond. µS cm^{-1}	Alkalinity meq L^{-1}	Cl^- µM	$SO_4^=$ µM	NO_3^- µM	NO_2^- µM	NH_4^+ µM	Total DIN[b] µM	DOC µM
Okeson Draw Reservoir	May-04	44.688	-105.978	7.96	13.5	2370	14	378	65	<5	<1	120	120	322
Shell Creek	May-04	44.767	-105.823	7.61	16.1	1502	9	281	15	<5	<1	95	96	133
LX Bar/Bar Creek	May-04	44.790	-105.831	8.25	16.7	1830	10	453	11	<5	<1	95	95	201
Big Reservoir	May-04	44.126	-106.156	6.90	20	3680	21	844	52	<5	<1	502	502	186
Beaver Creek	May-04	44.082	-105.991	7.48	20.8	1980	11	227	16	6	<1	135	141	383
Juniper Reservoir	May-04	44.209	-106.227	6.99	31.7	3170	18	1287	11	<5	<1	407	408	169
Burger Draw Discharge Sources[d]														
1	May-04	44.134	-106.099	7.64	21.5	3930	23	1111	12	6	<1	380	386	244
2	May-04	44.138	-106.099	7.52	23.6	3840	22	1150	47	<5	<1	229	230	202
3	Jun-04	44.121	-106.102	7.10	24.5	4470	26	886	9	<5	<1	455	456	233
4	May-04	44.133	-106.108	7.42	21.5	4200	25	1087	17	7	<1	445	452	244
5	Jun-04	44.134	-106.110	7.44	18.6	4290	25	1160	27	<5	<1	401	401	261
6	Jun-04	44.125	-106.113	7.16	23.2	3570	19	648	112	<5	<1	244	244	236
7	Jun-04	44.136	-106.117	7.12	20.1	3810	21	813	25	<5	<1	502	502	234
8	Jun-04	44.136	-106.117	7.67	20.3	4150	23	1075	225	<5	<1	446	446	245
9	Jun-04	44.126	-106.119	7.04	26.1	4110	23	650	7	<5	<1	439	439	249
10	Jun-04	44.137	-106.122	7.20	23.8	3750	21	738	<5	<5	<1	430	430	269
11	Jun-04	44.139	-106.126	6.93	n/a[e]	3720	21	887	7	6	<1	527	534	439
12	Jun-04	44.145	-106.133	n/a	n/a	n/a	20	899	8	<5	<1	447	448	246
13	Jun-04	44.147	-106.133	7.16	25.4	3530	19	929	7	<5	<1	472	472	245

Table 1A (continued)

Location	Date Collected	Lat[a] DD	Long[a] DD	Na^{+} µM	K+ µM	Ca^{+2} µM	Mg^{+2} µM	SAR[c]
Okeson Draw Reservoir	May-04	44.688	-105.978	27482	314	595	496	26.31
Shell Creek	May-04	44.767	-105.823	16553	271	486	234	19.51
LX Bar/Bar Creek	May-04	44.790	-105.831	20399	281	411	184	26.46
Big Reservoir	May-04	44.126	-106.156	40260	1241	1444	1108	25.20
Beaver Creek	May-04	44.082	-105.991	21175	358	832	514	18.25
Juniper Reservoir	May-04	44.209	-106.227	34764	903	711	476	31.91
Burger Draw Discharge Sources[d]								
1	May-04	44.134	-106.099	43286	1035	1509	1527	24.84
2	May-04	44.138	-106.099	41800	1226	1427	1518	24.36
3	Jun-04	44.121	-106.102	55910	1408	1316	1565	32.94
4	May-04	44.133	-106.108	46968	1137	1438	1394	27.91
5	Jun-04	44.134	-106.110	53834	993	1188	1141	35.27
6	Jun-04	44.125	-106.113	42442	1228	1607	1154	25.54
7	Jun-04	44.136	-106.117	46299	1218	1289	1143	29.69
8	Jun-04	44.136	-106.117	52176	1445	1245	1146	33.74
9	Jun-04	44.126	-106.119	50009	1387	1474	1448	29.25
10	Jun-04	44.137	-106.122	45855	1212	1235	1283	28.90
11	Jun-04	44.139	-106.126	45377	1254	1286	1159	29.02
12	Jun-04	44.145	-106.133	42579	1125	1470	1144	26.34
13	Jun-04	44.147	-106.133	42784	1180	1375	1089	27.25

[a]Decimal degrees (DD).
[b]Dissolved inorganic nitrogen (DIN); nitrate + nitrite + ammonium concentrations.
[c]Sodium adsorption ratio (SAR), calculated as described in (*1*).
[d]Locations for Burger Draw discharge points are shown in Figure 1.
[e]Not available (n/a).

