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Appendix A Mercury Solubility Result in Hydrocarbons

Table A1 Mercury solubility in single solvent system at 5°C

Solvent	Mercury solubility, ppb (wt)							
	Literature Value*	R1	R2	R3	Avg	SD	% CV	% Diff
<i>n</i> -pentane	549.95	134.22	158.05	143.75	145.34	11.99	8.25	73.57
<i>n</i> -hexane	568.89	330.99	359.39	308.58	332.99	25.46	7.65	41.47
<i>n</i> -heptane	570.37	131.34	119.97	131.17	127.49	6.52	5.11	77.65
<i>n</i> -octane	590.58	283.69	271.93	298.07	284.56	13.09	4.60	51.82
<i>n</i> -decane	N/A	195.48	183.40	186.03	188.00	5.85	3.11	N/A
2,2,4-trimethylpentane	372.82	104.36	98.83	88.61	97.27	7.99	8.22	73.91

* Calculated from the least square equation from Okouchi *et al.* (1981) except 2,2,4-trimethylpentane which was from Spencer *et al.* (1967).

Table A2 Mercury solubility in single solvent system at 15°C

Solvent	Mercury solubility, ppb (wt)							
	Literature Value*	R1	R2	R3	Avg	SD	% CV	% Diff
<i>n</i> -pentane	1016.21	215.93	225.51	201.53	214.32	12.07	5.63	78.91
<i>n</i> -hexane	1041.41	357.11	346.47	371.52	358.37	12.57	3.51	65.59
<i>n</i> -heptane	1049.45	159.04	158.91	159.65	159.20	0.40	0.25	84.83
<i>n</i> -octane	1058.05	307.91	339.39	310.27	319.19	17.53	5.49	69.83
<i>n</i> -decane	N/A	245.17	246.63	241.70	244.50	2.53	1.04	N/A
2,2,4-trimethylpentane	666.97	170.14	167.12	176.21	171.16	4.63	2.70	74.34

* Calculated from the least square equation from Okouchi *et al.* (1981) except 2,2,4-trimethylpentane which was from Spencer *et al.* (1967).

Table A3 Mercury solubility in single solvent system at 25°C

Solvent	Mercury solubility, ppb (wt)							
	Literature Value*	R1	R2	R3	Avg	SD	% CV	% Diff
<i>n</i> -pentane	1839.18	395.17	375.07	395.35	388.53	11.66	3.00	78.87
<i>n</i> -hexane	1867.50	500.24	511.63	522.94	511.60	11.35	2.22	72.60
<i>n</i> -heptane	1891.09	476.91	433.09	446.91	452.30	22.40	4.95	76.08
<i>n</i> -octane	1843.91	509.00	532.86	519.81	520.56	11.95	2.30	71.77
<i>n</i> -decane	1508.48	546.50	521.75	539.21	535.82	12.72	2.37	64.48
2,2,4-trimethylpentane	1166.23	371.15	342.78	368.11	360.68	15.58	4.32	69.07

* Calculated from the least square equation from Okouchi *et al.* (1981) except 2,2,4-trimethylpentane which was from Spencer *et al.* (1967).

Table A4 Mercury solubility in single solvent system at 40°C

Solvent	Mercury solubility, ppb (wt)							
	Literature Value*	R1	R2	R3	Avg	SD	% CV	% Diff
<i>n</i> -pentane	4315.05	1015.55	1054.22	1011.17	1026.98	23.69	2.31	76.20
<i>n</i> -hexane	4327.17	1407.50	1449.70	1318.05	1391.75	67.22	4.83	67.84
<i>n</i> -heptane	4412.40	1230.39	1121.26	1297.64	1216.43	89.01	7.32	72.43
<i>n</i> -octane	4177.78	1451.82	1436.55	1439.96	1442.78	8.02	0.56	65.47
<i>n</i> -decane	N/A	1009.23	1144.68	1055.87	1069.93	68.81	6.43	N/A
2,2,4-trimethylpentane	2606.06	968.67	949.97	963.22	960.62	9.62	1.00	63.14

* Calculated from the least square equation from Okouchi *et al.* (1981) except 2,2,4-trimethylpentane which was from Spencer *et al.* (1967).

