Table 5. Percent Differences of Quantitation Limits to the EPA/ACS QL for the Episode 6000 Dataset

Analyte	Method	Procedure	ISO LOQ/ML	SL-IQE/ML
Barium	1620		-5.7%	-19.3%
Barium	200.8	ICP/MS	46.6%	71.5%
Benzene	502.2	PID	53.7%	58.1%
Benzene	524.2		40.5%	-13.1%
Beryllium	1620		-61.9%	-68.5%
Beryllium	200.8	ICP/MS	-9.9%	75.0%
Boron	1620		-8.2%	2.2%
Bromobenzene	502.2	ELCD	18.0%	150.4%
Bromobenzene	502.2	PID	-0.9%	67.0%
Bromobenzene	524.2		-18.1%	-35.4%
Bromochloromethane	502.2	ELCD	25.8%	187.9%
Bromochloromethane	524.2		9.3%	-30.3%
Bromodichloromethane	502.2	ELCD	-25.6%	182.0%
Bromodichloromethane	524.2		-38.7%	-43.9%
Bromoform	502.2	ELCD	-12.0%	197.7%
Bromoform	524.2		-54.2%	-3.7%
Bromomethane	502.2	ELCD	N/A	176.9%
Bromomethane	524.2		23.2%	12.2%
Cadmium	1620		-36.4%	-19.7%
Cadmium	200.8	ICP/MS	79.2%	103.6%
Calcium	1620		60.4%	-0.0%
Carbon disulfide	524.2		-26.2%	1.3%
Carbon tetrachloride	524.2		23.9%	33.4%
Carbontet+1,1-dcp	502.2	ELCD	-74.3%	-37.3%
Chloroacetonitrile	524.2		70.3%	49.3%
Chlorobenzene	502.2	ELCD	15.7%	189.0%
Chlorobenzene	502.2	PID	35.2%	17.4%
Chlorobenzene	524.2		7.4%	-50.8%
Chloroethane	502.2	ELCD	-161.8%	168.4%
Chloroethane	524.2		-8.0%	24.2%
Chloroform	502.2	ELCD	-149.4%	-155.3%
Chloroform	524.2		31.7%	19.2%

Table 5. Percent Differences of Quantitation Limits to the EPA/ACS QL for the Episode 6000 Dataset

Analyte	Method	Procedure	ISO LOQ/ML	SL-IQE/ML
Chloromethane	502.2	ELCD	52.5%	158.6%
Chloromethane	524.2		-9.8%	-34.9%
Chromium	1620		-0.7%	22.9%
Chromium	200.8	ICP/MS	49.3%	134.9%
Cis-1,2-dce+2,2-dcp	502.2	ELCD	-9.5%	-24.7%
Cis-1,2-dichloroethene	524.2		42.4%	36.1%
Cis-1,3-dichloropropene	502.2	ELCD	-45.8%	181.6%
Cis-1,3-dichloropropene	502.2	PID	23.8%	-168.7%
Cis-1,3-dichloropropene	524.2		15.3%	34.2%
Cobalt	1620		-82.0%	-20.2%
Cobalt	200.8	ICP/MS	N/A	N/A
Copper	1620		31.6%	81.5%
Copper	200.8	ICP/MS	34.6%	179.2%
Dibromochloromethane	502.2	ELCD	41.1%	193.7%
Dibromochloromethane	524.2		-29.0%	36.0%
Dibromomethane	502.2	ELCD	34.7%	194.3%
Dibromomethane	524.2		-22.2%	-8.3%
Dichlorodifluoromethane	502.2	ELCD	-53.2%	192.8%
Dichlorodifluoromethane	524.2		36.7%	82.3%
Diethyl ether	524.2		11.9%	-21.3%
Ethyl methacrylate	524.2		-35.7%	-8.9%
Ethylbenzene	502.2	PID	-11.5%	44.6%
Ethylbenzene	524.2		20.4%	-25.4%
Hardness	130.2		39.1%	92.8%
Hexachlorobutadiene	502.2	ELCD	-114.4%	19.4%
Hexachlorobutadiene	524.2		-22.3%	13.3%
Hexachloroethane	524.2		14.8%	-17.7%
Hexchlobutadiene+naphthalene	502.2	PID	-82.3%	-25.9%
Iron	1620		152.7%	133.1%
Isopropylbenzene	502.2	PID	-10.4%	25.3%
Isopropylbenzene	524.2		11.9%	199.2%
Lead	1620		1.2%	13.1%

Table 5. Percent Differences of Quantitation Limits to the EPA/ACS QL for the Episode 6000 Dataset

Analyte	Method	Procedure	ISO LOQ/ML	SL-IQE/ML
Lead	200.8	ICP/MS	-145.2%	-98.0%
M+p xylene	502.2	PID	-98.3%	10.6%
M+p xylene	524.2		-17.7%	199.2%
Magnesium	1620		-9.6%	-60.7%
Manganese	1620		-86.2%	-26.9%
Manganese	200.8	ICP/MS	28.0%	84.1%
Mercury	200.8	ICP/MS	94.2%	63.6%
Methacrylonitrile	524.2		6.4%	180.1%
Methyl iodide	524.2		7.3%	-18.1%
Methyl tert-butyl ether	524.2		-31.2%	20.1%
Methylacrylate	524.2		-3.5%	-31.7%
Methylene chloride	502.2	ELCD	N/A	169.4%
Methylene chloride	524.2		55.6%	73.6%
Methylmethacrylate	524.2		-89.5%	181.6%
Molybdenum	1620		-2.5%	-27.3%
Molybdenum	200.8	ICP/MS	135.3%	193.5%
N-butylbenzene	502.2	PID	24.5%	152.7%
N-butylbenzene	524.2		42.2%	29.5%
N-propylbenzene	502.2	PID	-44.1%	-7.1%
N-propylbenzene	524.2		9.9%	198.7%
Naphthalene	524.2		-8.2%	-59.5%
Nickel	1620		-40.3%	-39.2%
Nickel	200.8	ICP/MS	-54.2%	-92.9%
O-xylene	524.2		21.3%	-21.4%
O-xylene+styrene	502.2	PID	4.9%	-10.0%
P-isopropol+1,4-dcb	502.2	PID	45.6%	78.1%
Pentachloroethane	524.2		-183.5%	-113.6%
Sec-butylbenzene	502.2	PID	-3.4%	-24.2%
Sec-butylbenzene	524.2		22.8%	-5.2%
Selenium	1620		63.5%	89.4%
Selenium	200.8	ICP/MS	46.8%	70.6%
Silver	1620		-17.8%	25.5%

Table 5. Percent Differences of Quantitation Limits to the EPA/ACS QL for the Episode 6000 Dataset

Analyte	Method	Procedure	ISO LOQ/ML	SL-IQE/ML
Silver	200.8	ICP/MS	-59.2%	94.7%
Sodium	1620		22.8%	51.2%
Styrene	524.2		6.9%	-20.6%
Tert-butylbenzene	502.2	PID	19.2%	67.9%
Tert-butylbenzene	524.2		-44.8%	-30.6%
Tetrachloroethene	502.2	ELCD	40.9%	83.5%
Tetrachloroethene	502.2	PID	19.6%	115.8%
Tetrachloroethene	524.2		61.5%	197.4%
Thallium	1620		60.8%	33.3%
Thallium	200.8	ICP/MS	3.8%	16.3%
Thorium	200.8	ICP/MS	90.3%	74.9%
Tin	1620		-7.9%	-6.1%
Titanium	1620		4.0%	-33.7%
Toluene	502.2	PID	-21.1%	-3.0%
Toluene	524.2		-57.9%	-9.1%
Total phosphorus	365.2		17.2%	39.9%
Total suspended solids	160.2		0.2%	29.5%
Trans-1,2-dichloroethene	502.2	ELCD	15.7%	-4.9%
Trans-1,2-dichloroethene	524.2		33.7%	41.7%
Trans-1,3-dichloropropene	502.2	ELCD	-101.5%	174.3%
Trans-1,3-dichloropropene	502.2	PID	19.8%	-13.4%
Trans-1,3-dichloropropene	524.2		-49.5%	8.7%
Trans-1,4-dichloro-2-butene	524.2		-10.4%	175.1%
Trichloroethene	502.2	ELCD	-144.3%	193.8%
Trichloroethene	502.2	PID	7.8%	120.2%
Trichloroethene	524.2		34.6%	-17.8%
Trichlorofluoromethane	502.2	ELCD	105.3%	161.3%
Trichlorofluoromethane	524.2		33.0%	198.1%
Uranium	200.8	ICP/MS	-33.2%	2.6%
Vanadium	1620		7.6%	19.6%
Vanadium	200.8	ICP/MS	27.1%	-3.4%
Vinyl chloride	502.2	ELCD	-116.4%	156.7%

Table 5. Percent Differences of Quantitation Limits to the EPA/ACS QL for the Episode 6000 Dataset

Analyte	Method	Procedure	ISO LOQ/ML	SL-IQE/ML
Vinyl chloride	524.2		-35.7%	9.3%
Wad cyanide	1677	WADCN	-80.5%	-20.8%
Xylene (total)	524.2		28.4%	199.7%
Yttrium	1620		27.2%	56.8%
Zinc	1620		-4.3%	4.4%
Zinc	200.8	ICP/MS	7.1%	111.4%

Note: ELCD or PID in the Procedure column indicates the photo-ionization detector (PID) or electrolytic conductivity detector (ELCD) in EPA Method 502.2

Summary Statistics for Table 5

	ISO LOQ/QL	SL-IQE/QL
Minimum	-194.7%	-174.7%
25th percentile	-35.0%	-18.1%
Median	-4.2%	19.6%
75th percentile	23.0%	111.4%
Maximum	152.7%	199.7%

Comparison	Sign Test p-value	Wilcoxon p-value
LOQ vs. QL	0.390	0.043
SL-IQE vs. QL	0.0001	<0.0001

Comparison	# analytes	Median % Difference	Sign Test p-value	Wilcoxon p-value
SL-IQE vs. QL (constant model used for SL-IQE)	32	179.6%	<0.0001	<0.0001
SL-IQE vs. QL (Linear model used for SL-IQE)	65	67.9%	<0.0001	<0.0001
SL-IQE vs. QL (Hybrid model used for SL-IQE)	100	-7.7%	0.533	0.160

Table 6. Detection and Quantitation Limits for EPA Methods 1631 and 1638 as Computed by EPA and by EPRI (ng/L)

Element[1]	Ambient WQC[2]	Detection limits			Quantitation limits		
		MDL in Method	IDE computed by		ML in Method	IQE computed by	
			EPA	EPRI		EPA	EPRI
Antimony	14000	9.7	170	110	20	270	270
Cadmium	370	25	160	150	100	540	380
Copper	2400	87	800	770	200	3800	3000
Lead	540	15	140	160	50	420	370
Mercury	12	0.2	0.81	0.43	0.5	0.55	1.6
Nickel	8200	330	230	130	1000	15000	330
Selenium	5000	450	810	600	1000	630	720
Silver	320	29	440	---	100	5500	---
Thallium	1700	7.9	28	20	20	88	50
Zinc	32000	140	1800	2100	500	21000	26100

[1] Mercury determined by EPA Method 1631; all others by EPA Method 1638

[2] Lowest ambient water quality criterion (WQC) in the National Toxics Rule (40 CFR 131.36)

Table 7. Comparison of IDEs and IQEs resulting from all model types for EPA Methods 1631 and 1638

Calculated IDEs					
Analyte	IDE, Based on Given Model				RSD (%)
	Constant	Linear	Exponential	Hybrid	
Antimony	2500	-80 [1]	170	100	148%
Cadmium	1200	130	160	150	129%
Copper	2700	1000	800	720	72%
Lead	400	150	140	150	61%
Mercury	8.3	0.058	0.81	0.52	162%
Nickel	7000	-48 [1]	230	120	161%
Selenium	4500	720	810	530	117%
Silver	2500	710	440	650	89%
Thallium	230	22	28	17	140%
Zinc	10,000	1600	1800	1700	110%
Calculated IQEs (10%)					
Analyte	IQE, Based on Given Model				RSD(%)
	Constant	Linear	Exponential	Hybrid	
Antimony	5400	-570 [1]	380	270	145%
Cadmium	2600	540	380	380	112%
Copper	5900	3800	2100	2300	50%
Lead	860	420	340	330	52%
Mercury	18	0.55	2.1	1.6	150%
Nickel	15,000	-160 [1]	500	270	190%
Selenium	9600	7600	2200	630 [3]	86%
Silver	5500	1500 [4]	1500	undefined [2]	82%
Thallium	500	88	67	47	124%
Zinc	22,000	21,000	4800	6700	67%

[1] Negative due to negative intercept estimate in precision model.
[2] IDE or IQE did not converge to a single value for estimated models.
[3] IQE 10% undefined, IQE 20% reported
[4] IQE 10% negative, IQE 20% reported

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
1,1,1,2-tetrachloroethane	502.2	ELCD	0.034	0.011	-99.6%	Exponential	Linear
1,1,1,2-tetrachloroethane	524.2		0.244	0.170	-35.8%	Exponential	Exponential
1,1,1-trichloroethane	502.2	ELCD	0.041	0.044	6.2%	Exponential	Exponential
1,1,1-trichloroethane	524.2		0.308	0.035	-159.4%	Exponential	Hybrid
1,1,2,2-tce+1,2,3-tcp	502.2	ELCD	0.179	3.548	180.8%	Exponential	Constant
1,1,2,2-tetrachloroethane	524.2		0.436	0.538	20.8%	Exponential	Exponential
1,1,2-trichloroethane	502.2	ELCD	0.032	0.013	-86.7%	Exponential	Linear
1,1,2-trichloroethane	524.2		0.319	0.229	-32.8%	Exponential	Exponential
1,1-dichloroethane	502.2	ELCD	0.083	0.036	-78.8%	Exponential	Exponential
1,1-dichloroethane	524.2		0.229	0.084	-92.7%	Exponential	Exponential
1,1-dichloroethene	502.2	ELCD	0.234	0.120	-64.0%	Exponential	Exponential
1,1-dichloroethene	524.2		0.335	0.080	-122.6%	Exponential	Hybrid
1,1-dichloropropanone	524.2		6.372	8.941	33.6%	Exponential	Exponential
1,1-dichloropropene	524.2		0.287	4.435	175.7%	Exponential	Constant [1]
1,2,3-trichlorobenzene	502.2	ELCD	0.134	0.169	23.1%	Exponential	Constant
1,2,3-trichlorobenzene	502.2	PID	0.115	0.069	-49.9%	Exponential	Exponential
1,2,3-trichlorobenzene	524.2		0.275	0.150	-59.2%	Exponential	Exponential
1,2,3-trichloropropane	524.2		1.263	16.238	171.1%	Exponential	Constant [1]
1,2,4-trichlorobenzene	502.2	ELCD	0.088	0.100	13.1%	Exponential	Constant
1,2,4-trichlorobenzene	502.2	PID	0.124	0.075	-48.9%	Exponential	Exponential
1,2,4-trichlorobenzene	524.2		0.224	0.115	-64.6%	Exponential	Exponential
1,2,4-trimethylbenzene	502.2	PID	0.125	0.143	12.8%	Exponential	Constant
1,2,4-trimethylbenzene	524.2		0.144	0.059	-84.6%	Exponential	Exponential
1,2-dibromo-3-chloropropane	524.2		1.749	0.432	-120.8%	Exponential	Hybrid
1,2-dibromoethane	502.2	ELCD	0.164	0.025	-147.8%	Exponential	Linear
1,2-dibromoethane	524.2		0.326	0.316	-3.1%	Exponential	Exponential
1,2-dichlorobenzene	502.2	ELCD	0.065	0.057	-13.4%	Exponential	Linear
1,2-dichlorobenzene	502.2	PID	0.148	0.077	-62.5%	Exponential	Exponential
1,2-dichlorobenzene	524.2		0.130	0.069	-61.3%	Exponential	Exponential
1,2-dichloroethane	502.2	ELCD	0.042	0.026	-48.3%	Exponential	Exponential

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
1,2-dichloroethane	524.2		0.258	0.211	-19.9%	Exponential	Exponential
1,2-dichloropropane	502.2	ELCD	0.043	0.087	67.5%	Exponential	Constant
1,2-dichloropropane	524.2		0.247	0.221	-11.1%	Exponential	Exponential
1,3,5-tmb+4-chlorotoluene	502.2	PID	0.114	0.141	21.4%	Exponential	Constant
1,3,5-trimethylbenzene	524.2		0.135	0.049	-94.1%	Exponential	Exponential
1,3-dichlorobenzene	502.2	ELCD	0.118	0.615	135.5%	Exponential	Constant
1,3-dichlorobenzene	502.2	PID	0.126	0.197	43.9%	Exponential	Constant
1,3-dichlorobenzene	524.2		0.143	0.038	-116.4%	Exponential	Exponential
1,3-dichloropropane	502.2	ELCD	0.047	0.020	-81.3%	Exponential	Exponential
1,3-dichloropropane	524.2		0.202	0.122	-49.2%	Exponential	Exponential
1,4-dichlorobenzene	502.2	ELCD	0.061	0.040	-40.5%	Exponential	Linear
1,4-dichlorobenzene	524.2		0.140	0.051	-93.7%	Exponential	Exponential
1-chlorobutane	524.2		0.220	0.061	-113.5%	Exponential	Linear
2,2-dichloropropane	524.2		0.691	0.122	-139.9%	Exponential	Hybrid
2-butanone	524.2		0.833	1.441	53.5%	Exponential	Exponential
2-chlorotduene	502.2	ELCD	0.175	0.117	-40.2%	Exponential	Exponential
2-chlorotduene	502.2	PID	0.230	0.409	56.2%	Exponential	Constant
2-chlorotduene	524.2		0.136	0.039	-111.2%	Exponential	Exponential
2-hexanone	524.2		0.902	0.904	0.3%	Exponential	Exponential
2-nitropropane	524.2		1.082	9.354	158.5%	Exponential	Constant
4-chlorotduene	502.2	ELCD	0.149	0.145	-3.2%	Exponential	Linear
4-chlorotduene	524.2		0.123	0.038	-105.5%	Exponential	Exponential
4-isopropyltoluene	524.2		0.117	0.038	-101.3%	Exponential	Exponential
4-methyl-2-pentanone	524.2		1.195	1.088	-9.3%	Exponential	Exponential
Acetone	524.2		2.120	30.183	173.8%	Exponential	Constant
Acrylonitrile	524.2		1.333	1.077	-21.3%	Exponential	Exponential
Allyl Chloride	524.2		0.229	0.073	-103.6%	Exponential	Hybrid
Aluminum	1620		206.975	73.421	-95.3%	Constant	Constant
Aluminum	200.8		12.747	22.654	56.0%	Exponential	Constant
Ammonia as Nitrogen [2]	350.3		0.014	0.040	94.0%	Exponential	Constant

