

Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

Disclaimer:

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U. S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

- 1) warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
- 2) representation that such use or results of such use would not infringe privately owned rights; or
- 3) endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.

**Integrating Regulatory, Programmatic and Technical Needs
for Modeling Tools to Support Decision-Making - 15219**

Roger Seitz^{*}, Paul Dixon^{**}, Justin Marble^{***}, Patricia Lee^{***}, and Mark Freshley^{****}

^{*} Savannah River National Laboratory, Savannah River Site, Bldg 773-43A, Aiken, SC 29808

^{**} Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87544

^{***} Department of Energy, Office of Environmental Management, 19901 Germantown Road,
Germantown, MD 20874-1290

^{****} Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99352

ABSTRACT

The U.S. Department of Energy (USDOE) Office of Environmental Management (EM), Office of Soil and Groundwater Remediation, is supporting development of the Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM provides a modeling workflow to support decision-making for site restoration, tank closure and waste management activities. Potential users involved in regulatory applications (e.g., performance and risk assessments and other activities supporting regulatory decisions) are a key target group for the toolset. Decision-making in these applications often requires consideration of multiple perspectives, including: regulators and the public, oversight and project management personnel, as well as practitioners involved in conducting the calculations, each with different interests.

From its inception, a key objective of the ASCEM project has been to actively seek input from these different user perspectives to help guide development. ASCEM formed a User Steering Committee (USC) with membership representing interests from management/staff at DOE Site Contractors, DOE-HQ and Field offices and Regulators (State and Federal). The project also provides opportunities for input from the broader user community through participation in meetings of the Performance & Risk Assessment (P&RA) Community of Practice (CoP), routine briefings and participation in meetings of the Low-Level Waste Disposal Facility Federal Review Group, and direct interactions with users involved in regulatory applications. Interactions with users involved in regulatory applications have influenced the requirements for the toolsets and are reflected in capabilities that have been and are being implemented.

INTRODUCTION

USDOE-EM, Office of Soil and Groundwater Remediation, is supporting development and implementation of a next generation workflow and modeling toolset to support decision-making via the ASCEM project [1,2,3]. End-user involvement has been an area of emphasis for the ASCEM team from the beginning of the project [4,5]. Early interactions with the team lead to the development of the initial requirements for the development of ASCEM. In addition, it was noted early in the development of ASCEM that frequent and consistent engagement is seen as critical to developing user acceptance and eventual deployment and application of the ASCEM toolsets at DOE sites. In the interest of seeking broad appeal for the developing tools, efforts have specifically targeted different classes of end-users recognizing their differing interests and needs. For the purposes of targeted interactions, three general categories of regulatory users have been identified: Performance Assessment (PA) and Risk Assessment (RA) practitioners, programmatic decision-makers and oversight personnel, and regulators who are engaged in the USDOE cleanup mission (see Fig. 1). The ASCEM team has sought to identify and implement capabilities and features that are of interest to all of these users.

There have been consistent interactions with the broader USDOE community, including researchers and USDOE staff involved in Office of Science and Office of Nuclear Energy activities. These interactions provide opportunities for sharing of collaborative development approaches that can be leveraged to

enhance capabilities in ASCEM in a cost effective manner. Consistent with recommendations from user interactions to date, user engagement includes a combination of direct outreach, including site-specific applications to provide experience working with the ASCEM tools, and engagement with regulators and management to gain their perspectives. The site-specific interactions provide the opportunity to identify and test specific capabilities that a site may need and demonstrate potential benefits of the use of ASCEM. These interactions are geared towards leading to a transition from code and toolset development towards more site contractors actively working with ASCEM. Examples of this targeted outreach are provided in separate papers [2, 3]. This paper includes a summary of the approaches that have been used to engage with the regulatory applications user community as ASCEM has matured and examples of feedback from those interactions to illustrate different interests.