Table A5 Mercury solubility in simulated condensate at various temperatures

Temperature (°C)	Mercury solubility, ppb (wt)					
	R1	R2	R3	Avg	SD	% CV
5	264.16	276.62	262.85	267.88	7.60	2.84
15	332.29	335.05	350.45	339.26	9.79	2.88
25	876.96	833.28	875.52	861.99	24.87	2.89
40	1787.97	1882.54	1782.83	1817.78	56.14	3.09

Appendix B Hysteresis of Mercury Solubility in Hydrocarbons

Table B1 Hysteresis of mercury solubility in single solvent system at 5°C

Solvent	Mercury solubility, ppb (wt)					
	R1	R2	R3	Avg	SD	% CV
<i>n</i> -pentane	126.24	118.91	130.03	125.06	5.65	4.52
<i>n</i> -hexane	223.93	207.66	223.90	218.50	9.38	4.30
<i>n</i> -heptane	164.74	179.31	170.21	171.42	7.36	4.29
<i>n</i> -octane	235.01	229.77	233.43	232.74	2.69	1.15
<i>n</i> -decane	194.21	199.29	185.12	192.87	7.18	3.72
2,2,4-trimethylpentane	111.60	117.61	102.84	110.68	7.43	6.71

Table B2 Hysteresis of mercury solubility in single solvent system at 15°C

Solvent	Mercury solubility, ppb (wt)					
	R1	R2	R3	Avg	SD	% CV
<i>n</i> -pentane	145.01	144.65	132.41	140.69	7.17	5.10
<i>n</i> -hexane	488.28	489.29	528.45	502.07	22.85	4.55
<i>n</i> -heptane	276.87	264.03	275.66	272.19	7.09	2.60
<i>n</i> -octane	311.67	314.67	319.85	315.40	4.14	1.31
<i>n</i> -decane	259.76	261.53	268.36	263.22	4.54	1.73
2,2,4-trimethylpentane	113.29	112.76	118.76	114.94	3.32	2.89

Table B3 Hysteresis of mercury solubility in single solvent system at 25°C

Solvent	Mercury solubility, ppb (wt)					
	R1	R2	R3	Avg	SD	% CV
<i>n</i> -pentane	353.81	394.74	399.91	382.82	25.26	6.60
<i>n</i> -hexane	615.36	644.96	613.51	625.28	17.15	2.74
<i>n</i> -heptane	468.01	435.54	451.47	451.67	16.24	3.59
<i>n</i> -octane	563.47	584.19	514.93	554.20	35.55	6.41
<i>n</i> -decane	577.57	506.86	505.31	529.91	41.28	7.79
2,2,4-trimethylpentane	379.57	339.58	369.93	363.03	20.87	5.75

Table B4 Hysteresis of mercury solubility in simulated condensate at various temperatures

Temperature (°C)	Mercury solubility, ppb (wt)					
	R1	R2	R3	Avg	SD	% CV
5	200.62	197.03	198.56	198.74	1.80	0.91
15	231.83	204.15	221.40	219.13	13.98	6.38
25	445.01	457.35	437.63	446.66	9.96	2.23

Appendix C Least Square Equation for the Temperature Dependence of the Solubility of Mercury

From Spencer *et al.* (1967) and Okouchi *et al.* (1981), the raw experimental data were not published, but the least square equations for the temperature dependence of the mercury solubility in hydrocarbons were given instead.

$$\text{Log } X = A \text{Log } T + B \quad (\text{C.1})$$

where X = the mole fraction of mercury
T = the absolute temperature.

From equation C.1, coefficients A and B for each hydrocarbon from previous works were tabulated in Table C.1.

Table C.1 Constants of equation C.1

Solvent	Spencer et al., 1967		Okouchi et al., 1981	
	A	B	A	B
n-pentane			17.375	-49.169
n-hexane	17.084 ± 0.420	-48.366	17.111	-48.432
n-heptane	17.462 ± 0.301	-49.234	17.250	-48.705
n-octane	16.583 ± 0.228	-47.003	16.500	-46.800
2,2,4-trimethylpentane	16.377 ± 0.451	-46.698		

However, the temperature range covered by this equation is about 0-40°C.

