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Supplemental Information for:

Exploring the Hydraulic Fracturing Parameter Space: A Novel High-Pressure, High-Throughput Reactor System for Investigating Subsurface Chemical Transformations

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Analytical details

All glassware was combusted in a muffle furnace for 8 hr at 450°C. Glass syringes with metal needles and plungers were used for sample transfer and preparation of standards and were rinsed with high purity solvents (hexane, dichloromethane (DCM), acetone, methanol) and HPLC-grade water prior to use.

LLE: The liquid-liquid extraction (LLE) method began with quenching the reactors on ice for rapid cooling. Reactors were then unsealed and contents were poured into separatory funnels. Each reactor was rinsed three times with 3mL of 90:10 dichloromethane/methanol, followed by a 30mL volume of solvent addition. All contents were then poured into the separatory funnels which were shaken vigorously (with venting as necessary) for 2 minutes. After 20 minutes, the bottom organic layer was deposited into a round bottom flask. This process was repeated two more times with 30mL solvent additions. The organic extracts were then dried with anhydrous Na_2SO_4 and rotary evaporated to approximately 10mL.

GC×GC TOF-MS: These analyses were performed on a LECO Pegasus 4D Comprehensive Two-Dimensional Gas Chromatography with Time-of-Flight Mass Spectrometer (GC×GC TOF MS) system (St. Joseph, MI, USA). The primary column was a Restek Rtx-1MS (60m length x 250µm d. x 0.25µm film thickness; 50°C, 2 min hold, 5°C min^{-1} ramp to 120°C, 10°C min^{-1} ramp to 250°C, 25°C min^{-1} ramp to 300°C, 2 min hold) and the secondary column was an SGE BPX50 (1.5m (0.21 m in the transfer line) x 100µm x 0.10µm; +5°C offset from the primary column and a 6 second modulation) under a flow rate of 1mL min^{-1} with a 200:1 split. The MS sampled an m/z range of 40-550 amu at a rate of 200 spectra/second.

Table S1: Complete parameter review data for all geological basins. Well temperature and depth data from SMU NGDS data and produced water composition and pH data are listed for all geological basins. See highlighted basins with geospatial plotting in main text, Figure 1a & b. Parameter values are reported as Median, 5th, and 95th percentiles. Sample sizes are reported and based on data availability.

