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# Using an Integrated, Multi-disciplinary Framework to Support Quantitative Microbial Risk Assessments

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**Abstract:** The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) provides the infrastructure to link disparate models and databases seamlessly, giving an assessor the ability to construct an appropriate conceptual site model from a host of modeling choices, so a number of modeling analyses can be supported and reproduced. FRAMES is a Windows-based system that can incorporate and communicate with a array of software models and databases and that is uniquely designed to allow users, by themselves, to visualize the problem and add and link disparate models – even older legacy models – and databases to the system. Quantitative Microbial Risk Assessment (QMRA) is a modeling approach that integrates a wide range of disparate data, including fate/transport, exposure, and human health effects' relationships, to characterize potential health impacts/risks from exposure to pathogenic microorganisms. Although QMRA does not preclude the use of source-term and fate and transport models, it most commonly has been applied where the “source term” is represented by the receptor location (i.e., exposure point), meaning that the full potential of a QMRA has not been realized traditionally. This paper describes unique attributes of FRAMES and demonstrates how open-system architecture can be used to link disparate models and databases to support a QMRA application, while addressing multiple microbial source types and organisms that impact downstream receptors.

**Keywords:** QMRA, Risk Assessment, Integrated Modeling, Pathogens, Watersheds

## 1. INTRODUCTION

Fecal bacteria are among the most common pollutants affecting rivers and streams. EPA [2002] revealed that 35% of impaired rivers and streams were polluted by fecal bacteria (generally indicated by fecal coliforms, enterococci, or *E. coli*) which could indicate the presence of pathogens. Due to large numbers of farm animals and wildlife, animal fecal matter may be an important source of contamination in rural areas. Among various animal fecal sources, poultry are responsible for 44% of the total feces production in the United States, followed by cattle (31%) and swine (24%) [Kellog et al. 2000]. Quantitative Microbial Risk Assessment (QMRA) uses information on the distribution and concentration of particular pathogens and infectivity data to determine risk to public health [Hunter et al. 2003; Haas et al. 1999; ILSI 2000, 1996]. Although QMRA does not preclude the use of source-term and fate and transport models, as demonstrated by Ferguson et al. [2007] and Signor et al. [2007], it has focused most commonly on the receptor location (i.e., exposure point), dose-response relationships, and health impacts, as

prescribed in Haas et al. [1999]. Thus, the full benefit of the QMRA paradigm traditionally has not been realized. Gaber et al. [2008] define integrated modeling as “a systems analysis-based approach to environmental assessment. It includes a set of interdependent science-based components ... capable of simulating the environmental stressor-response relationships relevant to a well specified problem statement.” This paper describes unique attributes of the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) and demonstrates how open-system architecture can link disparate models and databases to support a QMRA application, while addressing multiple microbial source types and organisms that impact downstream receptors.

## **2. FRAMEWORK FOR RISK ANALYSIS IN MULTIMEDIA ENVIRONMENTAL SYSTEMS**

FRAMES standardizes data exchange between models with different Input/Output (I/O) attributes [PNNL 2010]. The operation of the system is controlled by the Application Programming Interface (API) and Framework Development Environment (FDE), which use standardized dictionaries to describe the metadata associated with all data recognized by the system. A DICTIONARY (DIC) file is a comma-delimited text file that contains each parameter’s metadata, including name, description, units, measure (i.e., groupings of units), data type, range, stochastic, and indices (dependency on other parameters) [PNNL 2010]. The FRAMES API handles execution management and file I/O, and provides a series of editors that allows the user to register and operate components with and in the system, and helps facilitate the linking of disparate models. The editors help the user through the model and I/O registration processes. Editors and other tools include:

- DICTIONARY (i.e., DIC) Editor – Registers new or edits existing dictionaries.
- (Units) Conversion Editor – Registers additional or edits existing unit conversions supported by the system and allows legacy models to maintain their current use of units, relegating the responsibility of unit conversion between modules to the system.
- Module (DES) Editor – Registers attributes of the model in the system, such as the model’s icon pictogram; connection schemes with other models; input DICs consumed and output DICs produced by the model; folder location of executables, user interface, and related files; contact information; and software requirements.
- Domain Editor – Registers where the model fits in the system and is composed of a Domain, Group, and Subgroup. A Domain defines a grouping of components (e.g., models, databases, and related components).
- Simulation Editor – Allows the user to edit the Conceptual Site Model (CSM) work space, containing the drag-and-drop functionality of constructing a CSM, linking modules in a sequential order, and managing the sequential execution of the modules (Figure 1). The Simulation Editor is designed to be an intuitive interface for interaction with the CSM diagram and contains four user-interface areas. The upper left provides for a user-defined logo. The bottom left describes the Domain’s icon palette, from which the user chooses models, databases, viewers, or system tools. The top right is the “Global Workspace,” whose output can be accessed by all modules, and the bottom right is the “Local Workspace,” whose data flow is determined by physical connections.
- Data Client Editor (DCE) – Manipulates DICs. Because DICs represent the “monetary” exchange within FRAMES, the DCE can be used 1) as a user-defined module, allowing the user to provide input boundary conditions manually to any module; 2) to provide a relatively simple graphical user interface for those models whose UIs are not FRAMES-compliant; and 3) as a tabular viewer, providing the user with a simple means to view output in table form.
- Lock and Key Features – Allows “lock down” the CSM (i.e., picture containing linked icons), restricted access to certain models, or both, using password protection.
- Plus-Operator – Temporally combines multiple, like outputs, where appropriate, using linear superposition, to create a single input file for consumption by a downstream module (see Figure 1, icon titled “Sum SW Concentrations”).

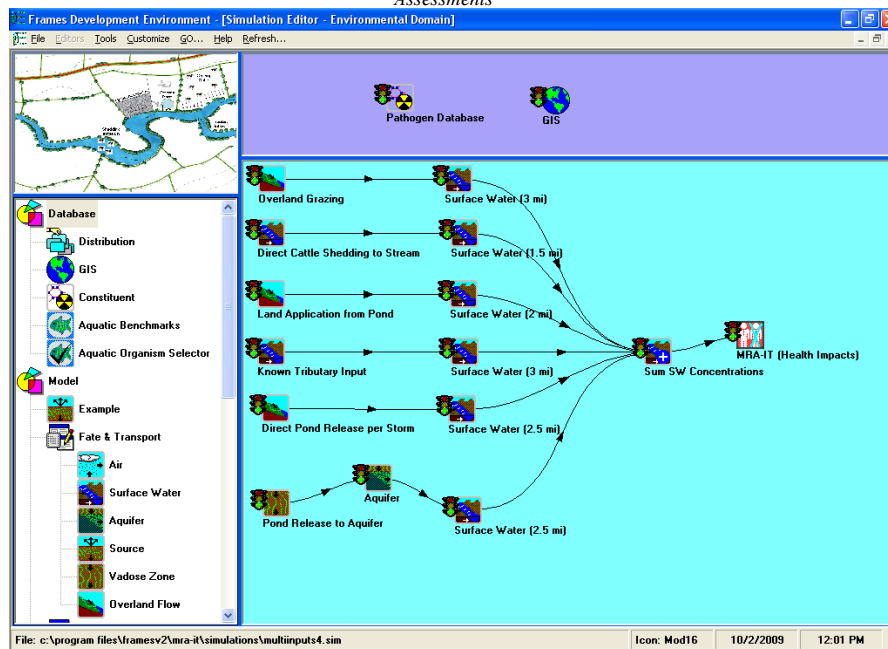


Figure 1. Simulation Editor, depicting the Conceptual Site Model for six source terms and their fate, transport, and health impacts at a receptor location

- Simulation Packager/UnPackager – Packages the entire simulation, so it can be sent to any remote computer, unpackaged, and then executed on that computer containing a compatible version of FRAMES to reproduce the entire simulation.
- Synchronization Operator –Transforms the output from multiple modules and creates new input boundary conditions by ensuring that each time-varying profile for each module output contains values at the same time steps, using linear interpolation to fill times in between time steps.
- Dictionary Registration Tool (DRT) – Uses a spreadsheet formatted to import and register the DICs automatically, while displaying warnings and errors on the status of the process. The DRT is written in Visual Basic for Applications (VBA) for Excel.
- Sensitivity/Uncertainty Modules – Supports Monte Carlo analyses. This module accesses model inputs and allows the user to alias them and assign statistical characteristics (i.e., distribution, correlation, and/or equation) to each. New features are being added, like the statistical package R, maximum likelihood or least-squares model parameter estimation, and the parameter estimation tool PEST.

FRAMES was originally designed to cater to three types of users. Model developers build or import DICs, define units, build/import modules/models, set-up domains, and define connection schemes, and FRAMES supports developers with the Conversion, Dictionary, Domain, and Module Editors. Users/Analysts select Domains and icons, connect icons when building CSMs, select modules/models and databases, populate user interfaces, and execute the CSM, and FRAMES supports users with the Simulation, Data Client, and Module Editors. Database owners map database schema and develop database extraction plans. Another software program, D4EM, now shoulders these responsibilities.

