INL/EXT-14-31935

OSPREY Model Development Progress Update to Support Transmittal to ORNL for Evaluation

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April 2014

The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

INL/EXT-14-31935

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Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

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Fuel Cycle Research & Development

Prepared for
U.S. Department of Energy
Separations and Waste Forms

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April 30, 2014

FCRD-SWF-2014-000458

SUMMARY

During the processing of used nuclear fuel, volatile radionuclides will be discharged to the atmosphere if no recovery processes are in place to limit their release. The volatile radionuclides of concern are ^{3}H, ^{14}C, ^{85}Kr, and ^{129}I. Methods are being developed, via adsorption and absorption unit operations, to capture these radionuclides. It is necessary to model these unit operations to aid in the evaluation of technologies and in the future development of an advanced used nuclear fuel processing plant. A collaboration between Fuel Cycle Research and Development Off-gas Sigma Team member INL and a NEUP grant including ORNL, Syracuse University, and Georgia Institute of Technology has been formed to develop off-gas models and support off-gas research. Georgia Institute of Technology is developing fundamental level model to describe the equilibrium and kinetics of the adsorption process, which are to be integrated with OSPREY. This report discusses the progress made on expanding OSPREY to be multiple components and the integration of macroscale and microscale level models. This update is being provided in conjunction with the transmittal of the OSPREY model to ORNL for evaluation. Also included in this report is a brief OSPREY user guide, which includes both how to initially gain access to OSPREY and how to use the model.

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ACRONYMS

INL	Idaho National Laboratory
UNF	Used Nuclear Fuel
ORNL	Oak Ridge National Laboratory
SU	Syracuse University
GIT	Georgia Institute of Technology
MOOSE	Multi Object Oriented Simulation Environment
OSPREY	Off-gas SeParation and RecoverY
NEUP	Nuclear Energy University Program

OSPREY Model Development Progress Update to Support Transmittal to ORNL for Evaluation

1. Introduction

The reprocessing of used nuclear fuel (UNF) generates off-gas containing several radioactive gases including $^{129}I_2$, ^{85}Kr, $^{3}H_2O$, and $^{14}CO_2$. The unit operations of adsorption and absorption are being developed for the removal of these off-gas constituents. It is necessary to model complex series of unit operations simulating the off-gas treatment system of a UNF reprocessing facility. These simulations will aid in the future design of advanced U.S. reprocessing plants as well as minimize waste, proliferation risk, environmental impact, process complexity and cost.

Currently, a generic dynamic adsorption model has been developed within Multi-physics Object Oriented Simulation Environment (MOOSE) developed at the Idaho National Laboratory (INL). Off-gas Separation and Recovery (OSPREY), a module generated within MOOSE, models the adsorption of off-gas constituents for dispersed plug flow in a packed bed under non-isothermal and non-isobaric conditions. Inputs to the model include gas composition, sorbent and column properties, equilibrium and kinetic data, and inlet conditions. The simulation outputs component concentrations along the column length as a function of time from which breakthrough data can be obtained. The breakthrough data can be used to determine bed capacity, which in turn can be used to size columns. The model also predicts temperature along the column length as a function of time and pressure drop along the column length.

OSPREY is a generic, dynamic adsorption model in which the user can change all parameters and species in order to simulate user specific systems. Submodels for simulating species-specific models are being developed within OSPREY for model development and validation. Experimental data collected at the INL and system parameters were input into the adsorption model to develop a model specific for krypton adsorption. A collaboration between Fuel Cycle Research and Development Off-gas Sigma Team member INL and a Nuclear Enegery University Program (NEUP) grant including ORNL, Syracuse University (SU), and Georgia Institute of Technology (GIT) has been formed to develop off-gas models and support off-gas research. Through this collaboration, OSPREY, a macroscale level model, is being integrated with microscale level models being developed at GIT to describe the equilibrium and kinetics of the system. This collaboration also aided in developing an initial tritium specific model and continues to aid in further developing this model.