Appendix D Certificate of Analysis of 3-methylpentane



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SIGMA-ALDRICH

Certificate of Analysis

Product Name	3-Methylpentane, purum ≥99.0% (GC)
Product Number	68322
Product Brand	Fluka
CAS Number	96-14-0
Molecular Formula	C ₆ H ₁₄
Molecular Weight	86.18

TEST	LOT 1146923 RESULTS
APPEARANCE (COLOR)	COLORLESS
APPEARANCE (FORM)	CLEAR LIQUID
ASSAY (GC AREA %)	99.3 % rel
REMARKS ON GC	0.7 % 2,3-Dimethylbutane
DENSITY D20/4	0.664
REFRACTIVE INDEX N20/D	1.377
INFRARED SPECTRUM	CORRESPONDS
DATE OF QC-RELEASE	18/NOV/04

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Appendix E Hysteresis Curve with the 10% Acceptable Deviation Range

In this work, the maximum acceptable deviation range for the mercury solubility was set to 10%. When we plotted the hysteresis curve with the 10% deviation range instead of the standard deviation for each point, the curve shows in Figures E.1 – E.7.

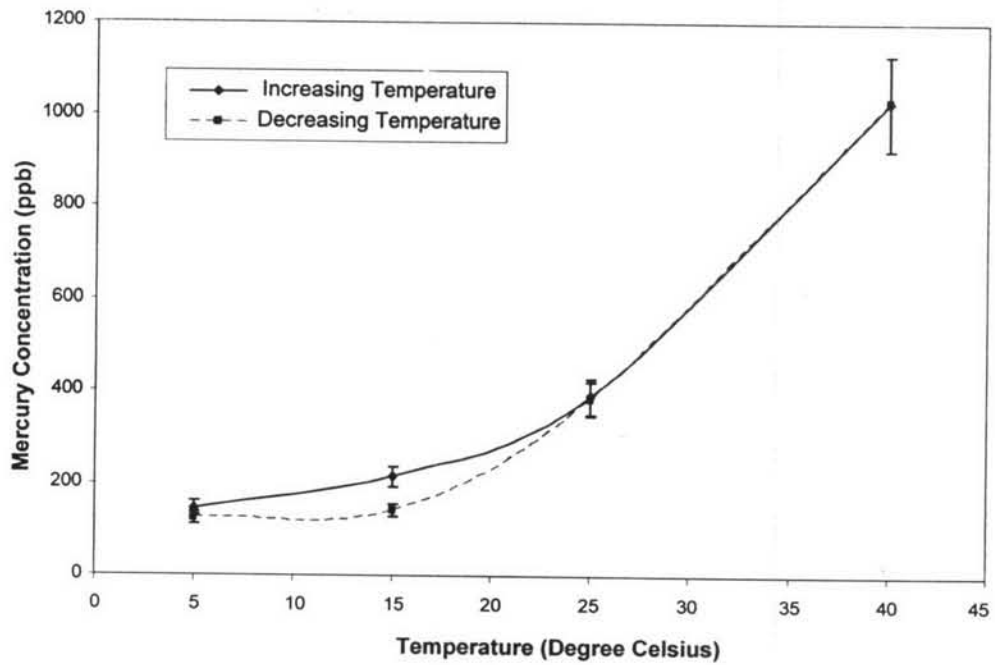


Figure E.1 Hysteresis study on mercury solubility in *n*-pentane.