### 3. EXAMPLE APPLICATION

FRAMES is a software structure for implementing an example QMRA that leverages and links disparate models in a unified framework for model integration. Source-to-outcome microbial exposure and risk modeling is demonstrated for an agriculturally contaminated runoff scenario in a conceptual watershed. The example consists of multiple adjacent fecal contamination sources, located within the same watershed.

### 3.1 Description

Six potential, but disparate sources of manure-based pathogen contamination, illustrated in Figure 2, are modeled in this multimedia example: tributary inflow (assumed boundary condition), grazing cattle on an open field (requiring overland runoff modeling), leaching from a waste storage basin (requiring subsurface modeling), pond overflow during precipitation events (inflow equals outflow directly to a stream), land application of disposal-pond contents (requiring overland runoff modeling), and cows directly shedding to the stream. Rainfall events drive contamination from sources related to runoff, while other sources are influenced by agricultural operations and practices. In each case, fecal contamination enters the appropriate stream segment and flows downstream to a recreational location; therefore, all sources require instream modeling. Figure 1 presents a CSM of the six potential disparate sources of manure-based pathogen contamination, routed from their sources to a receptor of concern, with each icon representing a separate model. Assumptions associated with the assessment are summarized in Tables 1 and 2.

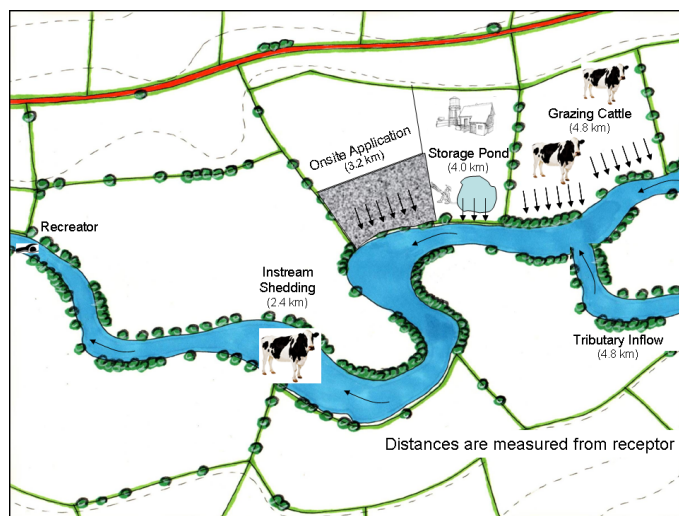


Figure 2. Example Schematic, Describing the Six Source Terms and Receptor

### 3.2 Models

To illustrate the ability of FRAMES to support a QMRA application, a series of reduced-form models, designed and built by different developers, are linked to FRAMES; these cover several components of the QMRA paradigm: source terms (e.g., ponded release), watershed, stream, aquifer, and human exposure/risk. The groundwater and surface water models were previously linked to FRAMES. For this particular effort, new linkages associated with the exposure/risk model and watershed results were performed.

It is assumed that a leak occurs in the disposal pond over 1% of the area. A unit hydraulic gradient is assumed below the pond, resulting in constant outflow to the soil medium [Hillel 1971]. A watershed model, based on kinematic wave theory [Eagleson 1970], was constructed and employed to account for runoff from 1) land application of pond waste and 2) grazing cattle with daily loadings. The watershed model results were exercised, using Data Client Editors (DCEs) within FRAMES. The MEPAS saturated zone model, based on the three-dimensional dispersive, one-dimensional advective equation with inactivation and soil-water partitioning, forms the basis for microbial movement from an area source through a porous medium [Whelan et al. 1999], recognizing that research is still required to more fully understand and substantiate the transport of non-virus pathogens in porous media. The MEPAS surface water model is used in the analysis and is based on a vertically integrated, steady-state solution to the one-dimensional advective, one-dimensional (lateral) dispersive equation with inactivation [Mills et al. 1997].

