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The Challenge of Model Implementation of Regulatory Models in Integrated Environmental Modeling Systems

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Abstract: This paper addresses an effort to develop a model for use both as a standalone regulatory model and as an operational module in an integrated modeling framework. As the state of the art of integrated environmental modeling advances, regulators have the opportunity to develop integrated modeling systems that have the capability of providing holistic overviews of potential environmental consequences. However because they are still bound by regulatory requirements, the implementation of regulatory models in integrated environmental modeling systems poses a number of special challenges. The component regulatory model must be able to be 1) documented as a separate entity, 2) implemented and used in a standalone mode, 3) meet the stringent quality control requirements for regulatory applications, 4) and for many applications have an expected operational lifetime on the order of decades. Implementation of a model (new or legacy) in integrated environmental modeling systems is usually accomplished either using direct coding or model wrapper approaches — both of which have major disadvantages for implementing regulatory models. During the process of developing a revised version of a regulatory facility emissions model for use in both standalone and integrated applications, a hybrid model implementation approach was developed. This hybrid approach enabled the authors to create an updated version of a regulatory model that has a single executable that performs both as 1) an independent standalone model and 2) a source-term module in an integrated environmental model system. Although the updated model is in the early stages of regulatory adoption, the experience to date indicate that the hybrid approach is meeting the special needs related to regulatory applications while still being operable in an integrated modeling environment.

Keywords*:* Integrated Modeling; FRAMES; GALE; Data Wrapper; Regulations.

1 INTRODUCTION

In recent years there have been a number of efforts directed at developing integrated environmental modeling systems as well as standards for their implementation (see for example Laniak et. al. (2013) and OpenMI (2014)). The state of the art includes reference models, services-based approaches and standard interfaces. The inclusion of models developed for regulatory purposes into integrated systems is seen in many cases as being highly desirable. Such is the case for the environmental emission model implementation considered in this paper.

With advances in integrated environmental modeling, regulators now have the opportunity to develop new integrated modeling systems that provide holistic overviews of potential environmental consequences. For example, when considering the release and movement of a contaminant through terrestrial and aquatic environments, regulatory emission, transport, and exposure models may be linked in an integrated system. However, the regulators are faced with assuring that these component models continue to meet the special requirements of regulatory activities.

Although focused on regulatory applications, this discussion also applies to models that are used to emulate a self-contained set of processes – models that produce a simulation of a sequence of events. An example would be a model for simulating emission rates from an industrial facility. The specific example considered in this paper is a set of models for estimating annual emissions from operating nuclear power plants.

The U.S. Nuclear Regulatory Commission (NRC) has developed models to estimate the long term airborne and waterborne effluents from operating nuclear power plants (published as NUREGs). These models are used to support calculations for licensing activities as well as for demonstrating operational compliance. NRC is in the process of updating these models and investigating the possibility of incorporation of these models into an integrated source-to-impact modeling environment. An important constraint is that the models they use to support their regulatory activities must be maintained in a form that meets the original regulatory requirements for which they were developed.

In this paper, the term 'regulatory models' is used to broadly refer to computer models developed to support regulatory, or similarly-based, computations. Such models often codify computations needed to support some aspect of guidance documents, regulations, or standards. For example, a model may be used in a licensing application to demonstrate regulatory compliance with some aspect of the applicable licensing regulations. Often once such a model has been developed and tested, the model source code is then codified to clearly define it as compliance tool. In addition, the integrity of such models often must be also maintained over an extended time period. As a result, the use of such a model in an integrated environmental modeling system has special constraints.

In comparison to research applications, many regulatory (or similarly-based) applications require higher levels of quality control for the model computations. A current major challenge to integrated environmental modeling systems is developing methods of conducting quality control for such applications.

The implementation of regulatory models in integrated environmental modeling systems thus poses a number of special challenges – beyond those encountered for research models. In particular, such models have application needs and requirements that must be met for them to be continued to be used as regulatory models. A hybrid model implementation approach has been developed specifically to address the special challenges of such models. The approach enables such models to be used both as independent regulatory models and as integrated environmental research models.

2 REGULATORY MODEL REQUIREMENTS

The spectrum of models that may be incorporated into integrated environmental systems range from 'research models' to 'regulatory models.' The distinction is that the former are models used in research applications and the latter are models that used in computations to support guidance documents, regulations, and standards. Typically research models have versions that are being constantly improved and updated whereby regulatory models typically have fixed/frozen versions. This paper addresses an approach for implementation of regulatory models.