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
Antimony	1620		4.260	6.467	41.2%	Constant	Linear
Antimony	200.8		0.019	0.304	176.5%	Exponential	Constant
Arsenic	1620		1.410	2.268	46.6%	Exponential	Constant
Arsenic	200.8		0.366	0.374	2.1%	Exponential	Exponential
Barium	1620		1.837	1.624	-12.3%	Constant	Constant
Barium	200.8		0.084	0.073	-13.7%	Exponential	Constant
Benzene	502.2	PID	0.079	0.061	-25.0%	Exponential	Exponential
Benzene	524.2		0.125	0.030	-122.6%	Exponential	Exponential
Beryllium	1620		0.448	0.438	-2.2%	Exponential	Exponential
Beryllium	200.8		0.024	0.017	-34.2%	Exponential	Constant
Boron	1620		21.161	22.333	5.4%	Exponential	Exponential
Bromobenzene	502.2	ELCD	0.765	0.348	-75.0%	Linear	Exponential
Bromobenzene	502.2	PID	0.050	0.025	-65.4%	Exponential	Exponential
Bromobenzene	524.2		0.211	0.165	-24.1%	Exponential	Exponential
Bromochloromethane	502.2	ELCD	0.482	0.044	-166.9%	Linear	Exponential
Bromochloromethane	524.2		0.345	0.507	38.1%	Exponential	Exponential
Bromodichloromethane	502.2	ELCD	0.075	0.026	-95.5%	Exponential	Exponential
Bromodichloromethane	524.2		0.205	0.088	-79.7%	Exponential	Exponential
Bromoform	502.2	ELCD	1.513	0.025	-193.5%	Constant	Linear
Bromoform	524.2		0.400	0.336	-17.4%	Exponential	Exponential
Bromomethane	502.2	ELCD	7.293	0.760	-162.3%	Constant	Exponential
Bromomethane	524.2		0.280	0.154	-57.8%	Exponential	Linear
Cadmium	1620		0.191	0.211	9.8%	Exponential	Exponential
Cadmium	200.8		0.022	0.016	-33.8%	Exponential	Constant
Calcium	1620		41.358	53.375	25.4%	Linear	Constant
Carbon Disulfide	524.2		0.239	0.087	-93.6%	Exponential	Linear
Carbon Tetrachloride	524.2		0.314	0.174	-57.3%	Exponential	Linear
Carbontet+1,1-dcp	502.2	ELCD	0.072	0.061	-15.5%	Exponential	Exponential
Chloroacetonitrile	524.2		1.569	2.079	28.0%	Exponential	Exponential
Chlorobenzene	502.2	ELCD	0.460	0.064	-151.5%	Linear	Exponential

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
Chlorobenzene	502.2	PID	0.064	0.059	-7.8%	Exponential	Exponential
Chlorobenzene	524.2		0.133	0.034	-118.1%	Exponential	Exponential
Chloroethane	502.2	ELCD	2.598	0.096	-185.7%	Constant	Linear
Chloroethane	524.2		0.395	0.303	-26.3%	Exponential	Exponential
Chloroform	502.2	ELCD	0.032	0.008	-117.3%	Exponential	Linear
Chloroform	524.2		0.225	0.104	-73.4%	Exponential	Exponential
Chloromethane	502.2	ELCD	0.250	0.520	70.3%	Exponential	Constant
Chloromethane	524.2		0.253	0.150	-51.2%	Exponential	Exponential
Chromium	1620		0.496	0.759	41.8%	Exponential	Constant
Chromium	200.8		0.408	0.491	18.5%	Linear	Constant
Cis-1,2-dce+2,2-dcp	502.2	ELCD	0.055	0.039	-35.0%	Exponential	Exponential
Cis-1,2-dichloroethene	524.2		0.234	0.201	-15.2%	Exponential	Exponential
Cis-1,3-dichloropropene	502.2	ELCD	0.074	0.024	-102.4%	Exponential	Exponential
Cis-1,3-dichloropropene	502.2	PID	0.082	0.111	30.2%	Exponential	Exponential
Cis-1,3-dichloropropene	524.2		0.173	0.119	-37.1%	Exponential	Exponential
Cobalt	1620		16.463	12.267	-29.2%	Exponential	Exponential
Cobalt	200.8		0.074	0.001	-195.2%	Constant	Exponential
Copper	1620		21.189	15.897	-28.5%	Constant	Constant
Copper	200.8		0.798	0.905	12.6%	Constant	Constant
Dibromochloromethane	502.2	ELCD	0.436	0.394	-10.1%	Linear	Constant
Dibromochloromethane	524.2		0.287	0.203	-34.3%	Exponential	Exponential
Dibromomethane	502.2	ELCD	0.460	0.298	-42.8%	Linear	Constant
Dibromomethane	524.2		0.388	0.439	12.5%	Exponential	Exponential
Dichlorodifluoromethane	502.2	ELCD	0.240	1.225	134.5%	Exponential	Constant
Dichlorodifluoromethane	524.2		0.560	0.591	5.4%	Exponential	Exponential
Diethyl Ether	524.2		0.376	0.330	-12.9%	Exponential	Exponential
Ethyl Methacrylate	524.2		0.273	0.259	-5.2%	Exponential	Exponential
Ethylbenzene	502.2	PID	0.078	0.050	-44.2%	Exponential	Exponential
Ethylbenzene	524.2		0.198	0.107	-59.5%	Exponential	Exponential
Hardness [2]	130.2		2.258	4.886	73.6%	Exponential	Constant

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
Hexachlorobutadiene	502.2	ELCD	0.094	0.073	-24.8%	Exponential	Linear
Hexachlorobutadiene	524.2		0.308	0.237	-26.0%	Exponential	Exponential
Hexachloroethane	524.2		0.288	0.260	-10.1%	Exponential	Exponential
Hexchlobutadiene+naphthalene	502.2	PID	0.597	0.592	-1.0%	Exponential	Constant
Iron	1620		373.590	1064.987	96.1%	Linear	Constant
Isopropylbenzene	502.2	PID	0.060	0.041	-37.0%	Exponential	Exponential
Isopropylbenzene	524.2		0.120	0.037	-104.7%	Exponential	Exponential
Lead	1620		2.423	2.951	19.6%	Exponential	Constant
Lead	200.8		0.204	2.872	173.5%	Exponential	Constant
M+p Xylene	502.2	PID	0.121	0.119	-1.2%	Exponential	Constant
M+p Xylene	524.2		0.142	0.031	-127.3%	Exponential	Exponential
Magnesium	1620		105.998	184.221	53.9%	Exponential	Constant
Manganese	1620		6.808	4.548	-39.8%	Constant	Constant
Manganese	200.8		0.109	0.077	-34.7%	Constant	Constant
Mercury	200.8		0.027	0.014	-63.8%	Exponential	Hybrid
Methacrylonitrile	524.2		0.718	0.552	-26.2%	Exponential	Hybrid
Methyl Iodide	524.2		0.193	0.109	-55.5%	Exponential	Exponential
Methyl Tert-butyl Ether	524.2		0.225	0.173	-26.3%	Exponential	Exponential
Methylacrylate	524.2		0.601	0.569	-5.5%	Exponential	Exponential
Methylene Chloride	502.2	ELCD	2.841	-1.381	-578.5%	Constant	Constant
Methylene Chloride	524.2		0.314	0.158	-66.1%	Exponential	Exponential
Methylmethacrylate	524.2		0.535	0.382	-33.3%	Exponential	Linear
Molybdenum	1620		3.034	6.028	66.1%	Exponential	Constant
Molybdenum	200.8		0.271	0.006	-191.8%	Constant	Constant
N-butylbenzene	502.2	PID	0.152	0.056	-93.0%	Exponential	Exponential
N-butylbenzene	524.2		0.092	0.105	13.9%	Exponential	Constant
N-propylbenzene	502.2	PID	25.560	41.908	48.5%	Exponential	Constant
N-propylbenzene	524.2		0.083	0.070	-16.1%	Exponential	Constant
Naphthalene	524.2		0.141	0.052	-91.4%	Exponential	Linear
Nickel	1620		0.284	0.052	-137.6%	Exponential	Hybrid

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
Nickel	200.8		0.186	0.194	4.1%	Exponential	Exponential
o-xylene	524.2		0.198	0.082	-82.9%	Exponential	Exponential
o-xylene+styrene	502.2	PID	0.116	0.151	26.8%	Exponential	Constant
P-isopropitol+1,4-dcb	502.2	PID	0.408	0.437	7.0%	Exponential	Linear
Pentachloroethane	524.2		0.159	0.150	-5.8%	Exponential	Constant
Sec-butylbenzene	502.2	PID	0.081	0.057	-35.3%	Exponential	Exponential
Sec-butylbenzene	524.2		0.140	0.040	-111.6%	Exponential	Exponential
Selenium	1620		1.975	1.801	-9.2%	Exponential	Exponential
Selenium	200.8		0.416	0.342	-19.5%	Exponential	Exponential
Silver	1620		10.668	11.589	8.3%	Exponential	Constant
Silver	200.8		0.012	-0.084	269.8%	Exponential	Constant [1]
Sodium	1620		138.768	140.860	1.5%	Exponential	Exponential
Styrene	524.2		0.141	0.048	-98.2%	Exponential	Exponential
Tert-butylbenzene	502.2	PID	0.074	0.051	-35.9%	Exponential	Exponential
Tert-butylbenzene	524.2		0.186	0.057	-106.6%	Exponential	Exponential
Tetrachloroethene	502.2	ELCD	0.061	0.054	-11.0%	Exponential	Exponential
Tetrachloroethene	502.2	PID	0.156	0.103	-40.6%	Exponential	Linear
Tetrachloroethene	524.2		0.469	0.550	15.9%	Exponential	Linear
Thallium	1620		1.153	1.249	8.0%	Exponential	Linear
Thallium	200.8		0.001	0.000	-76.1%	Exponential	Exponential
Thorium	200.8		0.001	0.000	-93.4%	Exponential	Constant
Tin	1620		3.932	4.651	16.8%	Exponential	Exponential
Titanium	1620		5.376	20.828	117.9%	Exponential	Constant
Toluene	502.2	PID	0.064	0.064	-1.3%	Exponential	Constant
Toluene	524.2		0.146	0.558	117.1%	Exponential	Constant [1]
Total Phosphorus [2]	365.2		0.013	0.011	-18.1%	Exponential	Exponential
Total Suspended Solids [2]	160.2		3.005	2.370	-23.6%	Exponential	Exponential
Trans-1,2-dichloroethene	502.2	ELCD	0.081	0.066	-21.7%	Exponential	Linear
Trans-1,2-dichloroethene	524.2		0.300	0.075	-119.7%	Exponential	Hybrid
Trans-1,3-dichloropropene	502.2	ELCD	0.098	0.033	-98.9%	Exponential	Exponential

Table 8. Comparison of 16-point and 5-point Single-laboratory IDEs (SL-IDEs) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE (16)	SL-IDE (5)	Percent Difference	SL-IDE 16 Model	SL-IDE 5 Model
Trans-1,3-dichloropropene	502.2	PID	0.092	0.116	22.7%	Exponential	Exponential
Trans-1,3-dichloropropene	524.2		0.223	0.132	-51.1%	Exponential	Exponential
Trans-1,4-dichloro-2-butene	524.2		1.250	1.448	14.7%	Exponential	Exponential
Trichloroethene	502.2	ELCD	0.059	0.020	-99.6%	Exponential	Exponential
Trichloroethene	502.2	PID	0.097	0.089	-8.5%	Exponential	Exponential
Trichloroethene	524.2		0.332	0.344	3.6%	Exponential	Linear
Trichlorofluoromethane	502.2	ELCD	2.079	0.688	-100.5%	Constant	Constant
Trichlorofluoromethane	524.2		0.384	0.384	0.1%	Exponential	Exponential
Uranium	200.8		0.000	0.000	-70.8%	Exponential	Exponential
Vanadium	1620		10.630	9.082	-15.7%	Exponential	Exponential
Vanadium	200.8		0.864	1.023	16.9%	Exponential	Linear
Vinyl Chloride	502.2	ELCD	3.672	0.387	-161.9%	Constant	Linear
Vinyl Chloride	524.2		0.365	0.188	-63.8%	Exponential	Linear
WAD Cyanide	1677		0.701	1.296	59.6%	Linear	Constant
Xylene (Total)	524.2		0.128	0.029	-126.9%	Exponential	Exponential
Yttrium	1620		3.247	13.972	124.6%	Exponential	Constant
Zinc	1620		4.500	6.943	42.7%	Exponential	Constant
Zinc	200.8		1.598	5.245	106.6%	Exponential	Constant

Note: ELCD or PID in the Procedure column indicates the photo-ionization detector (PID) or electrolytic conductivity detector (ELCD) in EPA Method 502.2

[1] Original model picked was Hybrid, but failed to converge

[2] Results reported as mg/L

Summary Statistics for Table 8

	SL-IDE(16) vs. SL-IDE (5) (all analytes)	SL-IDE(16) vs. SL-IDE (5) (same model used)	SL-IDE(16) vs. SL-IDE (5) (different models used)
Number of Analytes	198	108	90
Minimum:	-578.5%	-578.5%	-195.2%
25th percentile:	-79.5%	-80.1%	-72.2%
Median:	-24.9%	-35.6%	1.3%
75th percentile:	12.8%	-9.3%	55.5%
Maximum:	269.8%	53.5%	269.8%

	Number of analytes	Median % Difference	Sign Test p-value	Wilcoxon p-value
SL-IDE (16) vs. SL-IDE (5) (all analytes)	198	-24.9%	<0.0001	<0.0001
SL-IDE(16) vs. SL-IDE (5) (same model used)	108	-35.6%	<0.0001	<0.0001
SL-IDE(16) vs. SL-IDE (5) (different models used)	90	1.3%	>0.999	0.847

Table 9. Comparison of 16-point and 5-point Single-laboratory IQEs at 10% RSD (SL-IQEs 10%) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE10% (16)	SL-IQE10% (5)	Percent Difference	SL-IQE Model (16)	SL-IQE Model (5)
1,1,1,2-tetrachloroethane	502.2	ELCD	0.030	0.048	45.7%	Hybrid	Linear
1,1,1,2-tetrachloroethane	524.2		0.181	0.320	55.3%	Hybrid	Linear
1,1,1-trichloroethane	502.2	ELCD	0.830	0.055	-175.2%	Linear	Hybrid
1,1,1-trichloroethane	524.2		0.240	0.081	-98.6%	Hybrid	Hybrid
1,1,2,2-tce+1,2,3-tcp	502.2	ELCD	5.514	6.984	23.5%	Constant	Constant
1,1,2,2-tetrachloroethane	524.2		0.569	0.942	49.4%	Hybrid	Linear
1,1,2-trichloroethane	502.2	ELCD	0.060	0.046	-26.2%	Linear	Linear
1,1,2-trichloroethane	524.2		0.290	0.344	17.1%	Hybrid	Linear
1,1-dichloroethane	502.2	ELCD	0.527	0.058	-160.5%	Linear	Hybrid
1,1-dichloroethane	524.2		0.115	0.099	-14.8%	Hybrid	Hybrid
1,1-dichloroethene	502.2	ELCD	3.796	0.305	-170.3%	Linear	Hybrid
1,1-dichloroethene	524.2		0.129	0.199	42.6%	Hybrid	Hybrid
1,1-dichloropropanone	524.2		12.705	16.447	25.7%	Linear	Hybrid
1,1-dichloropropene	524.2		0.180	9.106[6]	192.2%	Hybrid	Constant
1,2,3-trichlorobenzene	502.2	ELCD	0.851	0.341	-85.6%	Linear	Constant
1,2,3-trichlorobenzene	502.2	PID	0.248	0.246	-0.9%	Hybrid	Hybrid
1,2,3-trichlorobenzene	524.2		0.216	0.147	-38.1%	Hybrid	Linear
1,2,3-trichloropropane	524.2		11.316	33.343[6]	98.6%	Linear	Constant
1,2,4-trichlorobenzene	502.2	ELCD	0.401	0.202	-65.9%	Linear	Constant
1,2,4-trichlorobenzene	502.2	PID	0.439	0.207	-72.0%	Linear	Hybrid
1,2,4-trichlorobenzene	524.2		0.141	3.760	185.6%	Hybrid	Constant
1,2,4-trimethylbenzene	502.2	PID	0.653	0.293	-76.2%	Linear	Constant
1,2,4-trimethylbenzene	524.2		20.896	0.119	-197.7%	Constant	Linear
1,2-dibromo-3-chloropropane	524.2		71.182[6]	0.877	-195.1%	Constant	Hybrid
1,2-dibromoethane	502.2	ELCD	0.592	0.065	-160.2%	Linear	Linear
1,2-dibromoethane	524.2		0.417	0.579	32.5%	Hybrid	Linear
1,2-dichlorobenzene	502.2	ELCD	0.183	0.109[3]	-50.9%	Linear	Linear
1,2-dichlorobenzene	502.2	PID	0.346	0.123	-94.7%	Hybrid	Hybrid
1,2-dichlorobenzene	524.2		0.085	0.117	32.3%	Hybrid	Linear
1,2-dichloroethane	502.2	ELCD	0.065	0.727[6]	167.2%	Hybrid	Constant
1,2-dichloroethane	524.2		0.222	0.327	38.4%	Hybrid	Linear
1,2-dichloropropane	502.2	ELCD	0.102	0.178	54.1%	Linear	Constant
1,2-dichloropropane	524.2		0.196	0.219	10.9%	Hybrid	Linear
1,3,5-tmb+4-chlorotoluene	502.2	PID	0.189	0.289	41.7%	Hybrid	Constant
1,3,5-trimethylbenzene	524.2		23.744	0.086	-198.6%	Constant	Linear
1,3-dichlorobenzene	502.2	ELCD	0.936	1.239	27.9%	Linear	Constant
1,3-dichlorobenzene	502.2	PID	0.465	0.404	-14.2%	Linear	Constant
1,3-dichlorobenzene	524.2		0.076	0.081	7.0%	Hybrid	Hybrid
1,3-dichloropropane	502.2	ELCD	0.054	0.448	157.0%	Linear	Constant
1,3-dichloropropane	524.2		0.139	0.154	10.0%	Hybrid	Hybrid
1,4-dichlorobenzene	502.2	ELCD	0.101	0.100	-1.3%	Hybrid	Linear
1,4-dichlorobenzene	524.2		0.078	0.068	-14.1%	Hybrid	Linear
1-chlorobutane	524.2		29.943	0.170	-197.7%	Constant	Linear
2,2-dichloropropane	524.2		38.009	0.361	-196.2%	Constant	Hybrid
2-butanone	524.2		0.893	39.665	191.2%		Constant
2-chlorotoluene	502.2	ELCD	0.493	0.357	-32.1%	Hybrid	Linear