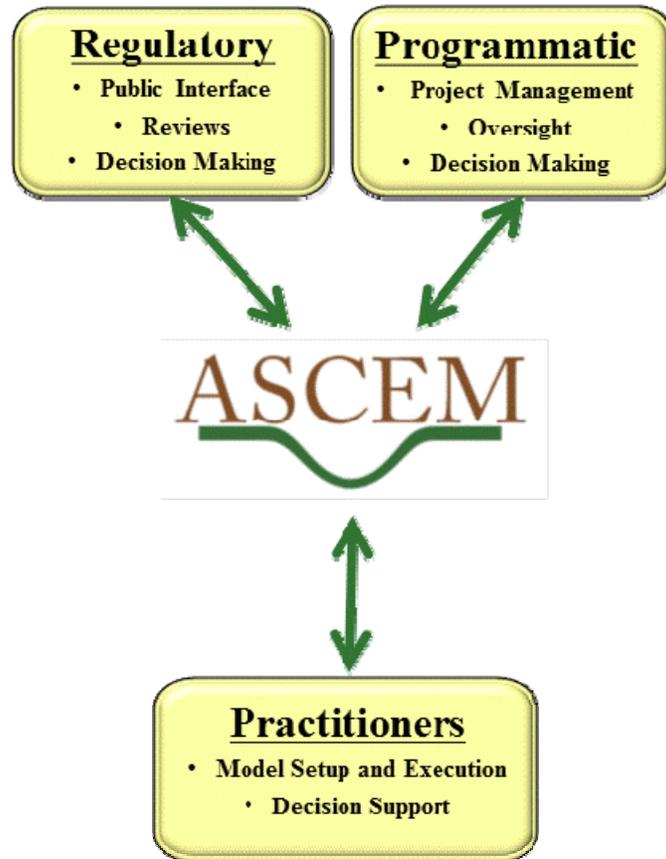


Fig. 1. General Perspectives of Targeted Users for the ASCEM Project.

SEEKING INPUT

ASCEM has taken a proactive approach to engage with potential regulatory users with the intent to make the regulatory user community part of the process as the tools are developed. This provides the opportunity to include features that will encourage users to want to use the new tools. The interactions have increasingly emphasized how the tools are being designed to help the different classes of users address their specific needs. Three primary audiences have consistently been involved from the beginning of ASCEM and a number of other *ad hoc* interactions continue to be pursued. The first audience is the User Steering Committee (USC) [6] directly reporting to the ASCEM management team. The USC was formed as a formal mechanism for the project to obtain input. The other two other groups represent the

broader user community: the DOE Low-level Waste Disposal Facility Federal Review Group (LFRG) and P&RA CoP.

As mentioned above, ASCEM also maintains routine interactions on USDOE Office of Science and Office of Nuclear Energy activities related to advanced modeling from the perspective of leveraging and sharing needs. ASCEM has also engaged with other groups involved with decision making on site restoration activities, including local stakeholders, the Interstate Technology and Regulatory Council (ITRC), and other government and industry groups. The ASCEM team also maintains active ties to activities associated with development and review of PAs around the DOE complex. Examples of interactions are provided below.

ASCEM User Steering Committee

The USC was formed at the beginning of the project to provide a formal mechanism for the ASCEM management team to seek feedback regarding the interests of the user community with responsibility for PA and RA efforts around the USDOE complex. The USC provides a higher-level forum to obtain input that will help encourage deployment and implementation. The USC was selected to represent specific interests from management and key technical staff at USDOE site contractors, regulators and USDOE Organizations that will be involved in application and review of analyses (see Table I). The members of the USC help to identify opportunities for applications of the tools, identify potential hurdles to implementation, provide suggestions regarding how to address those hurdles, and provide feedback and perspective from the view of those that will have to make decisions based on the results of modeling efforts.

ASCEM has interacted with the USC via a combination of face-to-face meetings and webinars. Generally, the meetings include an update on the status of the project, discussion of current capabilities and have also included demonstrations of the developing tools. The primary purpose of the meetings has been to seek feedback from the members of the committee and gain their insights to improve the future appeal of ASCEM. Members of the USC have also provided suggestions regarding potential applications for testing and demonstration. The USC has also provided formal written recommendations for the management team to consider during planning.

