Fugacity Framework 2.0: calculator and training applications for site assessment and rehabilitation

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Abstract

The Fugacity framework addresses multiple-media and multiple contaminant aspects of environmental site assessment based on a conceptual site model and a Fugacity Level I mathematical model. In an effort to help people use the Fugacity framework, a “Fugacity Calculator Tool” was developed and implemented to enable users to visualize the behavior of toxic chemicals at a contaminated site, the effect of site-specific characteristics on contaminant distribution, the behavior of daughter products of degradation, and the associated risks to humans and the environment. The framework has been used in U.S. EPA RCRA/CERCLA workshops for identifying alternatives and decisions, and the Calculator is freely available and can be downloaded from the internet at the following URL: http://www.engineering.usu.edu/uwrl/Fugacity/index.html. The Fugacity model was developed as a local application because extendibility was a major issue. Borland Delphi® (object Pascal) was used as the development tool. The Fugacity framework and Calculator were developed for several different Brownfield audiences and implementers. In addition to professional users in real-world contexts, the Fugacity Framework Version 2.0 is ideal for educating students and non-technical audiences. A “problem-based learning” classroom approach is described that utilizes the framework and Calculator. The framework can be used to make decisions regarding the protection of public health and the environment, site rehabilitation, and the sustainable development/economic recovery of impacted sites.

1 Introduction

The material presented here briefly reviews the Fugacity framework and Fugacity-based management system (Version 1.0) described by Sims et al. [1] in
2002, and emphasizes Fugacity Framework Version 2.0 that describes extensions and additions to Version 1.0, and identifies applications in training and educational settings. Contaminated site rehabilitation involves an assessment of contaminant distribution from source(s) to receptor(s) that may include humans and the environment. Contaminants within sources generally spread through release and migration that expands to larger volumes of soil, water, air, and/or oil phases that result in large-scale exposure and receptor scenarios (Figure 1) that must be controlled through costly risk management technologies of containment, removal, and/or destruction. The technologies selected often are not focused on the correct physical phase(s), resulting in inefficient or ineffective risk management and site rehabilitation efforts.

To address these issues of site rehabilitation, a Fugacity framework for assessment of multi-media distribution (air, water, soil, and oil) of chemical contaminants in subsurface environments was developed. The framework is utilized in an interactive mode and pedagogically designed for visual presentation to allow managers and decision makers to focus on making decisions regarding identification of information needs, site assessment, and site rehabilitation. This Fugacity-based management system has been implemented to allow easy web access to users worldwide. This paper describes Version 2.0 of the Fugacity-based management system and includes: (1) the Fugacity framework and linked database, (2) the Fugacity Calculator Tool, and (3) the Fugacity framework and calculator in training and educational settings.

![Figure 1: Linking sources to receptors including humans and the environment.](image)

2 Objectives

The overall objective of this paper is to describe Version 2.0 of a web-accessible tool for managers, senior personnel, and other decision makers who may or may
not have a technical background in mathematical modeling, multimedia contaminant behavior, and engineering treatment technologies.

The specific objectives of this paper include: (1) review of the Fugacity-based framework as a useful tool for multi-media contaminant evaluation, including chemical database and site characterization requirements; (2) example applications of the Fugacity framework; (3) description of the Fugacity Calculator Tool, (4) description of Version 3.0 under development for future enhancements to the Fugacity framework tool, and (5) use of the Fugacity framework and calculator in training and educational settings.

3 Fugacity-based framework

The Fugacity-framework is based on the conceptual site model (CSM) that consists of: (1) an Evaluative Site, (2) a chemical mass balance indicating distribution of contaminant(s) among physical phases at the evaluative site, and (3) a flow diagram to relate source(s) to receptor(s) pathways.

3.1 Evaluative site

The evaluator designs a “site,” then explores the likely behavior of chemicals in that site. The concept of “evaluative environments” was introduced by Baughman and Lassiter [2]. Physical phases of a subsurface evaluative site (Figure 2) include a solid phase and three fluid phases. The solid phase is composed of soil organic matter (SOM) and inorganic components including sand, silt, and clay that comprise the subsurface texture. Fluid phases include the water or leachate phase, the gas phase, and the oil or NAPL (non-aqueous phase liquid) phase.

![Figure 2: Evaluative site physical phases for Fugacity framework.](image)

3.2 Mass balance approach.

A chemical mass balance approach is directed at evaluating how contaminant chemicals are distributed among the physical phases at a site. Chemicals at
Brownfield sites are contained within the physical phases shown in Figure 2. One or more physical phases link contaminant sources to receptors. Chemical distribution among site phases can be determined through the application of Fugacity calculations.