Table 9. Comparison of 16-point and 5-point Single-laboratory IQEs at 10% RSD (SL-IQEs 10%) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE10% (16)	SL-IQE10% (5)	Percent Difference	SL-IQE Model (16)	SL-IQE Model (5)
2-chlorotoluene	502.2	PID	0.849	0.806	-5.2%	Hybrid	Constant
2-chlorotoluene	524.2		0.053	0.044	-19.1%	Hybrid	Linear
2-hexanone	524.2		0.442	61.796	197.2%	Hybrid	Constant
2-nitropropane	524.2		0.590	17.783	187.2%	Hybrid	Constant
4-chlorotoluene	502.2	ELCD	0.142[1]	0.485	109.4%	Hybrid	Linear
4-chlorotoluene	524.2		23.810	0.837	-186.4%	Constant	Constant
4-isopropyltoluene	524.2		0.016	1.194	194.6%	Hybrid	Constant
4-methyl-2-pentanone	524.2		1.785	14.514	156.2%	Hybrid	Constant
Acetone	524.2		2.741	59.415	182.4%	Hybrid	Constant
Acrylonitrile	524.2		28.056	19.275	-37.1%	Constant	Constant
Allyl Chloride	524.2		29.674	0.164	-197.8%	Constant	Hybrid
Aluminum	1620		464.069	144.530	-105.0%	Constant	Constant
Aluminum	200.8	ICP/MS	29.684	47.196	45.6%	Hybrid	Constant
Ammonia as Nitrogen[2]	350.3		0.035	0.082	78.8%	Hybrid	Constant
Antimony	1620		9.551	8.364[5]	-3.6%	Constant	Constant
Antimony	200.8	ICP/MS	0.034	0.633	179.8%	Hybrid	Constant
Arsenic	1620		3.097	4.656	40.2%	Hybrid	Constant
Arsenic	200.8	ICP/MS	0.798	0.847	6.1%	Hybrid	Hybrid
Barium	1620		4.118	3.334	-21.1%	Constant	Constant
Barium	200.8	ICP/MS	0.211	0.153	-32.1%	Linear	Constant
Benzene	502.2	PID	0.182	0.130	-33.2%	Linear	Linear
Benzene	524.2		0.044	0.029	-41.0%	Hybrid	Linear
Beryllium	1620		0.980	0.985	0.6%	Hybrid	Linear
Beryllium	200.8	ICP/MS	0.044	0.036	-19.9%	Hybrid	Constant
Boron	1620		51.134	46.392	-9.7%	Linear	Hybrid
Bromobenzene	502.2	ELCD	3.529	29.488	157.2%	Linear	Linear
Bromobenzene	502.2	PID	0.100	0.057	-55.4%	Linear	Hybrid
Bromobenzene	524.2		0.140	0.187	28.7%	Hybrid	Hybrid
Bromochloromethane	502.2	ELCD	1.598	0.057	-186.1%	Linear	Hybrid
Bromochloromethane	524.2		0.368	0.592	46.5%	Hybrid	Hybrid
Bromodichloromethane	502.2	ELCD	0.424	0.465	9.1%	Linear	Constant
Bromodichloromethane	524.2		0.128	0.111	-13.8%	Hybrid	Linear
Bromoform	502.2	ELCD	3.393	0.068	-192.1%	Constant	Linear
Bromoform	524.2		0.482	0.406	-17.1%	Hybrid	Hybrid
Bromomethane	502.2	ELCD	16.351	2.195	-152.7%	Constant	Hybrid
Bromomethane	524.2		0.226	0.412	58.4%	Hybrid	Linear
Cadmium	1620		0.410	0.400	-2.6%	Hybrid	Linear
Cadmium	200.8	ICP/MS	0.063	0.033	-63.4%	Hybrid	Constant
Calcium	1620		99.975	109.600	9.2%	Linear	Constant
Carbon Disulfide	524.2		0.101	0.268	90.3%	Hybrid	Linear
Carbon Tetrachloride	524.2		0.140	0.520	115.1%	Hybrid	Linear
Carbontet+1,1-dcp	502.2	ELCD	0.069	1.553	183.1%	Hybrid	Constant
Chloroacetonitrile	524.2		3.310	31.753	162.2%	Hybrid	Constant
Chlorobenzene	502.2	ELCD	1.766	1.558	-12.5%	Linear	Constant
Chlorobenzene	502.2	PID	0.119	0.034[3]	-110.6%	Hybrid	Linear
Chlorobenzene	524.2		0.059	0.831	173.3%	Hybrid	Constant

Table 9. Comparison of 16-point and 5-point Single-laboratory IQEs at 10% RSD (SL-IQEs 10%) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE10% (16)	SL-IQE10% (5)	Percent Difference	SL-IQE Model (16)	SL-IQE Model (5)
Chloroethane	502.2	ELCD	5.826	0.644	-160.2%	Constant	Linear
Chloroethane	524.2		0.255	0.207	-20.8%	Hybrid	Hybrid
Chloroform	502.2	ELCD	0.025	0.033	26.1%	Linear	Linear
Chloroform	524.2		0.121	0.092	-27.7%	Hybrid	Linear
Chloromethane	502.2	ELCD	1.734	1.049	-49.2%	Linear	Constant
Chloromethane	524.2		0.141	0.191	30.4%	Hybrid	Linear
Chromium	1620		1.259	1.558	21.2%	Linear	Constant
Chromium	200.8	ICP/MS	1.028	1.022	-0.6%	Linear	Constant
Cis-1,2-dce+2,2-dcp	502.2	ELCD	0.039	1.055	185.7%	Hybrid	Constant
Cis-1,2-dichloroethene	524.2		0.144	0.151	4.9%	Hybrid	Hybrid
Cis-1,3-dichloropropene	502.2	ELCD	0.415	0.447[6]	7.4%	Linear	Constant
Cis-1,3-dichloropropene	502.2	PID	0.017[1]	0.226	172.0%	Hybrid	Linear
Cis-1,3-dichloropropene	524.2		0.141	0.085	-49.3%	Hybrid	Linear
Cobalt	1620		40.837	25.933	-44.6%	Linear	Linear
Cobalt	200.8	ICP/MS	N/A[4]	0.001	0.0%	Linear	Hybrid
Copper	1620		47.509	32.643	-37.1%	Constant	Constant
Copper	200.8	ICP/MS	1.825	1.885	3.2%	Constant	Constant
Dibromochloromethane	502.2	ELCD	1.252	0.809	-43.0%	Linear	Constant
Dibromochloromethane	524.2		0.288	0.167	-53.2%	Hybrid	Hybrid
Dibromomethane	502.2	ELCD	1.395	0.587	-81.6%	Linear	Constant
Dibromomethane	524.2		0.460	0.498	7.9%	Hybrid	Hybrid
Dichlorodifluoromethane	502.2	ELCD	1.091[5]	2.470	77.4%	Linear	Constant
Dichlorodifluoromethane	524.2		0.480	0.442	-8.1%	Hybrid	Hybrid
Diethyl ether	524.2		0.404	0.525	26.0%	Hybrid	Hybrid
Ethyl methacrylate	524.2		0.183	0.141	-26.0%	Hybrid	Linear
Ethylbenzene	502.2	PID	0.157	0.007[3]	-182.9%	Hybrid	Linear
Ethylbenzene	524.2		0.077	0.064	-19.2%	Hybrid	Linear
Hardness[2]	130.2		5.465	10.032	58.9%	Linear	Constant
Hexachlorobutadiene	502.2	ELCD	0.243	0.582	82.2%	Hybrid	Linear
Hexachlorobutadiene	524.2		0.228	0.232	1.7%	Hybrid	Linear
Hexachloroethane	524.2		0.167	0.386	78.9%	Hybrid	Linear
Hexchlobutadiene+naphthalene	502.2	PID	1.542	1.193	-25.6%	Hybrid	Constant
Iron	1620		996.565[5]	2186.832	74.8%	Linear	Constant
Isopropylbenzene	502.2	PID	0.129	0.032	-120.6%	Linear	Linear
Isopropylbenzene	524.2		25.592	1.157	-182.7%	Constant	Constant
Lead	1620		5.698	6.059	6.1%	Linear	Constant
Lead	200.8	ICP/MS	0.685	5.983	158.9%	Linear	Constant
M+p xylene	502.2	PID	0.222	0.240	7.6%	Hybrid	Constant
M+p xylene	524.2		24.651	0.034	-199.4%	Constant	Hybrid
Magnesium	1620		267.199	378.277	34.4%	Linear	Constant
Manganese	1620		15.264	9.339	-48.2%	Constant	Constant
Manganese	200.8	ICP/MS	0.245	0.160	-41.8%	Constant	Constant
Mercury	200.8	ICP/MS	0.039	0.017[1]	-79.4%	Hybrid	Hybrid
Methacrylonitrile	524.2		19.062	1.111	-178.0%	Constant	Hybrid
Methyl Iodide	524.2		0.083	3.681	191.1%	Hybrid	Constant
Methyl tert-butyl ether	524.2		0.122	15.132[6]	196.8%	Hybrid	Constant

Table 9. Comparison of 16-point and 5-point Single-laboratory IQEs at 10% RSD (SL-IQEs 10%) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE10% (16)	SL-IQE10% (5)	Percent Difference	SL-IQE Model (16)	SL-IQE Model (5)
Methyla crylate	524.2		0.727	0.853	16.0%	Hybrid	Linear
Methylene Chloride	502.2	ELCD	6.033	N/A [4]	N/A	Constant	Constant
Methylene Chloride	524.2		0.433	0.293	-38.5%	Hybrid	Linear
Methylm ethacryl ate	524.2		20.773	0.873	-183.9%	Constant	Linear
Molybdenum	1620		7.597	11.866	43.9%	Linear	Constant
Molybdenum	200.8	ICP/MS	0.608	0.012	-192.4%	Constant	Constant
N-butylbenzene	502.2	PID	0.745	0.586	-24.0%	Linear	Linear
N-butylbenzene	524.2		0.067	1.287	180.1%	Hybrid	Constant
N-propylbenzene	502.2	PID	0.186	0.212	13.0%	Hybrid	Constant
N-propylbenzene	524.2		29.878	0.118	-198.4%	Constant	Hybrid
Naphthalene	524.2		0.108	0.256	81.1%	Hybrid	Hybrid
Nickel	1620		67.206	86.054	24.6%	Linear	Constant
Nickel	200.8	ICP/MS	0.183	0.147	-21.9%	Hybrid	Constant
O-xylene	524.2		0.040	0.016	-85.5%	Hybrid	Linear
O-xylene+styrene	502.2	PID	0.181	0.305	51.0%	Linear	Constant
P-isopreptol+1,4-dcb	502.2	PID	0.456	0.302	-40.8%	Linear	Constant
Pentachloroethane	524.2		0.551	1.036	61.1%	Hybrid	Linear
Sec-butylbenzene	502.2	PID	0.157	0.754	131.1%	Hybrid	Constant
Sec-butylbenzene	524.2		0.047	1.266	185.5%	Hybrid	Constant
Selenium	1620		5.235	4.076	-24.9%	Linear	Linear
Selenium	200.8	ICP/MS	1.045	0.707	-38.6%	Linear	Hybrid
Silver	1620		25.842	22.813	-12.5%	Linear	Constant
Silver	200.8	ICP/MS	0.056	N/A [4]	N/A	Linear	Linear
Sodium	1620		337.755	333.796	-1.2%	Linear	Linear
Styrene	524.2		0.041	0.067	49.3%	Hybrid	Linear
Tert-butylbenzene	502.2	PID	0.203	0.111	-58.9%	Linear	Hybrid
Tert-butylbenzene	524.2		0.073	0.074	1.1%	Hybrid	Linear
Tetrachloroethene	502.2	ELCD	0.122	0.182	39.7%	Hybrid	Linear
Tetrachloroethene	502.2	PID	0.750	0.385	-64.4%	Linear	Linear
Tetrachloroethene	524.2		30.554 [6]	1.643	-179.6%	Constant	Linear
Thallium	1620		2.799	2.745	-1.9%	Linear	Linear
Thallium	200.8	ICP/MS	0.002	0.001	-76.8%	Linear	Linear
Thorium	200.8	ICP/MS	0.004	0.001	-134.2%	Linear	Constant
Tin	1620		9.406	9.772	3.8%	Linear	Linear
Titanium	1620		14.236	42.768	100.1%	Linear	Constant
Toluene	502.2	PID	0.194	0.131	-39.1%	Linear	Constant
Toluene	524.2		0.046	1.145 [6]	184.7%	Hybrid	Constant
Total Phosphorus [2]	365.2		0.030	0.026	-15.8%	Hybrid	Linear
Total Suspended Solids [2]	160.2		6.729	6.929	2.9%	Hybrid	Linear
Trans-1,2-dichloroethene	502.2	ELCD	0.191	0.081 [5]	-80.6%	Hybrid	Linear
Trans-1,2-dichloroethene	524.2		0.153	0.171	11.3%	Hybrid	Hybrid
Trans-1,3-dichloropropene	502.2	ELCD	0.729	0.485	-40.2%	Linear	Constant
Trans-1,3-dichloropropene	502.2	PID	0.175	0.238	30.7%	Hybrid	Linear
Trans-1,3-dichloropropene	524.2		0.218	0.101	-73.5%	Hybrid	Hybrid
Trans-1,4-dichloro-2-butene	524.2		30.108	1.768	-177.8%	Constant	Hybrid
Trichloroethene	502.2	ELCD	3.169	1.010	-103.3%	Linear	Constant

Table 9. Comparison of 16-point and 5-point Single-laboratory IQEs at 10% RSD (SL-IQEs 10%) for the Episode 6000 Dataset (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE10% (16)	SL-IQE10% (5)	Percent Difference	SL-IQE Model (16)	SL-IQE Model (5)
Trichloroethene	502.2	PID	0.401	0.079	-134.4%	Linear	Linear
Trichloroethene	524.2		0.167	1.068	145.8%	Hybrid	Linear
Trichlorofluoromethane	502.2	ELCD	4.662	1.355	-109.9%	Constant	Constant
Trichlorofluoromethane	524.2		42.490[6]	0.301	-197.2%	Constant	Hybrid
Uranium	200.8	ICP/MS	0.001	0.000	-69.1%	Linear	Linear
Vanadium	1620		24.338	17.798	-31.0%	Hybrid	Linear
Vnadium	200.8	ICP/MS	1.933	2.225	14.1%	Hybrid	Linear
Vinyl Chloride	502.2	ELCD	8.234	3.258	-86.6%	Constant	Linear
Vinyl Chloride	524.2		0.219	0.652	99.2%	Hybrid	Linear
Wad Cyanide	1677	WADCN	1.624	2.661	48.4%	Linear	Constant
Xylene (total)	524.2		23.520	0.017	-199.7%	Constant	Hybrid
Yttrium	1620		8.962	28.689	104.8%	Linear	Constant
Zinc	1620		10.452	14.257	30.8%	Hybrid	Constant
Zinc	200.8	ICP/MS	7.024	10.927	43.5%	Linear	Constant

[1] IQE 10% undefined, IQE 20% reported

[2] Results reported as mg/L

[3] IQE 10% negative, IQE 20% reported

[4] IQE 10%, IQE 20%, IQE30% all negative based on chosen model (linear)

[5] IQE 10% and IQE 20% both negative, IQE 30% reported

[6] Hybrid model selected but did not converge; IQE 10% based on constant model instead

Summary Statistics for Table 9

	SL-IQE10 (16) vs. SL-IQE10 (5) (all analytes)	SL-IQE10 (16) vs. SL-IQE10 (5) (same model used)	SL-IQE10 (16) vs. SL-IQE10 (5) (different models used)
Number of Analytes	195	50	145
Minimum:	-19,971.5%	-19,237.7%	-19,971.5%
25th percentile:	-6,115.2%	-7,243.8%	-4,927.0%
Median:	-194.6%	-2,442.7%	613.9%
75th percentile:	4,562.6%	576.4%	6109.3%
Maximum:	19,715.8%	15724.6%	19,715.8%

	Number of analytes	Median % Difference	Sign Test p-value	Wilcoxon p-value
SL-IQE10 (16) vs. SL-IQE10 (5) (all analytes)	195	-194.600	0.567	0.345
SL-IQE10 (16) vs. SL-IQE10 (5) (same model used)	50	-2,442.7%	0.015	0.001
SL-IQE10 (16) vs. SL-IQE10 (5) (different models used)	145	613.9%	0.507	0.606

Table 10. Comparison of ACIL, USGS and EPA Limits Calculating using USGS Blank and Spiked data

Analyte	# blanks	# spikes	ACIL CRV		USGS LT-MDL (adding median)		USGS LT-MDL (adding mean)		EPA MDL (Randomly selected from simulated 7-replicate MDLs)	
			Limit	% exceeding	Limit	% exceeding	Limit	% exceeding	Limit	% exceeding
Ammonia (FCA)	52	24	0.022	0.0%	0.021	0.0%	0.021	0.0%	0.062	0.0%
Ammonia (FCC)	52	24	0.023	1.9%	0.011	11.5%	0.011	11.5%	0.012	9.6%
Ammonia Low Level (FCC)	52	15	0.006	1.9%	0.003	21.2%	0.004	7.7%	0.006	1.9%
Arsenic, Dissolved	26	24	1.068	3.8%	1.005	3.8%	1.071	3.8%	0.895	3.8%
Arsenic, Total	26	24	1.493	3.8%	0.829	7.7%	0.825	7.7%	1.298	3.8%
Cadmium, Dissolved by GFAA	26	24	0.082	0.0%	0.099	0.0%	0.095	0.0%	0.121	0.0%
Cadmium, Total by GFAA	26	24	0.075	0.0%	0.084	0.0%	0.089	0.0%	0.130	0.0%
Chromium, Dissolved by GFAA	26	24	0.441	3.8%	0.466	0.0%	0.475	0.0%	0.473	0.0%
Chromium, Total by GFAA	26	24	0.316	3.8%	0.341	3.8%	0.340	3.8%	3.540	0.0%
Cobalt, Dissolved by GFAA	26	24	1.287	0.0%	1.911	0.0%	1.847	0.0%	1.451	0.0%
Cobalt, Total by GFAA	26	24	1.639	3.8%	1.053	3.8%	1.093	3.8%	1.076	3.8%
Copper, Dissolved by GFAA	26	24	0.536	3.8%	0.408	3.8%	0.421	3.8%	1.102	0.0%
Copper, Total by GFAA	26	24	0.684	0.0%	0.766	0.0%	0.764	0.0%	26.384	0.0%
Lead, Dissolved by GFAA	26	24	0.609	3.8%	0.861	0.0%	0.857	0.0%	0.860	0.0%
Lead, Total by GFAA	26	24	0.774	3.8%	0.780	3.8%	0.736	3.8%	0.678	3.8%
Molybdenum (Wastewater) by GFAA	25	24	0.906	0.0%	0.779	0.0%	0.778	0.0%	0.639	4.0%
Molybdenum, Dissolved by GFAA	26	24	0.862	3.8%	1.098	0.0%	1.082	3.8%	1.190	0.0%
Nickel, Dissolved by GFAA	26	24	0.991	0.0%	1.014	0.0%	0.909	0.0%	2.568	0.0%
Nickel, Total by GFAA	26	24	1.765	0.0%	0.936	19.2%	1.167	11.5%	2.076	0.0%
Nitrate/Nitrite (FCA)	52	24	0.018	0.0%	0.009	21.2%	0.010	17.3%	0.009	21.2%

Table 10. Comparison of ACIL, USGS and EPA Limits Calculating using USGS Blank and Spiked data

Analyte	# blanks	# spikes	ACIL CRV		USGS LT-MDL (adding median)		USGS LT-MDL (adding mean)		EPA MDL (Randomly selected from simulated 7-replicate MDLs)	
			Limit	% exceeding	Limit	% exceeding	Limit	% exceeding	Limit	% exceeding
Nitrate/Nitrite (FCC)	52	15	0.023	3.8%	0.025	1.9%	0.026	1.9%	0.019	5.8%
Nitrate/Nitrite Low Level (FCC)	52	24	0.007	0.0%	0.008	0.0%	0.008	0.0%	0.006	11.5%
Nitrite (FCC)	52	15	0.003	0.0%	0.002	1.9%	0.002	1.9%	0.003	0.0%
Nitrite Low Level (FCC)	52	24	0.001	0.0%	0.002	0.0%	0.002	0.0%	0.002	0.0%
Orthophosphate (FCC)	52	24	0.022	3.8%	0.008	19.2%	0.010	15.4%	0.010	15.4%
Orthophosphate Low Level (FCC)	52	24	0.002	0.0%	0.000	26.9%	0.000	26.9%	0.001	0.0%
Phosphorus, Low Level Filtered	52	24	0.003	1.9%	0.003	0.0%	0.003	0.0%	0.003	0.0%
Phosphorus, Low Level Filtered	52	24	0.003	0.0%	0.003	0.0%	0.003	0.0%	0.004	0.0%
Phosphorus, Low Level in Wastewater	52	24	0.003	3.8%	0.004	1.9%	0.004	1.9%	0.009	0.0%
Selenium, Dissolved	26	24	1.174	0.0%	1.434	0.0%	1.410	0.0%	1.334	0.0%
Selenium, Total	26	24	2.123	3.8%	1.211	7.7%	1.324	7.7%	1.130	11.5%
Silver, Dissolved by GFAA	26	24	0.088	3.8%	0.159	0.0%	0.158	0.0%	0.122	0.0%
Silver, Total by GFAA	26	24	0.140	3.8%	0.125	3.8%	0.131	3.8%	0.196	0.0%
TKN/ Ammonia (FCA)	52	24	0.070	0.0%	0.092	0.0%	0.091	0.0%	0.071	0.0%
TKN/ Ammonia (FCC)	52	24	0.083	1.9%	0.056	3.8%	0.059	3.8%	0.049	7.7%
TKN/ Ammonia (WCA)	52	24	0.483	1.9%	0.081	1.9%	0.104	1.9%	0.071	1.9%
Total Phosphorus (FCA)	52	24	0.021	3.8%	0.026	0.0%	0.026	0.0%	0.022	1.9%
Total Phosphorus (FCC)	52	24	0.026	0.0%	0.025	0.0%	0.025	0.0%	0.023	0.0%
Total Phosphorus (WCA)	52	24	0.027	1.9%	0.023	1.9%	0.023	1.9%	0.021	3.8%

Summary Statistics for Table 10.

