ATTACHMENT 6: ISCO Screening Tool User's Manual

INTRODUCTION

The A5. ISCO Screening Tool is an Excel™ spreadsheet calculator that helps to automate the ISCO screening process. This tool accepts a limited amount of the user's site characterization data as input and returns semi-quantitative ratings on a number of ISCO approaches (oxidant / delivery method combinations), using effectiveness and implementability criteria.

The ISCO Screening Tool has an input sheet where users enter data by selecting ranges of values representative of their site from dropdown menus. A series of calculation spreadsheets and macros then take that data and determine the ability of an oxidant, activation approach, or injection method to work within the constraints of the values input by the user. To do this, the tool individually considers each factor and gives an output rating based on a weighted ranking system ("not recommended" / "poor" / "fair" / "good" / "excellent"), representing the ability of that ISCO approach to work within the confines of the user's inputs. Factors that are considered are broken into three general categories, which include "amenability" (representing the ability of a given oxidant to oxidize a given COC), "effectiveness" (representing the ability of the oxidant or activation method to work with site contaminant concentrations and geochemistry), and "implementability" (representing the ability of an injection method to function in a given hydrology). The three categories and the factors considered under them are summarized in Table A6-1.

Table A6-1. Factors Considered by the ISCO Screening Tool

Amenability	Effectiveness	Implementability
• Ability to degrade primary COCs • Ability to degrade co-contaminants • Reaction kinetics[1]	• Ability of approach to work with site COC concentration • Ability of approach to work with site chloride • Ability of approach to work with site alkalinity • Effectiveness with site f_{oc} • Effectiveness with site pH	• Implementability within site media type • Amenability of injection technique to site permeability • Ability to reach depth of contamination • Amenability to site heterogeneity • Ability to treat contaminant density • Disruption to surface activities • Disruption to subsurface

[1] Kinetics information is available at http://cgr.ebs.ogi.edu/isco/, which houses a database of oxidant-specific kinetic parameters for different oxidants and contaminants based on the following references:
Waldemer, R. H.; Tratnyek, P. G. Kinetics of contaminant degradation by permanganate. Environ. Sci. Technol. 2006, 40, 1055-1061. http://dx.doi.org/10.1021/es051330s.
Waldemer, R. H.; Tratnyek, P. G. The efficient determination of rate constants for oxidations by permanganate. In Proceedings of the Fourth International Conference on Remediation of Chlorinated and Recalcitrant Compounds, 24-27 May 2004, Monterey, CA; Battelle Press: Columbus, OH, 2004; Paper 2A-09.
Waldemer, R. H. Determination of the Rate of Contaminant Oxidations by Permanganate: Implications for In Situ Chemical Oxidation (ISCO). Thesis, OGI School of Science and Engineering, Oregon Health and Science University, 2004.)

The values that appear in the output table for each of these categories are determined from lookup tables, which have been prepared by the authors and represent their views for how well a given ISCO oxidant, activation method, or injection technology will work under the values input by the user. The three lookup table worksheets are titled "contaminant vs. oxidants", "Input vs. oxidant approach", and "input vs distribution method." For the tool to run properly, any modifications to the values must fall in line with the exact "excellent, good, fair, poor or not recommended" phrasing as used in the lookup tables. For informational purposes, the A8. ISCO Screening Tool Lookup Tables are provided, each on separate

Excel™ worksheets (tabs) that are used by the ISCO Screening Tool for determining viable and appropriate approaches based on site contaminant(s).

To prevent accidental alteration of these lookup tables that might result in erroneous performance of the tool, these lookup tables are hidden and password protected in the actual tool. However, if the user decides that he or she wishes to modify the values in the lookup tables to reflect their personal knowledge, experience, or preference; they may unhide and unlock these spreadsheets. To view these sheets in Excel™, go to “Format > Sheet > Unhide” and then select the sheet to modify. The three lookup tables are “Input vs. oxidant approach,” which includes the ability of an oxidant to function within geochemistry parameters, “Input vs. distribution technique,” which considers the ability of a distribution method to function within site hydrologic parameters, and “Contaminants vs. oxidant” which considers the amenability to different contaminant groups to be degraded by a given oxidant and activation method. To modify the values in these lookup tables, go to “Tools > Protection > Unprotect Sheet” and enter the password “ISCO”. Modifications of the values in the cells must conform to the terminology already in the lookup table, otherwise the tool will not function properly. It is recommended that you backup your work prior to modifying the tool in case of malfunction.