### 3.2.1 Fugacity

Fugacity is applicable to organic chemicals, but not to metals and other inorganic chemicals. Its convenience in environmental partitioning calculations became apparent after 1980. Donald Mackay introduced the concept of Fugacity in the 1970’s to express the distribution of organic pesticides among phases of the environment. His books “Multimedia Environmental Models – The Fugacity Approach” [3, 4] describe the basis and applications of Fugacity for handling chemical distribution, reaction, advective flow, and diffusive and nondiffusive transport in multimedia environments.

Fugacity modeling provides a way for conducting a chemical mass-balance analysis. Fugacity uses partition coefficients for a chemical contaminant between soil and water (Kd), air and water (Kh), and oil and water (Ko) to describe the distribution of chemicals among physical phases comprising a multi-phase evaluative site. Physical phases can be evaluated with regard to: (1) sources, (2) transport and transformation, and (3) exposure.

Fugacity has the units of pressure (Pa), and the basic equation for Level I Fugacity (equilibrium conditions among phases) is.

\[
Ci = fi \times Zi
\]

(1)

\(Ci\) = concentration of chemical in phase i, (moles/cubic meter)

\(fi\) = Fugacity in phase i (Pa)

\(Zi\) = Fugacity capacity of phase i (mole/Pa-cubic meter)

Relevant equations for Level I Fugacity calculations for subsurface assessments are provided in the publications by Sims et al. [1, 5, 6, 7].

![Site Conceptual Exposure Model](image)

**Figure 3:** Flow diagram identifies priority physical phases that connect source to receptor through migration and exposure. Risk management technology selection is based on priority phase management goals.

### 3.3 Flow diagram

A flow diagram incorporates site-specific data into an evaluative site and site specific mass balance information to assist in organizing the information to identify priority source phases with regard to release, secondary sources of...
contamination, exposure and the need for phase control to accomplish risk management and site rehabilitation (Figure 3). A flow diagram also serves as a common communication tool for site owners and operators, regulators, and consultants.

4 Chemical database and site characteristics required

Fugacity calculations require numerical values for properties of chemical substances for the calculation of Fugacity capacities. The chemical properties required are provided in an embedded chemical database as part of the Fugacity framework. The chemical database utilized in the Fugacity framework Version 2.0 was developed by the U.S. Environmental Protection Agency (U.S.EPA) [8] to provide information pertaining to fate and transport properties for contaminants commonly found at Superfund sites. The U.S. EPA database of approximately 70 chemicals therefore provides the values used for chemical properties required for Fugacity calculations for chemicals relevant to Brownfield and other sites, and also serves as a peer-reviewed reference.

Site characteristics required for Fugacity analysis include the volume (cubic meters) of each physical phase (air, water, soil or aquifer, and NAPL). If the volumes are not known, then relative percentages of the volumes can be estimated and used in the Fugacity calculations so the total percent of all phases equals 100. In addition, the soil organic carbon, as percent by weight of the soil phase, and the soil dry bulk density (kg/cubic meter) are required.

5 Example applications of the Fugacity framework

Examples of the applications of the Fugacity framework include: (1) distribution of trichloroethylene (TCE) in the subsurface as influenced by the NAPL phase, (2) distribution of TCE parent compound and daughter products dichloroethylene (DCE) and vinyl chloride (VC) within the same subsurface site conditions, and (3) Provo City Ironton Economic Redevelopment Project, Utah.

Figure 4 illustrates the distribution of TCE in a subsurface environment composed of 2% NAPL, 25% air, 23% water, and 50% soil by volume, and represents a source area of TCE contamination. The majority of TCE (87%) is located within the NAPL that comprises only 2% of the volume of the subsurface, while only 7% is present in the soil-solid phase.

Figure 5 represents the subsurface environment downgradient from the source where NAPL is absent (NAPL volume = 0%). With only air, water, and soil-solid phase present, the majority (55%) of TCE is present in the soil phase that represents a large increase in the %TCE in soil phase from 7% in Figure 4.

Using the same site characteristics as identified in Figure 4 for TCE, the distributions of daughter products of anaerobic biodegradation DCE and VC are shown in Figures 6 and 7, respectively. Figure 6 shows that DCE is present in air (34%) compared to 2% for TCE, and Figure 7 shows that VC is present almost exclusively in the air phase (96%). Therefore in the subsurface, anaerobic transformation from TCE to DCE to VC results in a different distribution of daughter products. These assessments have implications with respect to which
phases to monitor for which chemical, as well as the appropriate phase for control and treatment to prevent exposure to human health and the environment for each contaminant at a site.

