

H2 Equivalence and Release Profile

Provect-IR[™] Antimethanogenic ISCR Reagent

Provect-IR is a unique mixture of reagents combined into a single product that optimizes the *in situ* reductive dechlorination of chemicals present in soil, sediment, and groundwater. It acts by promoting synergistic interactions between:

- Natural antimethanogenic compounds
- Multiple hydrophilic, nutrient rich organic carbon sources
- Zero-Valent Iron (ZVI)
- Chemical oxygen scavengers
- Vitamin and mineral sources



This distinctive, patented combination of natural and food-grade chemicals promotes *In Situ* Chemical Reduction (ISCR) conditions for fast and effective destruction of targeted constituents of interest (COIs) such as chlorinated solvents, organochlorine pesticides, and other halogenated compounds (Brown *et al.*, 2009; Dolfing *et al.*, 2008; US Patent Office Scalzi *et al* 2012). Notably, Provect-IR is the only ISCR reagent to simultaneously inhibit the production of methane during the requisite carbon fermentation processes (US Patent Office Scalzi *et al*, 2013, 2014). This promotes more efficient use of the hydrogen donor (>30% more efficient which reduces amendment requirements) while avoiding negative issues associated with elevated methane (CH4) in groundwater, soil gas, and indoor air.

HYDROGEN EQUIVALENTS ANALYSIS

Under some circumstances it is desirable to compare remedial amendments based on their theoretical H₂ production. One limitation to such efforts is the uncertainty in values assigned to various carbon sources, and the rates of hydrogen release which is dependent on the site-specific conditions and groundwater quality. Nevertheless, the following calculations can be presented.

<u>Carbon Moiety</u>: The multiple, complex, hydrophilic organic components of Provect-IR can be viewed simply (although not accurately) as cellulose and hemicellulose which may therefore undergo hydrolysis to yield glucose. Hydrogen gas is produced during glucose fermentation via several enzymatic pathways, depending on site conditions and microbial assemblages:

$$Glucose + 6H_2O \rightarrow 6CO_2 + 12H_2 \tag{1}$$

 $Glucose + 2H_2O \rightarrow 2 \text{ Acetate} + 2CO_2 + 4H_2 + 2H^+$ (2)



As summarized below, the maximum amount of H_2 that can be generated from a carbon source is about 0.18 moles H_2/g substrate or 0.36 g H_2/g substrate.

	Atoms per Mole Substrate		Average	H ₂ Released	Moles H ₂ released per	
	с	Н	0	Molecular Weight	per mole Substrate	gram substrate
Acetate	2.0	4.0	2.0	60.1	4.0	0.0666
Lactate	3.0	6.0	3.0	90.1	6.0	0.0666
Glucose	6.0	12.0	6.0	180.2	12.0	0.0666
Soybean	56.3	99.5	6.0	873.1	156.5	0.1792
Corn	56.3	99.9	6.0	873.5	156.6	0.1793
Cottonseed	55.5	99.3	6.0	\$62.8	154.7	0.1792
Palm	54.2	100.8	6.0	848.5	152.8	0.1800
Peanut	56.8	102.7	6.0	881.4	158.9	0.1803
Olive	56.2	102.7	6.0	875.0	157.8	0.1804
Canola	57.1	102.3	6.0	884.6	159.3	0.1801
Butterfat	50.2	94.0	6.0	793.4	141.4	0.1782
Lard	55.2	102.4	6.0	862.4	155.6	0.1804
Beef Tallow	55.1	102.9	6.0	862.2	155.8	0.1807

Table 2.3. Average Composition of Different Edible Oils and Electrons Released
during Anaerobic Fermentation

<u>ZVI Moiety</u>: Provect-IR also contains ZVI which corrodes in water and produces hydrogen and hydroxide resulting in an increase in pH and decline in redox potential (Eh):

 $Fe^{\circ} + 2H_2O \rightarrow Fe^{2+} + H_{2(aq)} + 2OH^{-}$

(3)

Hydrogen gas evolution from ZVI will occur independently of the presence of organic compounds in the site water. Approximately 0.036 g H_2 (1/56) will be released from ZVI itself.