Basins	SMU NGDS Data								
		Bottom hole temperature, °C				Well Depth, m			
	n		Percentile				Percentile		
	(database)	n	Median	5th	95th	n	Median	5th	95th
TOTAL (all basins)	**964334**	**133031**	**77**	**23**	**148**	**643096**	**1780**	**265**	**4086**
Amarillo Arch	23788	562	77	36	102	12235	1000	673	3113
Anadarko	31084	6544	72	37	115	23011	2480	703	4587
Anadarko - Chautauqua Platform	0	0	-	-	-	0	-	-	-
Anadarko - Southern Oklahoma	0	0	-	-	-	0	-	-	-
Appalachian	17283	17017	37	25	73	17264	1273	647	2886
Arkla	0	0	-	-	-	0	-	-	-
Arkoma	198	195	53	29	116	195	1954	370	4216
Arkoma - Chautauqua Platform	0	0	-	-	-	0	-	-	-
Atlantic Coastal Plain	145	136	47	33	76	143	1370	895	3179
Bend Arch	0	0	-	-	-	0	-	-	-
Big Horn	0	0	-	-	-	0	-	-	-
Black Mesa	90	78	42	19	56	78	1375	90	2088
Black Warrior	11	11	60	37	68	11	1800	731	2262
Central Kansas Uplift	797	778	39	31	51	787	1045	550	1594
Central Monta- Uplift	0	0	-	-	-	0	-	-	-
Chadron Arch	932	922	50	15	72	930	1331	98	2156
Chautauqua Platform	1296	1177	56	34	99	1267	2138	555	4666
Cherokee	1	1	24	24	24	1	340	340	340
Cincin-ti Arch	0	0	-	-	-	0	-	-	-
Denver	528	454	57	11	99	481	1740	89	2928
Desha	0	0	-	-	-	0	-	-	-
Eagle	0	0	-	-	-	0	-	-	-
East Texas	0	0	-	-	-	0	-	-	-
Forest City	6	5	16	14	17	6	158	152	945
Fort Worth	0	0	-	-	-	0	-	-	-
Great Basin	9278	6435	23	11	121	7522	115	30	3008
Green River	61	25	141	30	202	39	544	73	2330
Gulf Coast	121467	38795	98	48	147	88361	3139	977	5125
Han-	0	0	-	-	-	0	-	-	-
Hoback	0	0	-	-	-	0	-	-	-
Illinois	1601	1559	35	25	48	1592	918	368	1899
Illinois - Michigan	8	8	35	22	40	8	1306	333	1345
Kerr	0	0	-	-	-	0	-	-	-
Laramie	0	0	-	-	-	0	-	-	-
Las Animas Arch	6	5	49	45	56	5	1629	1540	1656
Las Vegas - Raton	1202	1177	49	35	84	1177	811	613	1871
Llano Uplift	0	0	-	-	-	0	-	-	-
Los Angeles	26	2	38	26	50	25	2167	5	4100
Michigan	1090	1081	41	27	73	1090	1607	693	3565
Nemaha Uplift	0	0	-	-	-	0	-	-	-
North Park	0	0	-	-	-	0	-	-	-
Orogrande	0	0	-	-	-	0	-	-	-
Ozark Uplift	0	0	-	-	-	0	-	-	-
Pacific Coast	5	0	-	-	-	5	976	199	2163
Palo Duro	0	0	-	-	-	0	-	-	-
Paradox	160	47	21	17	36	120	1100	195	3045
Permian	730276	47049	91	42	161	471897	1646	287	3763
Permian - Bend Arch	0	0	-	-	-	0	-	-	-
Piceance	85	71	37	13	112	74	805	82	2335

Basins	SMU NGDS Data								
	n	Bottom hole temperature, °C				Well Depth, m			
			Percentile				Percentile		
	(database)	n	Median	5th	95th	n	Median	5th	95th
TOTAL (all basins)	**964334**	**133031**	**77**	**23**	**148**	**643096**	**1780**	**265**	**4086**
Powder River	1646	1581	62	27	99	1615	2282	274	3673
Powder River - Wind River	0	0	-	-	-	0	-	-	-
Puget Sound	0	0	-	-	-	0	-	-	-
Raton	0	0	-	-	-	0	-	-	-
Rocky Mountain	0	0	-	-	-	0	-	-	-
Sacramento	0	0	-	-	-	0	-	-	-
Sali-	0	0	-	-	-	0	-	-	-
San Joaquin	0	0	-	-	-	0	-	-	-
San Juan	864	555	56	20	99	556	2011	188	3437
Santa Maria	0	0	-	-	-	0	-	-	-
Sedgwick	0	0	-	-	-	0	-	-	-
Shirley	0	0	-	-	-	0	-	-	-
Sierra Grande Uplift	0	0	-	-	-	0	-	-	-
Sioux Uplift	0	0	-	-	-	0	-	-	-
S-ke River	265	238	29	9	101	240	137	27	3100
South Florida	143	141	79	52	110	143	3560	3000	4091
Southern Oklahoma	0	0	-	-	-	0	-	-	-
Strawn	0	0	-	-	-	0	-	-	-
Sweetgrass Arch	212	200	32	18	54	200	1149	426	2842
Uinta	0	0	-	-	-	0	-	-	-
Uinta - Piceance	0	0	-	-	-	0	-	-	-
Upper Mississippi Embayment	0	0	-	-	-	0	-	-	-
Ventura	0	0	-	-	-	0	-	-	-
Wasatch Uplift	0	0	-	-	-	0	-	-	-
Western Columbia	4	4	25	25	25	4	540	540	540
Williston	1245	1184	58	22	113	1186	1991	452	3850
Wind River	0	0	-	-	-	0	-	-	-
Wyoming Thrust Belt	3147	1719	23	8	81	1820	120	33	1954
Yellowstone	0	0	-	-	-	0	-	-	-

