

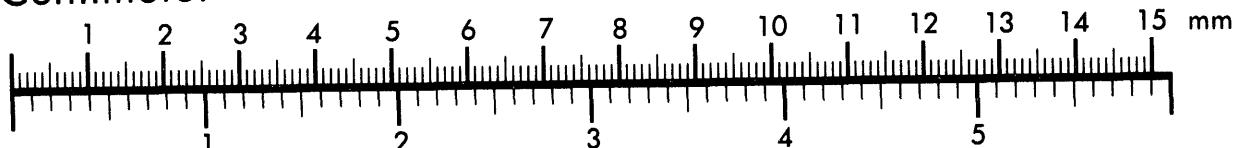


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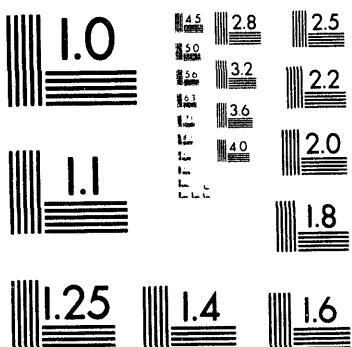
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## OVERVIEW OF TECHNOLOGY MODELING IN THE REMEDIAL ACTION ASSESSMENT SYSTEM (RAAS)

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## OVERVIEW OF TECHNOLOGY MODELING IN THE REMEDIAL ACTION ASSESSMENT SYSTEM (RAAS)

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### ABSTRACT

The Remedial Action Assessment System (RAAS) is a software tool designed to help complete the remedial investigation/feasibility study (RI/FS) of a hazardous waste site. The end goal of the RI/FS process is to identify sets of technologies that can be used to meet all remediation objectives established for the site. RAAS models over 100 remediation technologies that can be evaluated to determine if they can help remediate a site. Technology modeling is based on a description of the site created by RAAS from information supplied by the user. RAAS augments user-supplied data with static database information pertaining to contaminant and media properties. The first step of the technology modeling uses a set of applicability criteria to define a list of technologies that are potentially applicable to the site. The second step determines if there are technical constraints on implementation of a technology. The third step is calculation of the effectiveness of a technology. Effectiveness modeling is performed using three different approaches, depending on the type of technology and the amount of information available. The effectiveness may be zero (no effects on contaminant concentrations), based on a percent effectiveness value, or calculated based on contaminant-specific properties and the remediation objectives. The modeling of RAAS technologies provides the user with an automated screening tool that is useful for evaluating multiple remediation alternatives and for focusing the RI/FS on technologies that are most likely to work well for a specific contaminated site.

### I. INTRODUCTION

There are numerous hazardous waste sites under the jurisdiction of the U.S. Department of Energy (DOE). To assist the cleanup of these sites in a more consistent, timely, and cost-effective manner, the Remedial Action Assessment System (RAAS) is being developed by the Pacific Northwest Laboratory (PNL). RAAS is a software tool designed to automate the initial technology selection within the remedial investigation/feasibility study (RI/FS) process. The software does several things for the user: 1) provides information about available remedial technologies, 2) sorts possible technologies to recommend a list of technologies applicable to a given site, 3) points out technical issues which may prevent the implementation of a technology, and 4) provides an estimate of the effectiveness of a given technology at a particular site. Information from RAAS can be used to compare remediation options and guide selection of technologies for further study.

RAAS is organized to parallel the process of the RI/FS. The user characterizes the problem by responding to queries from RAAS about the waste site, the media to be remediated, the contaminants, and the risk to human health. Users may either input specific data or select default values provided by RAAS. The overall treatment strategy and remediation objectives are selected by the user. RAAS reduces the list of technologies to those that are applicable to the stated medium, contaminants, and remediation strategy. The user selects a sequence of

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technologies (i.e., a remediation alternative) from the shortened list and RAAS determines which alternatives are successful and which technologies fail to meet all of the criteria for implementation. The user evaluates and compares successful alternatives to see how the effectiveness differs.

RAAS is not intended to provide detailed design information for remediation technologies but instead was developed to help the user evaluate numerous technologies and identify those that are most likely to successfully remediate a site. As a result, the RAAS technology models are developed to a level that provides estimates of effectiveness rather than detailed design information.

The current version of RAAS has over 100 technologies that can be selected as a remedial action or as part of a treatment alternative. Many sources of information have been used to develop the RAAS technology models including literature, U.S. EPA documents, personal communication, and derivations from first principles.

