

# Prioritization of VOCs Emitted from Co-Processing Cement Kiln Using a Fuzzy Analytic Hierarchy Process Method

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## Assumption principles of estimation

### 1. OFP

1. For the compounds in the same category, their *MIR* decrease slightly with the growth of the carbon chain, and regardless of how long the carbon chain is, their *MIR* are still in the same order.
2. Functional groups and degree of unsaturation affect *MIR*. *MIR* reduces with an increase in the number of halogen groups in the organic compounds. Based on the *MIR* values of benzene, chlorin benzene, and 1,3-dichlorobenzene, the value drops roughly 50% when a chlorine group substitutes a hydrogen atom of the aromatic compound.
3. Based on our observation, we found that when the number of halogen groups is more than four in one compound, the *MIR* of the target compound is estimated as the value of 0 g O<sub>3</sub>/g VOCs. When the compound has three halogen groups, its *MIR* is less than 0.1 g O<sub>3</sub>/g VOCs. Notably, the OFP of tetrachloroethylene is 0.031 g O<sub>3</sub>/g VOCs, while the *MIR* of tetrachloromethane is 0 g O<sub>3</sub>/g VOCs. This discrepancy is due to the unsaturated bond in the tetrachloroethylene. The assumed *MIR* are listed in Table S1.

### 2. Odor Threshold

1. Isomerides have a similar odor threshold.
2. For the compounds in the same category, their odor threshold values are similar.
3. Halohydrocarbon has a much higher odor threshold.

The assumed odor threshold values are given in Table S1.

### 3. Saturated Vapor Pressure

Saturated vapor pressure is an important index to evaluate the diffusion of VOCs in multiple phases, and it was used to evaluate the influence ability of different VOCs. The saturated vapor pressure was obtained from the database of the National Institute of Standards and Technology.

The assumption is that compounds with similar structure and isomerides have similar saturated vapor pressure. Based on this assumption, the saturated vapor pressure of trans-1,3-dichloropropenem and cis-1,3-dichloropropene are represented by allyl chloride, which has a similar structure. Bromodichloromethane is represented by trichloromethane. The saturated vapor pressure of methyl t-butyl ether, hexachloro-1,3-butadiene, and methylcyclohexane are represented by their isomerides, which are pentanol, 1,3-Butadiene, and 1-heptene, respectively.

**Table S1.** Database and assumptions; Method: Assumption Principles of Estimation.

CAS	Compound	Average Concentration μg/m <sup>3</sup>	SD μg/m <sup>3</sup>	Odor Threshold mg/m <sup>3</sup>	Reference	MI g O <sub>3</sub> /g VOCs	Reference	Saturated Vapor Pressure kPa(25°C)	Reference	LC50, Fish mg/L	Reference	LC50, Mice ppm	Reference	IUR μg/m <sup>3</sup>	Reference	RfC mg/m <sup>3</sup>	Reference
75-28-5	isobutane	10.19	10.36	3113.70	Assumption	1.23	Carter2010	348.86	NIST	29.5	ECO-SAR						
106-97-8	n-butane	38.70	45.90	3113.70	Nagata2003	1.15	Carter2010	242.81	NIST	25.4	ECO-SAR	658000	MSDS				
78-78-4	isopentane	13.66	15.37	4.20	Nagata2003	0.37	Carter2010	91.76	NIST	13.3	ECO-SAR	1000	MSDS				
109-66-0	n-pentane	37.51	44.86	4.50	Nagata2003	1.31	Carter2010	68.33	NIST	11.4	ECO-SAR	364000	MSDS				
75-83-2	2,2-dimethylbutane	8.10	9.18	5.80	Assumption	1.17	Carter2010	42.56	NIST	6.21	ECO-SAR						
79-29-8	2,3-dimethylbutane	9.97	6.45	5.80	Assumption	0.97	Carter2010	31.34	NIST	6.69	ECO-SAR						
107-83-5	2-methylpentane	10.97	6.08	5.80	Assumption	1.5	Carter2010	28.23	NIST	5.74	ECO-SAR						
96-14-0	3-methylpentane	3.93	2.15	5.80	Assumption	1.8	Carter2010	25.31	NIST	5.74	ECO-SAR						
110-54-3	n-hexane	16.22	14.21	5.80	Nagata2003	1.24	Carter2010	20.17	NIST	4.93	ECO-SAR					0.7	EPA, IRIS
108-08-7	2,4-dimethylpentane	10.80	7.10	3.00	Assumption	1.55	Carter2010	13.12	NIST	2.82	ECO-SAR						
591-76-4	2-methylhexane	41.46	55.25	3.00	Assumption	1.19	Carter2010	8.79	NIST	2.42	ECO-SAR						
565-59-3	2,3-dimethylpentane	28.20	24.77	3.00	Assumption	1.61	Carter2010	9.18	NIST	2.82	ECO-SAR						
589-34-4	3-methylhexane	4.72	3.07	3.00	Assumption	1.61	Carter2010	8.21	NIST	2.42	ECO-SAR						
540-84-1	2,2,4-trimethylpentane	3.77	1.85	3.00	Assumption	1.26	Carter2010	6.58	NIST	1.26	ECO-SAR						
142-82-5	n-heptane	14.63	6.81	3.00	Nagata2003	1.07	Carter2010	6.09	NIST	2.08	ECO-SAR	75000	MSDS				
565-75-3	2,3,4-trimethylpentane	ND	ND	8.67	Assumption	1.03	Carter2010	3.57	NIST	1.35	ECO-SAR						