Basins	n (database)	Chloride, mg/L				Bromide, mg/L				Iodide, mg/L				pH			
			Percentile				Percentile				Percentile				Percentile		
		n	Median	5th	95th	n	Median	5th	95th	n	Median	5th	95th	n	Median	5th	95th
TOTAL (all basins)	**154117**	**129499**	**7340**	**9**	**174721**	**7638**	**13**	**0**	**1684**	**3663**	**8**	**0**	**77**	**116050**	**7**	**6**	**9**
Amarillo Arch	181	181	102000	16835	142375	3	172	139	343	3	18	5	18	163	7	4	8
Anadarko	2031	2030	86228	4686	162125	99	380	40	932	107	100	8	846	1439	6	5	8
Anadarko - Chautauqua Platform	97	97	127656	52118	176897	0	-	-	-	0	-	-	-	14	6	5	6
Anadarko - Southern Oklahoma	2603	2575	6957	2990	12000	0	-	-	-	0	-	-	-	2564	8	6	9
Appalachian	2414	1822	79950	8	206613	1327	692	12	2291	824	10	1	39	722	6	4	8
Arkla	2540	2540	65043	4466	205198	170	642	11	5705	162	16	4	65	2381	6	4	8
Arkoma	218	218	52573	989	114052	7	242	214	344	9	9	2	27	126	7	5	8
Arkoma - Chautauqua Platform	44	44	53942	3195	105068	0	-	-	-	0	-	-	-	1	7	7	7
Atlantic Coastal Plain	23	23	46909	24527	68989	2	114	106	121	2	1	0	2	17	7	6	8
Bend Arch	82	82	76907	35681	134485	5	223	181	322	5	14	13	51	77	6	4	7
Big Horn	2976	2962	392	21	12000	7	27	14	63	16	5	2	22	2601	8	7	9
Black Mesa	67	67	33031	5357	101752	1	20	20	20	1	20	20	20	67	7	6	8
Black Warrior	216	213	2800	140	49818	11	122	17	176	11	8	1	32	212	8	6	9
Central Kansas Uplift	4689	4633	30500	11096	122600	62	67	5	460	59	6	1	98	3281	7	6	8
Central Monta- Uplift	203	203	576	35	7307	0	-	-	-	0	-	-	-	193	8	6	9
Chadron Arch	71	71	3665	224	85000	3	5	5	5	0	-	-	-	63	8	6	9
Chautauqua Platform	5549	5549	105400	22070	159390	71	344	55	800	59	10	2	94	1278	6	5	8
Cherokee	29	29	36000	282	66458	1	72	72	72	0	-	-	-	17	7	6	7
Cincin-ti Arch	5	5	35428	10434	45461	0	-	-	-	0	-	-	-	5	7	7	8
Denver	1530	1527	4220	255	37258	2	51	44	57	26	2	1	37	1472	8	7	9
Desha	1	1	26100	26100	26100	0	-	-	-	0	-	-	-	1	7	7	7
Eagle	7	7	5934	1592	25960	0	-	-	-	0	-	-	-	7	8	7	9
East Texas	1739	1736	33484	3445	150038	13	630	10	2145	9	37	11	275	1700	7	5	8
Forest City	32	32	6464	2309	19767	0	-	-	-	0	-	-	-	0	-	-	-
Fort Worth	84	84	126650	39680	172027	5	646	411	693	5	17	13	22	65	6	4	7
Great Basin	45374	27086	36	3	1900	2763	0	0	23	755	0	0	0	30207	8	7	9
Green River	11820	11781	4000	140	23800	81	45	9	78	22	2	1	57	11274	7	6	9
Gulf Coast	14011	13966	45688	2478	140336	469	287	19	4877	381	18	4	31	12083	7	5	8
Han-	31	30	275	28	34398	0	-	-	-	0	-	-	-	30	9	7	10
Hoback	1	1	60	60	60	0	-	-	-	0	-	-	-	1	7	7	7
Illinois	1637	1388	66738	6727	94246	114	185	15	454	55	6	1	17	452	7	5	8
Illinois - Michigan	448	430	24300	1872	70830	223	89	11	196	0	-	-	-	301	7	5	8
Kerr	4	4	783	164	2898	0	-	-	-	0	-	-	-	4	7	7	8
Laramie	32	31	2020	20	12815	0	-	-	-	0	-	-	-	31	8	7	9
Las Animas Arch	108	108	7750	607	71819	0	-	-	-	0	-	-	-	89	8	6	9
Las Vegas - Raton	26	25	709	26	14573	0	-	-	-	0	-	-	-	25	9	7	10
Llano Uplift	47	47	39397	2150	67504	0	-	-	-	0	-	-	-	45	7	5	9
Los Angeles	300	299	17658	4243	20611	9	18	1	47	164	65	9	155	288	7	7	8
Michigan	581	415	175000	20348	238218	185	242	4	1303	33	12	8	27	226	6	4	7