In support of the DOE Fuel Cycle Research and Development Off-gas Sigma Team and the afore mentioned NEUP grant including, the OSPREY model is being provided to ORNL for evaluation. The delivery of this report, which supports the transmittal of OSPREY to ORNL for evaluation, satisfies milestones M4FT-14IN0312019.

2. Purpose and Scope

The purpose of this work was to update, maintain, and improve OSPREY as more data became available, integrate the Sigma Off-gas Team INL modeling effort with the NEUP grant off-gas modeling efforts, and provide the model to ORNL for evaluation. This report discusses the progress made on expanding OSPREY to be multiple components and the integration of macroscale and microscale level models. Also included in this report is a brief OSPREY user guide.

OSPREY has been modified to be multiple components. The user can now specify the number of components in a system and whether or not each component adsorbs. Integration of OSPREY and GIT's fundamental level models for kinetics and equilibrium predictions has been initiated. This integration of GIT and INL models, when fully complete, will allow for a much more flexible and higher level simulation capability for predicting behavior of off-gas adsorption.

3. OSPREY Progress, Status Update, and Ongoing Efforts

The OSPREY model is a generalized macroscale level model because the governing equations are generalized for adsorption and do not change based on the gas/sorbent system. A detailed description of the OSPREY model was previously reported[1]. It was initially developed and validated using data specific for krypton adsorption on hydrogen mordenite. In addition to this, the model has recently been verified, on a very simplistic and basic level utilizing the advection diffusion equation (Equation 1), in which there is no adsorption occurring.

$$\frac{\partial c_i}{\partial t} = D_{zi}\frac{\partial^2 c_i}{\partial z^2} - v\frac{\partial c_i}{\partial z};\ z \in (0, L) \qquad \textbf{Equation 1}$$

For verification, the OSPREY output was compared to an analytical solution for equation 1, shown in Figure 1.