592-27-8	2-methylheptane	ND	ND	8.67	Assumption	1.07	Carter2010	2.78	NIST	0.999	ECOSAR								
589-81-1	3-methylheptane	ND	ND	8.67	Assumption	1.24	Carter2010	2.62	NIST	0.999	ECOSAR								
111-65-9	n-octane	109.08	144.52	8.67	Na-gata2003	0.9	Carter2010	1.72	NIST	0.858	ECOSAR								
111-84-2	n-nonane	13.23	5.31	12.60	Na-gata2003	0.78	Carter2010	0.46	NIST	0.349	ECOSAR	16768	MSDS						
1120-21-4	n-undecane	12.12	4.38	6.07	Na-gata2003	0.61	Carter2010	0.05	NIST	0.056	ECOSAR								
112-40-3	n-dodecane	41.48	15.14	0.84	Na-gata2003	0.55	Carter2010	0.02	NIST	0.022	ECOSAR								
124-18-5	n-decane	1.90	1.74	3.94	Na-gata2003	0.68	Carter2010	0.12	NIST	0.14	ECOSAR	72300	MSDS						
115-07-1	propene	323.17	323.47	0.68	Na-gata2003	11.6	Carter2010	1155.13	NIST	67.2	ECOSAR								
106-98-9	1-butene	109.54	121.78	0.42	Na-gata2003	9.73	Carter2010	285.24	NIST	32.5	ECOSAR	420000	MSDS						
106-99-0	1,3-butadiene	81.46	82.77	0.56	Na-gata2003	12.6	Carter2010	281.74	NIST	41.5	ECOSAR	285000	MSDS	0.00003	EPA,IRIS	0.002	EPA,IRIS		
624-64-6	trans-2-butene	43.72	74.47	0.42	Assumption	16.1	Carter2010	234.55	NIST	38.2	ECOSAR								
590-18-1	cis-2-butene	14.43	13.29	0.42	Assumption	14.2	Carter2010	213.60	NIST	38.2	ECOSAR								
109-67-1	1-pentene	80.14	80.69	0.44	Na-gata2003	7.21	Carter2010	85.03	NIST	14.7	ECOSAR								
646-04-8	trans-2-pentene	9.62	10.42	0.15	Assumption	10.5	Carter2010	67.39	NIST	17.3	ECOSAR								
78-79-5	isoprene	2.31	2.30	0.15	Na-gata2003	10.6	Carter2010	73.65	NIST	16.9	ECOSAR	3400	MSDS						
627-20-3	cis-2-pentene	3.73	5.75	0.15	Assumption	10.3	Carter2010	65.95	NIST	17.3	ECOSAR								
592-41-6	1-hexene	52.39	38.78	0.53	Na-gata2003	5.49	Carter2010	24.79	NIST	6.39	ECOSAR	40000	MSDS						
287-92-3	cyclopentane	3.72	1.80	10.51	Assumption	1.96	Carter2010	42.32	NIST	14	ECOSAR	106000	MSDS						
96-37-7	methylcyclopentane	7.00	4.07	6.39	Na-gata2003	1.7	Carter2010	18.33	NIST	7.08	ECOSAR								
110-82-7	cyclohexane	9.02	3.61	10.51	Na-gata2003	1.25	Carter2010	13.01	NIST	6.08	ECOSAR	70000	MSDS			6	EPA,IRIS		
108-87-2	methylcyclohexane	55.61	22.11	0.66	Na-gata2003	1.7	Carter2010	13.01	NIST	2.99	Assumption	41500	MSDS						