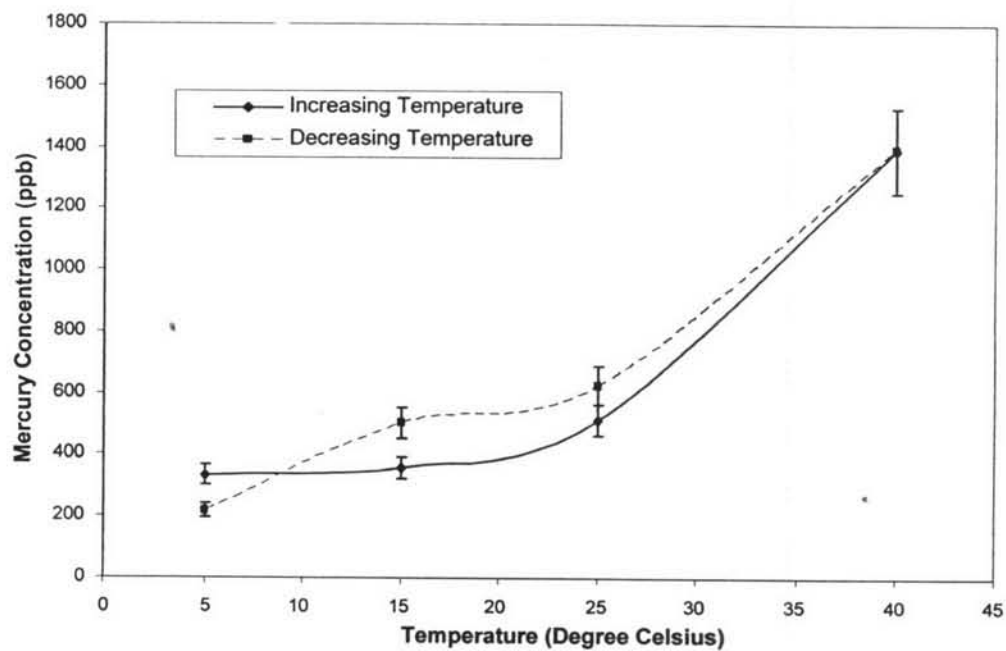


Figure E.2 Hysteresis study on mercury solubility in *n*-hexane.

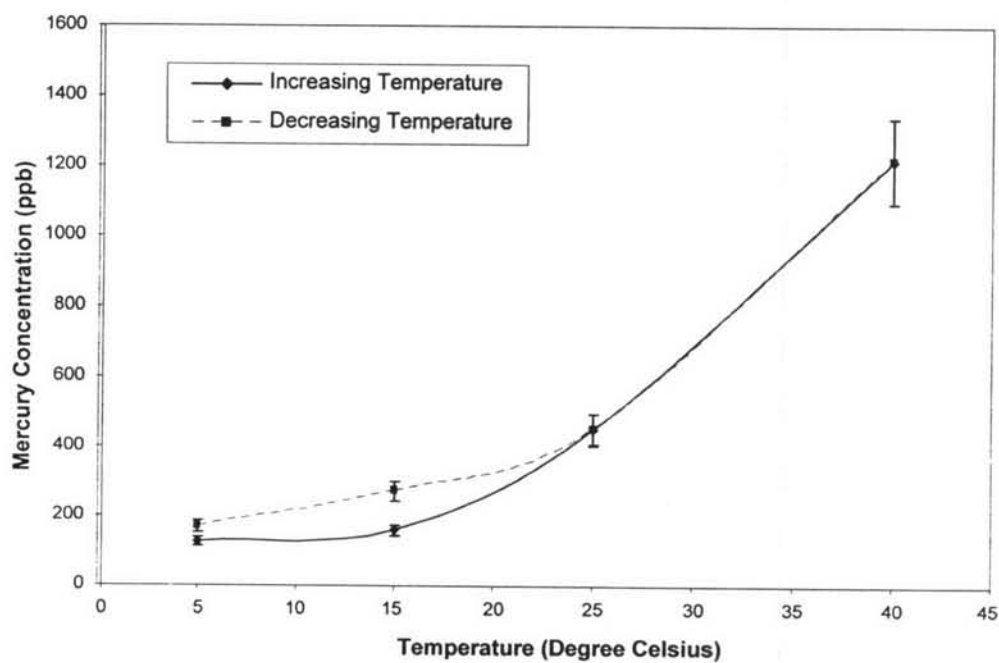


Figure E.3 Hysteresis study on mercury solubility in *n*-heptane.