The Provo City Ironton Economic Redevelopment Project was initiated in 1996 with a grant from the US EPA. The project involves the redevelopment of land contaminated with polycyclic aromatic hydrocarbons and metals, and includes citizens, local businesses, and local industry. The Fugacity framework is applicable to the evaluation of PAH source assessment and risk management with respect to human exposure and land rehabilitation.

6 A tool for using the Fugacity framework

In an effort to help people use the Fugacity framework, a “Fugacity Calculator” Tool was developed and implemented. The Fugacity Calculator was developed to evolve from a spreadsheet into a “local app” programmed in Delphi. It is now a stand-alone computer program based on the model of Fugacity detailed above. The Calculator is freely available and can be downloaded from the internet at the following URL: http://www.engineering.usu.edu/uwrl/Fugacity/index.html.

6.1 Features for Version 2.0 (PC only)

- **Small, downloadable program**
  The Fugacity model was developed as a local app because extendibility was a major issue. Borland Delphi® (object Pascal) was used as the development tool. Delphi provides a tight compiled module that can be easily downloaded and installed onto the local computer from the internet. Delphi is a powerful computer language with excellent interface components, and we have found that Delphi is good compromise between MS Visual Basic® and C++. Delphi combines much of the ease-of-use of Visual Basic with the programming power of C++.

- **Easy-to-use layout**
  The tool is proportioned into three sections. Reading left to right, top to bottom a user 1) defines characteristics of an evaluative site (i.e. percentage of air, water, soil, and NAPL composing the total volume of the site, percentage of organic carbon and the soil density), 2) selects one of the EPA chemicals to introduce into the site, and 3) interprets chemical distribution within the site.

- **EPA database**
  Users can choose from EPA priority pollutant chemicals to test.

- **Visual data display**
  Pie charts represent 1) the percentage of each phase comprising the site’s composition, and 2) the percentage of a chemical that distributes into each of those phases for each evaluative site. By design the pie charts are situated next to each other for easy comparison, the latter being noticeably larger so as to focus attention on the result, namely chemical distribution percentages.
Figure 4: Fugacity Analysis of TCE in a subsurface environment with 2% (volume) NAPL.

Figure 5: Fugacity analysis of TCE in a subsurface environment with 0% (volume) NAPL.
Six default sites with corresponding graphical displays of phases
If a user doesn’t know specific values for a site they are defining, they can choose from six default sites. These are dry, normal, and wet for sites with and without NAPL. Selecting a specific tab (upper right) automatically configures the program with corresponding values, and changes graphics.
• **User control over certain key variables and the plotting of results**  
Users can experiment with different values for Henry’s Law constant and Koc. They can also choose to plot the chemical distribution in units of mass or concentration.

• **Notes**  
This feature is a section for notes and information about different parts of the tool, specifically each field and what it means.

• **Ability to create, rename, and delete tabs**  
An important feature in the tool, this gives users the ability to run multiple tests using the same or different sites and chemicals. The tabs created are good as long as the tool is opened but cannot be saved.

• **Ability to print results**

6.2 **Upcoming features for Version 3.0**

• **Tutorial**  
Instructional content will be launched from the menu that includes demonstrations on how to use the tool and the Fugacity framework approach.

• **Tab duplication**  
For greater usability, there will be a feature that duplicates existing tabs. This will make it easier to run new tests based on previous ones.

• **Saving tabs and tab sets**  
The ability to save tabs and tab sets is one of the most important new features. Users will be able to call up, use, and extend previous work. Teachers will be able to create problem progressions that hold instructional value.

• **Improved notes**

7 **Using the Fugacity framework and calculator in training and educational settings**

The Fugacity framework and calculator system (Version 2.0) was developed with several different audiences in mind because it is not uncommon for people with varied backgrounds to be involved with site assessment, rehabilitation and development. Everyone from regulators and industry executives to other professionals, local officials and citizens need a common language as well as the ability to look at the same picture in order to effectively work together. In addition to users in real-world contexts, the Fugacity framework is ideal for educating students in a classroom setting. Meeting the needs of such diverse users requires appropriate instructional support.