71-43-2	benzene	1622.02	135 4.07	9.42	Na- gata200 3	0.72	Carter2 010	12.16	NIST	65.1	ECO- SAR	31900	MSDS	0.000 0022	EPA,I RIS	0.03	EPA,I RIS
108-88-3	toluene	166.93	136. 40	1.36	Na- gata200 3	4	Carter2 010	3.79	NIST	24.8	ECO- SAR	20003	MSDS			5	EPA,I RIS
108-90-7	chloro- ben- zene	111.56	36.0 9	5.70	As- sump- tion	0.32	Carter2 010	1.60	NIST	24.7	ECO- SAR						
100-41-4	ethylbe- nzene	11.24	3.89	0.81	Na- gata200 3	3.04	Carter2 010	1.26	NIST	10.3	ECO- SAR					1	EPA,I RIS
95-47-6	o-xylene	10.05	3.87	1.80	Na- gata200 3	7.64	Carter2 010	0.88	NIST	9.2	ECO- SAR						
100-42-5	styrene	12.27	20.2 9	0.16	Na- gata200 3	1.73	Carter2 010	0.87	NIST	13.4	ECO- SAR	24000	MSDS			1	EPA,I RIS
98-82-8	isopro- pyl ben- zene	1.81	0.26	0.05	Na- gata200 3	2.52	Carter2 010	0.61	NIST	4.93	ECO- SAR	24700	MSDS				
103-65-1	n-pro- pyl ben- zene	3.67	1.11	0.02	Na- gata200 3	2.03	Carter2 010	0.45	NIST	4.24	ECO- SAR	319150	MSDS				
620-14-4	3-ethyl- toluene	3.26	1.75	0.10	Na- gata200 3	7.39	Carter2 010	0.39	NIST	3.77	ECO- SAR						
622-96-8	4-ethyl- toluene	1.42	0.56	0.05	Na- gata200 3	4.44	Carter2 010	0.39	NIST	3.77	ECO- SAR						
108-67-8	1,3,5-tri- methylben- zene	1.63	0.50	0.91	Na- gata200 3	11.7 6	Carter2 010	0.32	NIST	3.36	ECO- SAR					4	EPA,I RIS
611-14-3	2-ethyl- toluene	2.56	0.92	0.40	Na- gata200 3	5.59	Carter2 010	0.33	NIST	3.77	ECO- SAR						
95-63-6	1,2,4-tri- methylben- zene	9.55	3.30	0.64	Na- gata200 3	8.87	Carter2 010	0.27	NIST	3.36	ECO- SAR	18000	MSDS			8	EPA,I RIS
541-73-1	1,3-di- chlor- benzene	2.03	0.00	5.70	As- sump- tion	0.17 8	Carter2 010	0.27	NIST	8.52	ECO- SAR						
106-46-7	1,4-di- chlor- benzene	5.05	0.13	5.70	As- sump- tion	0.17 8	Carter2 010	0.24	NIST	8.52	ECO- SAR						
526-73-8	1,2,3-tri- methylben- zene	3.29	1.44	0.64	As- sump- tion	11.9 7	Carter2 010	0.20	NIST	3.36	ECO- SAR					0.06	EPA,I RIS
100-44-7	benzyl chloride	0.96	0.00	5.70	As- sump- tion	2	As- sump- tion	0.16	NIST	0.825	ECO- SAR						
141-93-5	1,3-di- ethylben- zene	ND	ND	1.52	Na- gata200 3	7.1	Carter2 010	0.14	NIST	1.53	ECO- SAR						
105-05-5	1,4-di- ethylben- zene	ND	ND	0.01	Na- gata200 3	4.43	Carter2 010	0.13	NIST	1.53	ECO- SAR						

