LAWRENCE LIVERMORE NATIONAL LABORATORY 7000 EAST AVENUE, L-198, LIVERMORE, CALIFORNIA, 94550

LLNL-MI-838176

DATE: July 25, 2022

SUBJECT: Report of Foreign Travel for the FISPACT-II Training Course

TO: Dr. Angela Chambers, USDOE Nuclear Criticality Safety Program Manager, National Nuclear Security Administration, NA-511

FROM: Jesse Norris, Nuclear Criticality Safety Division, Lawrence Livermore National Laboratory

AUSPICES:

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

MEETING TITLE:

Training Course on FISPACT-II 2022: Inventory Simulation Platform for Nuclear Observables and Materials Science

MEETING LOCATION:

Organisation for Economic Cooperation and Development, Nuclear Energy Agency, 46 Quai Alphonse Le Gallo, Boulongne-Billancourt, Paris, France, 92100

MEETING DATES:

June 21-23, 2022

ATTENDEES ON BEHALF OF NCSP:

Catherine Percher and Jesse Norris

BENEFIT OF MEETINGS TO NCSP:

One of the many features of FISPACT-II is the solution of the Bateman equations for the time-dependent decay of radionuclide inventories. These calculations are based on initial abundances and decay rates of the radionuclides of interest. This type of calculation is necessary when modeling the current day composition of existing NCSP fissile material assets (e.g., PANN ZPPR plates, $^{233}U_3O_8$ ZPR plates, etc.). Furthermore, FISPACT-II provides an alternative to SCALE/ORIGEN, including additional capabilities.

Of particular interest were the lessons on Nuclear Data Selection (Tuesday afternoon) and the Uncertainties and Pathways feature (Wednesday morning):

Nuclear Data Selection: FISPACT-II allows the user to easily switch between which source of nuclear data is being used in the calculation. Furthermore, the developers of FISPACT-II curate the data and freely distribute many nuclear data libraries (TENDL, ENDF, JEFF, etc.) directly on their website:
https://fispact.ukaea.uk/nuclear-data/

Pathways Analysis: In addition to reporting the results of a radionuclide inventory irradiation or decay calculation, FISPACT-II has the capability to perform a "pathway" analysis. This is a unique feature that finds the significant pathways (reaction and/or decay chains) that may produce various target nuclides from the given source nuclides[1]. This has the ability to highlight the source (or sources) of any target nuclei, which may be otherwise be difficult to determine.

During the training course, the students were given time to construct their own problems of interest where the instructors were able to provide support and guidance. This allowed both Catherine Percher and myself to model the decay of the PANN ZPPR plates and the $^{233}U_3O_8$ ZPR plates. While this analysis had been performed beforehand as part of previous CED milestones, these exercises quickly showed the utility of FISPACT-II as we were able to reproduce our prior results within an hour.

The 2022 FISPACT-II Training Course Agenda is included as Appendix A.

PURPOSE OF THE MEETING:

FISPACT-II is "an enhanced multiphysics platform providing a wide variety of advanced simulation methods and employing the most up-to-date (TENDL-2019, ENDF/B-VIII.0, JENDL-4.0, JEFF-3.3, etc.) enhanced nuclear data forms for neutron, proton, alpha, deuteron, or gamma particle interactions." This 3-day training provided an introduction to the FISPACT-II software, examples of how to configure the data source and input files, exercises covering various problem types (irradiation, decay, etc.), and the unique features of the FISPACT-II software. The course was taught by two of the developers of FISPACT-II who were able to provide unique insights into the inner workings of the code and its typical applications.

[1] More on the Pathway Analysis methodology can be found in Sublet, J.-Ch. et. al., "FISPACT-II: An Advanced Simulation system for Activation, Transmutation and Material Modeling." Nucl. Data Sheets, **139**, 77-137 (2017).

APPENDIX A: 2022 FISPACT-II Training Agenda

Day 1 - Tuesday 21 June

9:30 - 10:00 Arrival
10:00 Coffee
10:00 - 11:00 Introduction to FISPACT-II. What is FISPACT-II, workshop_introduction_2022.pdf
12:00 - 14:00 Lunch
14:00 - 15:00 The work through FISPACT_Worked_example.pdf , combine.i , files , fluxes
15:00 Coffee
15:00 - 16:00 Exercises + files file ND example ND_DEMO.pdf , Standard.zip , API.zip
16:00 - 17:00 Exercises plus proton/neutron tungsten work through proton.zip , neutron.zip

19:30 Social Dinner at Brasserie Jean-Baptiste , 1, rond-point Rhin et Danube, Boulogne. How to get there .

Day 2 - Wednesday 22 June

9:00 - 10:00 Uncertainties and Pathways demo files3 , fluxes3 , Irradiation_Iron.i , Uncertainties_Pathways.i , FISPACT_Uncertainties_Pathways_worked_example.pdf
10:00 Coffee
10:00 - 11:00 External: Priti Talk
12:00 - 14:00 Lunch
14:00 - 15:00 FISPACT API work through example API_example.zip, APIanalysis.pptx
15:00 Coffee
15:00 - 15:30 Exercise + GG bins example ggbins_example.pptx , ggbins_example.zip

15:30 - 16:00 Example: Nuc graph files5 , fluxes5 , nuc_Graph_ex.i , ng_style (you need this as the gnuplot style file), nuc_Graph_ex.grn.ps
16:00 - 17:00 Exercise + Group convert groupconvert.pptx , groupconvert_example.zip

Day 3 - Thursday 23 June

9:00 - 10:00 Basic work through + tolerances Al-Be-151.i , files6 , fluxes6 , FISPACT_numerical_solver_tol.pdf
10:00 Coffee
10:00 - 11:00 External: Art group talk
12:00 - 14:00 Lunch
14:00 - 15:00 Self shielding FISPACT_Self_sheilding_demo.pdf , files7
15:00 Coffee
15:00 - 16:00 Exercises and final questions
16:00 - 17:00 Wrap up and end