Basins	n (database)	Chloride, mg/L				Bromide, mg/L				Iodide, mg/L				pH			
		n	Percentile			n	Percentile			n	Percentile			n	Percentile		
			Median	5th	95th		Median	5th	95th		Median	5th	95th		Median	5th	95th
TOTAL (all basins)	**154117**	**129499**	**7340**	**9**	**174721**	**7638**	**13**	**0**	**1684**	**3663**	**8**	**0**	**77**	**116050**	**7**	**6**	**9**
Nemaha Uplift	202	202	68007	17814	138285	18	170	29	217	16	3	1	6	91	7	6	8
North Park	93	93	410	90	3856	0	-	-	-	0	-	-	-	79	8	7	9
Orogrande	1	1	684	684	684	0	-	-	-	0	-	-	-	1	8	8	8
Ozark Uplift	2	2	1778	1678	1877	0	-	-	-	0	-	-	-	2	8	8	8
Pacific Coast	32	32	7357	441	16895	0	-	-	-	11	20	1	59	29	8	7	9
Palo Duro	283	283	108600	11029	158874	3	193	177	286	3	6	6	10	139	7	5	8
Paradox	640	640	30897	259	160234	15	41	3	278	10	12	2	42	608	7	6	9
Permian	14816	11225	53611	3479	156653	299	230	12	798	260	9	1	52	8585	7	5	8
Permian - Bend Arch	1	1	88200	88200	88200	0	-	-	-	0	-	-	-	1	3	3	3
Piceance	513	512	7061	215	65424	0	-	-	-	0	-	-	-	474	8	6	9
Powder River	6346	6288	2039	13	44000	64	0	0	23	10	11	2	48	6014	8	6	9
Powder River - Wind River	14	14	8375	245	10170	0	-	-	-	0	-	-	-	8	8	6	9
Puget Sound	1	1	381	381	381	0	-	-	-	0	-	-	-	1	9	9	9
Raton	2110	2095	7	2	55	600	1	0	18	0	-	-	-	2110	8	8	9
Rocky Mountain	3724	3724	2620	90	29480	2	237	126	348	5	4	1	89	3475	8	7	9
Sacramento	64	64	8530	2651	12870	61	35	10	74	60	26	7	58	54	7	7	8
Sali-	10	10	43793	5810	79265	1	37	37	37	0	-	-	-	9	7	6	7
San Joaquin	384	384	12143	300	24039	111	115	5	232	155	20	2	71	362	7	7	8
San Juan	4139	2800	705	7	25249	425	3	0	19	78	1	0	9	3369	8	6	9
Santa Maria	34	34	9960	3066	19924	0	-	-	-	2	6	1	10	32	8	5	8
Sedgwick	394	394	85682	12804	151935	14	201	15	392	2	7	3	11	101	7	5	8
Shirley	1	1	302	302	302	0	-	-	-	0	-	-	-	1	8	8	8
Sierra Grande Uplift	7	7	1350	158	23840	0	-	-	-	0	-	-	-	7	7	7	8
Sioux Uplift	2	2	78	74	82	0	-	-	-	0	-	-	-	2	8	8	8
S-ke River	7	7	224	145	1768	0	-	-	-	0	-	-	-	7	8	8	9
South Florida	60	60	148818	860	168246	1	695	695	695	0	-	-	-	55	6	5	9
Southern Oklahoma	1132	1131	86982	6997	153704	68	435	97	826	69	9	1	27	542	6	4	8
Strawn	1	1	47039	47039	47039	0	-	-	-	0	-	-	-	1	7	7	7
Sweetgrass Arch	612	612	800	134	7375	0	-	-	-	0	-	-	-	466	8	7	9
Uinta	879	877	4040	100	34000	58	21	3	196	56	13	2	32	857	8	7	9
Uinta - Piceance	41	41	2010	1270	17300	41	9	5	23	0	-	-	-	41	8	7	8
Upper Mississippi Embayment	1	1	72614	72614	72614	0	-	-	-	0	-	-	-	1	6	6	6
Ventura	31	31	15850	3443	19910	15	68	45	171	21	43	8	135	16	7	3	9
Wasatch Uplift	43	43	960	60	36590	1	3	3	3	1	9	9	9	39	8	7	9
Western Columbia	5	5	15788	13650	19119	5	36	29	112	5	16	13	20	5	7	6	8
Williston	10890	10879	164279	2120	213718	194	416	7	1312	175	13	1	88	10716	6	5	8
Wind River	4427	4399	1140	55	12450	9	3	2	620	15	6	1	196	3986	8	6	9
Wyoming Thrust Belt	171	171	14300	82	145000	0	-	-	-	1	7	7	7	155	7	4	10
Yellowstone	8	8	17100	110	21200	0	-	-	-	0	-	-	-	8	7	7	8