In addition to evaluating a given approach against these individual factors, the tool calculates weighted values for each category of criteria (amenability, effectiveness, implementability), as well as an overall weighted rating for an approach, noted in the matrix in the output table. An approach represents a given oxidant (and activation approach if applicable) coupled with a given injection technique. The weights for each factor within the three categories are located on the output table and the default value for all is 3, giving equal weight to every factor within the category. The sole exception to this is the default on disruption to surface and subsurface activities (defaults to zero). Here, the user must determine how much weight to give these factors as a function of how much disruption to the surface or subsurface of their site they can inflict (e.g., to utilities, foundations, active facilities, etc.). A zero indicates no weight to this factor and thus maximum disruption may occur with no change to the approach score. The higher this value is weighted, the more often techniques with high disruption are rejected as not favorable. For the calculation of the overall score, poor values are weighted more heavily than good or excellent values as the unfavorable values will typically represent the limiting conditions of a particular approach and thus carry more weight. Another weight input, on the input sheet, gives the overall percentage that each of the three categories contribute to the final overall weighted rating for an ISCO approach. For this input, starting values of 50% amenability, 35% for implementability, and 15% for effectiveness are recommended. These values do not ultimately reflect the overall priority of each of these categories but are reasonable values in the output table based on experience and the scoring formulas used. However, alterations to these values may be suitable depending on site conditions and objectives.

DEFAULT VALUES

There will occasionally be circumstances where a user will not have all of the values necessary to fill out the screening tool. Some inputs are absolutely necessary for the tool to yield informative results about a given site, while others may be set to default values. Field values are always preferable to default values as the ISCO technologies may encounter difficulties if field conditions deviate substantially from assumed values.

Values that users must absolutely know are the primary COC to be treated, some sense of COC concentration either in soil or groundwater samples, the average depth to contamination, the media type (unconsolidated porous media vs. consolidated bedrock), some indication of whether or not the site is heterogeneous, and some idea of the hydraulic conductivity that is to be expected. If field measurements of hydraulic conductivity are unavailable, a hydraulic conductivity range may be estimated from observation of other field parameters. For example, if the site is obviously permeable (e.g., a coarse sandy site or high groundwater velocities), then a hydraulic conductivity of $>10^{-3}$ cm/sec may be selected. If the site is obviously impermeable (e.g., a clay site), then a hydraulic conductivity of $<10^{-6}$ cm/sec may be selected. If the site is neither obviously permeable or impermeable (e.g., very fine sand, silt, loamy sand, etc), then a field estimation of hydraulic conductivity is highly recommended.

The default values below may be used if site specific data are not available.

- pH – Assume a range of 7-8 or 6-7.
- f_{oc} – In an aquifer, assume an foc of 0.001-0.003 unless clear evidence indicates that the foc is much higher.
- Co-contaminants – Set equal to none.
- Chloride – Set equal to 0-300 mg/L, unless a non-potable brackish groundwater is to be treated. Then set equal to 1000-3000 mg/L.
- Alkalinity – Set equal to 0-300 mg/L as $CaCO_3$, unless a non-potable brackish groundwater is to be treated. Then set equal to 1000-3000 mg/L as $CaCO_3$.

INTERPRETATION OF SCREENING TOOL OUTPUT

Once the user has input their site specific values into the screening tool, they then go to the output sheet and may evaluate the ISCO options available to them. On the output sheet, there is a color coded matrix that considers each injection technology and oxidant and activation approach separately, and then brings these together into an overall matrix. The overall matrix gives a qualitative rating (e.g., excellent, fair, poor, etc.) and numeric ranking (in parentheses) for each combined ISCO option (a specific oxidant coupled with a specific injection method). The qualitative color coded rating is based on the overall weighted score of all of the various factors considered in the two side matrices. Black cells are permanent and represent combinations of oxidants and injection methods that are technically impractical. The numeric ranking indicates where each approach stands relative to the others, with 1 representing the best ranking option, and lower ranking worse. When considering the output, many times there will be multiple good or excellent approaches, and some may even have the same rank as they may tie in the overall scoring system. These equal rankings reflect the fact that for many sites, multiple approaches may lead to a successful outcome. In addition to looking at the overall matrix, the user should look at the individual factors in the two side matrices and determine the strengths and weaknesses of each approach prior to selecting technologies to carry forward. It should be noted that any “not recommended” values in either the overall matrix or the two side matrices are used conservatively and represent instances where threshold criteria for successful implementation of the approach are not met; thus ISCO will not likely work.