Limit Type	% of Blanks Exceeding Limit for Dataset	
	Mean	Standard Error
ACIL CRV	1.9%	0.3%
USGS LT-MDL (adding median)	4.4%	1.2%
USGS LT-MDL (adding mean)	3.7%	0.9%
EPA MDL	2.9%	0.8%

Table 11. Comparison of SL-IDEs and MDLs calculated With and Without Outlier Removal, Episode 6000 Data
(µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE			MDL	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers dropped
1,1,1,2-tetrachloroethane	502.2	ELCD	0.034	0.024	E/E	0.041	0.006
1,1,1,2-tetrachloroethane	524.2		0.244	0.211	E/E	0.052	0.052
1,1,1-trichloroethane	502.2	ELCD	0.041	0.038	E/E	0.012	0.012
1,1,1-trichloroethane	524.2		0.308	0.311	E/E	0.055	0.055
1,1,2,2-tce+1,2,3-tcp	502.2	ELCD	0.179	0.123	E/E	0.064	0.064
1,1,2,2-tetrachloroethane	524.2		0.436	0.296	E/E	0.132	0.132
1,1,2-trichloroethane	502.2	ELCD	0.032	0.026	E/E	0.024	0.018
1,1-dichloroethane	502.2	ELCD	0.083	0.060	E/E	0.010	0.014
1,1-dichloroethane	524.2		0.229	0.187	E/E	0.033	0.033
1,1-dichloroethene	502.2	ELCD	0.234	0.165	E/E	0.038	0.028
1,1-dichloropropene	524.2		0.287	0.294	E/E	0.045	0.045
1,2,3-trichlorobenzene	502.2	ELCD	0.134	0.066	E/E	0.048	0.021
1,2,3-trichlorobenzene	502.2	PID	0.115	0.095	E/E	0.057	0.057
1,2,3-trichlorobenzene	524.2		0.275	0.256	E/E	0.070	0.070
1,2,3-trichloropropane	524.2		1.263	1.046	E/E	7.328	4.014
1,2,4-trichlorobenzene	502.2	ELCD	0.088	0.076	E/E	0.022	0.022
1,2,4-trichlorobenzene	502.2	PID	0.124	0.117	E/E	0.070	0.070
1,2,4-trimethylbenzene	502.2	PID	0.125	0.107	E/E	0.095	0.095
1,2,4-trimethylbenzene	524.2		0.144	0.134	E/E	0.012	0.026
1,2-dibromo-3-chloropropane	524.2		1.749	1.368	E/E	1.457	1.457
1,2-dibromoethane	502.2	ELCD	0.164	0.146	E/E	0.096	0.095
1,2-dibromoethane	524.2		0.326	0.290	E/E	0.127	0.127
1,2-dichlorobenzene	502.2	ELCD	0.065	0.061	E/E	0.035	0.035
1,2-dichlorobenzene	524.2		0.130	0.133	E/E	0.030	0.025
1,2-dichloroethane	502.2	ELCD	0.042	0.029	E/E	0.017	0.017
1,2-dichloroethane	524.2		0.258	0.237	E/E	0.039	0.059
1,2-dichloropropane	502.2	ELCD	0.043	0.031	E/E	0.023	0.029
1,2-dichloropropane	524.2		0.247	0.175	E/E	0.056	0.026
1,3,5-trimethylbenzene	524.2		0.135	0.127	E/E	0.011	0.011
1,3-dichlorobenzene	502.2	ELCD	0.118	0.073	E/E	0.035	0.014
1,3-dichlorobenzene	502.2	PID	0.126	0.106	E/E	0.093	0.067
1,3-dichloropropane	502.2	ELCD	0.047	0.037	E/E	0.016	0.014
1,3-dichloropropane	524.2		0.202	0.182	E/E	0.038	0.038
1,4-dichlorobenzene	502.2	ELCD	0.061	0.053	E/E	0.026	0.026
1,4-dichlorobenzene	524.2		0.140	0.130	E/E	0.023	0.023
2,2-dichloropropane	524.2		0.691	0.630	E/E	2.376	2.376
2-butanone	524.2		0.833	0.696	E/E	0.417	0.874
2-chlorotoluene	502.2	ELCD	0.175	0.161	E/E	0.108	0.108
2-chlorotoluene	502.2	PID	0.230	0.143	E/E	0.238	0.086
2-hexanone	524.2		0.902	0.753	E/E	1.316	0.426
4-chlorotoluene	502.2	ELCD	0.149	0.134	E/E	0.110	0.083
4-chlorotoluene	524.2		0.123	0.114	E/E	0.010	0.010
Allyl Chloride	524.2		0.229	0.213	E/E	0.032	0.029
Aluminum	1620		206.975	47.299	C/E	29.555	19.524
Aluminum	200.8	ICP/MS	12.747	9.371	E/E	19.145	0.839
Ammonia as Nitrogen [2]	350.3		0.014	0.013	E/E	0.010	0.010

Table 11. Comparison of SL-IDEs and MDLs calculated With and Without Outlier Removal, Episode 6000 Data
(µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE			MDL	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers dropped
Antimony	200.8	ICP/MS	0.019	0.014	E/E	0.178	0.008
Arsenic	200.8	ICP/MS	0.366	0.347	E/E	0.226	0.226
Barium	1620		1.837	1.441	C/C	1.702	1.702
Barium	200.8	ICP/MS	0.084	0.068	E/E	0.033	0.018
Benzene	502.2	PID	0.079	0.074	E/E	0.030	0.030
Beryllium	1620		0.448	0.430	E/E	0.528	0.528
Beryllium	200.8	ICP/MS	0.024	0.021	E/E	0.007	0.007
Bromobenzene	502.2	ELCD	0.765	0.242	L/E	0.131	0.131
Bromobenzene	502.2	PID	0.050	0.046	E/E	0.012	0.012
Bromobenzene	524.2		0.211	0.195	E/E	0.044	0.044
Bromochloromethane	502.2	ELCD	0.482	0.390	L/L	0.013	0.013
Bromodichloromethane	502.2	ELCD	0.075	0.065	E/E	0.004	0.004
Bromodichloromethane	524.2		0.205	0.190	E/E	0.043	0.043
Bromoform	502.2	ELCD	1.513	1.504	C/C	0.006	0.006
Bromoform	524.2		0.400	0.363	E/E	0.123	0.123
Bromomethane	502.2	ELCD	7.293	7.427	C/C	0.267	0.477
Cadmium	1620		0.191	0.159	E/E	0.127	0.127
Cadmium	200.8	ICP/MS	0.022	0.022	E/E	0.004	0.004
Calcium	1620		41.358	36.054	L/L	36.726	36.726
Carbon Tetrachloride	524.2		0.314	0.288	E/E	0.038	0.038
Carbontet+1,1-dcp	502.2	ELCD	0.072	0.068	E/E	0.029	0.029
Chlorobenzene	502.2	ELCD	0.460	0.378	L/L	0.011	0.011
Chlorobenzene	502.2	PID	0.064	0.055	E/E	0.030	0.026
Chloroethane	502.2	ELCD	2.598	2.357	C/C	0.108	0.011
Chloroethane	524.2		0.395	0.362	E/E	0.066	0.048
Chloroform	502.2	ELCD	0.032	0.026	E/E	0.043	0.043
Chloromethane	502.2	ELCD	0.250	0.150	E/E	0.070	0.070
Chloromethane	524.2		0.253	0.302	E/E	0.045	0.045
Chromium	1620		0.496	0.464	E/E	0.310	0.310
Chromium	200.8	ICP/MS	0.408	0.207	L/E	0.073	0.073
Cis-1,2-dce+2,2-dcp	502.2	ELCD	0.055	0.052	E/E	0.013	0.013
Cis-1,3-dichloropropene	502.2	ELCD	0.074	0.062	E/E	0.007	0.007
Cis-1,3-dichloropropene	502.2	PID	0.082	0.138	E/E	0.057	0.057
Cis-1,3-dichloropropene	524.2		0.173	0.145	E/E	0.038	0.036
Cobalt	1620		16.463	15.625	E/E	9.820	9.820
Cobalt	200.8	ICP/MS	0.074	0.074	C/C	0.001	0.001
Copper	1620		21.189	14.718	C/C	6.046	6.046
Copper	200.8	ICP/MS	0.798	0.160	C/E	0.037	0.037
Dibromochloromethane	502.2	ELCD	0.436	0.413	L/L	0.009	0.006
Dibromochloromethane	524.2		0.287	0.210	E/E	0.051	0.051
Dibromomethane	502.2	ELCD	0.460	0.344	L/L	0.007	0.007
Dibromomethane	524.2		0.388	0.319	E/E	0.102	0.102
Dichlorodifluoromethane	502.2	ELCD	0.240	0.069	E/E	0.009	0.071
Diethyl Ether	524.2		0.376	0.301	E/E	0.120	0.120
Ethyl Methacrylate	524.2		0.273	0.246	E/E	0.045	0.035
Ethylbenzene	502.2	PID	0.078	0.073	E/E	0.021	0.021

Table 11. Comparison of SL-IDEs and MDLs calculated With and Without Outlier Removal, Episode 6000 Data

(µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE			MDL	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers dropped
Ethylbenzene	524.2		0.198	0.184	E/E	0.033	0.023
Hexachlorobutadiene	502.2	ELCD	0.094	0.081	E/E	0.043	0.043
Hexchlobutadiene+naphthalene	502.2	PID	0.597	0.490	E/E	0.649	0.649
Iron	1620		373.590	42.840	L/E	90.409	19.188
Isopropylbenzene	502.2	PID	0.060	0.047	E/E	0.020	0.020
Isopropylbenzene	524.2		0.120	0.107	E/E	0.011	0.010
Lead	1620		2.423	1.855	E/E	1.647	1.288
Lead	200.8	ICP/MS	0.204	0.133	E/E	0.655	0.131
M+p xylene	502.2	PID	0.121	0.114	E/E	0.090	0.090
Magnesium	1620		105.998	100.489	E/E	103.033	103.033
Manganese	1620		6.808	2.183	C/E	6.856	1.176
Manganese	200.8	ICP/MS	0.109	0.018	C/E	0.031	0.012
Mercury	200.8	ICP/MS	0.027	0.024	E/E	0.004	0.004
Methacrylonitrile	524.2		0.718	0.492	E/E	0.356	0.336
Methylacrylate	524.2		0.601	0.477	E/E	0.220	0.220
Methylene Chloride	524.2		0.314	0.279	E/E	0.082	0.082
Methylmethacrylate	524.2		0.535	0.480	E/E	0.225	0.225
Molybdenum	1620		3.034	2.683	E/E	2.455	2.455
Molybdenum	200.8	ICP/MS	0.271	0.027 [1]	C/C	0.004	0.002
N-butylbenzene	502.2	PID	0.141	0.105	E/E	0.030	0.083
N-propylbenzene	502.2	PID	0.092	0.071	E/E	0.040	0.040
Naphthalene	524.2		0.186	0.219	E/E	0.048	0.048
Nickel	1620		25.560	23.853	E/E	20.219	20.219
Nickel	200.8	ICP/MS	0.083	0.057	E/E	0.146	0.075
O-xylene+styrene	502.2	PID	0.116	0.087	E/E	0.059	0.043
P-isoproptol+1,4-dcb	502.2	PID	0.159	0.131	E/E	0.073	0.054
Pentachloroethane	524.2		0.408	0.351	E/E	0.553	0.207
Sec-butylbenzene	502.2	PID	0.081	0.068	E/E	0.055	0.036
Selenium	200.8	ICP/MS	0.416	0.324	E/E	0.192	0.192
Silver	1620		10.668	10.718	E/L	4.907	4.250
Silver	200.8	ICP/MS	0.012	0.010	E/E	0.004	0.004
Tert-butylbenzene	502.2	PID	0.074	0.082	E/E	0.029	0.029
Tetrachloroethene	502.2	ELCD	0.061	0.054	E/E	0.018	0.018
Tetrachloroethene	502.2	PID	0.156	0.131	E/E	0.062	0.062
Tetrachloroethene	524.2		0.469	0.393	E/E	0.085	0.027
Thallium	200.8	ICP/MS	0.001	0.001	E/E	0.000	0.000
Thorium	200.8	ICP/MS	0.001	0.001	E/E	0.001	0.001
Tin	1620		3.932	3.700	E/E	3.670	3.670
Titanium	1620		5.376	4.732	E/E	4.777	4.663
Toluene	502.2	PID	0.064	0.056	E/E	0.070	0.071
Toluene	524.2		0.146	0.136	E/E	0.020	0.018
Total Suspended Solids [2]	160.2		3.005	3.060	E/E	1.170	0.980
Trans-1,2-dichloroethene	502.2	ELCD	0.081	0.073	E/E	0.041	0.041
Trans-1,3-dichloropropene	502.2	ELCD	0.098	0.083	E/E	0.012	0.012
Trans-1,3-dichloropropene	502.2	PID	0.092	0.088	E/E	0.058	0.058
Trans-1,3-dichloropropene	524.2		0.223	0.188	E/E	0.051	0.051

Table 11. Comparison of SL-IDEs and MDLs calculated With and Without Outlier Removal, Episode 6000 Data

(µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE			MDL	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers dropped
Trichloroethene	502.2	ELCD	0.059	0.049	E/E	0.012	0.012
Trichloroethene	502.2	PID	0.097	0.078	E/E	0.027	0.027
Trichloroethene	524.2		0.332	0.333	E/E	0.061	0.061
Trichlorofluoromethane	502.2	ELCD	2.079	1.762	C/C	0.108	0.012
Trichlorofluoromethane	524.2		0.384	0.528	E/E	0.087	0.087
Uranium	200.8	ICP/MS	0.000	0.000	E/E	0.000	0.000
Vinyl Chloride	502.2	ELCD	3.672	3.577	C/C	0.270	0.270
Wad Cyanide	1677	WADCN	0.701	0.665	L/L	0.572	0.550
Yttrium	1620		3.247	3.078	E/E	1.923	1.923
Zinc	1620		4.500	4.135	E/E	2.597	2.597
Zinc	200.8	ICP/MS	1.598	1.016	E/E	0.900	0.585

[1] Constant model used because IDE did not converge for chosen model (Exponential)

[2] Results reported as mg/L

Summary Statistics for Table 11.

Percent Difference (Positive if limit with outliers kept>limit with outliers removed)	# Analytes	Minimum	25th Percentile	Median	75th Percentile	Maximum
SL-IDE (all)	149	-51.6%	7.1%	14.3%	24.4%	164.2%
SL-IDE (same model used)	141	-51.6%	6.9%	13.7%	22.2%	164.2%
SL-IDE (different model used)	8	-0.5%	93.4%	114.7%	135.9%	158.9%
MDL	60	-115.4%	4.4%	30.2%	75.6%	183.7%

Table 12. Comparison of SL-IQEs and MLs calculated With and Without Outlier Removal, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE (10%)			ML	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers Dropped
1,1,1,2-tetrachloroethane	502.2	ELCD	0.030	0.023	H/H	0.2	0.02
1,1,1,2-tetrachloroethane	524.2		0.181	0.142	H/H	0.2	0.2
1,1,1-trichloroethane	502.2	ELCD	0.830	2.207	L/C	0.05	0.05
1,1,1-trichloroethane	524.2		0.240	0.157	H/H	0.2	0.2
1,1,2,2-tce+1,2,3-tcp	502.2	ELCD	5.514	5.290 [5]	C/C	0.2	0.2
1,1,2,2-tetrachloroethane	524.2		0.569	0.318	H/H	0.5	0.5
1,1,2-trichloroethane	502.2	ELCD	0.060	0.030	L/H	0.1	0.05
1,1-dichloroethane	502.2	ELCD	0.527	0.311	L/L	0.05	0.05
1,1-dichloroethane	524.2		0.115	25.620 [5]	H/C	0.1	0.1
1,1-dichloroethene	502.2	ELCD	3.796	3.827	L/L	0.1	0.1
1,1-dichloropropene	524.2		0.180	0.090	H/H	0.2	0.2
1,2,3-trichlorobenzene	502.2	ELCD	0.851	0.117	L/L	0.2	0.1
1,2,3-trichlorobenzene	502.2	PID	0.248	0.190	H/H	0.2	0.2
1,2,3-trichlorobenzene	524.2		0.216	0.217	H/H	0.2	0.2
1,2,3-trichloropropane	524.2		11.316	5.134	L/L	20	10
1,2,4-trichlorobenzene	502.2	ELCD	0.401	0.226	L/L	0.1	0.1
1,2,4-trichlorobenzene	502.2	PID	0.439	0.429	L/L	0.2	0.2
1,2,4-trimethylbenzene	502.2	PID	0.653	0.621	L/L	0.5	0.5
1,2,4-trimethylbenzene	524.2		20.896	21.013	C/C	0.05	0.1
1,2-dibromo-3-chloropropane	524.2		71.182 [5]	72.198 [5]	C/C	5	5
1,2-dibromoethane	502.2	ELCD	0.592	0.560	L/L	0.5	0.2
1,2-dibromoethane	524.2		0.417	0.418	H/H	0.5	0.5
1,2-dichlorobenzene	502.2	ELCD	0.183	0.114	L/H	0.1	0.1
1,2-dichlorobenzene	524.2		0.085	0.067	H/H	0.1	0.1
1,2-dichloroethane	502.2	ELCD	0.065	0.031	H/H	0.05	0.05
1,2-dichloroethane	524.2		0.222	0.168	H/H	0.1	0.2
1,2-dichloropropane	502.2	ELCD	0.102	0.038	L/H	0.1	0.1
1,2-dichloropropane	524.2		0.196	0.085	H/H	0.2	0.1
1,3,5-trimethylbenzene	524.2		23.744	23.877	C/C	0.05	0.05
1,3-dichlorobenzene	502.2	ELCD	0.936	0.463	L/L	0.1	0.05
1,3-dichlorobenzene	502.2	PID	0.465	0.401	L/L	0.2	0.2
1,3-dichloropropane	502.2	ELCD	0.054	0.059	L/H	0.05	0.05
1,3-dichloropropane	524.2		0.139	0.151	H/H	0.1	0.1
1,4-dichlorobenzene	502.2	ELCD	0.101	0.079	H/H	0.1	0.1
1,4-dichlorobenzene	524.2		0.078	0.077	H/H	0.1	0.1
2,2-dichloropropane	524.2		38.009	38.299	C/C	10	10
2-butanone	524.2		0.893	0.534	H/H	2	2
2-chlorotoluene	502.2	ELCD	0.493	0.439	H/H	0.5	0.5
2-chlorotoluene	502.2	PID	0.849	0.770	H/L	1	0.2
2-hexanone	524.2		0.442	0.518	H/H	5	2
4-chlorotoluene	502.2	ELCD	0.142 [1]	0.517	H/H	0.5	0.2
4-chlorotoluene	524.2		23.810	23.941	C/C	0.05	0.05
Allyl Chloride	524.2		29.674	29.866	C/C	0.1	0.1
Aluminum	1620		464.069	156.043	C/L	100	50
Aluminum	200.8	ICP/MS	29.684	31.466	H/L	50	2
Ammonia as Nitrogen [2]	350.3		0.035	0.032	H/H	0.05	0.05
Antimony	200.8	ICP/MS	0.034	0.020	H/H	0.5	0.02