Table S2: Reactor system components and design details. Part names, quantities and notes regarding purpose, materials, and design choices are listed.

Vendor	Part Name	Qty	Design details and notes
Swagelok			
	Sample vessel	15	316 stainless-steel 150mL batch reactors, rated to 5000 psi
	Tubing, joints	-	1/4" 316 stainless-steel tubing and fittings to construct pressure manifold
	Ball valves	15	valves to seal off reactors and maintain pressure during experiments
	Check valve	1	upstream valve to prevent backflow from system to pump line
	Pressure gauge	1	inline gauge to read pressure
	Bleed valve	1	valve for releasing pressure after experiment
Thermo-Fisher Scientific	Multipoint 15 Stirrer	1	15 point magnetic stir plate, 20 watt option to penetrate thick stainless steel reactors
Bel-Art			
	Rare Earth Spinbar	15	magnetics for sample stirring, rare earth strength necessary to penetrate reactors
McMaster-Carr			
	Strut channels	-	Aluminum frame for supporting scaffold to lift and submerge manifold
	Winch	1	Winch to raise and lower manifold from support scaffold
Cole-Parmer			
	Immersion Heater	1	Immersion heater to power water bath
Amazon			
	Bayite hot water pump	1	Pump and plastic tubing for water bath circulation
	Water cooler	1	10 gallon water reservoir for refilling bath
	Aquarium pump	1	Pump and plastic tubing for refilling bath from reservoir
	Water level sensor	1	Stainless-steel floating level sensor for actuating refill pump
	Arduino Uno	1	Micro-controller to read input from sensor and turn on/off refill pump
	Lipavi container	1	Polycarbonate tank for water bath
	"Sous vide" water balls	2	Bag of floating plastic balls to mitigate evaporation at high temperature operation

Figure S1: Time resolved experiments of cinnamaldehyde and epichlorohydrin. Concentrations are normalized to the initial loading (150 mg). These figures are provided to demonstrate our understanding of the time-scale for chemicals at the concentrations and temperatures used in this study. In general, equilibrium occurs within a day or two, justifying our decision to terminate the experiment after a week.