Table 2A. Selected water constituents for synoptic sample collection in Burger Draw Trib. B, July 2003 and Trib. C, March 2005.

Sample Name	Location[a]	Date Collected	Time Collected	Distance meters	pH	Temp ºC	Specific cond. µS cm^{-1}	Alk meq/L	Cl^- µM	$SO_4^=$ µM	NO_3^- µM	NO_2^- µM	NH_4^+ µM	Total DIN[b] µM	DOC µM
Trib. B	1	7/31/2003	16:10	0	7.30	26.9	3940	24	990	165	<5	<1	351	351	304
Trib. B	2	7/31/2003	16:12	4	7.65	26.8	3940	24	1048	196	<5	<1	413	413	343
Trib. B	3	7/31/2003	16:13	6	7.72	26.7	3940	23	986	160	<5	<1	386	386	320
Trib. B	4	7/31/2003	16:14	11	7.80	26.6	3820	23	987	161	11	<1	384	396	314
Trib. B	5	7/31/2003	16:16	24	7.90	26.7	3680	23	993	170	12	5	399	417	308
Trib. B	6	7/31/2003	16:40	62	8.03	26.2	3910	23	1000	167	9	30	284	323	316
Trib. B	7	7/31/2003	16:51	77	8.15	25.9	3890	23	1013	159	15	63	230	308	346
Trib. B	8	7/31/2003	17:35	113	8.31	23.9	3840	23	918	121	33	132	100	265	341
Trib. B	9	7/31/2003	17:45	136	8.40	23.4	3850	23	1030	143	84	123	86	293	341
Trib. B	10	7/31/2003	17:53	166	8.36	22.9	3880	23	1001	135	107	68	46	222	385
Trib. B	11	7/31/2003	18:02	243	8.69	24.2	3920	23	938	128	121	<1	<5	122	400
Trib. B	12	7/31/2003	18:10	322	8.78	24.2	3940	24	1036	126	125	<1	<5	125	433
Trib. B	13	7/31/2003	18:18	389	8.82	24.0	3960	24	1007	121	112	<1	<5	112	439
Trib. B	14	7/31/2003	18:00	450	8.86	23.8	3980	24	1044	139	113	<1	<5	114	523
Trib. C	1	3/9/2005	12:38	0	7.15	23.1	4140	51	822	9	<5	<1	197	197	315
Trib. C	2	3/9/2005	n/a[c]	50	n/a	n/a	n/a	48	831	96	16	25	178	219	300
Trib. C	3	3/9/2005	n/a	250	n/a	n/a	n/a	47	836	635	26	34	149	208	364
Trib. C	4	3/9/2005	n/a	735	n/a	n/a	n/a	47	862	1115	47	41	112	200	405
Trib. C	5	3/9/2005	n/a	955	n/a	n/a	n/a	40	793	2460	70	34	52	157	451
Trib. C	6	3/9/2005	n/a	1255	n/a	n/a	n/a	41	797	2435	79	31	47	157	448
Trib. C	7	3/9/2005	13:40	1555	n/a	n/a	n/a	39	777	2484	84	28	39	150	431

[a]Location for sampling station 1 in Trib. B and Trib. C are shown in Figure 1. Other stations are downstream from station 1 according to the distance given.
[b]Dissolved inorganic nitrogen (DIN); nitrate + nitrite + ammonium concentrations.
[c]Not available (n/a).

Table 3A. Selected water constituents for synoptic sample collection in the Burger Draw main channel in May 2002, July 2003, June 2004, and March 2005.