Table 12. Comparison of SL-IQEs and MLs calculated With and Without Outlier Removal, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE (10%)			ML	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers Dropped
Arsenic	200.8	ICP/MS	0.798	0.747	H/H	1	1
Barium	1620		4.118	3.231	C/C	5	5
Barium	200.8	ICP/MS	0.211	0.191	L/L	0.1	0.05
Benzene	502.2	PID	0.182	0.149	L/H	0.1	0.1
Beryllium	1620		0.980	0.975	H/H	2	2
Beryllium	200.8	ICP/MS	0.044	0.038	H/H	0.02	0.02
Bromobenzene	502.2	ELCD	3.529	0.594	L/H	0.5	0.5
Bromobenzene	502.2	PID	0.100	0.022	L/L	0.05	0.05
Bromobenzene	524.2		0.140	0.143	H/H	0.2	0.2
Bromochloromethane	502.2	ELCD	1.598	1.344	L/L	0.05	0.05
Bromodichloromethane	502.2	ELCD	0.424	0.323	L/L	0.02	0.02
Bromodichloromethane	524.2		0.128	0.131	H/H	0.2	0.2
Bromoform	502.2	ELCD	3.393	3.350	C/C	0.02	0.02
Bromoform	524.2		0.482	0.484	H/H	0.5	0.5
Bromomethane	502.2	ELCD	16.351	16.541	C/C	1	2
Cadmium	1620		0.410	0.422	H/L	0.5	0.5
Cadmium	200.8	ICP/MS	0.063	0.068	H/H	0.02	0.02
Calcium	1620		99.975	88.075	L/L	100	100
Carbon Tetrachloride	524.2		0.140	0.061	H/H	0.1	0.1
Carbontet+1,1-dcp	502.2	ELCD	0.069	4.481	H/C	0.1	0.1
Chlorobenzene	502.2	ELCD	1.766	1.514	L/L	0.05	0.05
Chlorobenzene	502.2	PID	0.119	0.100	H/H	0.1	0.1
Chloroethane	502.2	ELCD	5.826	5.285	C/C	0.5	0.05
Chloroethane	524.2		0.255	0.202	H/H	0.2	0.2
Chloroform	502.2	ELCD	0.025	0.006	L/H	0.2	0.2
Chloromethane	502.2	ELCD	1.734	0.766	L/L	0.2	0.2
Chloromethane	524.2		0.141	0.187	H/H	0.2	0.2
Chromium	1620		1.259	1.072	L/L	1	1
Chromium	200.8	ICP/MS	1.028	0.636	L/L	0.2	0.2
Cis-1,2-dce+2,2-dcp	502.2	ELCD	0.039	0.038	H/H	0.05	0.05
Cis-1,3-dichloropropene	502.2	ELCD	0.415	0.131	L/H	0.02	0.02
Cis-1,3-dichloropropene	502.2	PID	0.017 [1]	0.262	H/H	0.2	0.2
Cis-1,3-dichloropropene	524.2		0.141	0.070	H/H	0.1	0.1
Cobalt	1620		40.837	39.614	L/L	50	50
Cobalt	200.8	ICP/MS	N/A [3]	N/A [3]	N/A	0.005	0.005
Copper	1620		47.509	33.000	C/C	20	20
Copper	200.8	ICP/MS	1.825	1.706	C/C	0.1	0.1
Dibromochloromethane	502.2	ELCD	1.252	1.189	L/L	0.02	0.02
Dibromochloromethane	524.2		0.288	0.177	H/H	0.2	0.2
Dibromomethane	502.2	ELCD	1.395	1.099	L/L	0.02	0.02
Dibromomethane	524.2		0.460	0.473	H/H	0.5	0.5
Dichlorodifluoromethane	502.2	ELCD	1.091 [4]	5.023	L/C	0.02	0.2
Diethyl Ether	524.2		0.404	0.400	H/H	0.5	0.5
Ethyl Methacrylate	524.2		0.183	0.109	H/H	0.2	0.1
Ethylbenzene	502.2	PID	0.157	0.149	H/H	0.1	0.1
Ethylbenzene	524.2		0.077	0.047	H/H	0.1	0.1
Hexachlorobutadiene	502.2	ELCD	0.243	0.194	H/H	0.2	0.2

Table 12. Comparison of SL-IQEs and MLs calculated With and Without Outlier Removal, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE (10%)			ML	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers Dropped
Hexchlobutadiene+naphthalene	502.2	PID	1.542	1.216	H/H	2	2
Iron	1620		996.565 [4]	151.265	L/H	200	50
Isopropylbenzene	502.2	PID	0.129	1.928	L/C	0.1	0.1
Isopropylbenzene	524.2		25.592	25.726	C/C	0.05	0.05
Lead	1620		5.698	4.449	L/L	5	5
Lead	200.8	ICP/MS	0.685	0.281	L/H	2	0.5
M+p xylene	502.2	PID	0.222	0.217	H/H	0.2	0.2
Magnesium	1620		267.199	259.424	L/L	500	500
Manganese	1620		15.264	5.629	C/L	20	5
Manganese	200.8	ICP/MS	0.245	0.071	C/L	0.1	0.05
Mercury	200.8	ICP/MS	0.039	0.033	H/H	0.02	0.02
Methacrylonitrile	524.2		19.062	19.451	C/C	1	1
Methylacrylate	524.2		0.727	0.586	H/H	1	1
Methylene Chloride	524.2		0.433	0.390	H/H	0.2	0.2
Methylmethacrylate	524.2		20.773	20.951	C/C	1	1
Molybdenum	1620		7.597	6.737	L/L	10	10
Molybdenum	200.8	ICP/MS	0.608	0.011	C/H	0.01	0.005
N-butylbenzene	502.2	PID	0.745	0.397	L/L	0.1	0.2
N-propylbenzene	502.2	PID	0.186	0.128	H/H	0.2	0.2
Naphthalene	524.2		0.108	0.166	H/H	0.2	0.2
Nickel	1620		67.206	58.049	L/L	100	100
Nickel	200.8	ICP/MS	0.183	0.116	H/H	0.5	0.2
O-xylene+styrene	502.2	PID	0.181	0.140	L/H	0.2	0.2
P-isopropitol+1,4-dcb	502.2	PID	0.456	0.330	L/L	0.2	0.2
Pentachloroethane	524.2		0.551	0.406	H/H	2	1
Sec-butylbenzene	502.2	PID	0.157	0.101	H/H	0.2	0.1
Selenium	200.8	ICP/MS	1.045	0.607	L/H	0.5	0.5
Silver	1620		25.842	25.005	L/L	20	20
Silver	200.8	ICP/MS	0.056	0.027	L/L	0.02	0.02
Tert-butylbenzene	502.2	PID	0.203	0.121	L/L	0.1	0.1
Tetrachloroethene	502.2	ELCD	0.122	0.092	H/H	0.05	0.05
Tetrachloroethene	502.2	PID	0.750	0.664	L/L	0.2	0.2
Tetrachloroethene	524.2		30.554 [5]	0.275	C/H	0.2	0.1
Thallium	200.8	ICP/MS	0.002	0.002	L/L	0.002	0.002
Thorium	200.8	ICP/MS	0.004	0.001	L/H	0.002	0.002
Tin	1620		9.406	8.651	L/L	10	10
Titanium	1620		14.236	13.166	L/L	20	20
Toluene	502.2	PID	0.194	0.084	L/L	0.2	0.2
Toluene	524.2		0.046	0.039	H/H	0.05	0.05
Total Suspended Solids [2]	160.2		6.729	7.441	H/L	5	5
Trans-1,2-dichloroethene	502.2	ELCD	0.191	0.159	H/H	0.2	0.2
Trans-1,3-dichloropropene	502.2	ELCD	0.729	0.610	L/L	0.05	0.05
Trans-1,3-dichloropropene	502.2	PID	0.175	0.173	H/H	0.2	0.2
Trans-1,3-dichloropropene	524.2		0.218	0.124	H/H	0.2	0.2
Trichloroethene	502.2	ELCD	3.169	0.041 [1]	L/L	0.05	0.05
Trichloroethene	502.2	PID	0.401	0.332	L/L	0.1	0.1
Trichloroethene	524.2		0.167	0.237	H/H	0.2	0.2

Table 12. Comparison of SL-IQEs and MLs calculated With and Without Outlier Removal, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE (10%)			ML	
			Outliers Kept	Outliers Dropped	Model Used (Kept/Dropped)	Outliers Kept	Outliers Dropped
Trichlorofluoromethane	502.2	ELCD	4.662	3.950	C/C	0.5	0.05
Trichlorofluoromethane	524.2		42.490[5]	0.228	C/H	0.2	0.2
Uranium	200.8	ICP/MS	0.001	0.001	L/H	0.001	0.001
Vinyl Chloride	502.2	ELCD	8.234	8.020	C/C	1	1
Wad Cyanide	1677	WADCN	1.624	1.543	L/L	2	2
Yttrium	1620		8.962	8.501	L/L	5	5
Zinc	1620		10.452	11.630	H/L	10	10
Zinc	200.8	ICP/MS	7.024	2.291	L/H	2	2

[1] IQE 10% undefined, IQE 20% reported

[2] Results reported as mg/L

[3] IQE 10%, IQE 20% and IQE 30% all negative based on chosen model (linear)

[4] IQE 10% and IQE 20% both negative, IQE 30% reported

[5] Hybrid model selected but did not converge; IQE 10% based on constant model instead

Summary Statistics for Table 12

Percent Difference (Positive if limit with outliers kept> limit with outliers removed)	# Analytes	Minimum	25th Percentile	Median	75th Percentile	Maximum
SL-IQE (all)	148	-198.2%	1.0%	16.3%	50.2%	197.9%
SL-IQE (same model used)	117	-176.3%	0.0%	2.8%	23.7%	194.9%
SL-IQE (different model used)	31	-198.2%	-7.7%	53.1%	107.1%	197.9%
ML	31	-163.6%	66.7%	66.7%	120.0%	184.6%

Table 13. Comparison of SL-IDEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE, Based on Given Model				RSD
			Constant	Linear	Exponential	Hybrid	
1,1,1,2-tetrachloroethane	502.2	ELCD	0.687	0.000	0.034	0.010	184%
1,1,1,2-tetrachloroethane	524.2		11.051	-1.234	0.244	0.078	166%
1,1,1-trichloroethane	502.2	ELCD	0.985	0.016	0.041	0.010	183%
1,1,1-trichloroethane	524.2		14.141	-0.836	0.308	0.098	166%
1,1,2,2-tce+1,2,3-tcp	502.2	ELCD	2.597	-0.222	0.179	N/A [1]	123%
1,1,2,2-tetrachloroethane	524.2		12.456	-1.517	0.436	0.248	160%
1,1,2-trichloroethane	502.2	ELCD	0.476	0.016	0.032	0.016	169%
1,1,2-trichloroethane	524.2		7.245	-0.407	0.319	0.127	158%
1,1-dichloroethane	502.2	ELCD	0.801	0.083	0.083	0.067	140%
1,1-dichloroethane	524.2		11.355	-0.642	0.229	0.049	167%
1,1-dichloroethene	502.2	ELCD	1.167	0.305	0.234	0.213	96%
1,1-dichloroethene	524.2		18.473	-2.042	0.335	0.050	168%
1,1-dichloropropanone	524.2		15.292	4.713	6.372	6.513	58%
1,1-dichloropropene	524.2		13.573	-0.554	0.287	0.073	167%
1,2,3-trichlorobenzene	502.2	ELCD	0.942	0.117	0.134	0.117	125%
1,2,3-trichlorobenzene	502.2	PID	0.640	0.134	0.115	0.083	109%
1,2,3-trichlorobenzene	524.2		18.047	-1.759	0.275	0.090	168%
1,2,3-trichloropropane	524.2		12.464	3.599	1.263	0.041	129%
1,2,4-trichlorobenzene	502.2	ELCD	0.739	0.082	0.088	0.069	135%
1,2,4-trichlorobenzene	502.2	PID	0.688	0.113	0.124	0.100	112%
1,2,4-trichlorobenzene	524.2		14.387	-1.058	0.224	0.059	168%
1,2,4-trimethylbenzene	502.2	PID	0.889	0.125	0.125	0.108	123%
1,2,4-trimethylbenzene	524.2		9.319	-0.074	0.144	0.020	169%
1,2-dibromo-3-chloropropane	524.2		34.167	-7.305	1.749	N/A [1]	128%
1,2-dibromoethane	502.2	ELCD	0.543	0.184	0.164	0.160	71%
1,2-dibromoethane	524.2		8.173	-0.811	0.326	0.184	158%
1,2-dichlorobenzene	502.2	ELCD	0.653	0.037	0.065	0.045	151%
1,2-dichlorobenzene	502.2	PID	0.895	0.136	0.148	0.121	117%
1,2-dichlorobenzene	524.2		12.369	-1.392	0.130	0.036	170%
1,2-dichloroethane	502.2	ELCD	0.951	-0.041	0.042	0.022	157%
1,2-dichloroethane	524.2		7.061	-0.485	0.258	0.097	161%
1,2-dichloropropane	502.2	ELCD	0.733	0.015	0.043	0.024	173%
1,2-dichloropropane	524.2		9.388	-0.729	0.247	0.085	164%
1,3,5-tmb+4-chlorotoluene	502.2	PID	1.526	0.084	0.114	0.073	160%
1,3,5-trimethylbenzene	524.2		10.590	-0.059	0.135	0.016	170%
1,3-dichlorobenzene	502.2	ELCD	0.775	0.230	0.118	0.103	103%
1,3-dichlorobenzene	502.2	PID	0.773	0.102	0.126	0.099	121%
1,3-dichlorobenzene	524.2		12.273	-1.099	0.143	0.033	170%
1,3-dichloropropane	502.2	ELCD	0.578	0.015	0.047	0.028	164%
1,3-dichloropropane	524.2		6.432	-0.320	0.202	0.061	163%
1,4-dichlorobenzene	502.2	ELCD	0.654	0.050	0.061	0.033	152%
1,4-dichlorobenzene	524.2		11.443	-1.116	0.140	0.034	169%
1-chlorobutane	524.2		13.444	-0.406	0.220	0.024	169%
2,2-dichloropropane	524.2		17.294	-0.134	0.691	0.152	161%
2-butanone	524.2		14.170	-1.296	0.833	0.384	153%
2-chlorotoluene	502.2	ELCD	1.533	0.051	0.175	0.166	146%
2-chlorotoluene	502.2	PID	0.977	0.272	0.230	0.187	90%
2-chlorotoluene	524.2		11.146	-0.639	0.136	0.023	170%

Table 13. Comparison of SL-IDEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE, Based on Given Model				RSD
			Constant	Linear	Exponential	Hybrid	
2-hexanone	524.2		22.744	-5.136	0.902	0.188	161%
2-nitropropane	524.2		18.337	-3.854	1.082	0.254	156%
4-chlorotoluene	502.2	ELCD	1.792	-0.022	0.149	0.112	140%
4-chlorotoluene	524.2		10.619	-0.329	0.123	0.013	170%
4-isopropyltoluene	524.2		9.108	0.162	0.117	0.007	192%
4-methyl-2-pentanone	524.2		20.121	-5.006	1.195	0.773	150%
Acetone	524.2		22.659	-1.723	2.120	1.092	141%
Acrylonitrile	524.2		13.467	-1.190	1.333	0.715	139%
Allyl Chloride	524.2		13.324	-0.815	0.229	0.051	168%
Aluminum	1620		206.975	88.830	51.697	N/A [1]	70%
Aluminum	200.8	ICP/MS	41.919	12.689	12.747	12.961	73%
Ammonia as Nitrogen [2]	350.3		0.078	0.009	0.014	0.013	114%
Antimony	1620		4.260	3.728	3.562	3.596	9%
Antimony	200.8	ICP/MS	0.229	0.027	0.019	0.015	144%
Arsenic	1620		2.131	1.510	1.410	1.390	22%
Arsenic	200.8	ICP/MS	2.023	0.257	0.366	0.345	114%
Barium	1620		1.837	1.522	1.300	1.306	17%
Barium	200.8	ICP/MS	0.257	0.085	0.084	0.079	69%
Benzene	502.2	PID	0.802	0.036	0.079	0.060	152%
Benzene	524.2		8.619	-0.122	0.125	0.019	169%
Beryllium	1620		1.587	0.365	0.448	0.431	83%
Beryllium	200.8	ICP/MS	0.170	0.013	0.024	0.018	134%
Boron	1620		38.617	20.625	21.161	20.805	35%
Bromobenzene	502.2	ELCD	1.685	0.765	0.499	0.515	65%
Bromobenzene	502.2	PID	0.569	0.028	0.050	0.032	157%
Bromobenzene	524.2		12.851	-1.691	0.211	0.060	168%
Bromochloromethane	502.2	ELCD	0.939	0.482	0.162	0.157	85%
Bromochloromethane	524.2		8.929	-0.807	0.345	0.161	159%
Bromodichloromethane	502.2	ELCD	0.617	0.111	0.075	0.060	125%
Bromodichloromethane	524.2		8.020	-0.455	0.205	0.056	165%
Bromoform	502.2	ELCD	1.513	1.161	0.381	0.381	66%
Bromoform	524.2		10.207	-1.309	0.400	0.211	159%
Bromomethane	502.2	ELCD	7.293	5.796	4.313	N/A [1]	26%
Bromomethane	524.2		12.379	-1.072	0.280	0.096	166%
Cadmium	1620		0.364	0.208	0.191	0.180	37%
Cadmium	200.8	ICP/MS	0.040	0.022	0.022	0.026	31%
Calcium	1620		54.321	41.358	37.020	37.410	19%
Carbon Disulfide	524.2		14.835	-1.181	0.239	0.040	168%
Carbon Tetrachloride	524.2		15.266	-1.197	0.314	0.056	167%
Carbontet+1,1-dcp	502.2	ELCD	1.998	-0.007	0.072	0.020	162%
Chloroacetonitrile	524.2		11.548	-0.814	1.569	1.453	119%
Chlorobenzene	502.2	ELCD	0.982	0.460	0.189	0.183	83%
Chlorobenzene	502.2	PID	0.749	0.020	0.064	0.048	160%
Chlorobenzene	524.2		10.276	-0.665	0.133	0.026	169%
Chloroethane	502.2	ELCD	2.598	2.161	1.091	1.053	45%
Chloroethane	524.2		14.465	-0.836	0.395	0.104	165%
Chloroform	502.2	ELCD	0.732	0.006	0.032	0.004	185%
Chloroform	524.2		9.385	-0.399	0.225	0.051	166%