95-50-1	1,2-dichlorobenzene	ND	ND	5.70	Assumption	0.178	Carter2010	0.19	NIST	8.52	ECO-SAR						
120-82-1	1,2,4-trichlorobenzene	ND	ND	5.70	Assumption	0.089	Assumption	0.06	NIST	2.77	ECO-SAR						
91-20-3	naphthalene	253.37	504.45	9.42	Assumption	3.3	Carter2010	0.03	NIST	9.39	ECO-SAR			0.003	EPA,IRIS		
75-71-8	dichlorodifluoromethane	0.60	0.22	20.25	Assumption	0	Assumption	641.91	NIST	145	ECO-SAR						
1320-37-2	dichlorotetrafluoroethane	ND	ND	20.25	Assumption	0	Assumption	216.96	NIST	27.9	ECO-SAR						
74-87-3	chloromethane	498.85	483.49	20.25	Assumption	0.038	Carter2010	575.66	NIST	274	ECO-SAR			0.02	EPA,IRIS		
75-01-4	vinyl chloride	22.33	18.61	5.70	Assumption	2.83	Carter2010	391.51	NIST	26.7	ECO-SAR		0.0000088	EPA,IRIS	0.1	EPA,IRIS	
74-83-9	methyl bromide	114.86	119.60	20.25	Assumption	0.187	Carter2010	219.51	NIST	429	ECO-SAR	1540	MSDS				
75-00-3	chloroethane	10.15	9.72	20.25	Assumption	0.29	Carter2010	160.29	NIST	127	ECO-SAR			10	EPA,IRIS		
75-69-4	trichlorofluoromethane	2.05	1.85	20.25	Assumption	0	Assumption	106.05	NIST	86.5	ECO-SAR						
75-35-4	vinylidene chloride	ND	ND	5.70	Assumption	1.79	Carter2010	80.03	NIST	14.8	ECO-SAR	25210	MSDS				
26523-64-8	trichlorotrifluoroethane	0.25	0.00	20.25	Assumption	0	Assumption	48.72	NIST	160	ECO-SAR						
75-09-2	dichloromethane	12.89	9.79	606.64	Nagata2003	0.041	Carter2010	57.27	NIST	273	ECO-SAR		0.00000001	EPA,IRIS	0.6	EPA,IRIS	
156-60-5	trans-1,2-dichloroethylene	ND	ND	5.70	Assumption	1.7	Carter2010	44.37	NIST	19.6	ECO-SAR						
75-34-3	1,1-dichloroethane	ND	ND	20.25	Assumption	0.069	Carter2010	29.84	NIST	134	ECO-SAR	16000	MSDS				
156-59-2	cis-1,2-dichloroethene	0.17	0.00	5.70	Assumption	1.7	Carter2010	27.05	NIST	19.6	ECO-SAR						
67-66-3	trichloromethane	2.35	1.60	20.25	Nagata2003	0.022	Carter2010	25.90	NIST	264	ECO-SAR	47702	MSDS	0.000023	EPA,IRIS		
71-55-6	1,1,1-trichloroethane	ND	ND	20.25	Assumption	0.0049	Carter2010	17.78	NIST	26.9	ECO-SAR	97920	MSDS		7	EPA,IRIS	