Table 1. Microbial Characteristics

Parameter	Units	Salmonella	EColi0157	Cryptosporidium	Reference
Inactivation Rate (in soils)	1/d	0.23	0.16	0.04	Soller et al. [2009]
Inactivation (in surface water)	1/d	1.30	0.54	10	Soller et al. [2009]
Distribution Coefficient	mL/g	9	9	9	Pachepsky et al. [2006]
Prevalence	%	10	20	30	Soller et al. [2009]
Tributary Inflow	g/yr	6.00E-03	6.00E-03	1.39E+00	Assumed, 2-day lag
Excretion Density (Log10)	#/g manure	3	2	2	Soller et al. [2009]
Pathogen Pond Concentrations	mg/L	8.85E-03	1.77E-03	6.14E-01	Assumed, after Rogers et al. [2009]

Table 2. Source and Media Characteristics

Parameter	Value	Units	Reference
<b>Animal Characteristics</b>			
Cow Density	5	cow/ha	Duhigg [2009], Butler et al. [2008a]
Number of Cows	360	#	Assumed
Shedding Rate of Cow	24	kg/d	Soller et al. [2009]; Duhigg [2009]; Butler et al. [2008a]
# of Cows Shedding to Stream	36	#	Assumed 10%
<b>Soil Characteristics</b>			
Soil Type	Sandy Loam		Assumed
Land Bulk Density	1.58	g/cm <sup>3</sup>	Meyer et al. [1997]
Land Porosity	0.41	fraction	Meyer et al. [1997]
Saturated Hydraulic Conductivity	1.17E-03	cm/s	Meyer et al. [1997]
<b>Overland Flow Characteristics</b>			
Mannings Constant	1.49		Eagleson [1970]
Mannings Coefficient	0.20		Whelan [1980]
Friction Slope (S <sub>f</sub> )	0.005		Assumed
Precipitation Intensity (i)	9.68	cm/d	NOAA [2009]
Mannings exponent (m)	1.67		Eagleson [1970]
Size of Overland Areas	72.8	ha	Assumed square
Precipitation Events per year	10	#/yr	Assumed
<b>Pond and Land Application Characteristics</b>			
Depth of Pond	3	m	Assumed
Area of Pond	1.44E+03	m <sup>2</sup>	Assumed square
Fraction of Pond that Leaks	0.010	fraction	Assumed
Storage Basin <i>E coli</i> Concentration	3.16E+06	MPN <i>E. coli</i> /100mL	Rogers et al. [2009]
Flow into/out of Pond/event	133	L/d/cow	Duhigg [2009], Butler et al. [2008a]
Pond Land Applications/yr	4	#/yr	Assumed
<b>Groundwater Characteristics</b>			
Soil characteristics			Meyer et al. [1997]
Darcy Velocity	1	cm/d	Assumed
<b>Surface Water Characteristics</b>			
Discharge	42.5	m <sup>3</sup> /s	Assumed
Width	30.5	m	Assumed
Velocity	0.91	m/s	Assumed
<b>Tributary Characteristics</b>			
Lag time	2	d	Assumed
Maximum Tributary Discharge	6.8	m <sup>3</sup> /s	Assumed

Microbial Risk Assessment Interface Tool (MRA-IT) is an open-source, MathCad- and event-based, integrated software tool for characterizing human-health impacts from ingestion of reclaimed water, based on the pathogen of interest, exposure, intake, and dose [Soller and Eisenberg 2008; Soller et al. 2007]. As a stand-alone, it does not contain a fate and transport component, nor does it accept inputs of microbial densities from multiple upstream models. FRAMES provides the upstream fate and transport models and the ability to combine multiple inputs, as illustrated by the “Plus-Operator” (see module titled “Sum SW Concentrations” in Figure 1), forming a time-varying input density curve for consumption by MRA-IT. A pathogen list (i.e., *Salmonella*, *Cryptosporidium*, and *E coli 0157*) is supplied from the FRAMES Constituent Database Selection module. After calculations are complete and output written, the MRA-IT MathCad-based UI presents graphical and tabular results to the user, as with its stand-alone version.

### 3.3 Results and Discussion

Figure 3 presents typical time-varying pathogen densities for the first four rainfall events (i.e., peaks A, B, E, and F) associated with *Cryptosporidium* at the receptor location; the results account for contamination from all six sources, with point C being tributary inflow. These results are very similar to those exhibited by *Salmonella* and *E coli 0157* and are indicative of the entire one-year simulation. This is the density curve exiting from the Plus-Operator module. The only sources contributing to contamination at the receptor at all times are leakage from the Pond and cows shedding directly to the stream (D in Figure 3). Closer inspection of the results indicates that the manure application method (e.g., shedding, spreading, pond leakage, etc.); pathogen rate of release; timing of the manure loading; sequence and type of transporting media; pathogen characteristics (e.g., prevalence, excretion density, inactivation rate, and distribution coefficient); timing of rainfall events; duration and intensity of rainfall; antecedent moisture conditions; and landscape characteristics all play important roles in identifying which source contributes to the contamination and pathogen density at the receptor location, and to what degree.