Table 13. Comparison of SL-IDEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE, Based on Given Model				RSD
			Constant	Linear	Exponential	Hybrid	
Chloromethane	502.2	ELCD	1.130	0.453	0.250	0.233	82%
Chloromethane	524.2		19.617	-2.484	0.253	0.056	169%
Chromium	1620		1.090	0.528	0.496	0.471	46%
Chromium	200.8	ICP/MS	0.672	0.408	0.284	0.290	44%
Cis-1,2-dce+2,2-dcp	502.2	ELCD	1.893	-0.048	0.055	0.012	164%
Cis-1,2-dichloroethene	524.2		11.249	-0.960	0.234	0.062	167%
Cis-1,3-dichloropropene	502.2	ELCD	0.716	0.083	0.074	0.061	138%
Cis-1,3-dichloropropene	502.2	PID	0.933	0.039	0.082	0.013	167%
Cis-1,3-dichloropropene	524.2		7.072	-0.454	0.173	0.062	165%
Cobalt	1620		30.100	16.339	16.463	16.102	35%
Cobalt	200.8	ICP/MS	0.074	-0.012	-0.004	-0.001	192%
Copper	1620		21.189	16.989	14.754	14.861	18%
Copper	200.8	ICP/MS	0.798	0.404	0.205	0.207	69%
Dibromochloromethane	502.2	ELCD	0.784	0.436	0.144	0.141	81%
Dibromochloromethane	524.2		8.159	-0.667	0.287	0.126	161%
Dibromomethane	502.2	ELCD	0.836	0.460	0.192	0.184	73%
Dibromomethane	524.2		7.135	-0.585	0.388	0.203	153%
Dichlorodifluoromethane	502.2	ELCD	2.194	0.348	0.240	0.153	133%
Dichlorodifluoromethane	524.2		24.275	-4.798	0.560	0.183	166%
Diethyl Ether	524.2		12.008	-1.243	0.376	0.175	162%
Ethyl Methacrylate	524.2		10.053	-0.957	0.273	0.079	164%
Ethylbenzene	502.2	PID	0.888	0.020	0.078	0.060	160%
Ethylbenzene	524.2		11.939	-0.776	0.198	0.032	168%
Hardness [2]	130.2		3.658	2.362	2.258	2.385	25%
Hexachlorobutadiene	502.2	ELCD	0.997	0.105	0.094	0.065	144%
Hexachlorobutadiene	524.2		17.734	-2.203	0.308	0.092	167%
Hexachloroethane	524.2		18.095	-2.155	0.288	0.069	168%
Hexchlobutadiene+naphthalene	502.2	PID	1.442	0.793	0.597	0.523	50%
Iron	1620		486.971	373.590	125.364	124.648	66%
Isopropylbenzene	502.2	PID	0.856	0.025	0.060	0.033	168%
Isopropylbenzene	524.2		11.414	-0.141	0.120	0.012	170%
Lead	1620		3.976	2.396	2.423	2.437	28%
Lead	200.8	ICP/MS	1.007	0.265	0.204	0.200	94%
M+p xylene	502.2	PID	1.701	0.005	0.121	0.088	170%
M+p xylene	524.2		10.994	-0.206	0.142	0.016	170%
Magnesium	1620		145.717	112.074	105.998	106.575	16%
Manganese	1620		6.808	4.201	2.993	3.033	42%
Manganese	200.8	ICP/MS	0.109	0.065	0.034	0.034	59%
Mercury	200.8	ICP/MS	0.827	0.006	0.027	0.016	185%
Methacrylonitrile	524.2		8.883	-0.181	0.718	0.356	145%
Methyl Iodide	524.2		12.103	-0.866	0.193	0.035	168%
Methyl tert-butyl ether	524.2		10.845	-1.117	0.225	0.053	167%
Methylacrylate	524.2		13.820	-1.522	0.601	0.315	157%
Methylene Chloride	502.2	ELCD	2.841	1.822	-3.178	N/A [1]	651%
Methylene Chloride	524.2		8.787	-0.455	0.314	0.188	159%
Methylmethacrylate	524.2		9.597	-0.342	0.535	0.244	154%
Molybdenum	1620		4.908	3.163	3.034	3.042	26%
Molybdenum	200.8	ICP/MS	0.271	0.096	0.180	-0.007	88%

Table 13. Comparison of SL-IDEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE, Based on Given Model				RSD
			Constant	Linear	Exponential	Hybrid	
Naphthalene	524.2		14.829	-0.891	0.186	0.044	169%
N-butylbenzene	502.2	PID	0.714	0.215	0.141	0.135	92%
N-butylbenzene	524.2		10.237	-0.145	0.152	0.028	169%
Nickel	1620		50.587	26.333	25.560	24.898	39%
Nickel	200.8	ICP/MS	1.023	0.176	0.083	0.072	136%
N-propylbenzene	502.2	PID	0.785	0.075	0.092	0.066	139%
N-propylbenzene	524.2		13.415	-0.751	0.284	0.061	167%
o-xylene	524.2		11.622	-0.802	0.198	0.017	168%
o-xylene+styrene	502.2	PID	1.372	0.043	0.116	0.082	160%
Pentachloroethane	524.2		11.186	-0.793	0.408	0.237	159%
P-Isopropitol+1,4-dcb	502.2	PID	1.583	0.091	0.159	0.118	150%
Sec-butylbenzene	502.2	PID	0.942	0.053	0.081	0.052	156%
Sec-butylbenzene	524.2		11.240	0.080	0.140	0.020	194%
Selenium	1620		4.161	2.054	1.975	1.971	43%
Selenium	200.8	ICP/MS	2.090	0.406	0.416	0.364	104%
Silver	1620		13.219	11.098	10.668	10.801	10%
Silver	200.8	ICP/MS	0.048	0.020	0.012	0.010	77%
Sodium	1620		169.136	141.290	138.768	140.811	10%
Styrene	524.2		10.516	-0.600	0.141	0.017	169%
Tert-butylbenzene	502.2	PID	0.854	0.038	0.074	0.050	158%
Tert-butylbenzene	524.2		11.706	-0.323	0.186	0.030	169%
Tetrachloroethene	502.2	ELCD	0.927	0.029	0.061	0.031	169%
Tetrachloroethene	502.2	PID	1.027	0.114	0.156	0.127	126%
Tetrachloroethene	524.2		13.627	-0.451	0.469	N/A [1]	132%
Thallium	1620		1.726	1.185	1.153	1.161	21%
Thallium	200.8	ICP/MS	0.003	0.001	0.001	0.001	73%
Thorium	200.8	ICP/MS	0.032	0.002	0.001	0.000	176%
Tin	1620		5.755	3.991	3.932	3.986	20%
Titanium	1620		8.500	6.012	5.376	5.419	23%
Toluene	502.2	PID	0.731	0.044	0.064	0.051	152%
Toluene	524.2		9.778	-0.303	0.146	0.019	169%
Total Phosphorus [2]	365.2		0.018	0.014	0.013	0.013	16%
Total Suspended Solids [2]	160.2		4.317	3.195	3.005	2.977	19%
trans-1,2-dichloroethene	502.2	ELCD	0.922	0.067	0.081	0.060	151%
trans-1,2-dichloroethene	524.2		13.734	-0.953	0.300	0.062	167%
trans-1,3-dichloropropene	502.2	ELCD	0.666	0.201	0.098	0.087	104%
trans-1,3-dichloropropene	502.2	PID	0.650	0.052	0.092	0.068	135%
trans-1,3-dichloropropene	524.2		6.714	-0.432	0.223	0.096	161%
trans-1,4-dichloro-2-butene	524.2		14.301	-1.059	1.250	0.782	141%
Trichloroethene	502.2	ELCD	1.006	0.035	0.059	0.038	169%
Trichloroethene	502.2	PID	0.914	0.066	0.097	0.069	146%
Trichloroethene	524.2		12.510	-0.619	0.332	0.065	165%
Trichlorofluoromethane	502.2	ELCD	2.079	1.656	1.107	1.076	32%
Trichlorofluoromethane	524.2		19.248	-2.147	0.384	N/A [1]	136%
Uranium	200.8	ICP/MS	0.002	0.000	0.000	0.000	116%
Vanadium	1620		22.721	9.967	10.630	10.693	46%
Vanadium	200.8	ICP/MS	2.762	0.730	0.864	0.840	75%
Vinyl Chloride	502.2	ELCD	3.672	3.036	1.756	1.690	39%

Table 13. Comparison of SL-IDEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IDE, Based on Given Model				RSD
			Constant	Linear	Exponential	Hybrid	
Vinyl Chloride	524.2		22.292	-3.345	0.365	0.083	168%
Wad Cyanide	1677	WADCN	1.023	0.701	0.620	0.638	25%
Xylene (total)	524.2		10.490	-0.264	0.128	0.008	170%
Yttrium	1620		4.569	3.520	3.247	3.279	17%
Zinc	1620		14.628	3.804	4.500	4.425	76%
Zinc	200.8	ICP/MS	7.561	2.537	1.598	1.610	86%

[1] Hybrid model failed to converge

[2] Results reported as mg/L

Summary Statistics for Table 13

Method	# Analytes	Minimum	25th Percentile	Median	75th Percentile	Maximum
All	198	8.5%	81.8%	151.1%	166.7%	650.6%
502.2	65	25.7%	103.5%	140.1%	159.9%	650.6%
524.2	81	58.2%	159.2%	166.0%	168.5%	194.5%
1620	26	8.5%	18.1%	26.8%	42.4%	83.0%
200.8	21	31.0%	72.5%	88.0%	134.5%	191.6%

Table 14. Comparison of SL-IQEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE 10%, Based on Given Model				RSD [1]
			Constant	Linear	Exponential	Hybrid	
1,1,1,2-tetrachloroethane	502.2	ELCD	1.541	0.000	0.078	0.030	182.6%
1,1,1,2-tetrachloroethane	524.2		24.612	-4.974	0.556	0.181	165.7%
1,1,1-trichloroethane	502.2	ELCD	2.208	0.830	0.096	0.058	126.0%
1,1,1-trichloroethane	524.2		31.494	-4.112	0.704	0.240	165.7%
1,1,2,2-tce+1,2,3-tcp	502.2	ELCD	5.514	-1.416	0.430	N/A [2]	120.9%
1,1,2,2-tetrachloroethane	524.2		27.377	-5.971	1.001	0.569	159.1%
1,1,2-trichloroethane	502.2	ELCD	1.067	0.060	0.075	0.040	162.6%
1,1,2-trichloroethane	524.2		15.923	-1.175	0.726	0.290	157.7%
1,1-dichloroethane	502.2	ELCD	1.795	0.527	0.200	0.178	113.2%
1,1-dichloroethane	524.2		25.290	-2.390	0.521	0.115	166.8%
1,1-dichloroethene	502.2	ELCD	2.617	3.796	0.627	0.886	75.6%
1,1-dichloroethene	524.2		41.142	-28.559	0.767	0.129	167.7%
1,1-dichloropropanone	524.2		30.102	12.705	15.558	15.041	43.2%
1,1-dichloropropene	524.2		30.229	-2.582	0.655	0.180	166.2%
1,2,3-trichlorobenzene	502.2	ELCD	2.113	0.851	0.334	0.341	92.1%
1,2,3-trichlorobenzene	502.2	PID	1.435	0.482	0.279	0.248	91.5%
1,2,3-trichlorobenzene	524.2		40.193	-12.045	0.628	0.216	167.9%
1,2,3-trichloropropane	524.2		27.394	11.316	2.981	0.166	117.0%
1,2,4-trichlorobenzene	502.2	ELCD	1.658	0.401	0.212	0.186	114.4%
1,2,4-trichlorobenzene	502.2	PID	1.544	0.439	0.303	0.276	94.7%
1,2,4-trichlorobenzene	524.2		32.041	-5.251	0.510	0.141	168.0%
1,2,4-trimethylbenzene	502.2	PID	1.993	0.653	0.309	0.291	99.2%
1,2,4-trimethylbenzene	524.2		20.896	-0.243	0.326	0.048	168.6%
1,2-dibromo-3-chloropropane	524.2		71.182	-145.715	4.217	N/A [2]	125.6%
1,2-dibromoethane	502.2	ELCD	1.218	0.592	0.401	0.381	60.5%
1,2-dibromoethane	524.2		17.963	-2.444	0.743	0.417	157.5%
1,2-dichlorobenzene	502.2	ELCD	1.465	0.183	0.154	0.121	136.6%
1,2-dichlorobenzene	502.2	PID	1.992	0.638	0.367	0.346	93.6%
1,2-dichlorobenzene	524.2		27.734	-6.758	0.294	0.085	169.7%
1,2-dichloroethane	502.2	ELCD	2.132	0.266	0.100	0.065	155.8%
1,2-dichloroethane	524.2		15.586	-1.407	0.585	0.222	160.5%
1,2-dichloropropane	502.2	ELCD	1.643	0.102	0.101	0.065	162.6%
1,2-dichloropropane	524.2		20.909	-2.433	0.562	0.196	164.1%
1,3,5-tmb+4-chlorotoluene	502.2	PID	3.422	0.396	0.268	0.189	147.0%
1,3,5-trimethylbenzene	524.2		23.744	-0.208	0.305	0.037	169.5%
1,3-dichlorobenzene	502.2	ELCD	1.738	0.936	0.289	0.267	85.9%
1,3-dichlorobenzene	502.2	PID	1.732	0.465	0.309	0.288	99.3%
1,3-dichlorobenzene	524.2		27.518	-4.866	0.324	0.076	169.5%
1,3-dichloropropane	502.2	ELCD	1.287	0.054	0.110	0.067	159.5%
1,3-dichloropropane	524.2		14.324	-0.934	0.458	0.139	162.8%
1,4-dichlorobenzene	502.2	ELCD	1.467	0.218	0.144	0.101	136.4%
1,4-dichlorobenzene	524.2		25.657	-5.226	0.316	0.078	169.3%
1-chlorobutane	524.2		29.943	-1.682	0.499	0.060	168.5%
2,2-dichloropropane	524.2		38.009	-15.752	1.607	0.464	159.8%
2-butanone	524.2		30.407	-4.569	1.934	0.893	151.2%
2-chlorotoluene	502.2	ELCD	3.438	1.364	0.452	0.493	97.4%
2-chlorotoluene	502.2	PID	2.176	1.249	0.597	0.849	56.9%
2-chlorotoluene	524.2		24.990	-2.436	0.308	0.053	169.5%

Table 14. Comparison of SL-IQEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE 10%, Based on Given Model				RSD [1]
			Constant	Linear	Exponential	Hybrid	
2-hexanone	524.2		47.881	-30.174	2.102	0.442	160.2%
2-nitropropane	524.2		38.203	-16.221	2.531	0.590	153.7%
4-chlorotoluene	502.2	ELCD	4.017	0.161	0.383	N/A [3]	142.4%
4-chlorotoluene	524.2		23.810	-1.231	0.278	0.032	169.9%
4-isopropyltoluene	524.2		20.421	0.528	0.265	0.016	189.9%
4-methyl-2-pentanone	524.2		41.919	-23.810	2.804	1.785	147.6%
Acetone	524.2		47.703	-8.481	5.137	2.741	136.5%
Acrylonitrile	524.2		28.056	-3.845	3.129	1.651	135.6%
Allyl Chloride	524.2		29.674	-3.694	0.521	0.121	167.7%
Aluminum	1620		464.069	255.899	130.746	N/A [2]	59.4%
Aluminum	200.8	ICP/MS	93.989	37.673	30.404	29.684	64.5%
Ammonia as Nitrogen [4]	350.3		0.175	0.052	0.035	0.035	90.3%
Antimony	1620		9.551	8.719	8.275	8.104	7.5%
Antimony	200.8	ICP/MS	0.525	0.073	0.044	0.034	140.8%
Arsenic	1620		4.705	3.542	3.240	3.097	20.0%
Arsenic	200.8	ICP/MS	4.629	0.692	0.859	0.798	110.3%
Barium	1620		4.118	3.475	2.973	2.934	16.4%
Barium	200.8	ICP/MS	0.589	0.211	0.197	0.183	66.6%
Benzene	502.2	PID	1.798	0.182	0.189	0.155	139.7%
Benzene	524.2		19.325	-0.385	0.284	0.044	168.9%
Beryllium	1620		3.559	0.964	1.044	0.980	78.3%
Beryllium	200.8	ICP/MS	0.382	0.041	0.057	0.044	127.8%
Boron	1620		86.584	51.134	49.514	47.266	31.9%
Bromobenzene	502.2	ELCD	3.704	3.529	1.408	1.417	50.7%
Bromobenzene	502.2	PID	1.277	0.100	0.118	0.079	149.8%
Bromobenzene	524.2		28.621	-7.963	0.479	0.140	167.7%
Bromochloromethane	502.2	ELCD	2.106	1.598	0.399	0.379	77.6%
Bromochloromethane	524.2		19.625	-2.531	0.787	0.368	158.8%
Bromodichloromethane	502.2	ELCD	1.384	0.424	0.178	0.148	108.8%
Bromodichloromethane	524.2		17.863	-1.404	0.465	0.128	164.9%
Bromoform	502.2	ELCD	3.393	2.540	0.922	0.877	64.3%
Bromoform	524.2		22.334	-4.327	0.914	0.482	157.9%
Bromomethane	502.2	ELCD	16.351	5.779	N/A [3]	N/A [2]	67.6%
Bromomethane	524.2		27.570	-5.134	0.637	0.226	165.3%
Cadmium	1620		0.816	0.505	0.445	0.410	34.1%
Cadmium	200.8	ICP/MS	0.090	0.065	0.054	0.063	23.1%
Calcium	1620		121.796	99.975	86.815	84.600	17.4%
Carbon Disulfide	524.2		33.263	-7.679	0.545	0.101	168.3%
Carbon Tetrachloride	524.2		34.000	-7.521	0.718	0.140	166.8%
Carbontet+1,1-dcp	502.2	ELCD	4.480	0.105	0.167	0.069	181.2%
Chloroacetonitrile	524.2		24.059	-2.331	3.679	3.310	114.7%
Chlorobenzene	502.2	ELCD	2.202	1.766	0.477	0.458	72.9%
Chlorobenzene	502.2	PID	1.679	0.092	0.151	0.119	152.8%
Chlorobenzene	524.2		23.041	-2.418	0.300	0.059	169.2%
Chloroethane	502.2	ELCD	5.826	4.368	2.730	2.613	39.2%
Chloroethane	524.2		31.932	-4.186	0.907	0.255	164.1%
Chloroform	502.2	ELCD	1.640	0.025	0.075	0.011	183.1%
Chloroform	524.2		20.902	-1.329	0.511	0.121	165.6%