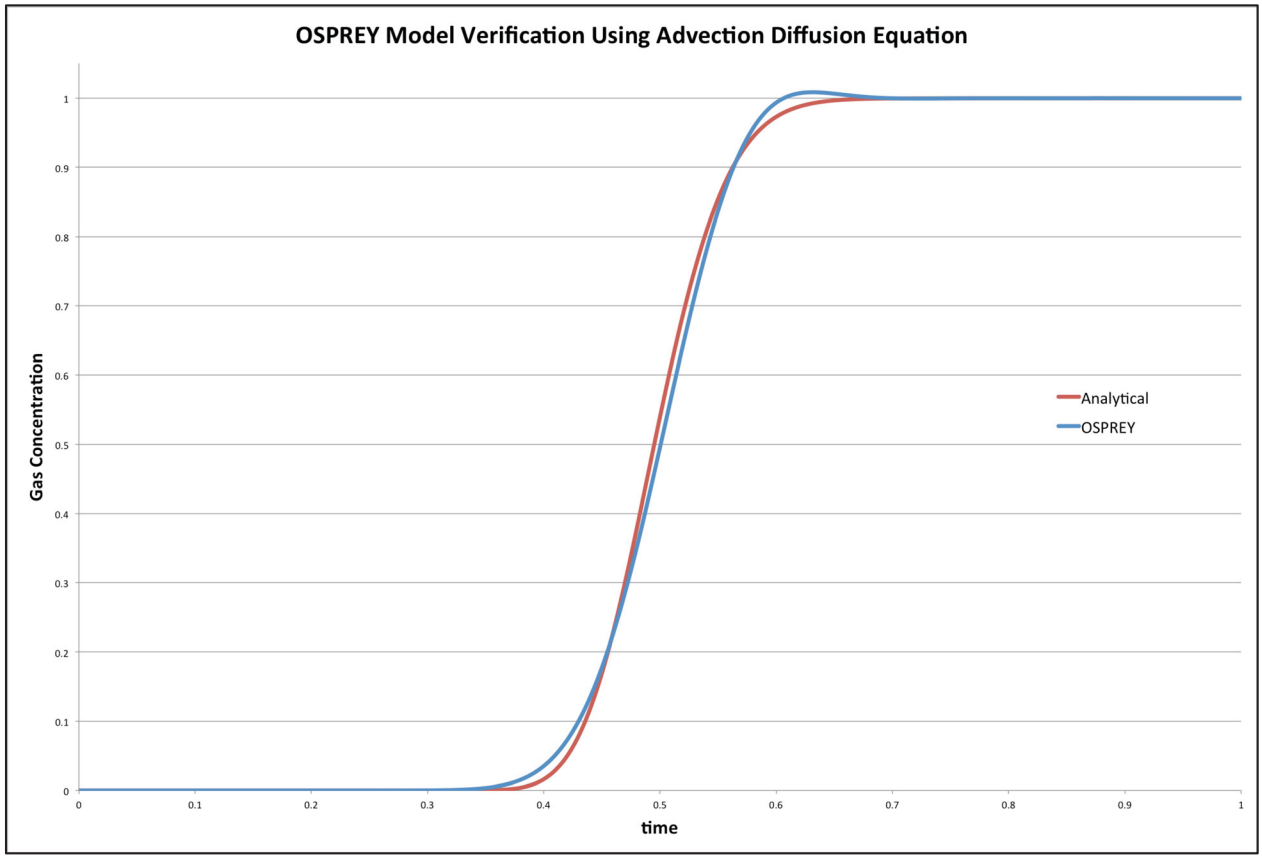

Figure 1: Advection Diffusion verification of the OSPREY model.

The analytical solution of the advection diffusion equation was obtained from literature[2] and is valid for the same boundary conditions as used in OSPREY. Results from OSPREY show that there is more diffusion occurring in the simulation than in the analytical solution. This artificial diffusion is due to the timestepping algorithm being used. Oscillations and negative concentrations are a well-known issue with the Galerkin finite element method and pure advection problems. Artificial diffusion is added on the order of the timestep size (dt). Decreasing dt lessens this artificial diffusion, however, if decreased too much, oscillations will occur. This oscillation is beginning to show in Figure 1 at approximately t=0.6 where the gas concentration is greater than 1.

To minimize this artificial diffusion that is occurring in the OSPREY simulation, initially different time integrators are being tried and dt is being modified. Once the best possible solution is reached with those efforts, the mesh will be refined and/or adapted to remove spurious oscillations and catch the advancing front. This is currently an ongoing effort.

Another upgrade to OSPREY that has occurred is that it has been modified from being for a single component in a carrier gas to being for multiple components. The user can now specify how many components the system includes and whether or not each component adsorbs. The expansion to multiple components has made OSPREY an even more dynamic model. This version of OSPREY has been set up using the same data/information for the initial single component version that was generated. Two species have been specified – 1 adsorbing (krypton) and 1 not adsorbing (helium). The multiple components version of OSPREY has not been validated with more than 1 adsorbing species yet, as there is not sufficient deep bed experimental data that has been provided to this date. Experimental data is currently being obtained and evaluated for use for model validation.

Even though the governing equations remain the same for different gas adsorption systems, changes that may occur due to changing the gas/sorbent system being modeled are the isotherm model and the kinetic equations; therefore, having fundamental level models to describe this behavior would be beneficial. GIT has developed microscale level models to describe these phenomena and continue to develop them to be more dynamic and general. OSPREY was previously loosely coupled with the GIT developed equilibrium model[3]. This loose coupling simply used the GIT model output in OSPREY and did not include any exchange of variables or parameters between the macroscale and microscale models.

OSPREY is now in the initial stages of being tightly integrated with a suite of GIT developed fundamental level models describing both the equilibria and kinetics of the adsorption process. In this integration, OSPREY and the microscale models pass information back and forth to predict the system's behavior. Information that is being passed between the macroscale and microscale models are the variables gas concentration, solid concentration (amount adsorbed), temperature, and pressure and multiple parameters necessary for both GIT's and INL's models. This integration is not complete, however, much progress has been made. It is also an ongoing effort in which many challenges are being faced. This integration of GIT and INL models, when fully complete, will allow for a much more flexible and higher level simulation capability for predicting behavior of off-gas adsorption.