56-23-5	tetra-chloro-methane	0.76	0.26	31.59	Na-gata2003	0	Carter2010	15.22	NIST	50.6	ECO-SAR	50400	MSDS	0.000006	EPA,I RIS		
107-06-2	1,2-di-chloro-ethane	57.31	63.30	20.25	As- sump- tion	0.21	Carter2010	10.49	NIST	115	ECO-SAR						
79-01-6	trichlo-roe-thene	1.53	0.82	20.78	Na-gata2003	0.64	Carter2010	9.20	NIST	9.48	ECO-SAR			0.0000041	EPA,I RIS	0.02	EPA,I RIS
78-87-5	1,2-di-chloro-propane	ND	ND	20.25	As- sump- tion	0.29	Carter2010	6.71	NIST	55.4	ECO-SAR					0.004	EPA,I RIS
75-27-4	bro-mo-di-chloro-methane	ND	ND	20.25	As- sump- tion	0.22	As- sump- tion	25.90	As- sump- tion	301	ECO-SAR						
10061-02-6	trans-1,3-di-chloro-propene	0.25	0.00	5.70	As- sump- tion	0.03	Carter2010	49.16	As- sump- tion	11.8	ECO-SAR			0.000004	EPA,I RIS	0.02	EPA,I RIS
10061-01-5	cis-1,3-di-chloro-propene	0.40	0.00	5.70	As- sump- tion	3.7	Carter2010	49.16	As- sump- tion	11.8	ECO-SAR			0.000004	EPA,I RIS	0.02	EPA,I RIS
79-00-5	1,1,2-tri-chloro-ethane	4.87	1.89	20.25	As- sump- tion	0.086	Carter2010	2.91	NIST	107	ECO-SAR			0.0000016	EPA,I RIS		
127-18-4	tetra-chloro-ethylene	0.91	0.44	5.70	Na-gata2003	0.031	Carter2010	2.48	NIST	4.27	ECO-SAR			0.00000026	EPA,I RIS	0.04	EPA,I RIS
124-48-1	di-bromo-mono-chloro-methane	ND	ND	20.25	As- sump- tion	0.022	As- sump- tion	25.90	NIST	318	ECO-SAR						
106-93-4	1,2-di-bromo-ethane	ND	ND	20.25	As- sump- tion	0.102	Carter2010	1.90	NIST	151	ECO-SAR			0.000003	EPA,I RIS	0.009	EPA,I RIS
75-25-2	bromo-form	ND	ND	30.00	Ro-cen1920	0.05	As- sump- tion	0.72	NIST	321	ECO-SAR			0.0000011	EPA,I RIS		
79-34-5	1,1,2,2-tetra-chloro-ethane	ND	ND	20.25	As- sump- tion	0	As- sump- tion	0.53	NIST	92.6	ECO-SAR	4500	MSDS				
87-68-3	hexa-chloro-1,3-bu-tadiene	0.48	0.15	5.70	As- sump- tion	0	As- sump- tion	281.74	As- sump- tion	0.171	ECO-SAR						
64-17-5	ethanol	ND	ND	1.07	Na-gata2003	1.53	Carter2010	7.87	NIST	3170	ECO-SAR						
107-02-8	acrolein	1105.45	1343.59	0.01	Na-gata2003	7.45	Carter2010	36.67	NIST	0.123	ECO-SAR					0.000002	EPA,I RIS
67-64-1	acetone	584.24	720.14	108.90	Na-gata2003	0.36	Carter2010	30.60	NIST	4850	ECO-SAR						

67-63-0	isopropyl alcohol	1.02	0.00	69.75	Na-gata2003	0.61	Carter2010	5.70	NIST	1740	ECO-SAR				
1634-04-4	methyl t-butyl ether	0.51	0.00	0.10	Assumption	0.73	Carter2010	0.29	Assumption	236	ECO-SAR	85000	MSDS		
108-05-4	vinyl acetate	ND	ND	3.42	Assumption	3.2	Carter2010	15.30	NIST	63.7	ECO-SAR	11400	MSDS	0.02	EPA,IRIS
78-93-3	2-butanone	62.53	35.11	1.42	Na-gata2003	1.48	Carter2010	12.00	NIST	2180	ECO-SAR				
141-78-6	ethyl acetate	33.83	21.46	3.42	Na-gata2003	0.63	Carter2010	12.62	NIST	54.3	ECO-SAR				
109-99-9	tetrahydrofuran	10.86	9.71	31.87	Na-gata2003	3.22	Carter2010	21.62	NIST	534	ECO-SAR	61740	MSDS	2	EPA,IRIS
80-62-6	methyl methacrylate	21.37	10.90	0.94	Na-gata2003	15.61	Carter2010	4.81	NIST	73.5	ECO-SAR	78000	MSDS		
123-91-1	1,4-dioxane	19.88	2.40	3.42	Assumption	2.62	Carter2010	4.98	NIST	8770	ECO-SAR	46000	MSDS		
108-10-1	4-methyl-2-pentanone	3.46	1.38	0.11	Assumption	3.88	Carter2010	2.62	NIST	463	ECO-SAR	32720	MSDS		
591-78-6	2-hexanone	14.39	4.57	0.11	Na-gata2003	3.14	Carter2010	0.51	NIST	398	ECO-SAR	8000	MSDS	0.03	EPA,IRIS
75-15-0	carbon disulfide	47.84	54.26	0.71	Na-gata2003	0.25	Carter2010	48.12	NIST	70.8	ECO-SAR			0.7	EPA,IRIS