TABLE I. Organizations currently represented on ASCEM USC

Bechtel National, Gov't Services – Environmental (Chair)
Savannah River National Laboratory (ASCEM Liaison)
US NRC, Performance Assessment Branch
DOE EM, Co-Chair of the LFRG
DOE Office of Environment, Health, Safety and Security
Los Alamos, Environmental Programs
Washington Dept. Of Ecology
Hanford, CHPRC and WRPS
DOE Oak Ridge
DOE Portsmouth Paducah Project Office
Savannah River, SRNS and SRR
DOE Nevada National Security Site
DOE EM, Office of Tank Waste Management
DOE EM, Office of Soil & Groundwater

The USC has provided a number of recommendations both formally and informally that contributed to development efforts and are reflected in the current approach. The recommendations have largely focused on fostering engagement with the user community and thus helping to gain acceptance. The USC has encouraged the ASCEM team to seek out opportunities to deploy the tools to demonstrate capabilities for on-going EM work and provided input regarding potential applications that could be pursued. ASCEM has used working groups as a means start this process (e.g., [1,2,3]). These applications demonstrate the developing capabilities and their value to support improved decision-making and also serve as testing opportunities. The committee also emphasized the importance of engaging directly with end users and regulators so they can experience firsthand, the benefits of ASCEM. The outreach activities described below, working directly with users at Savannah River and Hanford are examples of initial ASCEM implementation of these recommendations. The project is also engaged with the ITRC to share information with the regulator community.

The USC has also provided programmatic suggestions, such as the need to identify near term goals to continually demonstrate progress towards deployment of the tools. Engagement with the USC has provided a means for the project to obtain direct and candid feedback from people that would be involved in decision-making related to site cleanup and waste disposal activities and selection of modeling tools that would be used for those efforts.

Performance Assessment and Risk Assessment Community of Practice

The P&RA CoP, formerly the PA CoP, provides a forum for PA and RA practitioners to share information on on-going activities related to regulatory applications. Participants in the CoP cover the whole spectrum of potential users (i.e., programmatic, regulatory and practitioners). In the past, the PA CoP involved annual technical exchanges including presentations on a variety of topics of current interest to the PA and RA community [7]. The P&RA CoP has recently expanded to include topical webinars in addition to annual technical exchanges.

The ASCEM project has actively participated in the PA&RA CoP, including serving on the Steering Committee and providing presentations about ASCEM development and applications. Early in the ASCEM project, the CoP technical exchanges provided an important opportunity to present the plans for ASCEM and to seek input regarding desirable features for the new tools. At one CoP exchange, panel sessions were held with a group of regulators and a group of practitioners to identify their areas of interest for new modeling tools. Another technical exchange featured presentations about the status and plans for the ASCEM tools. A number of suggestions were obtained from that meeting (see Table II). ASCEM received many valuable suggestions from these interactions that are reflected in the current capabilities (e.g., [7]). The panel sessions tended to address higher level considerations associated with decision-making. When users were interviewed directly, there were more insights into specific modeling needs (see discussion later in this paper). The following paragraphs include a few examples of suggestions from the panel discussions, many of which have been addressed in the current tools.

TABLE II. Examples of topical suggestions from a PA CoP technical exchange

- | |
|---|
| <ul style="list-style-type: none">• Address prospective challenges – consider modeling needs for major EM challenges• Integrated approach – modeling and field/lab activities (data, characterization, monitoring, etc.)• Compatibility and ease of use – transparency, range of users, existing accepted tools• Range of complexity – graded approach, add detail when needed• Source term – barriers, waste forms• Exploit computing advances – leverage high performance computing to consider added detail• Involve users and decision makers to gain acceptance• Address exposure assessment – ability to consider exposure via multiple pathways and dose/risk |
|---|

The regulator panel emphasized the importance of being able to effectively communicate the basis for decision making. Visualization, such as plume maps and movies of simulations, has been particularly effective for public communication to help explain often complex topics in a more understandable manner. Integration of data/monitoring activities and modeling has also been an important consideration with a view towards demonstrating a thoughtful process that is informed by both data and models. Advanced visualization capabilities have been an important focus for development of the ASCEM tools and examples of those capabilities are routinely used for presentations and papers (e.g., [1,2,3,8]).