Technology models are structured to accommodate a wide range of input parameter values so that RAAS can be effectively applied to many scenarios. The models respond to any input with an output of either 1) technology is not applicable, 2) technology is applicable but not technically implementable, or 3) technology is applicable and has a calculated effectiveness. In the first case, the technology does not show up on the list of applicable technologies. In the second case, the technology is applicable, but an effectiveness is not calculated because the technology cannot be implemented for technical reasons. In the third case, the technology is applicable and has an effectiveness ranging from 0% to 100%.

This paper describes how technologies are modeled in RAAS. The first section describes the inputs that are needed for the technology models. These inputs consist of user-supplied information about the scenario and data from the RAAS database (which augments the user-supplied information). The second section discusses the screening logic that determines whether a technology can be applied to a given scenario. The third section discusses logic for determining if a technology can be implemented (from a technical standpoint). The fourth section discusses approaches for modeling technology effectiveness. The three approaches discussed in this paper are based on no change in concentration, a percent effectiveness calculation, or an objective-driven effectiveness calculation.

## II. MODEL INPUTS

Inputs to a technology model describe the media to be processed and provide the remediation objectives. Models use this data to determine whether a technology can meet the input constraints/objectives. These inputs to the model are a combination of user-supplied information and information from the RAAS database. User-supplied information is needed to establish the scenario to be analyzed. RAAS database information augments user input so models can determine outputs. The minimum amount of information required to adequately estimate the effectiveness of the technology is collected and processed.

### A. User Input

User input characterizes the scenario that RAAS will address. The location and type of medium to be remediated, physical/chemical properties, contaminants present, and the strategy/objectives of remediation all specify the scenario. This information is the framework for calculating effectiveness with the technology models. Default information is available for many of the inputs, based on typical values found in many field conditions. Engineering judgement help is available to provide background information about inputs and typical ranges of values for the inputs.

The location ("situness") and type of media are specified as user inputs. A distinction is made between technologies that can treat media *in situ* and those that act on *ex situ* media. An *in situ* treatment can be applied directly to the media as it exists in the environment. On the other hand, an *ex situ* technology can only be applied to media that have been removed from their natural environment and transported to the processing location. The main types of media (which can be specified as *in situ* or *ex situ*) available in RAAS are as follows:

- Unsaturated soil
- Saturated sediment
- Groundwater
- Aqueous stream
- Organic liquid
- Gas or air

Medium information such as bulk density and moisture content are entered by the user and processed to generate the medium parameters necessary for the technology models. The main medium parameters include the total volume of contaminated medium and the relative quantities of solid, liquid, immiscible (free organic liquid), and gas phases present in the medium. Additional parameters describe the particle size distribution, hydraulic conductivity, and other physical parameters.

RAAS has a database of over 500 contaminants that can be chosen as constituents in a given scenario. Contaminants in RAAS are grouped into 10 organic and 4 inorganic categories based on U.S. Environmental Protection Agency (EPA) categories. Contaminants are divided into these categories of similar compounds to facilitate the modeling of technologies and the applicability sorting.

Contaminant concentration information is supplied by the user for each contaminant that is present in a scenario. Concentrations may be entered as a total concentration or as a concentration in each individual phase of the contaminated medium. If the scenario is for an *in situ* contaminated medium, the baseline risk to human health and the environment can be specified. Remediation objectives for each contaminant are specified by the user in terms of concentration or risk.

The user specifies a strategy for remediation of the scenario. The strategy determines which technologies could be used in a remediation alternative. The technologies are divided into groups based on their general function and the strategies correspond to these technology functions. Strategies include removal/recovery, treatment (volume reduction, toxicity reduction, mobility reduction), containment, institutional control, disposal, materials handling and no action (i.e., no remediation technology is used). There are a number of combinations of strategies that can be pursued, but RAAS includes logic to block any unrealistic combinations. Each contaminant can have a different strategy because the same strategy may not make sense for all contaminants. Examples of two possible strategies that might be compared for an *in situ* medium with both inorganic and organic contaminants are: 1) recovery/removal of the medium and both types of contaminants, and 2) *in situ* treatment to reduce the toxicity of all the organic contaminants and the mobility of the inorganic contaminants.