4. Conclusions

The off-gas adsorption model is continually being improved and becoming a more dynamic and generalized model. The current version of OSPREY is ready for evaluation and the appendix includes a user guide on how to access and use the model. A significant amount of

progress has been made on integrating the macro scale level OSPREY with the microscale level models describing the fundamental concepts of equilibrium and kinetics through the NEUP collaboration. This collaboration will continue as the off-gas adsorption modeling further develops.

5. References

1. VERONICA RUTLEDGE, "OSPREY Model," FCRD-SWF-2013-000086, January 2013.
2. ATUL KUMAR, et.al. "Analytical solutions of one-dimensional advection-diffusion equation with variable coefficients in a finite domain," *J. Earth Syst. Sci.*, **2009,** 118, 539-549.
3. VERONICA RUTLEDGE, "Tritium Specific Adsorption Simulation Utilizing the OSPREY Model," FCRD-SWF-2013-000384, September 2013.

Appendix – OSPREY User Guide

Introduction

Off-gas Separation and REcoverY (OSPREY) models the adsorption of off-gas constituents for dispersed plug flow in a packed bed under non-isothermal and non-isobaric conditions. Inputs to the model include gas, sorbent, and column properties, equilibrium and kinetic data, and inlet conditions. The simulation outputs component concentrations along the column length as a function of time from which breakthrough data are obtained. The breakthrough data can be used to determine bed capacity, which in turn can be used to size columns. It also outputs temperature along the column length as a function of time and pressure drop along the column length.

Gaining access to OSPREY

1. To gain access to OSPREY, MOOSE must be set up and the MOOSE repository must be checked out.
    a. Contact Derek Gaston (Derek.gaston@inl.gov) to begin this process and be added to MOOSE users.
        i. Let him know you will be using, not developing, OSPREY and Peacock and need to get MOOSE setup on your computer. When performing this step also request Peacock and cylindrical visualization in Peacock.
    b. The MOOSE wiki has instructions on setting it up on your computer (http://www.mooseframework.com/getting-started/)
        i. Follow the instructions on this page
2. Once you have OSPREY on your computer, to enable Peacock to be used with OSPREY, you must add peacock to your .bash_profile Path
        i. Open terminal
        ii. Navigate to moose/gui directory
        iii. Type “pwd”
            1. Whatever is printed out, that is your path to Peacock
        iv. Type “export PATH=pwd:$PATH
            1. pwd is what was printed out in the previous step
        v. Refer to http://www.mooseframework.com/wiki/Peacock/ for additional information
    b. These first 2 should be a one-time step. Each time using OSPREY after initial set up, start at step 3.

Using OSPREY

3. Open bash profile (i.e. Terminal)
4. Open the trunk directory.
    a. The trunk is the folder in which the MOOSE repository checked out in step 1 is located.
    b. Line of code to type into bash: cd <address>
        i. Should be: cd ~/projects
5. Update the repository.
    a. Type: svn update