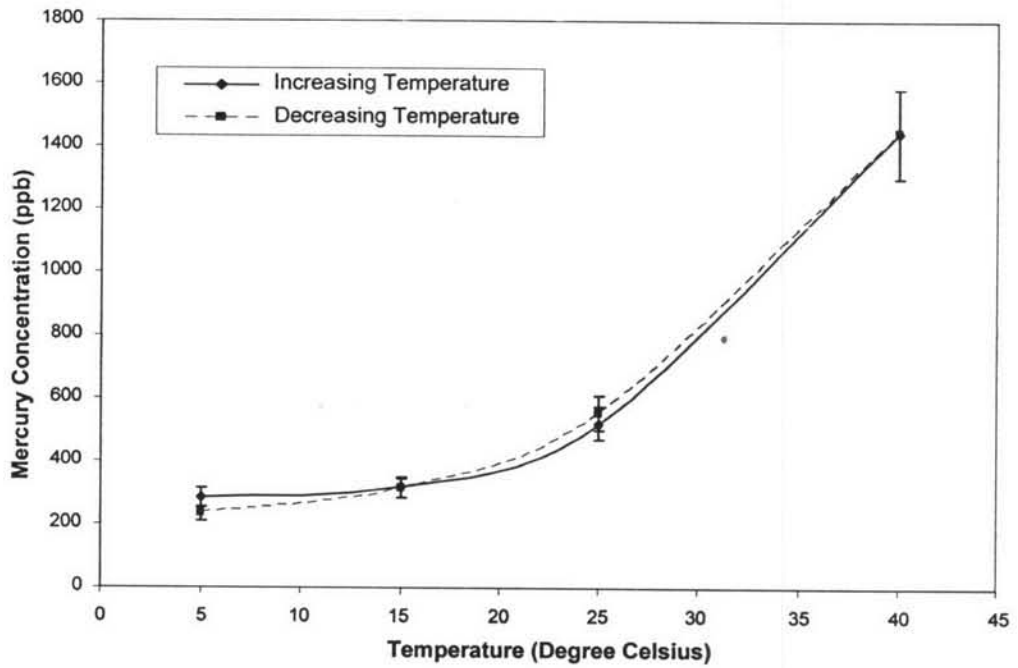


Figure E.4 Hysteresis study on mercury solubility in *n*-octane.

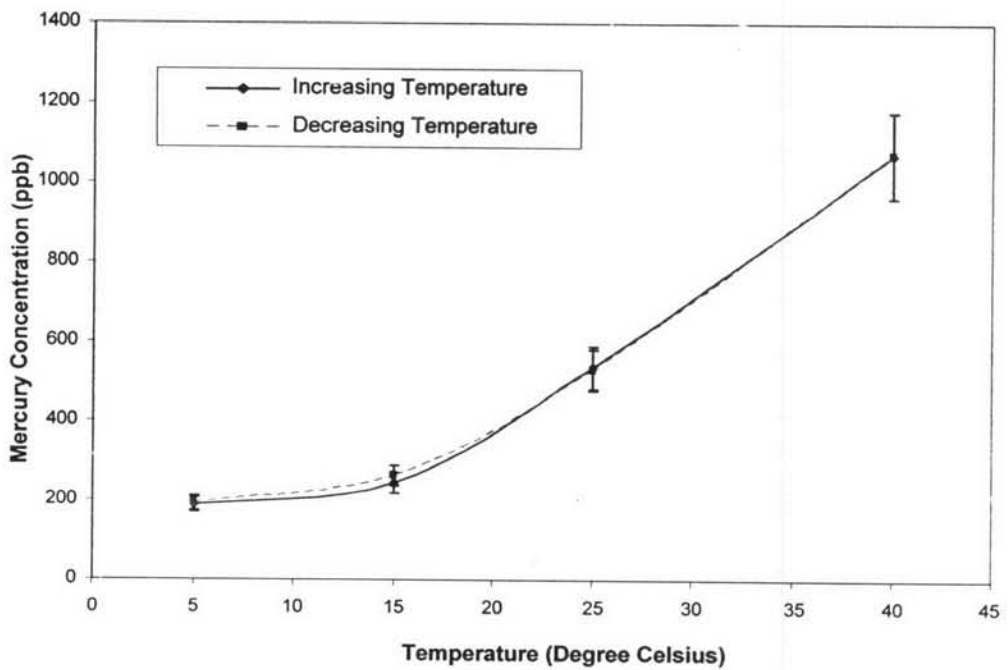


Figure E.5 Hysteresis study on mercury solubility in *n*-decane.