#### B. Database Information

The RAAS database contains physical/chemical property information for each contaminant. Table 1 lists the contaminant properties available from the database. Data is included in the database where appropriate (e.g., inorganic contaminants don't have an octanol/water partitioning coefficient). Contaminant information is used to help assess contaminant applicability for specific technologies and to model the technology effectiveness.

TABLE 1. CONTAMINANT PROPERTIES IN THE RAAS DATABASE.

Property	Symbol	Units
Chemical Formula	--	--
Chemical Abstract Number	--	--
Physical State (gas, liquid, solid)	--	--
Molecular Weight	MW	g/gmole
Boiling Point	BP	°C
Melting Point	MP	°C
Vapor Pressure at a Known Temperature	VP	mm Hg
Water Solubility at a Known Temperature	WS	mg/L
Henry's Law Constant	HLC	atm·m <sup>3</sup> /gmole
Octanol/Water Partition Coefficient	K <sub>ow</sub>	unitless (ppm/ppm)
Organic Carbon/Water Partition Coefficient	K <sub>oc</sub>	L/g

#### III. SORTING APPLICABLE TECHNOLOGIES

RAAS has rules and logic to sort technologies into a short list of applicable technologies known as the Selected Technologies List (STL). Determination of the STL reduces the number of technologies to consider and focuses the RI/FS evaluation on the proper technologies.

The four sorting criteria (medium location, medium type, applicable contaminants, technology function) that define the STL are generated by supplying the following information for each technology:

1. Is the technology intended for *in situ* or *ex situ* treatment?
2. What type(s) of media can the technology treat?
3. What types of contaminants can the technology treat?
4. What type of function does the technology perform?

The first sorting criterion refers to whether the medium is *in situ* or *ex situ*. This is an important distinction that greatly reduces the number of technologies that are applicable to a scenario.

Most technologies cannot treat all types of media. For example, Soil Vapor Extraction will only treat

unsaturated soil. The second sorting criterion is answered based on a description of the technology.

The third sorting criterion is also determined by a description of the technology and literature information on treatability tests or actual operation. If a technology is known to be effective for a contaminant or group of contaminants, then the contaminant applicability is based on this information. Some technologies use contaminant properties to determine contaminant applicability. For example, Air Stripping is only applicable to contaminants having a Henry's Law Constant (HLC) above a certain minimum. At least one applicable contaminant must be present in the scenario for the technology to be applicable.

The fourth sorting criterion (technology function) relates to the remediation strategy chosen by the user. If a given strategy is not chosen, the technologies performing the corresponding function are not applicable to the scenario. For example, if the user has chosen a strategy of immobilization, then a destruction technology such as Incineration will not be applicable.

#### IV. TECHNICAL IMPLEMENTABILITY

Technologies on the STL are applicable to a scenario, but there may be technology-specific limitations on the medium, contaminants, etc. Disabling conditions are engineering rules-of-thumb and other technical issues that determine if a technology can be implemented. Disabling conditions do not consider implementability issues such as permitting or schedule. However, issues regarding operation of the technology are considered. For example, if contamination is too deep, Electrokinetic Separation will be disabled (unimplementable) because the electrodes have a maximum length. Additionally, there are disabling conditions that are in place to prevent calculational errors (e.g., division by zero) in the effectiveness model for a technology.

Disabling conditions are modeled as logical decisions based on calculation of appropriate equations. Where equations cannot be calculated from the available data, the user is asked for additional information. When a technology is disabled, the user knows that either the problem must be corrected by using another technology first (pretreatment) or that the technology generally cannot be implemented in the given scenario. There may be special conditions which would, in reality, allow a technology to be implemented. However, the disabling conditions are based on a set of assumptions that emulate the general application of the technologies.

#### V. EFFECTIVENESS MODELING

Remediation technologies are modeled in RAAS with the intent of providing realistic results for a multitude of scenarios. The purpose of RAAS is to be an automated tool for screening remediation alternatives in the RI/FS process. Thus, the models do not provide a remedial design, but calculate outputs with sufficient detail for use in screening remediation alternatives or determining effectiveness.

Because RAAS is a screening tool, the technology models try to be as broad as possible in representing a type of technology yet still provide a given level effectiveness estimates. Some types of technologies can be operated in a variety of ways. Different operational methods for the same type of technology may have similar or different effects on a given scenario. When different operational methods have a similar effectiveness, the technology model represents all of the operational methods. For example, Incineration can be operated as a rotary kiln, multiple hearth, etc. However, the effectiveness is the same for all of these operational methods so there is one model in RAAS that encompasses all variations of Incineration.