It should also be noted that this tool and the values in its lookup tables have been developed as a result of the best understanding the authors have of ISCO processes based on what is currently available in the literature, the field case study experience, engineering intuition and professional opinion. However, ISCO is an evolving technology and new innovations may require periodic revision to present state of understanding with the technology. Some technologies currently thought to be impractical in some circumstances may eventually prove to be effective. Also, the tool only considers a limited number of specific factors, and yet for any particular remediation site, there may be many more that may need to be taken into consideration before selecting a technology for implementation. Such factors may include the size of the contaminated area to be treated, regulatory constraints, costs, previous experience with specific technologies and others. Furthermore, even with the number of factors considered by this tool, there are many thousands of possible combinations of these variables, not all of which have been tested, and thus some may give unexpected results. Thus, judgment is still required on behalf of the user to determine the best option. The tool is merely provided to help compare and evaluate technologies rapidly on the same platform to assist informed decision-making, but is not intended to replace sound judgment.

At this stage, a user should select several (e.g., 3-10) of the various ISCO options to carry forward for consideration during the remainder of the screening process. Additional considerations (see attachment) and other site-specific concerns about a given approach should be carried forward as well. It may be helpful at this stage to consult with either engineering consultants or technology vendors about the possibility of any of the various approaches recommended by the screening tool.

EXAMPLE PROBLEM

The screening tool can be used to quickly evaluate ISCO options for a particular site. The screening tool can be used to apply to the entire site, or the site could be divided up into specific units or compartments and the screening tool run separately for each compartment. The latter option allows the user to determine which compartments might require more aggressive approaches. For example, a site consisting of a permeable sand, underlain by a impermeable but contaminated clay might be treated as one heterogeneous treatment zone, or two homogeneous treatment zones. The recommendations of the tool will likely be different for the two compartments, and may impact the technologies selected for further screening. The following example problem is based on a hypothetical "Site X," but is based on a real site where ISCO was applied. The properties and parameters of Site X are given below.

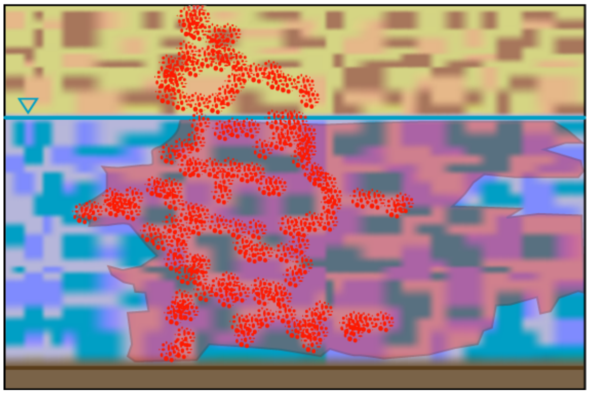
Conditions at Site X

Contaminant conditions:

- Chlorobenzenes
- Total VOCs max. 30,500 ug/L in groundwater
- Total VOCs max. 40,500 mg/kg in soil
- 1,794 kg of contaminants
- DNAPL inferred to be present

Aquifer Characteristics:

- Glacial till (dense mixture of sands, clays and gravel)
- Geology Type C (heterogeneous and permeable)
- Saturated Hydraulic Conductivity: 10 ft/day
- Depth to groundwater: 10 ft
- Groundwater flow velocity: 0.1 ft/day
- Depth of contamination: 10-30 ft



Geochemistry:

- pH: 7.5
- ORP: -60 mV
- Temperature: 14ºC
- DO: 0.1 mg/L
- Chloride: 190 mg/L
- Sulfate: 160 mg/L

Remedial action objective:

- The objective is to reduce the mass of contamination in areas that were inaccessible to previous excavation.

Inputs Into the Screening Tool

Open the A5. ISCO Screening Tool and click on the tool input sheet. Observe the entry fields. To screen site X in the tool, enter values in these fields as described below.