There was also a desire for transparency where regulators are able to independently work with the modeling tools that are used for decision making. In this case, the emphasis is less on actually setting up new models, but more focused on interrogating existing models to identify the basis for assumptions and perhaps varying individual parameters to gain insights. “Player” versions of models were mentioned. The panel also encouraged a graded approach to modeling, where relatively simple approaches can be used when adequate for a decision, but more complexity and detail can be added, when needed, to help support improved decision making on the more complex challenges around the DOE Complex. The server-based structure implemented for ASCEM provides an integrated framework linking data management and the modeling tools to provide for improved transparency [1].

Emphasis was placed on using models not only to help decision-making at the end of the process, but also to support decision making regarding what is important in the model and prioritizing data collection in those areas. The importance of demonstrating an understanding of the system was also a topic of much discussion. Sensitivity and uncertainty analysis tools are included in ASCEM that provide the capability to gain insights into the dominant assumptions in a model and to develop a better understanding of the uncertainties and the assumptions that most contribute to the uncertainty.

Low-Level Disposal Facility Federal Review Group

The DOE-EM LFRG is the organization that provides oversight of DOE disposal facilities and the PAs that are conducted as part of the process to obtain the Disposal Authorization for operation of a facility. The LFRG also serves a forum for exchange of information between the sites involved in waste disposal. The LFRG reflects the views of DOE’s regulatory authority, programmatic oversight as well as practitioners, which provides a good cross-section of interests to provide input for ASCEM. ASCEM provides routine briefings to this group and maintains active involvement in their activities. This provides the opportunity to maintain awareness of current challenges and needs for this community. The LFRG has provided feedback to the ASCEM project during the briefings and as part of interviews that have been conducted with users. This feedback is included as part of the overall summary provided later in this paper.

End-users responsible for PAs and composite analyses at DOE sites are required to generate maintenance plans and annual reports upon receiving a Disposal Authorization Statement. The LFRG representatives also review these documents on an annual basis. The maintenance plans outline commitments for activities intended to help address uncertainties associated with PAs and long-term performance of a disposal facility. Routine maintenance activities include surveillance and monitoring at the facility, comparing monitoring results with model results, and special analyses to address unique waste disposal requests not directly addressed in the PA. Other maintenance activities are a direct result of the LFRG and NRC review findings. Examples of these types of maintenance activities include: laboratory studies to confirm assumptions about material properties, demonstrations/experiments to confirm or refine assumptions for key parameters, improved sensitivity and uncertainty analyses, and geochemical assumptions (e.g., solubility, sorption). These types of activities reflect areas where further work was deemed necessary by reviewers and are good indicators for potential ASCEM needs.

Direct Outreach with Site Users

The ASCEM project conducted focused user outreach sessions for the Research and Development Release of ASCEM. The purpose of the outreach sessions was to engage directly with end users and provide an opportunity for hands-on experience with the ASCEM toolsets. The outreach also provided an opportunity to receive direct feedback regarding the tools. Outreach sessions were conducted at the Hanford Site in Richland, Washington and at the Savannah River Site (SRS) in Aiken, South Carolina. Additional more focused user interactions occurred at Lawrence Berkeley National Laboratory and at Los Alamos National Laboratory. In addition, an international project in Argentina funded through DOE EM included an outreach session in Buenos Aires, Argentina and there have been interactions with staff at the Chalk River Laboratories in Canada.

Both the Hanford and SRS outreach sessions were well attended and included participants from DOE, national laboratories, and site contractors responsible for modeling and simulation. At both sessions, an introduction to the ASCEM toolset was provided as well as a demonstration of using Akuna and the associated utilities. Following the introduction, the ASCEM team led participants through hands-on use of model setup and executing a single run. The UQ and SA toolsets were explored as well as visualization in Akuna. Open sessions were conducted with further exploration of the toolsets as well as discussion and feedback from the users. The users appreciated the direct outreach sessions and the opportunity to gain hands-on experience with the tools.