If the effects of different operational methods are notably different, separate models have been developed to represent specific operational methods. These different models of operational methods are termed "process options" of a remediation technology. Process options allow RAAS to better model a method of operation by making the model more specific. For example, Soil Vapor Extraction is a type of remediation technology that can be operated as Soil Vapor Extraction: Ambient Air Stripping or Soil Vapor Extraction: Hot Air/Steam Stripping. The hot air process option operates at a higher temperature and can effectively treat a larger number of contaminants and remove contaminants at a higher rate than ambient air stripping, so the two methods are modeled as separate process options.

The development of RAAS technology models uses a typical chemical engineering approach. A mass balance is drawn around the system and stream (media) properties are determined. A flow diagram representing inlet and outlet streams is shown in Figure 1. Stream parameters are the information of interest because the stream parameters show conditions before and after application of a technology.

There are 23 parameters tracked to represent a stream. These parameters are listed in Table 2. Note that the mass is not explicitly tracked. Rather, the volume,

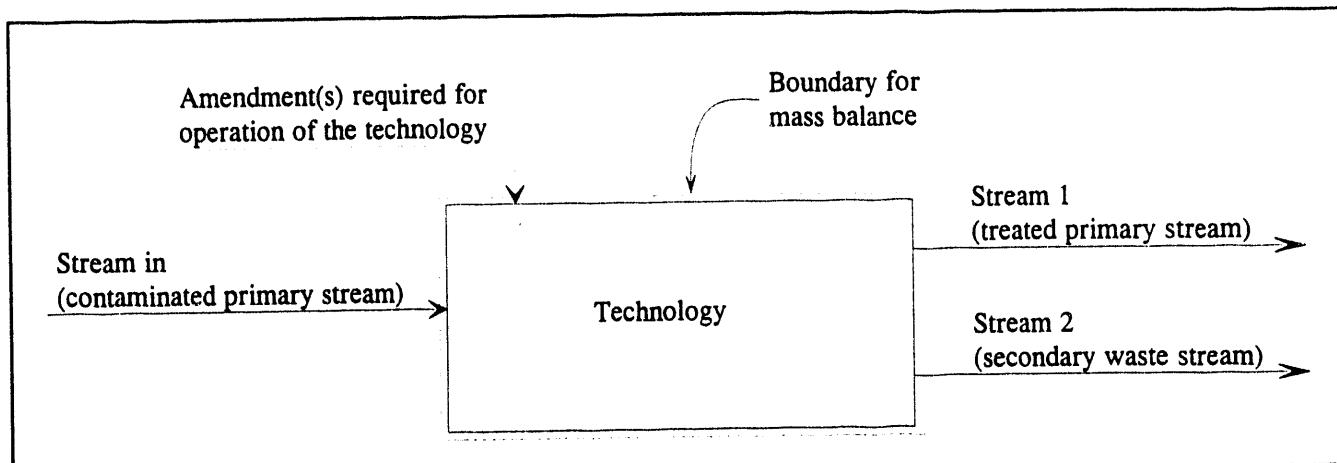


Figure 1. General flow diagram for a technology depicting inlet and outlet streams.

TABLE 2. PARAMETERS DESCRIBING EACH PROCESS STREAM IN RAAS.

Stream Parameter	Symbol	Units
Location of medium	--	--
Type of medium	--	--
Temperature	T	Kelvin
Pressure	P	Atm
pH	pH	pH units
Mass average particle diameter	D	m
Standard deviation of the logarithmic particle distribution	logsigma	--
Hydraulic Conductivity	HC	m/s
Total volume of the medium	V	m <sup>3</sup>
Volumetric flowrate	F	m <sup>3</sup> /s
Solids phase volume fraction of the medium	VS	--
Immiscible phase volume fraction of the medium	VO	--
Aqueous phase volume fraction of the medium	VA	--
Gas phase volume fraction of the medium	VG	--
Solids phase density of the medium	$\rho_S$	kg/m <sup>3</sup>
Immiscible phase density of the medium	$\rho_O$	kg/m <sup>3</sup>
Aqueous phase density of the medium	$\rho_A$	kg/m <sup>3</sup>
Gas phase density of the medium	$\rho_G$	kg/m <sup>3</sup>
Concentration of the $i^{\text{th}}$ contaminant in the solid phase	CS <sub>i</sub>	kg/m <sup>3</sup>
Concentration of the $i^{\text{th}}$ contaminant in the immiscible phase	CO <sub>i</sub>	kg/m <sup>3</sup>
Concentration of the $i^{\text{th}}$ contaminant in the aqueous phase	CA <sub>i</sub>	kg/m <sup>3</sup>
Concentration of the $i^{\text{th}}$ contaminant in the gas phase	CG <sub>i</sub>	kg/m <sup>3</sup>
Toxicity Characteristic Leaching Procedure concentration for the $i^{\text{th}}$ contaminant	TCLP <sub>i</sub>	ppm