1. Site Conditions – This gives a rough description of the type of hydrologic unit to be screening for ISCO. Options include consolidated rock, or unconsolidated soil, and varied degrees of heterogeneity within.
    a. For "media type" under the site conditions tab, select "unconsolidated" (meaning the site is unconsolidated soils, not consolidated bedrock).
    b. For "media", select heterogeneous and permeable. Heterogeneous indicates that the groundwater permeability field is inferred to be non-uniform. This is common in glacial till as it is a mixture of sands, silts and clays.
2. Contaminants – This is one of the major criteria in selecting an oxidant. Many contaminants are degradable by ISCO oxidants and activation methods, but some will be much more effective than others depending on the contaminant characteristics.
    a. For the primary contaminant, under "class/group" select "chlorinated aromatic contaminants.
    b. Then in the second cell where it now says "chlorinated aromatic contaminants", select "chlorobenzenes."

   c. (Optional) - A second contaminant or a degradation byproduct can be added under the co-contaminants tab. Select "chlorinated aromatic contaminants" again, and then select di- and trichlorobenzenes.

3. Geochemistry parameters – These parameters relate to oxidant and activation effectiveness, as some oxidants are more effective than others under certain chemical conditions.
   a. Under "pH range," select 7-8.
   b. No alkalinity value was available from site X, but it was inferred to be low, so select "0-300."
   c. Under chloride, the background concentration was reported to be 190 mg/L, which is low. However, since there is a large amount of halogenated contaminant, and chloride will be produced by the oxidation reaction, this should be considered. Chloride background levels may be important to some oxidants because as chloride concentrations increase, the oxidation reaction may become less efficient with free radical processes. If all 40500 mg/kg of contaminant are assumed to be chlorobenzene, and chlorobenzene contains 1 mole chloride per mole chlorobenzene, then this 40500 mg/kg chlorobenzene may be converted to an effective chloride concentration via the following mass balance, assuming a dry bulk density of 1.6 kg/L and porosity of 0.3.

$$\frac{40500\,mg\,CB}{kg\,soil}\times\frac{1.6\,kg\,soil}{L\,soil}\times\frac{1\,L\,soil}{0.30\,L\,pores}\times\frac{1\,mmol\,CB}{112.5\,mg\,CB}\times\frac{1\,mmol\,Cl^-}{1\,mmol\,CB}\times\frac{35.45\,mg\,Cl^-}{1\,mmol\,Cl^-}\approx 62000\,mg/L$$

   With this a very high chloride effective chloride concentration is calculated (62000 mg/L in 1 pore space). However, this is based on the maximum single concentration rather than a spatially weighted concentration which would yield a better estimation. This also assumes no dilution from adding a volume of oxidant. Assuming the effective chloride concentration over the treatment zone would be an order of magnitude lower if spatially weighted, (e.g. 6000), enter "3000-10000" mg/L for chloride.

   d. A f_{oc} value from the site was not reported, but observations of the aquifer material indicate that organic matter is a not a significant fraction of the media. Enter "<0.1%"
   e. Under contaminant concentration, enter "very high" as concentrations over 10000 mg/kg have been measured for this treatment zone.

4. Hydrology parameters – this section relates to oxidant deliverability in the saturated zone, and provides for a rough screening of injection methods.
   a. The "media type" should display that which was entered previously under site conditions (unconsolidated media). No "consolidated media properties" are displayed, as consolidated was not selected. Under "unconsolidated media properties", "hydraulic conductivity" and "scale of heterogeneities" is displayed.
   b. The hydraulic conductivity relates to the ability to inject an oxidant, and should represent the average hydraulic conductivity of the site. A saturated conductivity of 10 ft/day was reported for Site X, so enter ">10-3 cm/s or >3 ft/day".
   c. "Scale of heterogeneities" is a parameter that relates to the effective distance that the oxidant may need to diffuse into low permeability layers within a treatment zone. If clay lenses observed from soil cores are observed to be a foot in thickness (e.g. <0.3 m), then enter "small." If they are thicker, then enter medium or large accordingly. In this case, we will assume that the heterogeneities are small. In the case of large or very large clay layers, consider treating these as entirely separate units.
   d. "Depth of delivery" is always displayed, and refers to the depth of the injection. In the case of site X, the treatment zone is from 10 to 30 ft bgs, so enter "<10 m bgs but >5 m bgs (15-35 ft)

5. User's weighting factors – this section allows the user to weight certain aspects of ISCO application higher than another. Amenability refers to the ability of the oxidant / activation approach to degrade a particular contaminant, effectiveness describes the efficiency of that oxidant within the geochemical matrix it will be applied to, and implementability refers to the performance of a particular injection technology in the selected hydrology. For starting values, a value of 50% for amenability, 30% for implementability and 20% for effectiveness are recommended.