As would be expected, hands-on experience during the outreach sessions resulted in very specific feedback to the ASCEM team by participants with suggestions for capabilities and functionality. In the area of capabilities, examples of some of this specific feedback included: support for the concept of file-read capabilities for incorporating current models and data, the ability to echo or print a listing of model inputs for QA, integration of unstructured mesh development with model setup, and importing multiple overlapping data and mesh features. In the area of functionality, examples of feedback included: a need for alerts when input is needed or errors in inputs are observed, ability to check job queue status, need to install and run standalone versions of the full set of ASCEM tools on their local systems for sensitive applications, desire to view parameter values in traditional units, and a variety of suggestions for graphical output capabilities. Many of these specific recommendations have already been implemented.

Examples of Other Interactions

The ASCEM team continues to seek input in a variety of different ways in addition to the three main areas described above. There are continuing discussions at a working level with practitioners and oversight personnel involved in PA and RA modeling activities around the DOE Complex. These tend to be more informal and often in the course of other work in which the ASCEM team is involved. Nevertheless, these direct interactions often provide the most specific indication of the day-to-day needs to be considered for ASCEM. As mentioned earlier, ASCEM also directly supports working group activities that provide the opportunity to apply and test the tools on specific applications at SRS, NTS and for waste tank performance assessment. This work is discussed in more detail in separate papers [1, 2, 3].

The ASCEM team also maintains ties with other advanced modeling groups within the USDOE (NE: NEAMS and CASL). This interaction is primarily through Advanced Computing Tech Team (ACTT) bi-monthly meetings where computing topics of mutual interest are discussed and program updates presented. In addition the ASCEM team closely interacts with the USDOE Office of Science and Office of Nuclear Energy in the areas of Biological and Environmental Research and advanced computing. These interactions serve as a means to leverage mutually beneficial research developments and share information about ASCEM. Also, it provides a venue for insights into current activities that may be

leveraged for capabilities in ASCEM. ASCEM team members are also active participants in other crossover USDOE Office of Science activities.

As ASCEM has matured, the team has increased efforts on targeted presentations for stakeholders and regulators at a local level as well as industry groups involved in site restoration activities. There have been a number of presentations including the EM Advisory Board, local Citizen's Advisory Boards, State regulators and other stakeholders to share information about ASCEM and how it can be used to improve decision making. ASCEM has also engaged with organizations like the Electric Power Research Institute, Federal Remediation Technologies Roundtable, and the ITRC. There have also been presentations for the international community (e.g., International Atomic Energy Agency and international conferences). These presentations are used to provide more opportunities to build interest and seek feedback and input about the features/capabilities of interest from user communities beyond the DOE.

FEEDBACK

The ASCEM team has received large amounts of feedback via these different interactions. The feedback has ranged from very specific suggestions regarding individual components of the tools to higher level suggestions intended to steer the project in productive directions and identify key areas of interest. This feedback is considered by the project leadership and has proven to be very valuable to help guide development of the tools. Many of the capabilities that have been incorporated into the tools directly reflect input and suggestions that have been received. The current capabilities of the ASCEM tools are described in more detail in [1,8].

Many high-level suggestions are common to different user groups. These areas of interest were identified early in the project and have been reinforced as the project has proceeded. The importance of recognizing the role of modeling to specifically support regulatory decision-making has been a recurring theme that is the driver for many of the interests of the regulatory applications user community. Important considerations towards that end that have been addressed during development and are provided in the ASCEM tools include a need for:

- flexible modeling tools that can be applied in a graded manner depending on the level of detail needed to support a decision,
- advanced computing capability to allow for efficient consideration of additional details and avoid the need to compromise with simplifying assumptions and potential over-conservatism,
- integrated sensitivity and uncertainty analysis capabilities to provide a better understanding of the uncertainties and assumptions that drive those uncertainties,
- visualization tools to help explain complex information in a manner that is understandable to a variety of stakeholders,
- data management tools to provide transparency of assumptions and sources of information and facilitate integration of model setup and results with characterization and monitoring information, and
- user friendly interface and collaborative environment to provide accessibility for a variety of users with different interests (e.g., practitioners, reviewers).