Sample Name	Location[a]	Date Collected	Time Collected	Distance meters	pH	Temp ºC	Specific cond. µS cm^{-1}	Alk meq/L	Cl^- µM	$SO_4^=$ µM	NO_3^- µM	NO_2^- µM	NH_4^+ µM	Total DIN[b] µM	DOC µM
Burger Draw	1	5/29/2002	n/a[c]	0	8.14	25.9	4210	24	925	52	53	57	304	414	283
Burger Draw	2	5/30/2002	n/a	265	8.16	27.9	4040	24	910	86	77	80	167	324	268
Burger Draw	3	5/30/2002	n/a	555	8.24	25.0	4020	24	1010	52	73	67	204	344	273
Burger Draw	4	5/30/2002	n/a	1181	7.94	28.5	4090	25	862	94	56	122	202	381	275
Burger Draw	5	5/30/2002	n/a	2136	8.26	31.9	4220	25	838	31	76	131	160	367	296
Burger Draw	6	5/30/2002	n/a	2695	8.23	31.6	4160	25	781	47	69	131	186	387	328
Burger Draw	7	5/30/2002	n/a	4369	8.24	31.0	4060	24	692	112	90	127	178	395	372
Burger Draw	8	5/29/2002	n/a	5130	8.23	25.4	4160	24	748	212	199	70	90	359	413
Burger Draw	1	7/30/2003	n/a	0	8.41	n/a	3910	23	961	149	85	58	127	271	357
Burger Draw	2	7/30/2003	n/a	265	8.57	25.0	3870	23	975	145	99	115	70	284	336
Burger Draw	3	7/30/2003	n/a	555	8.61	26.0	3840	23	1006	147	138	80	<5	218	341
Burger Draw	4	7/30/2003	13:10	1181	8.46	27.0	3960	24	791	260	175	40	<5	215	n/a
Burger Draw	5	7/30/2003	15:25	2136	8.79	29.0	4020	24	894	362	192	30	<5	222	401
Burger Draw	6	7/30/2003	16:00	2695	8.77	29.0	3960	23	858	478	167	47	103	317	446
Burger Draw	7	7/30/2003	16:50	4369	8.80	28.0	3900	23	789	303	159	59	98	316	436
Burger Draw	8	7/30/2003	17:25	5230	8.69	n/a	3870	23	781	276	163	59	68	290	443
Burger Draw	1	6/22/2004	n/a	0	8.45	19.0	3920	23	1078	14	41	42	113	195	342
Burger Draw	2	6/22/2004	n/a	265	8.55	18.1	3920	23	1078	14	37	35	171	242	335
Burger Draw	3	6/22/2004	n/a	555	8.59	19.0	3930	23	1098	14	34	25	101	160	400
Burger Draw	4	6/22/2004	n/a	1181	8.31	24.6	4010	23	1019	21	37	46	217	300	320
Burger Draw	5	6/22/2004	n/a	2136	8.61	24.9	4160	24	1012	176	142	53	50	245	394
Burger Draw	6	6/22/2004	n/a	2695	8.52	24.6	4040	23	960	285	113	39	79	231	393
Burger Draw	7	6/22/2004	n/a	4369	8.73	23.8	4020	23	888	288	123	52	44	218	423
Burger Draw	8	6/22/2004	n/a	5230	8.54	22.0	3880	22	802	130	53	38	210	302	372

Table 3A (continued)

Sample Name	Location[a]	Date Collected	Time Collected	Distance meters	pH	Temp ºC	Specific cond. µS cm^{-1}	Alk meq/L	Cl^- µM	$SO_4^=$ µM	NO_3^- µM	NO_2^- µM	NH_4^+ µM	Total DIN[b] µM	DOC µM
Burger Draw	1	3/9/2005	10:08	0	8.64	13.4	3710	46	1077	20	43	24	119	186	439
Burger Draw	2	3/9/2005	9:35	265	8.77	10.9	3700	46	1093	20	62	24	92	179	312
Burger Draw	3	3/9/2005	10:40	555	8.71	12.1	3710	46	1096	19	68	23	79	170	324
Burger Draw	4	3/9/2005	11:05	1181	8.57	16.9	3720	45	1010	15	48	27	74	149	312
Burger Draw	5	3/9/2005	14:34	2136	8.57	15.6	3770	45	967	389	91	28	16	135	387
Burger Draw	6	3/9/2005	14:46	2695	8.85	14.1	3760	44	944	645	115	22	9	147	434
Burger Draw	8	3/9/2005	15:11	5230	8.65	13.1	3700	43	833	399	100	22	119	241	500