Considering the above, the tables below show that various ISCR reagents will exhibit total H_2 production or Hydrogen Equivalents ranging from 0.23 g $H_2/g_{provect-IR40}$ to 0.32 g $H_2/g_{provect-IR10}$ and other non-ISCR substrates contain as low as 0.07 g $H_2/g_{lactate}$.



Provect-IR™ and Provect-IRM™

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Component	EHC 10% ZVI	Provect-IR 10% ZVI	EHC 40% ZVI	Provect-IR 40% ZVI
ZVI	10%	<mark>10%</mark>	40%	40%
ZVI Surface Area	0.71ft ² /lb _{substrate}	2.27ft ² /lb _{substrate}	0.71ft ² /lb _{substrate}	2.27ft ² /lb _{substrate}
Carbon	90%	<mark>90%</mark>	60%	60%
H equivalents	0.18 gH2/gsubstrate	<mark>0.32 g_{H2}/g_{substrate}</mark>	0.12 g _{H2} /g _{substrate}	0.23 g _{H2} /g _{substrate}

• From EHC published literature

Compound	Average MW	Moles of H ₂ per mole	g of H₂ per g NON ISCR substrate
LACTATE	90	6	0.07
Emulsified			
Soybean Oils	873	156	0.18*
HRC® +			
unknowns	956	212	0.22**
	ZVI (56 MW)	1	
EHC [®] with			0.40
40% ZVI	C component =		0.12
	180	12	

Assumes suspension of 50% oil

** As reported by vendor but we could not substantiate via the scientific literature.

Compound	Weight %C	Weight %N	Weight %H	Notes
Na Lactate	32	0	4.5	NaC₃H₅O₃
Soybean Oils	77	0	11	Standard Agricultural formulas
HRC®	41	0	4.8	C ₃₉ H ₅₆ O ₃₉ (AFCEE report)
Provect-IR™	<mark>36 to 40</mark>	<mark>1 to 3</mark>	<mark>5 to 6</mark>	80% C + 20% ZVI
EHC®	36 to 40	0.08 to 0.8	5 to 6	80% C + 20% ZVI

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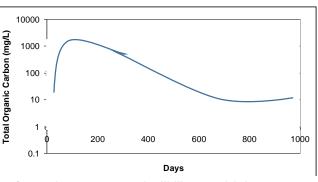
Provect-IR[™] and Provect-IRM[™]



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HYDROGEN AND CARBON (DOC) RELEASE RATES

The rate of release of hydrogen is as more important as the total amount of hydrogen released. Provect-IR has multiple sources of organic hydrogen donor designed to provide short, medium and long-term release profiles designed to maintain >20 ppm TOC over an estimated 3 to 5 years period of time. To quickly establish reducing conditions, the



readily biodegraded calcium propionate provides a fast release rate and will liberate high amounts of TOC (>1,000 ppm) for an estimated 100 to 200 days. Next, the relatively more biodegradable components of the kelp and organic plant materials will liberate moderate levels of TOC (>200 ppm) for the next ca. 400 days. Subsequently, the more slowly degraded carbon moieties will liberate lower levels of TOC (e.g. >50 ppm) over the following 800+ days. Based on the AFCEE recommendation to maintain at least 20 ppm TOC to support reductive dechlorination reactions, this is sufficient to maintain effective treatment as the contaminant concentrations decrease and the TOC demand is lowered.

SUMMARY

There are many site-specific factors that will influence the actual H₂ release kinetics and longevity. In general, the standard formulations of Provect-IR and Provect-IRM containing 10% to 40% ZVI (weight basis) will have a hydrogen equivalence of 0.23 g H₂/g_{provect-IR40} to 0.32 g H₂/g_{provect-IR10}. This exceeds the amount of H₂ liberated from other ISCR amendments while uniquely offering the safety and economic benefits of antimethanogenic ISCR treatment. The TOC release characteristics are very favorable, maintaining >20 ppm TOC over a 3 to 4 year period.

CONTACT US FOR A COMPLIMENTARY SITE EVALUATION

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