6. If it has been a week or more since last using the model, re-configure and rebuild Libmesh just to be sure an important MOOSE or libmesh update was not missed.
    a. Type: cd moose
    b. Type: scripts/update_and_rebuild_libmesh.sh
        i. this configures and builds libmesh
7. Rebuild OSPREY
    a. Every day OSPREY is used, it should be updated in case I have modified or added anything to the repository.
    b. Type: cd ../osprey
        i. This will take you to the osprey directory/folder
    c. Type: make cleanall
    d. Type: make –j8
        i. 8 is the number of processors being used. Adjust this number based on the number of processors you have available.
        ii. This will build the OSPREY application
        iii. Final line of build should say "Linking /<address>/osprey/osprey-opt"
    e. Run Tests to make sure they are working properly
        i. Type: ./run_tests
        ii. No tests should fail, however, some might get skipped
        iii. If tests fail, let me know (veronica.rutledge@inl.gov)
8. Open input file in peacock
    a. Input files are the file I created that brings together all equations and parameters and information needed to run a particular simulation
    b. Must go to osprey gas adsorption problems directory
        i. Type: cd ../problems/osprey/gas_adsorption
    c. List all the files in the directory so you see all available input files (.i files)
        i. Type: ls
    d. Open input file you want to run in Peacock
        i. Type: peacock –i <input_file.i>
            1. Example: peacock –i GasAdsorption.i
                a. Currently GasAdsorption.i is set up with parameters to simulate krypton sorption
        ii. As modifications are made to the model to include other component specific simulations, new input files will be created and show up in this folder for use when an update is performed.
            1. There will be 3 main input files of interest initially
                a. GasAdsorption_single_comp.i
                    i. This is set up as single component in carrier gas
                    ii. Same as GasAdsorption.i
                b. GasAdsorption_multi_comp.i
                    i. This is set up as a multiple component version of GasAdsorption_single_comp.i
                    ii. User is able to specify number of components and whether or not each adsorbs
                c. GasAdsorption_skua.i

i. This is set up for integration with fundamental level models to describe equilibrium and kinetics
ii. Still working on completion of this integration
iii. This command will open a window that is shown in figure 1.

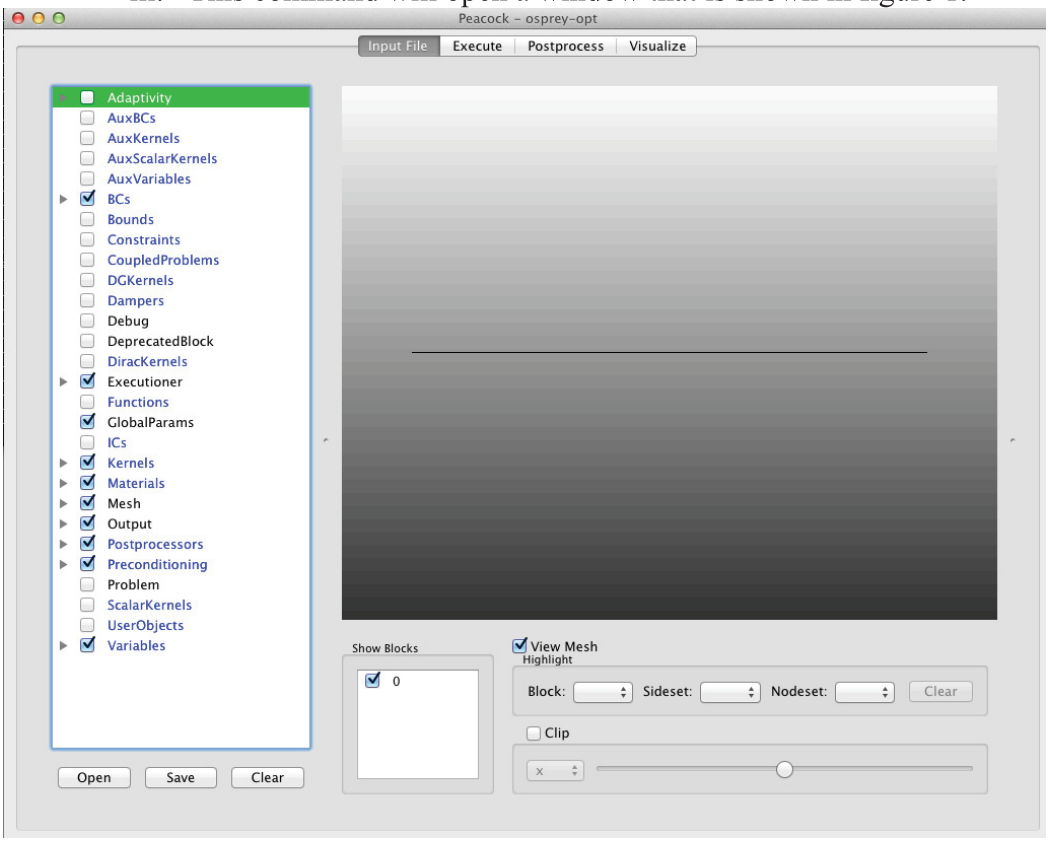

Figure 1: Peacock will look like this when it is opened.