6. Click "go to output sheet"

Screening Tool Output

The output sheet should display as on in Figure A6-1 which also gives an overview of the organization of the output sheet. Highlighted in the green rectangles, the oxidants and activation methods are listed at top right, and the injection methods are listed at bottom left. Highlighted in black rectangles to the left and center are the criteria that each oxidant, activation method and injection technology are evaluated against. The amenability, effectiveness and implementability scores are listed in color coded tables below or to the right of these criteria. The rectangles at bottom right represent the overall scores for each ISCO approach.

In the square containing the overall scores for the approach, this represents the combined, weighted score for a specific ISCO approach based on the weighting factors and input given on the input sheet. For example, the square at top left represents permanganate with direct push injection, and it is rated as “fair”. The small number listed in the cell gives the overall rank of the option versus the 93 possible options in the tool (not two rows of options are truncated from the right side of the figure below, but are visible in the tool). In this case, permanganate with probe injection is the 86th ranked option, and thus is one of the lowest scoring in the screening tool for this site. The next square down represents permanganate with vertical well injection, and is the 88th ranked option, also low scoring. These low scores are mainly due to permanganate’s very limited reactivity with the contaminant. However, soil mixing with persulfate and alkaline activation is rated as “excellent” and is the number 1 ranked option. Hence, the tool anticipates that this option may perform well for this site and it may be valuable to consider it for further screening. In this case, this option performs well as mixing is presumed to achieve effective oxidant contact in this heterogeneous environment, and alkaline activation is anticipated to work well with regards to degrading chlorobenzenes and function effectively in this site’s geochemistry. However, other options may merit consideration as well. In this case, the 3rd ranked option is listed as “excellent” and represents Persulfate with chelated iron and soil mixing. Again mixing is assumed to deliver well to heterogeneous formations and the persulfate with chelated iron activation is assumed to work well in this geochemistry. The 21st ranked option is listed as “good” and is persulfate with chelated iron activation and vertical well injection. As this example is based on a real site, this is the actual option that was implemented. The site implemented this option as follows:

Initial ISCO Design:

- Target Treatment Zone: 60,000 cubic feet
- Oxidant: Persulfate at 199 g/L
- Activation Method: chelated iron
- Pore Volumes Delivered: 0.5 (does not include activator)
- Oxidant Dose (g ox./kg media): 10
- Number Delivery Events: 2
- Delivery Method: Well Injection.

Process Monitoring:

- Groundwater Quality Parameters (pH, ORP, iron, chloride, and persulfate).
- After injections both monitoring wells and injection wells were sampled for VOCs.
- Soil sampling for VOCs.

Mid-Course Corrections:

- Additional injection events were performed to address the high level of contamination in the area. These injection events were designed in a similar manner to the first two events described above.

ISCO Effectiveness:

- Contaminant mass was reduced by ~75%
- Maximum groundwater concentrations reduced 16% in TTZ
- Case Status: Open

Post-ISCO Coupling:

- ISCO may be planned for the area and underlying bedrock in the future.
- MNA will be a component of the long term remedy.

Since the remediation action objective was to reduce the contaminant mass, and an approximate 75% mass reduction was observed, this site concluded that they had a good result from ISCO. Certainly, given the high concentrations and DNAPL assumed to be present, getting large concentration reductions would be presumably very difficult for nearly any remediation technology at this site. The tool does suggest that several other potential methods ranked higher in score, but this does not mean that lower ranked options cannot work. It might perhaps indicate that a mixing approach might have achieved even better results, if it is presumed that the remaining mass was due to delivery challenges in the heterogeneous material. However, mixing can also suffer other pitfalls, so it is impossible to know if the top ranked options truly would result in better ISCO resulfs.

Further Customization of the Screening Tool Results

The results on the output sheet can be further modified according to unique user criteria. Note that in Figure A6-1, highlighted in blue below the criteria, are input fields for user-assigned importance factors. These allow the user custom weight the criteria against which the ISCO options are evaluated. As a default, these input fields area all assigned a value of 3 (equal weighted), except for the entry fields under the “disruption of surface and subsurface activities”, which default to zero. These fields may be changed to any value from 0 (no importance) to 5 (high importance). The values in these fields impact how each criteria impacts the overall amenability, effectiveness and implementability scores, and overall score for the approach, and represents a weighted average score. Depending on the nature of a given site, some factors might matter to a user much more than others. For instance, say that site X is an active industrial facility and part of the treatment zone is underneath a busy road that cannot be disrupted for extended ISCO injections. Thus the user may choose to set the importance factor for “disruption of subsurface activities” to 3, meaning that this criterion is weighted equal to all others (the default, being zero, means it is not considered). Now the mixing and surface application options kick out as not recommended, since they require intensive disruption to the surface to implement. The overall rankings also shift because of this. Note that Persulfate with chelated iron activation and vertical well injection is now the 3rd ranked option, and this is what was implemented at the site.