[a]Location for sampling station 1 is shown in Figure 1. Other stations are downstream from station 1 according to the distance given.
[b]Dissolved inorganic nitrogen (DIN); nitrate + nitrite + ammonium concentrations.
[c]Not available (n/a).

Table 4A. Selected water constituents for diel sample collection in Burger Draw Trib. B, location 14, in July 2003.

Date Sampled	Time Sampled	pH	Temp C	O_2 µM	Light watts/m^2	Cl^- µM	$SO_4^=$ µM	NO_3^- µM	NO_2^- µM	NH_4^+ µM	Total DIN[a] µM
7/28/2003	1600	8.66	31.0	230	725	1010	99	153	<1	<5	153
7/28/2003	1800	8.60	29.2	167	77	1022	105	134	<1	<5	134
7/28/2003	2000	8.49	26.2	118	5	1019	104	112	1	<5	113
7/28/2003	2200	8.43	23.4	143	0	1014	101	75	8	<5	83
7/29/2003	0000	8.40	21.5	160	0	1006	106	89	30	<5	119
7/29/2003	200	8.40	20.5	167	0	1003	97	108	37	<5	145
7/29/2003	400	8.40	19.4	176	0	1024	93	120	38	<5	158
7/29/2003	600	8.40	18.3	186	7	1034	89	125	39	<5	165
7/29/2003	800	8.43	18.9	240	340	1035	79	145	35	<5	180
7/29/2003	1000	8.50	21.3	301	772	1031	77	202	5	<5	208
7/29/2003	1200	8.60	25.1	345	943	1028	71	197	<1	<5	197
7/29/2003	1400	8.69	28.5	341	1075	1045	90	160	<1	<5	160
7/29/2003	1600	8.77	27.7	246	217	1098	187	133	<1	<5	133
7/29/2003	1800	8.59	25.7	232	460	1120	920	132	<1	<5	133
7/29/2003	2000	8.44	22.8	173	21	1041	278	137	4	<5	141
7/29/2003	2200	8.39	20.2	176	0	1034	127	120	22	<5	142
7/30/2003	0000	8.39	18.7	187	0	1046	95	115	33	<5	148
7/30/2003	200	8.39	17.4	198	0	1054	85	125	37	<5	163
7/30/2003	400	8.40	16.5	206	0	1045	92	132	39	<5	171
7/30/2003	600	8.40	15.9	214	8	1025	103	139	40	<5	179
7/30/2003	800	8.41	16.6	243	316	1027	114	148	37	<5	185
7/30/2003	1000	8.48	20.7	292	788	1028	123	196	13	<5	209
7/30/2003	1200	8.57	26.3	322	1075	1020	119	205	<1	<5	206
7/30/2003	1400	8.63	30.4	305	1071	1039	150	177	<1	<5	177
7/30/2003	1600	8.65	30.4	262	752	1049	143	155	<1	<5	155
7/30/2003	1800	8.61	27.6	184	417	1046	149	131	<1	<5	131
7/30/2003	2000	8.54	24.5	132	21	1053	175	93	<1	<5	94
7/30/2003	2200	8.48	21.2	133	0	1092	183	67	<1	<5	68

Table 4A (continued).