7.1 **Training**

Justification for using the overall Fugacity framework with diverse groups can be found from cognitive psychologists and educational researchers who advocate
using conceptual structures to help learners organize new knowledge. It has been
found among other things that “Providing learners with a conceptual model can
facilitate the acquisition of problem-solving skills....” [10] If they are equipped
with a “big picture,” then users are able to ask important questions about what is
known and what needs to be known. Because trainers should provide cues and
questions that help others use what they already know about a topic [11],
different kinds of questions are built into the calculator’s tutorial and can be used
to great advantage during problem-solving activities (see figure 9).

<table>
<thead>
<tr>
<th>Questions</th>
<th>Site Characterization</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>General</strong></td>
<td></td>
</tr>
<tr>
<td>• What phases are present and in what relative amounts?</td>
<td></td>
</tr>
<tr>
<td>• Where are the primary and secondary sources?</td>
<td></td>
</tr>
<tr>
<td>• Which chemicals or intermediates are or may be at the site and what are their properties?</td>
<td></td>
</tr>
<tr>
<td><strong>Probing</strong></td>
<td></td>
</tr>
<tr>
<td>• What is the cubic volume of your site?</td>
<td></td>
</tr>
<tr>
<td>• Are there “sub-sites” that need to be sampled?</td>
<td></td>
</tr>
<tr>
<td>• What industry activities have occurred in the area?</td>
<td></td>
</tr>
<tr>
<td><strong>Reflective</strong></td>
<td></td>
</tr>
<tr>
<td>• Do you understand where a contaminant is and how it got there?</td>
<td></td>
</tr>
<tr>
<td>• How much confidence do you have in the characterization?</td>
<td></td>
</tr>
</tbody>
</table>

Figure 9: Sample questions pertaining to site characterization are built into the Fugacity Calculator’s tutorial.

<table>
<thead>
<tr>
<th>Problem Format</th>
<th>Givens</th>
<th>Goal(s)</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>conventional problems</td>
<td>+</td>
<td>+</td>
<td>?find</td>
</tr>
<tr>
<td>worked-out examples</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>completion problems</td>
<td>+</td>
<td>+</td>
<td>?complete</td>
</tr>
<tr>
<td>goal-free</td>
<td>+</td>
<td>?define</td>
<td>?find</td>
</tr>
<tr>
<td>reverse problems</td>
<td>?predict</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>imitation problems</td>
<td>+analog</td>
<td>+analog</td>
<td>+ analog</td>
</tr>
</tbody>
</table>

Figure 10: Different problem formats that can help guide problem preparation.

Instructional support provided with the Fugacity Calculator also takes the
form of trainer guidance. Because using the Calculator depends on entering data
for specific problems, trainers will need to generate problem sets, which is key in
working with adult-learners. Figure 10 provides an overview of different
problem formats that can help guide problem preparation as an example of
trainer guidance.
7.2 A problem-based classroom approach

It is critical that students become proficient in working with and building models, and the Fugacity Framework and the Fugacity Calculator Version 2.0 are valuable resources for education. Instructional designers have also come to appreciate the value of building instruction and learning around models. In what he calls Model-Centered Instruction Gibbons [11] prescribes methods for making human/model interactions effective by promoting model observation, interaction, and problem solving. These prescriptions have guided the design of both the Fugacity calculator and the associated instruction.

In the winter semester of 2003 we integrated the Fugacity framework into a problem-based learning approach for USU’s Soil Based Hazardous Waste Management graduate course. Traditionally the classroom portion of the course was primarily lecture. The problem-based learning approach required the instructor to assume a more facilitative role. By presenting the students an extended case study based on the book *A Civil Action* [12], students were expected to work as a team through a site characterization and remediation proposal problem. The instructor served as a process facilitator instead of a dispenser of knowledge. Instead of directly answering questions his role was to make sure that students were formulating hypotheses, evaluating known facts, documenting learning issues and creating action plans. They in turn had to divide up learning tasks, seek appropriate information resources, and then collaborate in recommending a solution.

The final test was partly an oral exam that took on a real-world form in which students were individually asked to respond to the instructor who played the role of an industry owner and prospective client. Students acted as consultants by responding to the instructor problems and concerns. The outcome of this experience was characterized by the instructor as driving the students to go “deeper and farther [into the subject by].” This format required the instructor to constantly observe what the students actually comprehended and required the students to take initiative for their learning.

Acknowledgement

Support for this project was provided by a grant from the Huntsman Environmental Research Center (HERC) at Utah State University, Utah, U.S.A. (Dr. Maurice Thomas, Director), and by support provided by the Utah Water Research Laboratory, and the Department of Biological & Irrigation Engineering at USU.

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