volume fractions, and concentrations are tracked; these can be used to do a mass balance around the process.

Each stream can be represented by four phases of matter: solid, aqueous liquid, immiscible (organic) liquid, and gas. RAAS tracks contaminants in each phase and models the effects on contaminants depending on which phase contains contaminants. The user of RAAS will see the phase concentrations as well as the environmental concentration (EC) of the contaminant in the medium (i.e., total mass of contaminant in the total volume of the medium).

The technology models use first principles as much as possible to estimate the effectiveness of the technologies. A number of models tie the effectiveness to contaminant properties, thereby producing results that reflect how a variety of contaminants could be affected. All technology models make assumptions to simplify the model. Many assumptions are technology specific and relate to how the process is operated. Some assumptions are common throughout a majority of models. For example, it is assumed that there are no contaminant interactions; the technology affects each contaminant but does not account for differences stemming from treating a mixture of contaminants. The underlying assumptions of technology models represent the general application of the technology. Hence, the modeling basis may not be valid for specific scenarios and the user must adjust the evaluation of remediation alternatives accordingly.

There are several approaches to determining the effects of a technology on the contaminated medium. There may be no effect on the contaminants, a percentage of the contaminant mass may be treated, or the effectiveness of a technology may be driven by the concentration objective.

#### A. No Effect on Contaminant Concentrations

Containment and institutional control technologies do not change the contaminants or medium, so most of the stream properties remain unchanged. The major effects of control technologies are on the risk and the contamination release mechanisms. Control technologies generally prevent the spread of contamination or prevent additional exposure of people or the environment to the contamination by affecting contaminant mobility. The modeling of the control technologies is trivial with respect to the contaminant mass balance ( $\text{mass}_{\text{in}} = \text{mass}_{\text{out}}$ ). Modeling the effects on risk is complex, however, and will be discussed in a future paper.

#### B. Percent Effectiveness Approach

The next step up in complexity (with respect to the mass balance) is to employ a percent-effectiveness value. Technologies using this approach assume that the process is a given percent effective. For example, a technology may be 98% effective at destroying a class of contaminants (toxicity reduction) or 80% effective at achieving a separation of phases (volume reduction).

The percent-effectiveness approach is used in two cases: when there is not enough information to model contaminant-specific effects and when the technology is best represented with a percent effectiveness. There is not enough information available about partitioning and solubility of contaminants in supercritical fluids, so a percent-effectiveness approach must be used for modeling Solvent Extraction: Supercritical Fluid Extraction. Incineration is an example of where a percent-effectiveness approach is appropriate. Because incineration is only operated in a manner such that specific destruction and removal efficiencies (DRE) are achieved (as mandated by regulatory agencies), it makes sense to model the effectiveness with a percent-effectiveness approach.

The percent effectiveness approach is relatively easy to implement. Literature information reporting percent effectiveness is used as a basis to determine a conservative value for use in modeling. When reasonable, the percent effectiveness is used for a category of similar contaminants. Assuming that similar contaminants will be affected in a like manner broadens the applicability of the technology model. The effectiveness is used in a contaminant mass balance around the process to determine how much contaminant is in each of the output streams.

#### C. Concentration Objective Approach

The most complex modeling of effectiveness in RAAS uses concentration objectives. The concentration objective approach is based on contaminant-specific properties such as partitioning between phases or biodegradation rate, as well as inlet and objective concentrations. The concept is one of determining the quantity of solvent or the length of time that it would take to remediate the hardest-to-remove contaminant down to the concentration objective. This quantity can be used to back-calculate the amount of contamination remaining with the treated medium. All of the applicable contaminants can meet or exceed their respective concentration objectives because, by definition, the hardest-to-remove contaminant meets its objective.