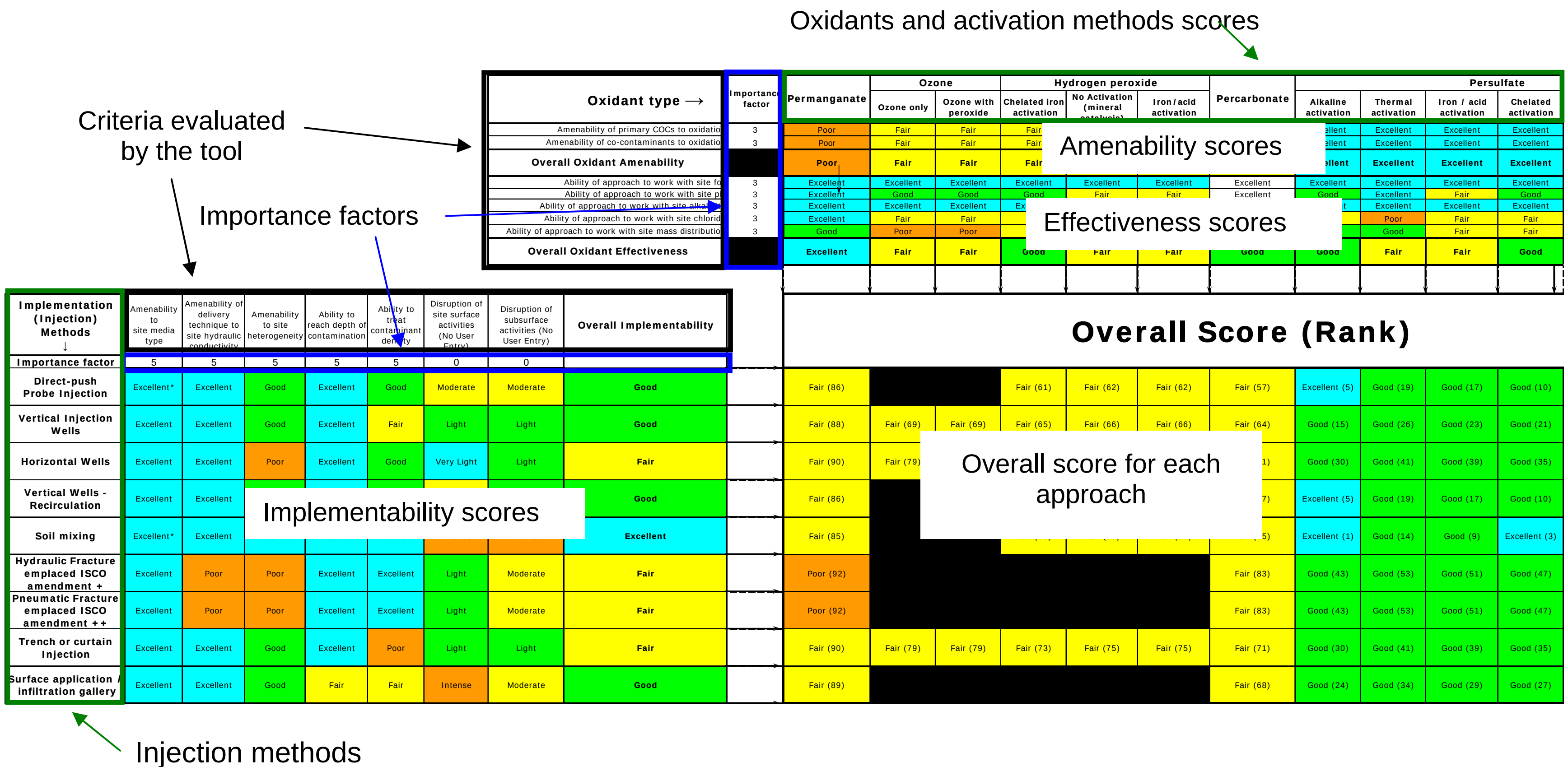


Figure A6-1: Example ISCO Screening Tool Output.