The U.S. Nuclear Regulatory Commission (NRC) model codes for estimating potential routine air and water effluent rates for an operating boiling water reactor (BWR) and pressured water reactor (PWR) are referred to as GALE BWR and GALE PWR codes. As part of an effort to update these models whose original development which was in the 1970s, revised FORTRAN source codes are being developed. In addition to updating the codes to recent regulatory guidance, the revised GALE model source codes will include the capability of operating in an integrated environmental modeling framework called FRAMES (PNNL 2012, Droppo et al 2010, Whelan et al 1997). Calls are to be made in FRAMES V2 application program interface (API) based on data-dictionary files for 1) model input and output data exchanges, 2) initialization of model parameters, and 3) conducting simulations (Gelston et al. 2004).

There are major challenges for versions of regulatory models that are to also be incorporated into an integrated modeling system.

- For use in regulatory applications, a model's source code must be clearly defined such that it will endure in a useable form (for at least a decade), and as such can be codified (i.e., published) in regulations.
- The regulatory model must be implemented in a manner such that it can be easily tested and verified (for quality assurance purposes).

To meet these challenges, the authors propose that an integrated regulatory model must be also able to be used as a standalone model – in a form that is independent of the complexity of the integrated modeling system.

3 MODEL IMPLEMENTATION APPROACHES

A major challenge in the development of a functional integrated modeling framework is being able to design an effective system for incorporating models. There is no one best approach. Instead, there are a variety of approaches that have various strengths and weaknesses. Major considerations for designing a system-specific model incorporation system are related to the origin of models, the approach for linking models, the desired flexibility for model implementations, and limitations related to obtaining the desired level of performance for the integrated modeling system.

When integrating (or connecting) two models together, the challenge is in accurately passing output data from the first model such that it can be used as input data for the second model. Implementation of a model (new or legacy) in integrated environmental modeling systems is usually accomplished either using model wrapper approach or direct coding. Figures 1 and 2 compare the modules and model-to-model information flow associated with using these two approaches.

A model wrapper approach (Figure 1) involves writing external codes to handle input/output activities with the wrapped model. While this approach has been the one of better choices for regulatory models because the unmodified model is in a form that can best meet the regulatory requirements listed above, actual implementations tend to be problematic in that the implementations are relatively fragile. With the occurrence of model and framework updates, they often become non-functional. Also there often are limited ranges of applicability tied to using modeling wrapping approach.

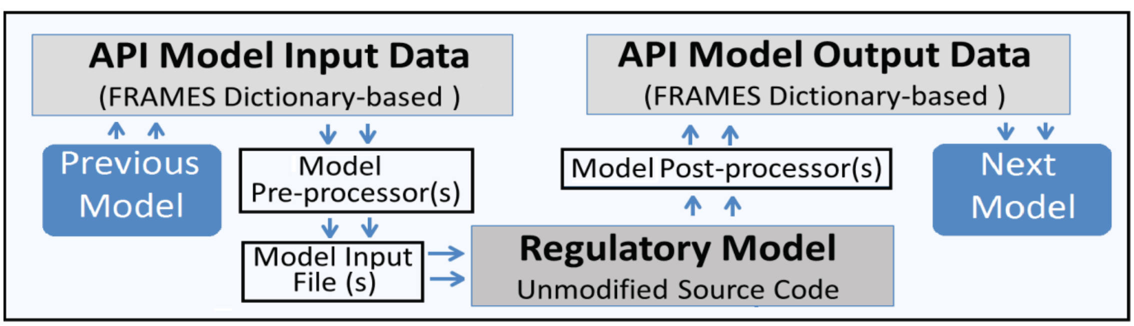

Figure 1. Wrapper-based Model Implementation Approach Schematic

A model wrapper approach was used to implement the legacy and updated versions of the U.S. Nuclear Regulatory Commission's GALE codes in FRAMES (Droppo et al., 2010). Figure 2 shows the step-by-step details on how wrapper-based modeling linking was accomplished. The Figure shows the multiple wrapper modules and intermediate files that were required. The result was an fully functional implementation that involved a fairly complex set of modules and data-exchanges.