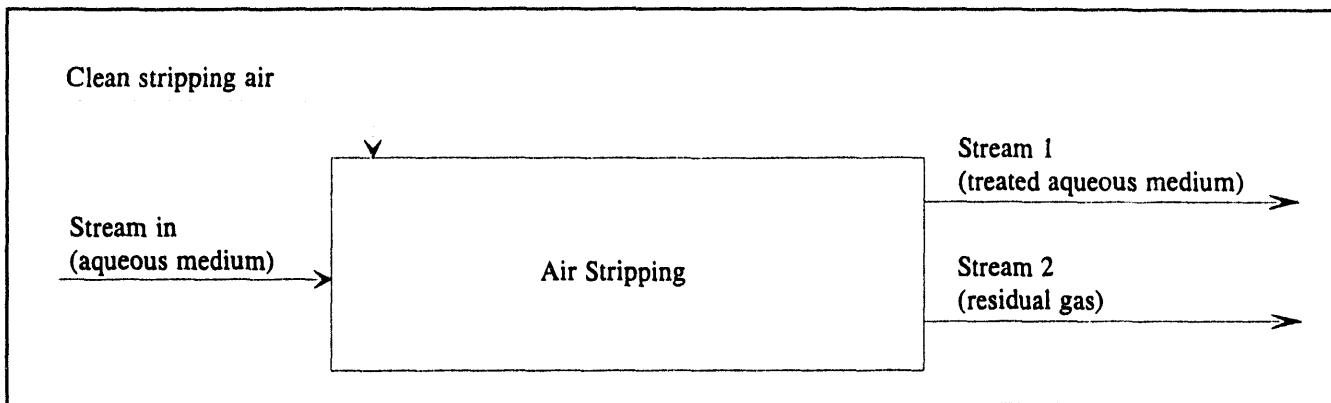


Figure 2. Box flow diagram for Air Stripping.

However, a user-defined practicality limit on operation of the technology regulates whether the objectives are achieved. If the practicality limit is reached first, the effectiveness is reported at that point in the process.

Technologies that perform an extracting process can use the objective concentrations of the contaminants to estimate how much solvent will be required to remove the hardest-to-remove applicable contaminant (and, hence, all of the other applicable contaminants). Calculations are done, based on first principles, to estimate the number of equilibrium contacts of solvent with the contaminated medium that are required to remove a contaminant to its objective. Air Stripping will be used to illustrate this approach to modeling of effectiveness. The concentration objective approach is similar for all technologies where the approach is used.

The flow diagram for Air Stripping is shown in Figure 2. An aqueous stream enters a packed column from the top and distributes over the packing as it travels downward. Air is the "solvent" that enters the packed column from the bottom and contacts the water in a countercurrent fashion. There are two outlet streams: the treated water and the contaminated air. The contaminant mass balance is  $mass_{in} = mass_{out}$  for this technology because there is no destruction or generation of contaminant.

The Air Stripping model looks at how many equilibrium contacts are required to remove the hardest-to-remove applicable contaminant. An arbitrary unit of 1 kg of air is used for each equilibrium contact with the total volume of the contaminated aqueous medium. The unitless HLC is the partitioning coefficient that governs distribution of contaminant between the contaminated medium (water) and the solvent (air) for this technology.

Equation 1 shows the definition of the unitless HLC.

$$HLC^* = \frac{\left( \frac{kg \text{ cont. in air}}{kg \text{ air}} \right)}{\left( \frac{kg \text{ cont. in } H_2O}{kg \text{ } H_2O} \right)} = \frac{(HLC)(\rho A)(1000)}{(P)(MW_{air})} \quad (1)$$

The mass balance and the definition of the HLC are used to derive an equation for the number of contacts,  $n_i$ , for each applicable contaminant (Equation 2). Equation 2 calculates how many contacts are required to reach a given concentration objective when starting with a known equilibrium partitioning (HLC). The inlet stream is assumed to be a dilute system, the volume of the contaminated medium is assumed to be unchanged after the air stripping process, and the effect of multiple contaminants is assumed to be negligible.