Table 14. Comparison of SL-IQEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE 10%, Based on Given Model				RSD [1]
			Constant	Linear	Exponential	Hybrid	
Chloromethane	502.2	ELCD	2.533	1.734	0.650	0.678	65.0%
Chloromethane	524.2		43.690	-89.292	0.577	0.141	169.0%
Chromium	1620		2.444	1.259	1.141	1.062	44.0%
Chromium	200.8	ICP/MS	1.538	1.028	0.681	0.669	41.7%
Cis-1,2-dce+2,2-dcp	502.2	ELCD	4.244	0.218	0.127	0.039	178.0%
Cis-1,2-dichloroethene	524.2		25.054	-3.865	0.532	0.144	166.4%
Cis-1,3-dichloropropene	502.2	ELCD	1.604	0.415	0.177	0.151	117.3%
Cis-1,3-dichloropropene	502.2	PID	2.077	0.222	0.196	N/A [3]	129.7%
Cis-1,3-dichloropropene	524.2		15.751	-1.358	0.391	0.141	164.7%
Cobalt	1620		67.490	40.837	38.691	36.682	31.5%
Cobalt	200.8	ICP/MS	0.166	-0.022	-0.009	0.002	138.6%
Copper	1620		47.509	39.683	34.348	33.546	16.6%
Copper	200.8	ICP/MS	1.825	0.984	0.487	0.477	67.2%
Dibromochloromethane	502.2	ELCD	1.757	1.252	0.349	0.330	76.3%
Dibromochloromethane	524.2		18.012	-2.066	0.653	0.288	160.3%
Dibromomethane	502.2	ELCD	1.874	1.395	0.475	0.447	67.3%
Dibromomethane	524.2		15.614	-1.663	0.885	0.460	152.6%
Dichlorodifluoromethane	502.2	ELCD	4.918	-0.244	0.732	0.654	116.1%
Dichlorodifluoromethane	524.2		53.352	30.938	1.297	0.480	118.6%
Diethyl Ether	524.2		26.391	-4.619	0.860	0.404	161.4%
Ethyl Methacrylate	524.2		22.094	-3.192	0.621	0.183	164.1%
Ethylbenzene	502.2	PID	1.991	0.128	0.188	0.157	148.8%
Ethylbenzene	524.2		26.591	-3.326	0.450	0.077	168.2%
Hardness [4]	130.2		8.005	5.465	5.109	5.258	23.0%
Hexachlorobutadiene	502.2	ELCD	2.236	0.753	0.228	0.243	109.3%
Hexachlorobutadiene	524.2		39.496	-21.961	0.703	0.228	167.2%
Hexachloroethane	524.2		40.301	-19.924	0.657	0.167	168.0%
Hexchlobutadiene+naphthalene	502.2	PID	3.234	2.358	1.524	1.542	37.5%
Iron	1620		1091.863	-281.500	N/A [3]	N/A [3]	N/A
Isopropylbenzene	502.2	PID	1.919	0.129	0.141	0.088	158.1%
Isopropylbenzene	524.2		25.592	-0.498	0.270	0.029	170.2%
Lead	1620		8.914	5.698	5.587	5.489	25.9%
Lead	200.8	ICP/MS	2.305	0.685	0.478	0.462	90.4%
M+p xylene	502.2	PID	3.813	0.031	0.285	0.222	167.3%
M+p xylene	524.2		24.651	-0.743	0.321	0.037	169.5%
Magnesium	1620		326.719	267.199	247.396	240.982	14.4%
Manganese	1620		15.264	10.195	7.113	6.899	39.5%
Manganese	200.8	ICP/MS	0.245	0.156	0.079	0.076	57.3%
Mercury	200.8	ICP/MS	1.854	0.019	0.063	0.039	183.8%
Methacrylonitrile	524.2		19.062	-0.518	1.655	0.815	143.5%
Methyl Iodide	524.2		26.956	-3.833	0.439	0.083	168.3%
Methyl tert-butyl ether	524.2		23.940	-4.171	0.511	0.122	166.5%
Methylacrylate	524.2		29.913	-5.560	1.386	0.727	156.1%
Methylene Chloride	502.2	ELCD	6.033	5.201	-4.095	N/A [2]	10.5%
Methylene Chloride	524.2		19.701	-1.528	0.717	0.433	158.9%
Methylmethacrylate	524.2		20.773	-1.043	1.228	0.561	152.7%
Molybdenum	1620		11.003	7.597	7.049	6.869	23.9%
Molybdenum	200.8	ICP/MS	0.608	0.260	N/A [3]	0.026	98.3%

Table 14. Comparison of SL-IQEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE 10%, Based on Given Model				RSD [1]
			Constant	Linear	Exponential	Hybrid	
N-butylbenzene	502.2	PID	1.601	0.745	0.343	0.325	79.3%
N-butylbenzene	524.2		22.952	-0.521	0.345	0.067	168.6%
N-propylbenzene	502.2	PID	1.759	0.351	0.221	0.186	120.2%
N-propylbenzene	524.2		29.878	-3.650	0.647	0.148	166.5%
Napthalene	524.2		33.249	-4.704	0.422	0.108	169.1%
Nickel	1620		113.424	67.206	60.455	57.072	35.2%
Nickel	200.8	ICP/MS	2.341	0.800	0.202	0.183	115.1%
O-xylene	524.2		25.884	-3.313	0.450	0.040	168.4%
O-xylene+styrene	502.2	PID	3.077	0.181	0.272	0.202	153.2%
P-isopropitol+1,4-dcb	502.2	PID	3.550	0.456	0.380	0.312	134.9%
Pentachloroethane	524.2		24.914	-3.372	0.934	0.551	158.6%
Sec-butylbenzene	502.2	PID	2.112	0.346	0.196	0.157	134.2%
Sec-butylbenzene	524.2		25.203	0.279	0.316	0.047	193.4%
Selenium	1620		9.268	5.235	4.657	4.474	38.3%
Selenium	200.8	ICP/MS	4.686	1.045	0.957	0.829	99.7%
Silver	1620		29.640	25.842	24.547	24.294	9.5%
Silver	200.8	ICP/MS	0.107	0.056	0.030	0.034	62.6%
Sodium	1620		379.229	337.755	323.935	317.747	8.1%
Styrene	524.2		23.420	-2.180	0.318	0.041	169.3%
Tert-butylbenzene	502.2	PID	1.916	0.203	0.177	0.135	143.6%
Tert-butylbenzene	524.2		26.246	-1.197	0.423	0.073	168.4%
Tetrachloroethene	502.2	ELCD	2.078	0.415	0.145	0.122	135.5%
Tetrachloroethene	502.2	PID	2.303	0.750	0.392	0.400	94.7%
Tetrachloroethene	524.2		30.554	-2.553	1.080	N/A [2]	131.8%
Thallium	1620		3.870	2.799	2.661	2.614	19.9%
Thallium	200.8	ICP/MS	0.007	0.002	0.002	0.002	70.9%
Thorium	200.8	ICP/MS	0.074	0.004	0.003	0.001	174.7%
Tin	1620		12.904	9.406	9.064	8.971	18.7%
Titanium	1620		19.058	14.236	12.443	12.213	21.9%
Toluene	502.2	PID	1.640	0.194	0.153	0.124	140.6%
Toluene	524.2		21.925	-1.050	0.330	0.046	168.8%
Total Phosphorus [4]	365.2		0.040	0.032	0.030	0.030	14.1%
Total Suspended Solids [4]	160.2		9.679	7.570	6.985	6.729	17.3%
Trans-1,2-dichloroethene	502.2	ELCD	2.068	0.795	0.197	0.191	108.7%
Trans-1,2-dichloroethene	524.2		30.588	-4.773	0.684	0.153	166.3%
Trans-1,3-dichloropropene	502.2	ELCD	1.492	0.729	0.237	0.212	89.8%
Trans-1,3-dichloropropene	502.2	PID	1.457	0.206	0.221	0.175	122.1%
Trans-1,3-dichloropropene	524.2		14.821	-1.254	0.506	0.218	161.1%
Trans-1,4-dichloro-2-butene	524.2		30.108	-3.685	2.938	1.819	137.8%
Trichloroethene	502.2	ELCD	2.256	3.169	0.141	0.120	108.1%
Trichloroethene	502.2	PID	2.049	0.401	0.235	0.209	122.7%
Trichloroethene	524.2		27.861	-2.666	0.759	0.167	164.9%
Trichlorofluoromethane	502.2	ELCD	4.662	5.166	3.222	3.308	23.8%
Trichlorofluoromethane	524.2		42.490	-50.543	0.881	N/A [2]	135.7%
Uranium	200.8	ICP/MS	0.005	0.001	0.001	0.001	112.1%
Vanadium	1620		50.943	26.049	25.112	24.338	40.8%
Vanadium	200.8	ICP/MS	6.320	1.828	2.022	1.933	72.6%
Vinyl Chloride	502.2	ELCD	8.234	4.775	3.544	3.828	42.3%

Table 14. Comparison of SL-IQEs calculated using different Model Types, Episode 6000 Data (µg/L except where footnoted)

Analyte	Method	Procedure	SL-IQE 10%, Based on Given Model				RSD [1]
			Constant	Linear	Exponential	Hybrid	
Vinyl Chloride	524.2		49.647	49.158	0.837	0.219	113.0%
Wad Cyanide	1677	WADCN	2.277	1.624	1.414	1.424	24.2%
Xylene (total)	524.2		23.520	-0.952	0.290	0.019	169.8%
Yttrium	1620		10.244	8.962	7.839	7.516	14.3%
Zinc	1620		32.799	12.850	10.999	10.452	64.0%
Zinc	200.8	ICP/MS	17.301	7.024	3.817	3.741	80.4%

[1] Calculation includes positive IQEs only

[2] Given model did not converge

[3] IQE 10% could not be calculated based on given model

[4] Results reported as mg/L

Summary Statistics for Table 14

Method	# analytes	Minimum	25th Percentile	Median	75th Percentile	Maximum
All	197	7.5%	72.6%	135.6%	165.3%	193.4%
502.2	65	10.5%	79.3%	114.4%	142.4%	183.1%
524.2	81	43.2%	157.9%	165.7%	168.4%	193.4%
1620	25	7.5%	16.6%	23.9%	38.3%	78.3%
200.8	21	23.1%	66.6%	90.4%	115.1%	183.8%

Table 15. Comparison of SL-IDEs and SL-IQEs Calculated Using Different Software

Analyte	Model Type	Limit	QCalc	Excel	SAS [1]
1,1-dichloroethene (502.2)	Hybrid	IDE	-0.0338	**0.3180** [2]	0.2135
		IQE 10	-0.87	**2.006**	0.886
	Exponential	IDE	0.2307	0.2367	**0.2337**
		IQE 10		0.622	0.627
	Linear	IDE		0.3059	0.3051
		IQE 10	3.7	3.693	**3.796**
	Constant	IDE		1.169	1.167
		IQE 10		2.604	2.617
1,2,4-trichlorobenzene (502.2, ELCD)	Hybrid	IDE	0.0688	**0.1072**	0.0694
		IQE 10	0.19	**0.297**	0.186
	Exponential	IDE	0.0874	0.0888	**0.0880**
		IQE 10		0.212	0.212
	Linear	IDE		0.0821	0.0817
		IQE 10	**0.40**	0.399	**0.401**
	Constant	IDE		0.741	0.740
		IQE 10		1.651	1.658
1,3,5-trimethylbenzene (524.2)	Hybrid	IDE	0.0157	-4.10E-07	0.0157
		IQE 10	0.04	-6.00E-06	0.037
	Exponential	IDE	0.1345	0.1367	**0.1349**
		IQE 10		not calc [3]	0.305
	Linear	IDE		**-0.0595**	-0.0586
		IQE 10	**not calc** [3]	**not calc** [3]	-0.208
	Constant	IDE		10.448	10.590
		IQE 10		23.269	**23.744**
Antimony (1620) [4]	Hybrid	IDE	3.5724	3.8364	3.5960
		IQE 10	8.10	8.578	8.104
	Exponential	IDE	3.5380	3.5853	3.5616
		IQE 10		8.270	8.275
	Linear	IDE		**3.7511**	3.7283
		IQE 10	8.72	**8.713**	8.719
	Constant	IDE		4.266	**4.260**
		IQE 10		9.502	**9.551**
Arsenic (200.8)	Hybrid	IDE	**0.3433**	**0.3675**	0.3449
		IQE 10	**0.80**	**0.837**	**0.798**
	Exponential	IDE	0.3643	0.3734	**0.3661**
		IQE 10		0.858	0.859
	Linear	IDE		0.2623	0.2570
		IQE 10	0.69	0.691	0.692
	Constant	IDE		2.056	2.023
		IQE 10		4.611	4.629

Table 15. Comparison of SL-IDEs and SL-IQEs Calculated Using Different Software

Analyte	Model Type	Limit	QCalc	Excel	SAS [1]
Bromoform (524.2)	Hybrid	IDE	**0.2165**	-0.0094	0.2113
		IQE 10	**0.48**	-0.132	**0.482**
	Exponential	IDE	0.4097	0.4157	**0.3998**
		IQE 10		not calc [3]	0.914
	Linear	IDE		**-1.3717**	-1.3091
		IQE 10	not calc [3]	**not calc** [3]	-4.327
	Constant	IDE		10.355	10.207
		IQE 10		22.220	22.334
Chloroethane (524.2)	Hybrid	IDE	**0.1048**	-0.0035	0.1036
		IQE 10	**0.25**	-0.057	**0.255**
	Exponential	IDE	0.3999	0.4028	**0.3953**
		IQE 10		not calc [3]	0.907
	Linear	IDE		**-0.8594**	-0.8365
		IQE 10	not calc [3]	**not calc** [3]	-4.186
	Constant	IDE		14.518	14.465
		IQE 10		31.769	31.932
Cis-1,3-dichloropropene (502.2 ELCD)	Hybrid	IDE	0.0600	**0.1254**	0.0606
		IQE 10	0.15	**0.351**	0.151
	Exponential	IDE	0.0734	0.0750	**0.0740**
		IQE 10		0.176	0.177
	Linear	IDE		0.0833	0.0830
		IQE 10	**0.41**	0.412	**0.415**
	Constant	IDE		0.718	0.716
		IQE 10		1.598	1.604
Dibromochloromethane (502.2)	Hybrid	IDE	0.1397	**0.4531**	0.1406
		IQE 10	0.33	**1.081**	0.330
	Exponential	IDE	0.1430	0.1502	0.1441
		IQE 10		0.348	0.349
	Linear	IDE		0.4389	**0.4359**
		IQE 10	**1.25**	1.252	**1.252**
	Constant	IDE		0.786	0.784
		IQE 10		1.750	1.757
Lead (200.8)	Hybrid	IDE	0.2001	**0.3318**	0.2005
		IQE 10	0.46	**0.752**	0.462
	Exponential	IDE	0.2033	0.2086	**0.2038**
		IQE 10		0.477	0.478
	Linear	IDE		0.2705	0.2650
		IQE 10	**0.68**	0.684	**0.685**
	Constant	IDE		1.024	1.007
		IQE 10		2.296	2.305

Table 15. Comparison of SL-IDEs and SL-IQEs Calculated Using Different Software

Analyte	Model Type	Limit	QCalc	Excel	SAS [1]
M+p Xylene (502.2)	Hybrid	IDE	0.0876	0.0872	0.0883
		IQE 10	0.22	0.255	0.222
	Exponential	IDE	0.1197	0.1208	0.1205
		IQE 10		0.285	0.285
	Linear	IDE		0.0053	0.0052
		IQE 10	0.03	0.030	0.031
	Constant	IDE		1.704	1.701
		IQE 10		3.795	3.813
Methylmethacrylate (524.2)	Hybrid	IDE	0.2522	-0.0267	0.2441
		IQE 10	0.56	-0.364	0.561
	Exponential	IDE	0.5528	0.5615	0.5350
		IQE 10		not calc [3]	1.228
	Linear	IDE		-0.3617	-0.3415
		IQE 10	not calc [3]	not calc [3]	-1.043
	Constant	IDE		9.734	9.597
		IQE 10		20.667	20.773
Sec-butylbenzene (524.2)	Hybrid	IDE	0.0194	0.0205	0.0195
		IQE 10	0.05	0.050	0.047
	Exponential	IDE	0.1388	0.1403	0.1397
		IQE 10		0.316	0.316
	Linear	IDE		0.0803	0.0798
		IQE 10	0.28	0.279	0.279
	Constant	IDE		11.258	11.240
		IQE 10		25.074	25.203
Selenium (200.8)	Hybrid	IDE	0.3565	0.4600	0.3637
		IQE 10	0.83	1.045	0.829
	Exponential	IDE	0.4076	0.4159	0.4159
		IQE 10		0.957	0.957
	Linear	IDE		0.4057	0.4059
		IQE 10	1.04	1.044	1.045
	Constant	IDE		2.082	2.090
		IQE 10		4.668	4.686
Selenium (1620)	Hybrid	IDE	-0.3256	2.2850	1.9709
		IQE 10	-4.47	5.107	4.474
	Exponential	IDE	1.9742	2.0045	1.9754
		IQE 10		4.653	4.657
	Linear	IDE		2.0809	2.0539
		IQE 10	5.23	5.231	5.235
	Constant	IDE		4.195	4.161
		IQE 10		9.221	9.268
Sodium (1620)	Hybrid	IDE	139.8852	145.2512	140.8112
		IQE 10	317.64	326.198	317.747
	Exponential	IDE	137.8479	139.6656	138.7678
		IQE 10		323.711	323.935

Table 15. Comparison of SL-IDEs and SL-IQEs Calculated Using Different Software

Analyte	Model Type	Limit	QCalc	Excel	SAS [1]
	Linear	IDE		142.1564	141.2901
		IQE 10	337.63	337.515	**337.755**
	Constant	IDE		169.406	169.136
		IQE 10		377.295	379.229
Styrene (524.2)	Hybrid	IDE	**0.0175**	-5.70E-08	0.0174
		IQE 10	**0.04**	-8.40E-07	**0.041**
	Exponential	IDE	0.1407	0.1423	**0.1405**
		IQE 10		not calc [3]	0.318
	Linear	IDE		**-0.6099**	-0.6000
		IQE 10	not calc [3]	**not calc** [3]	-2.180
	Constant	IDE		10.555	10.516
		IQE 10		23.301	23.420
Vanadium (1620)	Hybrid	IDE	**10.6227**	11.4032	10.6931
		IQE 10	**24.33**	25.889	**24.338**
	Exponential	IDE	10.5597	**10.7036**	**10.6304**
		IQE 10		**25.094**	25.112
	Linear	IDE		10.0290	9.9671
		IQE 10	26.04	26.029	26.049
	Constant	IDE		22.757	22.721
		IQE 10		50.684	50.943
Vinyl Chloride (524.2)	Hybrid	IDE	**0.0840**	-2.30E-07	0.0834
		IQE 10	**0.22**	-9.78E-07	**0.219**
	Exponential	IDE	0.3671	0.3701	**0.3649**
		IQE 10		not calc [3]	0.837
	Linear	IDE		**-3.4286**	-3.3451
		IQE 10	49.30	**not calc** [3]	49.158
	Constant	IDE		22.474	22.292
		IQE 10		49.394	49.647
Yttrium (1620)	Hybrid	IDE	3.2571	**3.6382**	3.2787
		IQE 10	7.51	**8.305**	7.516
	Exponential	IDE	3.2251	3.2726	**3.2468**
		IQE 10		7.833	7.839
	Linear	IDE		3.5420	3.5202
		IQE 10	**8.96**	8.955	**8.962**
	Constant	IDE		4.576	4.569
		IQE 10		10.192	10.244

[1] Calculated using SAS programs written by EPA to run IDE and IQE calculations. Results are the same as those presented in Tables 2 and 4.

[2] Limits in bold indicate the calculated IDE or IQE based on the model suggested as most appropriate based on the given software.

[3] No value could be calculated due to model not converging.

[4] Based on statistical tests, QCalc determined that the constant model should be used to calculate the IDE and IQE. However, determination of the IDE and IQE using the constant model is not run by this program.