The direct coding approach (Figure 3) involves modifying the model's source code to implement the model. This approach typically provides a more robust linking of a model than the model wrapper approach – but such a "hard-wired" model implementation can make the source code and model testing documentation required in regulatory applications difficult to accomplish.

For the updated GALE codes, we were faced with the challenge of developing new codes that both maintained the regulatory advantages of standalone codes (wrapper approach) and provide direct linkages in integrated modeling efforts (direct coding approach). To meet this challenge a hybrid model implementation approach was developed that combines the best features of both the wrapper and direct coding approaches. The approach is based on having both standalone and direct linkage capabilities in each of the updated GALE codes.

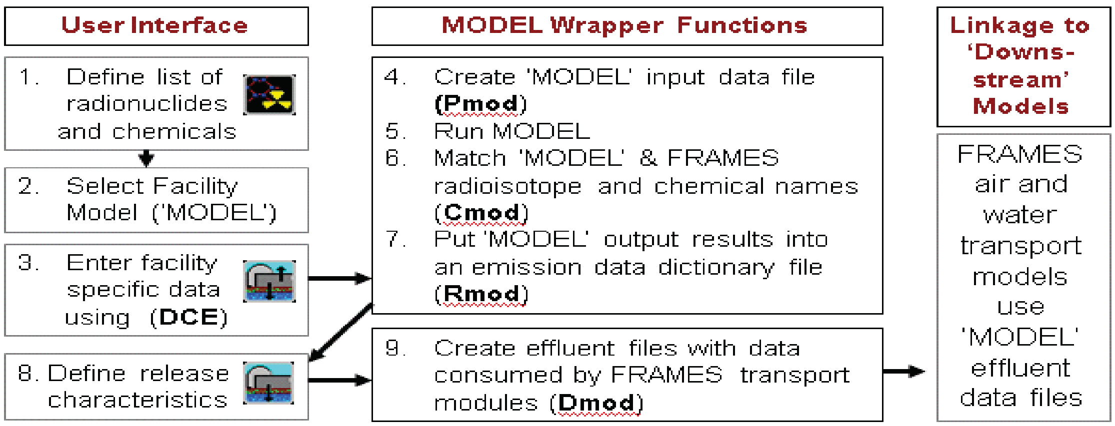

Figure 2. Complex Wrapper-based Implementation of the GALE Models

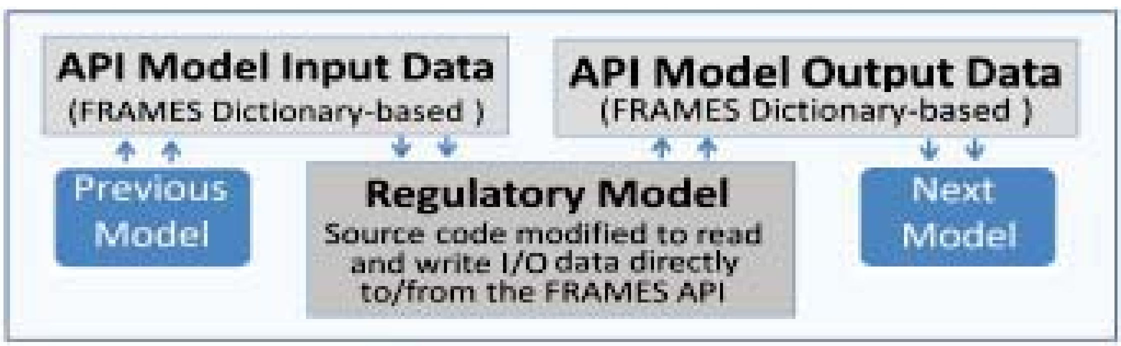

Figure 3. Directly Linked Model Implementation Schematic

The modules and the data exchanges for the hybrid approach are shown in Figure 4. For integrated modeling operations (shown across the lower portion of Figure 4), the hybrid approach uses direct calls with the integrated modeling API to exchange run-time data. For standalone operation (shown across the upper portion of Figure 4), the hybrid approach supports a file-based input-output capability. To minimize the possibility of different model behaviour between integrated and standalone model runs, the same file-based input-output capability is utilized by the GALE codes in both types of runs.