$$n_i = \frac{\ln\left(\frac{C_{obj,i}}{CA_{in,i}}\right)}{\ln\left(\frac{\rho A_{in} V A_{in} V_{in}}{HLC^* + \rho A_{in} V A_{in} V_{in}}\right)} \quad (2)$$

The contaminant that takes the largest number of contacts (maximum of the  $n_i$  values) to reach its objective is the contaminant that is hardest to remove. This largest number of contacts ( $n_e$ ) could be used to back-calculate residual concentrations (and all applicable contaminants would meet the objectives). However, it may take an unreasonable amount of time or volume of solvent to do the largest number of equilibrium contacts ( $n_e$ ). The user-defined practicality limit is used to keep the estimate of the effectiveness within reasonable limits. If it takes more

equilibrium contacts than could be done within the practicality limit, the practicality limit is used to determine how many equilibrium contacts ( $n_p$ ) will be done. Note that for the Air Stripping model, the practicality limit is on the amount of air used because time is less constraining for *ex situ* processes.

Setting  $n_{max} = \min(n_c, n_p)$ , and rearranging Equation 2 gives Equation 3 for determining the concentration of all of the contaminants in the outlet aqueous stream. Note that only applicable contaminants were used in determining the  $n_i$  values, but Equation 3 is used to determine concentrations for all organic contaminants because there will be some effect on any organic contaminant even if the HLC is below the contaminant applicability cutoff of 0.003. All non-applicable inorganic contaminants are assumed to be unaffected by the air stripping technology.

$$CA_{1,i} = (CA_{in,i}) \left( \frac{\rho A_{in} V A_{in} V_{in}}{HLC^* + \rho A_{in} V A_{in} V_{in}} \right)^{n_{max}} \quad (3)$$

A mass balance can now be drawn around the air stripper and the concentration of contaminants in the stripping gas can be determined. Most of the other parameters that describe each stream are unchanged by the process.

A summary of the concentration objective approach is given for clarity. For each applicable contaminant, the quantity (time, volume of solvent, number of equilibrium contacts) required to remediate the contaminant to its concentration objective is calculated. The hardest-to-remove contaminant is determined from the first step. The maximum value of the quantity determined in the first step is compared to the user-defined practicality limit and the lesser value is used to back-calculate residual contaminant concentrations.

#### IV. SUMMARY

The current version of RAAS models remediation technologies using a set of inputs and a mass balance approach. Data is available as part of either the user input or the contaminant property database. The technology model sorts technologies based on four applicability criteria (medium location, media treated, contaminants treated, strategy/technology function) to produce a list of technologies potentially applicable to a given scenario. The technology model further evaluates technology-specific disabling conditions to determine technical implementability in a given scenario.

Using the model inputs that characterize a scenario, the effectiveness of a technology is estimated from a mass balance around the process. Three approaches for determining effectiveness are employed: no effect on concentration, a percent effectiveness, and concentration objective-driven effectiveness. Containment and institutional control technology models have no effect on concentrations, but do impact the risk and exposure mechanisms. The percent effectiveness is used in situations where not enough information is available to model effects on specific contaminants or where the method of operation indicates that a percent effectiveness is appropriate. A quantity (volume of solvent or time) is calculated such that concentration objectives are achieved in the objective-driven effectiveness approach (unless the practicality limit is reached first).

The modeling approaches are sophisticated enough to realistically represent the technologies for the purpose of screening remediation alternatives. As more information becomes available in the literature, technology models will be refined. Some technologies using the percent effectiveness approach will be upgraded to use the concentration objective approach. Additional models will be developed and included in RAAS to represent new technologies and variations in operating procedure.

#### ACKNOWLEDGEMENTS

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#### NOMENCLATURE

$C_{obj,i}$	= objective concentration of the $i^{th}$ contaminant ( $\text{kg}/\text{m}^3$ )
cont.	= abbreviation for "contaminant"
$HLC^*$	= unitless Henry's Law Constant
$\ln()$	= natural logarithm of the quantity in parentheses
$MW_{air}$	= molecular weight of air = 29 (g/gmole)
$n_c$	= maximum number of equilibrium contacts calculated from Equation (2) based on all applicable contaminants
$n_i$	= number of equilibrium contacts needed to reach the objective concentration of the $i^{th}$ contaminant
$n_p$	= number of equilibrium contacts calculated based on the maximum period of operation (i.e., the practicality limit)

Additional nomenclature is found in Tables 1 and 2.

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