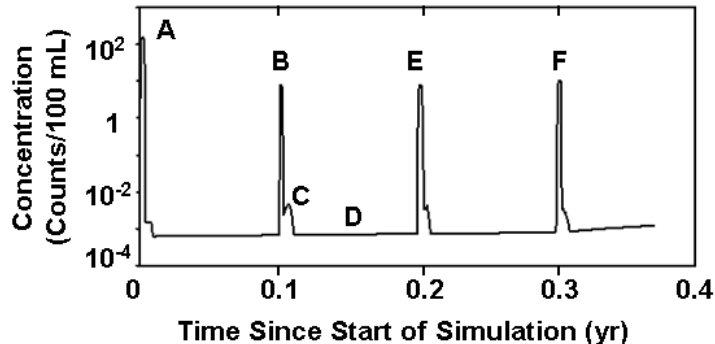


Figure 3. Time-varying *Cryptosporidium* Concentrations at the Receptor location for the First Four Rainfall Events

MRA-IT is used to estimate risks where a receptor potentially is exposed to contaminated water (e.g., swimming for the day at a beach); hence, an event window needs to be defined. In this example, an exposure event was chosen during the recession limb of the pollution hydrograph after the second storm event, and it is assumed to last 1.46 days. Figure 4 presents the time-varying densities associated with *Cryptosporidium*, *E coli 0157*, and *Salmonella* during the event window of 0.102 – 0.106 yr at the receptor. These data represent the input boundary conditions produced by the transport modeling for consumption by MRA-IT. The Monte Carlo-based risk assessment for the three pathogens indicates that the risk for infection to *Cryptosporidium* is slightly larger than that of *E coli 0157* and significantly larger than *Salmonella*. For example, there is a 50% probability of exceeding an individual risk of  $1.4 \times 10^{-4}$  and  $8.0 \times 10^{-5}$  for *Cryptosporidium* and *Salmonella*, respectively, and there is a 10% probability of exceeding an individual risk of  $3.8 \times 10^{-2}$  and  $1.5 \times 10^{-2}$  for *Cryptosporidium* and *Salmonella*, respectively.

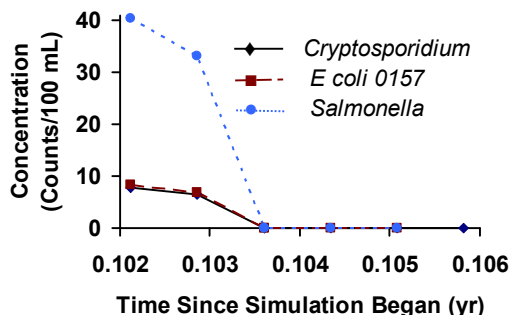


Figure 4. Time-varying Concentrations at Receptor for Event Window 0.102-0.106 yr for *Cryptosporidium*, *E coli 0157*, and *Salmonella*

#### 4. SUMMARY

Quantitative Microbial Risk Assessment (QMRA) is a modeling approach that integrates fate/transport, exposure, and dose-response relationships, to characterize potential health impacts/risks from exposure to pathogenic microorganisms. FRAMES facilitates a user's linkage of disparate models and databases to support a custom assessment and to provide a structure that better leverages the capabilities of QMRA beyond the point of exposure. A series of models and databases were linked to assess six potential sources of manure-based pathogen contamination, thereby simulating the fate, transport, and health impacts from three pathogens to a recreational receptor at a downstream exposure point. By combining fate and transport modeling with point-of-exposure calculations, an analyst can begin to evaluate importance of the components more holistically, including manure application method, pathogen rate of release, timing of the manure loading, sequence and type of transporting media, pathogen characteristics, timing of rainfall events, duration and intensity of rainfall, antecedent moisture conditions, and landscape characteristics. Past user experience (e.g., hazardous or radioactive risk assessments) has indicated that the mechanics of building Conceptual Site Models are straight-forward. Training though is advised for the more involved operations (e.g., registering models, parameters, and connection schemes, and constructing dictionaries), which is not an atypical requirement for a sophisticated modeling system. The user also needs to have some familiarity with the models, as the system takes no responsibility to train the users in their operation.

The views expressed in these Proceedings are those of the individual authors and do not necessarily reflect the views and policies of the United States Environmental Protection Agency. Scientists in EPA have prepared the EPA sections, and those sections have been reviewed in accordance with EPA's peer and administrative review policies and approved for presentation and publication.

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