Table 16. Summary Statistics of Ratios Comparing IDEs/IQEs using different Software Packages

Comparison Ratio	Model Type	Limit	Minimum	25th Percentile	Median	75th Percentile	Maximum
QC_{Calc}/ SAS	Hybrid	IDE	-0.17	0.99	0.99	1.00	1.03
		IQE 10	-1.00	0.99	1.00	1.00	1.07
	Exponential	IDE	0.98	0.99	0.99	1.00	1.03
	Linear	IQE 10	0.97	0.99	1.00	1.00	1.00
Excel/ SAS	Hybrid	IDE	-0.11	-0.000003	1.10	1.32	3.22
		IQE 10	-0.65	-0.000009	1.06	1.35	3.27
	Exponential	IDE	1.00	1.01	1.01	1.02	1.05
		IQE 10	0.99	1.00	1.00	1.00	1.00
	Linear	IDE	1.00	1.01	1.01	1.02	1.06
		IQE 10	0.97	1.00	1.00	1.00	1.00
	Constant	IDE	0.99	1.00	1.00	1.01	1.02
		IQE 10	0.98	0.99	0.99	1.00	1.00
QC_{Calc}/ Excel	Hybrid	IDE	-365,000	-12.85	0.54	0.93	1.01
		IQE 10	-225,000	-2.07	0.52	0.91	1.01
	Exponential	IDE	0.96	0.98	0.99	0.99	0.99
	Linear	IQE 10	0.99	1.00	1.00	1.00	1.00

Table 17. Comparison of Simulated 7-replicate ACIL CRVs to Overall CRV, ACIL Blanks

Analyte	# Blanks *	Overall CRV	# simulated 7-replicate CRVs	Mean of Simulated 7-replicate CRVs	Range of Simulated 7-replicate CRVs	Range of Days between 1st and Last of 7 consecutive replicates	% short-term CRVs exceeding Overall CRV
Barium	26	0.0039	20	0.0039	0.0011 to 0.0083	7 to 26	30
Cadmium	33	0.0012	27	0.0014	0.00044 to 0.0019	11 to 24	67
Chromium	55	0.0048	49	0.0051	0.0014 to 0.0117	7 to 20	29
Copper	52	0.0035	46	0.0039	0.0010 to 0.0059	7 to 20	78
Silver	45	0.0105	39	0.0100	0.0019 to 0.0326	7 to 20	28

* Analyzed over a period of 3 months

Table 18. Comparison of Simulated 7-replicate ACIL CRVs to Overall CRV, ACIL Blanks After Outlier Removal

Analyte	# Blanks *	Overall CRV	# simulated 7-replicate CRVs	Mean of Simulated 7-replicate CRVs	Range of Simulated 7-replicate CRVs	Range of Days between 1st and Last of 7 consecutive replicates	% short-term CRVs exceeding Overall CRV
Barium	25	0.0020	19	0.0021	0.0011 to 0.0029	11 to 26	74
Chromium	54	0.0040	48	0.0044	0.0014 to 0.0080	7 to 20	56
Silver	42	0.0031	36	0.0038	0.0019 to 0.0058	8 to 21	72

* Analyzed over a period of 3 months

This Appendix is included to support Appendices B of this Assessment Document, by providing example calculations of the single-laboratory variants of the Interlaboratory Detection Estimate (SL-IDE) and Interlaboratory Quantitation Estimate (SL-IQE) as described in ASTM D6091 and ASTM D6512, respectively. Example calculations of the method detection limit (MDL) and minimum level of quantitation (ML) also are included. The example calculations provided in this Appendix were used in the data analyses presented in Appendix B.

All abbreviations and symbols used in the SL-IDE and SL-IQE calculations match those given in the ASTM procedures. The linear and exponential standard deviation models and all recovery models were fit using the PROC REG procedure in SAS Version 8.1. The hybrid standard deviation model was fit using Newton's Non-Linear Least Squares procedure as described in ASTM D6512, programmed using SAS Version 8.1. The dataset used in these examples is that included for 1,1,1,2- tetrachloroethane in EPA's Episode 6000 (see Chapter 1 and Appendix B of this document for descriptions of datasets).

Single-Laboratory IDE (SL-IDE)

The procedure for calculating the IDE that is described in ASTM D6091 stipulates use of data from multiple laboratories. However, because analytes in the Episode 6000 dataset were only measured by a single laboratory, EPA calculated a variant of the IDE which was called the single-laboratory IDE (SL-IDE). The SL-IDE and the analyses performed using the SL-IDE are described in greater detail in Appendix B of this Assessment document.

In order to calculate the SL-IDE, means and standard deviations are needed for each spike level. The means and standard deviations for 1,1,1,2-tetrachloroethane are listed in Table 1.

Table 1. Mean and Standard Deviation Calculated at each Spike Level

Spike (ug/L)	N	Mean (ug/L)	SD (ug/L)
0.01	7	0.0016	0.0018
0.015	7	0.001	0.0017
0.02	7	0.0007	0.0010
0.035	7	0.0057	0.0036
0.05	7	0.0081	0.0024
0.075	7	0.0263	0.0202
0.1	6	0.0295	0.0039
0.15	7	0.0536	0.0046
0.20	7	0.0991	0.0158

Spike (ug/L)	N	Mean (ug/L)	SD (ug/L)
0.35	7	0.235	0.0078
0.50	7	0.3744	0.0257
0.75	6	0.6193	0.0262
1.0	8	0.8368	0.0814
2.0	7	1.9560	0.0980
5.0	8	5.0994	0.2382
10.0	7	10.4453	0.5469

In order to choose the appropriate model to calculate the IDE, significance tests were used.

The fitted unweighted linear model was:

S = 0.000039515 + 0.05326 * T, where T corresponds to spike concentration

The slope of this model was significantly greater than 0, and therefore the constant model was rejected.

The fitted unweighted exponential model (fit by natural log-transforming standard deviations) was:

Log(S)= -5.02407 + 0.54851 * T

The slope of this model was significantly greater than 0, thus, the linear model was rejected.

Based on this assessment, the exponential model was used in Appendix B to calculate the IDE for this analyte. While the exponential model was chosen as the most appropriate model for this analyte, the calculation of the SL-IDE using all four model types is presented in this Appendix. This was done to provide a step-by-step example for the calculation of the SL-IDE using all of the different model types.

Constant model: The pooled within-spike variance was first calculated using the equation below:

$$g^2 = \frac{\sum_{i=1}^{16}[(n_i - 1) * s_i^2]}{\sum_{i=1}^{16} n_i - 16}$$

where: s_i is the standard deviation of the results for spike level i, and
n_i is the number of replicates for spike level i.

The calculated pooled within-spike variance (g^2) is 0.024, and the square root of this value, g, equals 0.155.

A linear regression model was then fit for the mean results for the 16 spike levels. The estimates of slope and intercept for this model are: a = -0.089 and b=1.0478, respectively.

Based on these results:

$YC = (k1 * g) + a = (0.155 * k1) - 0.089 = (0.155 * 2.6) - 0.089 = 0.3137$

where: YC = the recovery critical value as defined in ASTM D6091, and
k1 = 2.6 (a conservative number based on the total n of 112)

$LC = (YC - a)/b = (0.3137 + 0.089) / 1.0478 = 0.3848$

where: LC = the true concentration critical value as defined in ASTM D6091.

$IDE = LC + (k2 * g)/b = 0.3848 + (1.86 * 0.155)/1.0478 = 0.660$

where: k2 = 1.86 (a conservative number based on the total n of 112).

Linear Model:

An unweighted linear regression model was fit, predicting standard deviation based on concentration, using PROC REG in SAS Version 8.1. The estimated parameters are: g = 0.0000392 and h = 0.05326. Based on these parameters, weights for the recovery model were calculated for each spike value. For each concentration, the weight was calculated as:

$$weight = \frac{1}{\hat{s}_i^2} = \frac{1}{(g + h * T_i)^2}$$, for each true concentration T_i.

The calculated weights are given in Table 2.

Table 2. Calculated Weights based on Linear Model

Spike (ug/L)	Est. SD (ug/L)	Weight
0.01	0.00057	3,058,709
0.015	0.00084	1,423,673
0.02	0.00110	819,854
0.035	0.00190	276,031
0.05	0.00270	136,940
0.075	0.00403	61,454
0.1	0.00537	34,736
0.15	0.00803	15,514

Spike (ug/L)	Est. SD (ug/L)	Weight
0.20	0.01069	8,748
0.35	0.01868	2,865
0.50	0.02667	1,406
0.75	0.03999	625.4
1.0	0.05330	352.0
2.0	0.10657	88.1
5.0	0.26635	14.1
10.0	0.53267	3.52

Using these weights, the fitted recovery model estimates were a = -0.00898 and b = 0.6860. Based on these results:

YC = (k1 * g) + a = (0.0000392 * 2.6) - 0.00898 = -0.00888, and

LC = (YC - a)/b = (-0.00888 + 0.00898) / 0.6860 = 0.00015

For the linear model, the SL-IDE must be calculated recursively. The initial estimate of the SL-IDE, LD_0, was:

$LD_0 = LC + (k_2 * s(0)) / b = 0.00025$.

Each following estimate was calculated using the recursive formula:

$$LD_{i+1} = [k_1 * \hat{s}(0) + k_2 * (g + h * LD_i)] / b$$

Results of the recursive LD calculations are given in Table 3.

Table 3. Recursive SL-IDE Calculations, Linear Model

LD estimate run	LD estimate
0	0.000255
1	0.000291
2	0.000297
3	0.000297

The recursive estimates of LD converge to 6 decimal places by the third iteration. Therefore, the linear model estimate of the IDE = 0.000297 ug/L.

Exponential Model:

An unweighted linear regression model was fit, predicting natural log-transformed standard deviation based on concentration. The estimated parameters are: g = 0.00658 and h = 0.54851. Based on these parameters, weights for the recovery model were calculated for each spike value. For each concentration, the weight was calculated as:

$$weight = \frac{1}{\hat{s}_i^2} = \frac{1}{(g * e^{h*T_i})^2}$$, for each true concentration T_i.

The calculated weights are given in Table 4.

Table 4. Calculated Weights based on Exponential Model

Spike (ug/L)	Est. SD (ug/L)	Weight
0.01	0.00661	22,861
0.015	0.00663	22,736
0.02	0.00665	22,611
0.035	0.00671	22,242
0.05	0.00676	21,879
0.075	0.00685	21,287
0.1	0.00695	20,711
0.15	0.00714	19,606
0.20	0.00734	18,560
0.35	0.00797	15,744
0.50	0.00865	13,355
0.75	0.00993	10,152
1.0	0.01138	7,717
2.0	0.01970	2,576
5.0	0.10213	96
10.0	1.58566	0.40

Using these weights, the fitted recovery model estimates were a = -0.04585, and b = 0.91696. Based on these results:

YC = (k1 * g) + a = (0.00658 * 2.6) - 0.04585 = -0.0287, and

LC = (YC - a)/b = (-0.0287 + 0.04585) / 0.91696 = 0.0187

For the Exponential model, the SL-IDE must be calculated recursively. The initial estimate of the SL-IDE, LD_0, was:

$LD_0 = LC + (k_2 * s(0)) / b = 0.03199.$

Each following estimate was calculate using the recursive formula:

$$LD_{i+1} = [k_1 * \hat{s}(0) + k_2 * (g * e^{h*LD_i})] / b$$

Results of the recursive LD calculation are given in Table 5, below.

Table 5. Recursive SL-IDE Calculations, Exponential Model

LD estimate run	LD estimate
0	0.031993
1	0.032229
2	0.032231

The recursive estimates of LD converge to 6 decimal places by the second iteration. Therefore, the exponential model estimate of the IDE = 0.032231 ug/L.

Hybrid Model:

The Hybrid model was fit using Newton's Method for Non-linear Least Squares. Summary statistics from this fit of the hybrid model are presented in Table 6, using the same notation as shown in ASTM D6512-00.

Table 6. Summary Statistics from Newton's Non-Linear Least Squares

Run	g	h	u	v	c	d	p	q	Δg	Δh	dg%	dh%
0	0.00095	0.05465	1,254330	4,285	19,889	2×10^{-10}	555.95	-0.592	0.00048	-0.00237	50.5	43.4
1	0.00143	0.05228	981,892	4,275	15,368	3×10^{-10}	41.83	-1.132	0.00005	-0.00044	3.45	8.5
2	0.00148	0.05184	958,193	4,309	15,092	3×10^{-10}	4.47	-0.123	5×10^{-6}	-0.00005	0.37	0.9

Because dg% (the percent difference between the last 2 estimates of g) and dh% (the percent difference between the last 2 estimates of h) were both less than 1% in run 2, the model converged, and the estimated parameters of the hybrid model were:

$$g = g_{run\,2} + \Delta g_{run\,2} = 0.00148 + 0.000005 = 0.00149$$
$$h = h_{run\,2} + \Delta h_{run\,2} = 0.05184 - 0.00005 = 0.05179$$

Using these fitted parameters, the weights for the recovery model were calculated as shown in Table 7.

Table 7. Calculated Weights, Hybrid Model

Spike (ug/L)	Est. SD (ug/L)	Weight
0.01	0.00158	403,037
0.015	0.00168	355,066
0.02	0.00181	304,351
0.035	0.00234	181,881
0.05	0.00299	112,141
0.075	0.00416	57,811
0.1	0.00539	34,447
0.15	0.00791	15,987
0.20	0.01046	9,134
0.35	0.01819	3,024
0.50	0.02594	1,487
0.75	0.03887	662
1.0	0.05181	373
2.0	0.10358	93.2
5.0	0.25893	14.9
10.0	0.51786	3.73

Using these weights, the fitted recovery model estimates were a = -0.01471, and b = 0.74338. Based on these results:

YC = (k1 * g) + a = (0.00149 * 2.6) - 0.01471 = -0.01085, and

LC = (YC - a)/b = (-0.01085 + 0.01471) / 0.74338 = 0.00520

LD had to be calculated recursively. The initial estimate of LD was:

$LD_0 = LC + (k_2 * s(0)) / b = 0.00893.$

Each following estimate was calculated using the recursive formula:

$$LD_{i+1} = [k_1 * \hat{s}(0) + k_2 * (g * e^{h * LD_i})] / b$$

Results of the recursive LD calculation are given in Table 8.

Table 8. Recursive SL-IDE Calculations, Hybrid model

LD estimate run	LD estimate
0	0.008925
1	0.009101
2	0.009108
3	0.009108

The recursive estimates of LD converge to 6 decimal places by the third iteration. Therefore, the hybrid model estimate of the IDE = 0.009108 ug/L.

Single-Laboratory IQE (SL-IQE)

The procedure for the IQE described in ASTM D6512 stipulates use of data from multiple laboratories. However, because analytes in the Episode 6000 dataset were only measured by a single laboratory, EPA calculated a variant of the IQE which was called the single-laboratory IDE (SL-IQE). The SL-IQE and the analyses performed using the SL-IQE are described in greater detail in Appendix B of this Assessment document.

Fitting and selection of models in the IQE calculation process are identical to the IDE calculation process except:

- The Hybrid model was considered in model selection instead of the Exponential model, based on significance tests for curvature as described in 6.3.3.2 (g) - (i) of ASTM D6512.
- A bias-correction adjustment factor is applied to calculated standard deviations prior to modeling as described in 6.3.3.2 (b) of ASTM D6512.

Therefore, the example calculation begins with the fitted model parameters for each model type, and demonstrates the calculation of each IQE value.

Constant model:

Using the same steps for fitting the constant model as described in the SL-IDE example, the fitted precision and recovery model parameters are determined to be:

g = 0.1615
a = -0.0894, and b = 1.0478.

The IQE (10%) was calculated as: IQE (10%) = (g/b)*(100/10) = 1.541

The IQE (20%) was calculated as: IQE (20%) = (g/b)*(100/20) = 0.770

The IQE (30%) was calculated as: IQE (30%) = (g/b)*(100/30) = 0.514

Linear model:

Using the same steps for fitting the linear model as described in the SL-IDE example, the fitted precision and recovery model parameters are determined to be:

$g = 4.2 \times 10^{-7}$, h = 0.0555
a = -0.0087, b = 0.6810

The IQE (10%) was calculated as: IQE (10%) = $g/(b*(10/100)-h) = 3.3 \times 10^{-5}$

The IQE (20%) was calculated as: IQE (20%) = $g/(b*(20/100)-h) = 5.2 \times 10^{-6}$

The IQE (30%) was calculated as: IQE (30%) = $g/(b*(30/100)-h) = 2.8 \times 10^{-6}$

Hybrid model:

Using the same steps for fitting the hybrid model as described in the SL-IDE example, the fitted precision and recovery model parameters are determined to be:

g = 0.00155, h = 0.0540
a = -0.0147, b = 0.7434

The IQE (10%) was calculated as:

$$IQE(10\%) = \frac{g}{\sqrt{\left(\frac{10*b}{100}\right)^2 - h^2}} = 0.0304$$

The IQE (20%) was calculated as:

$$IQE(20\%) = \frac{g}{\sqrt{(\frac{20 * b}{100})^2 - h^2}} = 0.0112$$

The IQE (30%) was calculated as:

$$IQE(30\%) = \frac{g}{\sqrt{(\frac{30 * b}{100})^2 - h^2}} = 0.0072$$

Exponential model:

Using the same steps for fitting the constant model as described in the SL-IDE example, the fitted precision and recovery model parameters are determined to be:

g = 0.0069, h = 0.5482
a = -0.0459, b = 0.9170

For the Exponential model, the IQE must be solved recursively. The initial estimate of the IQE was set to the IDE (re-calculated using bias-corrected standard deviations, and therefore not matching the IDE presented in the example above). The IQE was then re-calculated using the estimate from the prior round, based on the equation below:

$$IQE(Z)_{i+1} = \frac{100g * e^{h * IQE(Z)_i}}{Zb},$$

where: Z i = 10, 20 or 30, depending on the IQE being calculated.

Results of the recursive calculations for the IQEs are given in Table 9.

Table 9. Recursive SL-IDE Calculations, Exponential model

Run	IQE (10%)	IQE (20%)	IQE (30%)
0	0.0355	0.0355	0.0355
1	0.0763	0.0381	0.0254
2	0.0780	0.0382	0.0253
3	0.0781	0.0382	0.0253
4	0.0781	0.0382	0.0253

MDL/ML

This section gives an example calculation of the MDL and ML determined using the Episode 6000 data, and presented in Appendix B. Due to the nature of the study design, MDLs could not be determined following the MDL procedure directly. Therefore, the MDL was calculated based on the results of the two lowest spike levels with all positive results for which the standard deviations were not significantly different.

The lowest two spike levels with all positive, non-zero results are 0.050 µg/L and 0.075 µg/L. From Table 1, the standard deviations at these concentrations are 0.0024 µg/L and 0.0202 µg/L, respectively. The F test was then run on the variances at these two spike levels:

$$F = \frac{(0.0202)^2}{(0.0024)^2} = \frac{0.0004}{0.000006} = 70.385$$

The critical value for the F test at α=0.10, where both variances are based on 7 results, is 3.05. Because 70.385 > 3.05, the variance at the higher concentration is significantly greater than the variance at the lower concentration, and these two concentrations cannot be used to calculate the MDL.

The next lowest spike level (0.10 µg/L) has only 6 results, but all results are greater than 0. Therefore, an F test was run comparing variances at 0.075 µg/L and 0.10 µg/L. From Table 1, the standard deviation at 0.10 µg/L is 0.0039 µg/L. The results of the F test are:

$$F = \frac{(0.0039)^2}{(0.0202)^2} = \frac{0.00002}{0.0004} = 0.037$$

The critical value for this F test is 3.11, slightly higher than for the prior comparison due to the fewer number of results at the higher spike level. Because $0.037 < 3.11$, the variance at the higher spike level is not significantly greater than the variance at the lower spike level. Therefore, the MDL is calculated based on these two spike levels:

$$MDL = \sqrt{\frac{(6-1)*(0.0039)^2+(7-1)*(0.0202)^2}{(6-1)+(7-1)}} * t_{(0.99,7+6-2)}$$

$$= 0.015 * 2.71$$

$$= 0.041$$

The ML is determined by first multiplying the pooled standard deviation (0.015 µg/L from the calculation above) by 10. This yields a result of 0.15 µg/L. Based on the ML rounding scheme, this becomes 0.2 µg/L.