9. Modify Parameters
    a. Double click on GlobalParams in list on left side of window
    b. Go through list of parameters and change Value to system specific parameters
        i. Comment section shows units used and has brief description of parameter
    c. Click on "Apply" button
10. Currently the input file for mutiple components is set up for 2 components, 1 adsorbing and 1 not adsorbing
    a. If this changes will need to add variables, initial conditions, kernels, and parameters for each species added.
    b. To do this click on each corresponding label on the left side of the window and click add.
        i. Go through each box that comes up and input system information.
        ii. With multiple components, each species has a comp_index, starting with 0. This is how each component is identified within the model so anytime asked for the comp_index, indicate with the number which species you are referring to.
11. Modify xmax in Mesh
    a. If changed bed length in GlobalParams, must also change xmax
        i. xmax = bed length

b. Double click on Mesh in list on the left
c. Scroll to xmax and input Value to be that of bed length
d. Can also modify the number of spatial steps (in the x direction) by changing nx value, however 50 seems to work well so do not change unless simulation fails to run.
e. Click "Apply"

12. Modify initial conditions
    a. Click on arrow next to Variables in the list on the left side of the window
    b. Double click on a variable to set the initial condition for that particular variable
    c. Input initial_condition in Value column
    d. Click "Apply"
    e. Go through and set initial conditions for each variable
13. Modify simulation run time
    a. Double click Executioner in the list on the left side of the window
    b. Locate end_time and change Value to be that of desired simulation time
    c. Can change times step here also by changing value for dt
    d. Click "Apply"
14. Running the simulation
    a. Click on Execute tab at the top of the window. The new window will look like shown in figure 2.

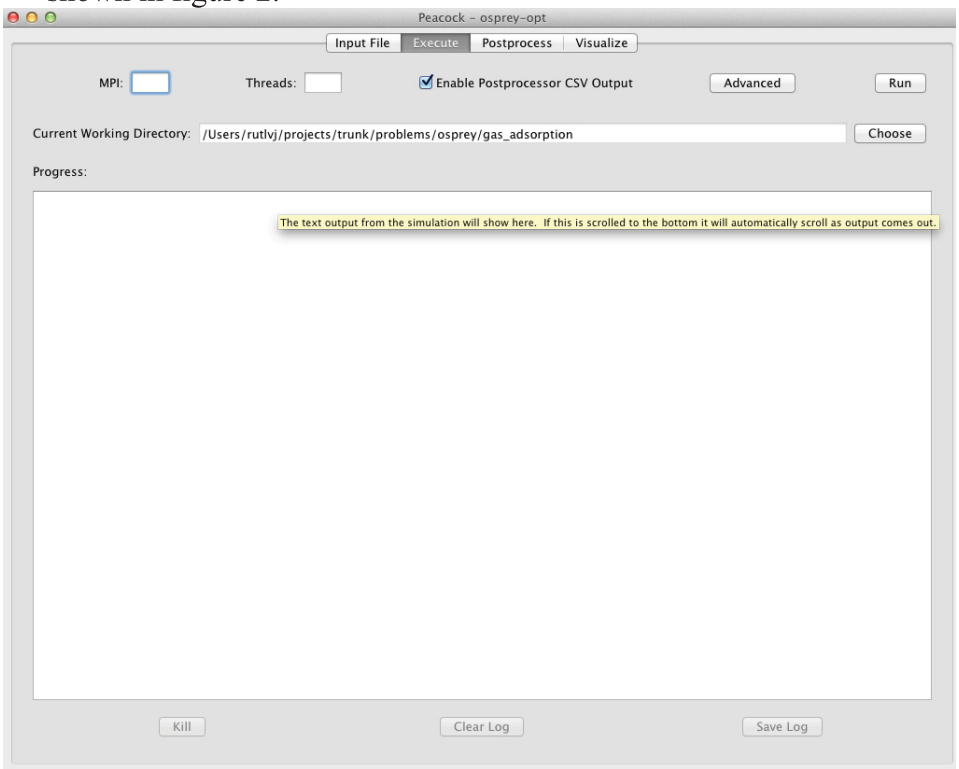

Figure 2: Execute tab of Peacock.