Date Sampled	Time Sampled	pH	Temp C	O_2 µM	Light watts/m^2	Cl^- µM	$SO_4^=$ µM	NO_3^- µM	NO_2^- µM	NH_4^+ µM	Total DIN[a] µM
7/31/2003	0000	8.41	19.0	183	0	1091	133	93	18	<5	111
7/31/2003	200	8.40	17.5	195	0	1031	129	117	33	<5	150
7/31/2003	400	8.40	16.7	202	0	771	82	105	29	<5	134
7/31/2003	600	8.41	16.2	196	5	973	101	143	27	<5	170
7/31/2003	800	8.45	17.2	246	278	1020	117	154	16	<5	170
7/31/2003	1000	8.51	20.5	304	745	828	122	153	<1	<5	154
7/31/2003	1200	8.60	25.7	333	919	740	101	131	<1	<5	131
7/31/2003	1400	8.65	26.7	191	68	1058	139	146	<1	<5	146
7/31/2003	1600	8.66	29.8	279	599	1082	157	131	<1	<5	132
7/31/2003	1800	8.60	24.5	156	89	1044	139	113	<1	<5	114

[a]Dissolved inorganic nitrogen (DIN); nitrate + nitrite + ammonium concentrations.

Table 5A. Ammonium and DIN uptake parameters for Burger Draw Tributaries B and C calculated from synoptic sampling events[1].

Date	Time		NH_4^+ Uptake[2,3] $[NH_4^+]>50$ µM			DIN Uptake[2,3] $[NH_4^+]>50$ µM		DIN Uptake[2,3] $[NH_4^+]<50$ µM	
			S_w m	v_f m hr^{-1}	$k1$ day^{-1}	S_w m	$k1$ day^{-1}	S_w m	$k1$ day^{-1}
Tributary B									
31-Jul-03	1600		63	0.083	28.5	256	9.2	2000	0.9
1-Aug-03	700		91	0.058	19.8	196	7.0	833	2.2
23-Jun-04	1100		14	0.369	126.4	182	9.9	256	7.0
23-Jun-04	1700		21	0.256	87.7	75	24.1	79	22.9
23-Jun-04	2300		25	0.209	71.7	49	36.6	147	12.2
8-Mar-05	1100		70	0.075	25.6	333	5.4	1000	1.8
11-Sep-05	2200		50	0.106	36.4	271	8.3	1250	1.4
		Avg	48	0.165	56.6	195	14.4	795	6.9
		Std dev	29	0.117	40.0	104	11.6	698	8.1
Tributary C									
8-Mar-05	1100		909	0.031	14.7	5000	2.7	n/a	n/a
11-Sep-05	1300		714	0.039	18.8	-25000	-0.5	n/a	n/a
		Avg	812	0.035	16.8	-10000	1.1		
		Std dev	138	0.006	2.8	21213	2.3		

[1]DIN (dissolved inorganic nitrogen) = $[NO_3^-] + [NO_2^-] + [NH_4^+]$.
[2]Ammonium uptake calculated for up-stream reach of tributary where $[NH_4^+] > 50$ µM. DIN uptake calculated for same reach and for reach in which $[NH_4^+] < 50$ µM.
[3]Uptake parameters were defined and calculated as described in (*1, 2*):

S_w = uptake length, or average distance traveled by a solute molecule before being removed or reacted. S_w was determined as the negative inverse of the slope of the natural log of the solute concentration as a function of transport distance down-gradient. Inorganic nitrogen was treated as a point source discharge, concentration changes were normalized relative to chloride in the discharge water. Groundwater input was assumed to be zero.

v_f, the mass transfer coefficient = uz/S_w. Where u is the average reach depth and z is average stream velocity, determined using rhodamine tracer tests.

$k1$, the first order rate constant for solute concentration decrease = v_f/u.

Table 6A. Nitrogen loads in Powder River above and below Burger Draw.

Date	Above Burger Draw USGS Station 6313590			Below Burger Draw USGS Station 6313605	
	Q[a] (m^3 sec^{-1})	DIN[b] (mg L^{-1})	N load (kg day^{-1})	DIN (mg L^{-1})	N load (kg day^{-1})
Sept 8, 2004	0.31	0.14	3.76	1.93	51.81
July 13, 2005	0.59	0.19	9.82	0.38	19.51

[a]Daily average discharge from station 6313590 (*3*) used for both stations. See Fig. 1 for station locations.
[b]Dissolved inorganic nitrogen (DIN), sum of dissolved concentrations of nitrate, nitrite, and ammonium. Samples were collected as depth- and width-integrated composites, as previously described (*4*).

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