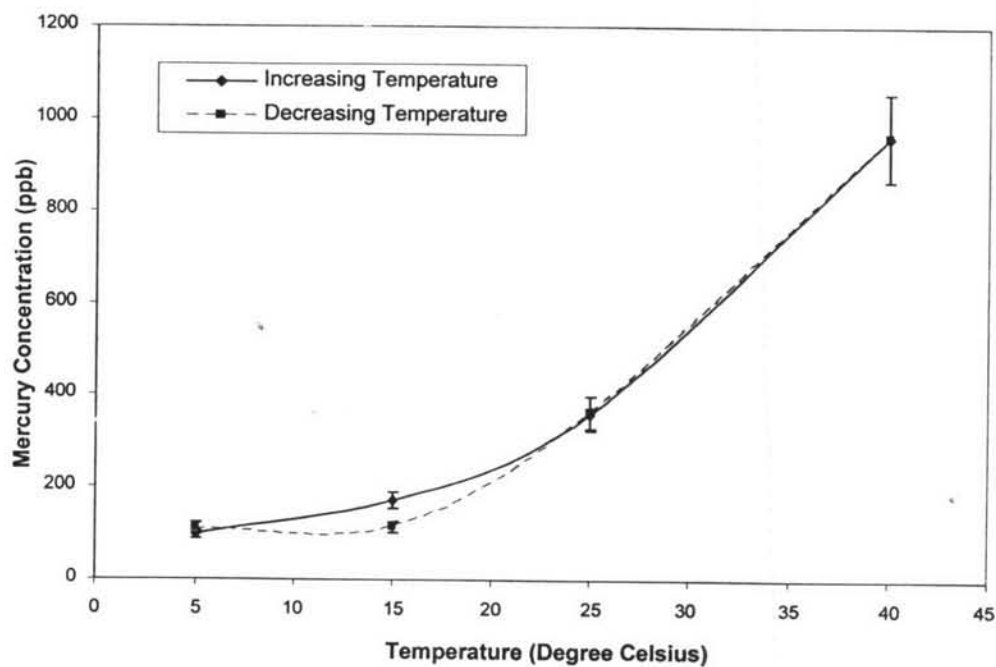


Figure E.6 Hysteresis study on mercury solubility in 2,2,4-trimethylpentane.

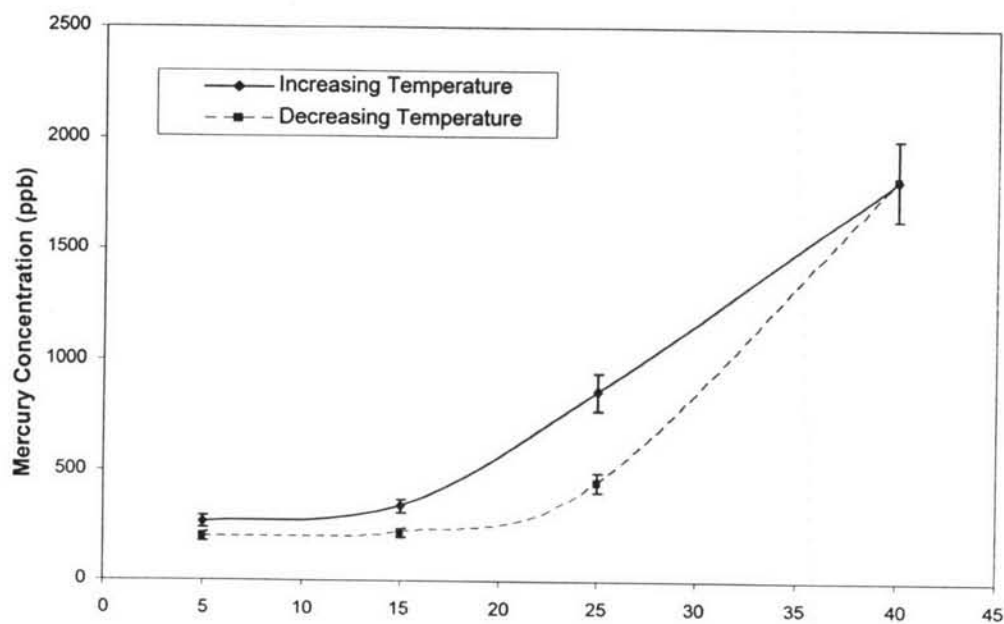


Figure E.7 Hysteresis study on mercury solubility in simulated condensate.

It can be concluded that hysteresis did not exist in *n*-octane and *n*-decane since the differences between the increasing and decreasing temperature curves were

insignificant, whereas the other solvents and simulated condensate show the occurrence of hysteresis.

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