    b. Enter 1 in MPI box
    c. Ensure "Enable Postprocessor CSV Output" is checked
    d. Click "Run" button
        i. Simulation as it's set up prior to any modifications to parameters, will run in a few seconds.

e. If you want to end simulation early, click “Kill”.

15. Viewing graphical results as output by simulation
    a. Click on Postprocess tab at top of window. It will look like shown in figure 3.

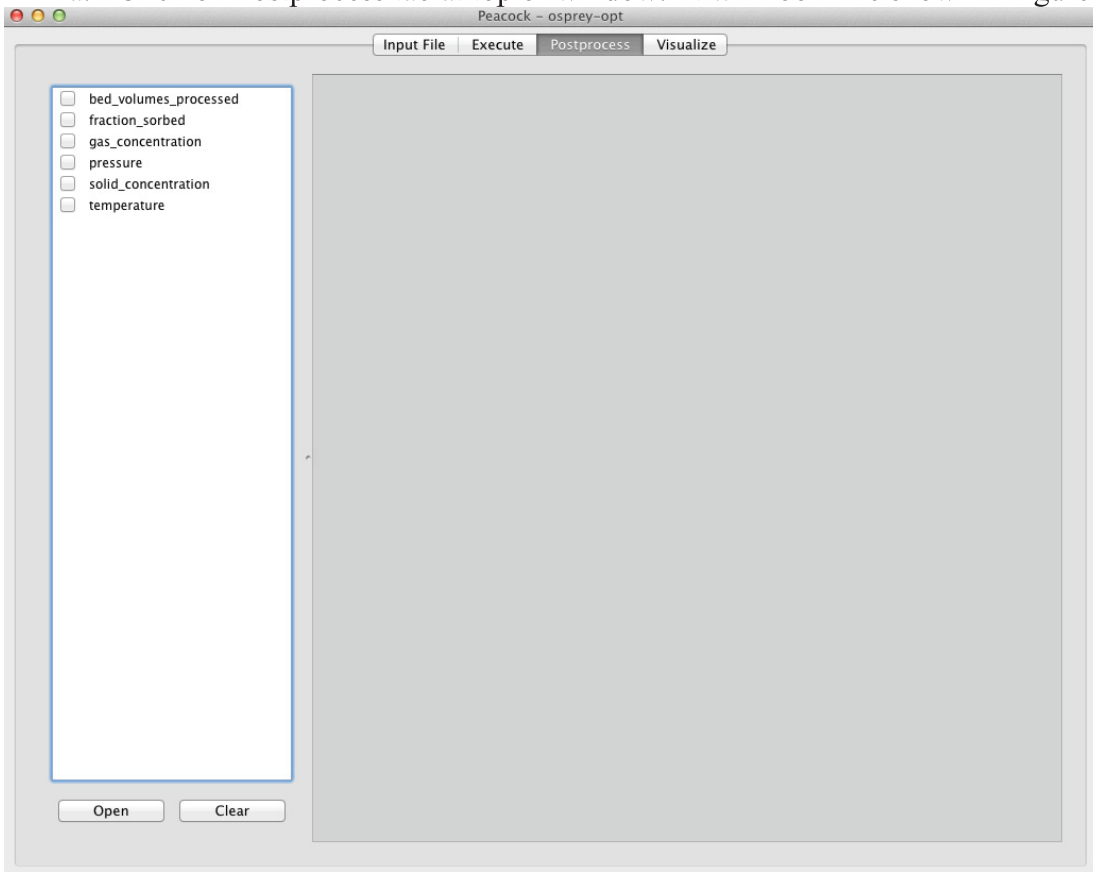

Figure 3: Postprocess window of Peacock.

    b. To view plots of variables, check the box next to the variable listed on the left of the window and the plots will be generated in the grey area.
        i. All plots are a function of time.
    c. This can be done while simulation is running

16. Viewing the gradient along the bed length with time
    a. Click on the visualize tab at the top of the window. It will look as shown in figure 4.