Each of these topics has proven to be an important consideration and has influenced the design and approach reflected in the ASCEM workflow. The ASCEM user needs reports [4,5] provide a more comprehensive summary of higher-level and very specific suggestions that have been received. Likewise, the 2011 PA CoP Technical Exchange summary [7] also documents areas of interest from the regulatory applications user community discussed during the panel sessions.

CONCLUSIONS

Actively engaging end-users and decision-makers in the development process for ASCEM was recognized as a critical need from the inception of the project. Significant emphasis has been placed on developing a tool that is focused on user needs as well as improving the modeling capabilities that are currently available. This approach is targeted at helping to enhance user acceptance of the tools prior to implementation. It was recognized early in the project that there are different classes of users that have differing priorities in terms of capabilities. From a general perspective, ASCEM has considered three different classes of users (regulatory, programmatic and practitioner). The project has deliberately sought opportunities to engage with groups that reflect these different interests in order to address the broad range of needs from the community. It was interesting to find that there were many high-level considerations that were of common interest across the different groups, although with somewhat different focus.

Collaborations with other DOE and industry organizations have also been recognized as an important aspect of the project. There are two key benefits from these collaborations: obtaining input from a broader population of users with different interests and also identifying opportunities for leveraging efforts that have already been completed and site-specific opportunities to demonstrate and test the capabilities of the tools. A number of the ASCEM tools are derived from existing tools that have been developed in other organizations. These interactions have helped the ASCEM team to better understand the interests and priorities of users and have helped to guide development of capabilities that are targeted to those needs.

REFERENCES

1. Dixon, P. et al., 2015, “Advanced Simulation Capability for Environmental Management, Integrated Toolsets and Simulator to Enhance Public Communication,” Proceedings of Waste Management ’15, March 15-19, 2015, Phoenix, AZ.
2. Freshley, M. et al., 2015, “Collaborating with End Users to Add Realism in Performance Assessments,” Proceedings of Waste Management ’15, March 15-19, 2015, Phoenix, AZ.
3. Wainwright, H. et al., 2015, “Using ASCEM Modeling and Visualization to Inform Stakeholders of Contaminant Plume Evolution and Remediation Efficacy at F-Basin Savannah River Site,” Proceedings of Waste Management ’15, March 15-19, 2015, Phoenix, AZ.
4. Seitz, R. et al., 2010, “User Suggestions and State of Practice for Development of ASCEM Requirements,” ASCEM-SITE-2010-02-1, Advanced Simulation Capability for Environmental Management, United States Department of Energy, Germantown, MD.
5. Seitz, R. et al., 2011, “ASCEM User Needs Report – FY 2011,” ASCEM-SITE-11-02, Advanced Simulation Capability for Environmental Management, United States Department of Energy, Germantown, MD.
6. USDOE, 2010, “ASCEM User Steering Committee Charter,” ASCEM-PM-2010-02-1, Advanced Simulation Capability for Environmental Management, United States Department of Energy, Germantown, MD.
7. Seitz, R. et al., 2011, “2011 Performance Assessment Community of Practice Technical Exchange – Summary,” SRNL-STI-2011-00752, Savannah River National Laboratory, Aiken, SC.

8. Freedman VL, X Chen, SA Finsterle, MD Freshley, I Gorton, LJ Gosink, E Keating, C Lansing, WAM Moeglein, CJ Murray, GSH Pau, EA Porter, S Purohit, ML Rockhold, KL Schuchardt, C Sivaramakrishnan, VV Vesselinov, and SR Waichler. 2014. "A high-performance workflow system for subsurface simulation." *Environmental Modelling & Software* 55:176-189. doi:10.1016/j.envsoft.2014.01.030