The result of our code integration efforts are revised versions of the GALE codes that work both as 1) research models for use in integrated applications and standalone models for compliance applications. The standalone versions are ideal for licensing and compliance computation – largely because the applications can be made independently of the complexity of the FRAMES modeling platform. On the other hand, the research version implemented in FRAMES provides an ideal platform for developing updated versions of these codes.

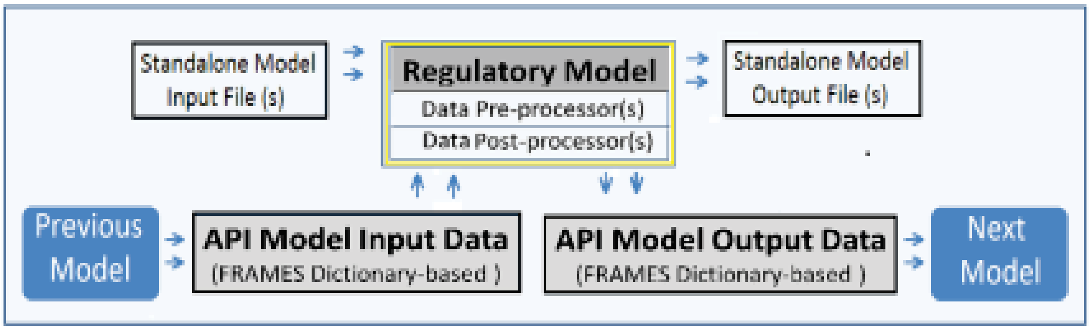

Figure 4. Hybrid Model Implementation in FRAMES

The key aspect of the implementation of the hybrid approach is to carefully separate the model computations source code from the model integration source code. The model computations section of the implemented model source code needs to:

- Be able to be compiled and run as a standalone model outside the integrated modeling system,
- Be used as source code listing that codify model computations in regulations,
- Be able to remain fixed/unmodified over time (that is, not affected by updates/changes to the integrated modeling system), and
- Be implemented in an unmodified form in alternative integrated modeling systems.

The model integration source code section of the source code needs to:

- Define user-interface variables and their properties
- Have 'Input Data Pre-processor(s)'
- Define output variables
- Have an 'Output Data Post-processor(s)'
- Support writing/reading of data to/from the FRAMES API
- Have replaceable code for model implementation in an alternative integrated modeling system.

Note that the hybrid approach does not propose to use an unmodified legacy code – but instead to use a new version of model (regulatory computations section of source code) that is updated to allow the required integrated modeling data exchanges (model implementation section of source code). The separation of data transfer components from computation will allow the use of common ETL tools to achieve the former.

An important distinction between the contents of these two source code sections from a quality assurance standpoint is that all computations are done in the first section and only data exchanges are performed in the second section. Different quality assurance requirements will apply for the different functionalities. In general, a higher level of quality assurance is required for codes that do computations.

A comparison of the direct, wrapper, and hybrid linkage approaches shows only the wrapper and hybrid linkage meet the regulatory need to maintain an independent capability of doing computations with the model. In addition, the hybrid linkage greatly simplified the complexity of conducting the linkage by consolation of the linkage activities within model source code.

An additional benefit of the hybrid linkage was the ability to easily load data from the model source code back to the FRAMES API within the data pre-processor. This capability was used to allow the user the option of loading hard-codified model default values into the FRAMES user data input interfaces.

4 CONCLUSIONS

The near term need is to allow the use of regulatory models both as standalone compliance versions and as integrated model system versions. The hybrid implementation approach meets that need without creating a complex system of interacting modules and files. The one model executable file runs in both integrated systems and standalone mode.

In terms of the major challenges for regulatory models, the proposed approach will help ensure that the model's computation source code can endure in a useable form once it has been codified in guidance, regulations, or standards. The key is the clear separation of the source code into model computations and data-transfer sections. This approach means that the code version can be easily run (as well as tested and verified) as a standalone model that runs independently of the integrated modeling system. Such a capability for the model computation code section is needed both for quality assurance as well as for compliance computations.

The hybrid model implementation approach supports the capability of an implemented model to be run both 1) as a standalone model and 2) as an integrated model. While developed specially for regulatory model applications, the approach has broader applications for situations where it is desirable to be able to run implemented models in both modes. This capability will be needed for future integrated regulatory systems that address the performance of holistic systems.
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