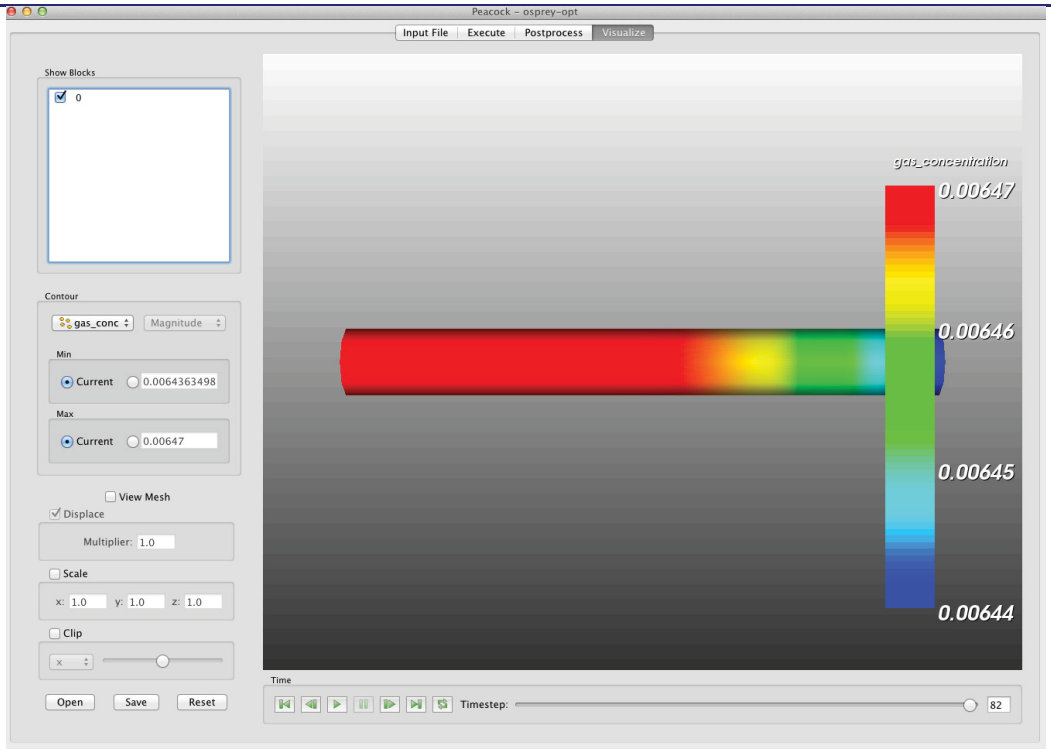

Figure 4: Visualize tab of peacock.

b. Choose the variable to visualize from the drop down list in the Contour box on the left side.
c. The min and max can be changed in the Contour box also.
d. Click on the play button at the bottom of the window to watch the gradient move along with bed length with each time step.
e. This can be done while simulation is running.

17. Viewing results in tabular form
    a. Results shown in graphical form in the postprocess tab are saved as a .csv file that can be open in excel.
        i. They will be saved in the same folder that the input file was located in.
18. Any modifications you made to the input file by changing parameters and other values, can be saved as a new input file.
    a. Go to the input file tab in Peacock.
    b. Click the "save" button.
    c. Choose name and directory to be saved under.
        i. If want to be able to open in Peacock at a later time must save in the osprey folder in the problems directory.
    d. Click save.
19. A different input file can be opened directly from Peacock.
    a. Go to input file tab.
    b. Click the "open" button.
    c. Locate the input file to open and run in peacock.
20. If need help with running OSPREY, contact veronica.rutledge@inl.gov