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Standardized verification of fuel cycle modeling

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ABSTRACT

A nuclear fuel cycle systems modeling and code-to-code comparison effort was coordinated across multiple national laboratories to verify the tools needed to perform fuel cycle analyses of the transition from a once-through nuclear fuel cycle to a sustainable potential future fuel cycle. For this verification study, a simplified example transition scenario was developed to serve as a test case for the four systems codes involved (DYMOND, VISION, ORION, and MARKAL), each used by a different laboratory participant. In addition, all participants produced spreadsheet solutions for the test case to check all the mass flows and reactor/facility profiles on a year-by-year basis throughout the simulation period. The test case specifications describe a transition from the current US fleet of light water reactors to a future fleet of sodium-cooled fast reactors that continuously recycle transuranic elements as fuel. After several initial coordinated modeling and calculation attempts, it was revealed that most of the differences in code results were not due to different code algorithms or calculation approaches, but due to different interpretations of the input specifications among the analysts. Therefore, the specifications for the test case itself were iteratively updated to remove ambiguity and to help calibrate interpretations. In addition, a few corrections and modifications were made to the codes as well, which led to excellent agreement between all codes and spreadsheets for this test case. Although no fuel cycle transition analysis codes matched the spreadsheet results exactly, all remaining differences in the results were due to fundamental differences in code structure and/or were thoroughly explained. The specifications and example results are provided so that they can be used to verify additional codes in the future for such fuel cycle transition scenarios.

1. Introduction

Numerous nuclear fuel cycle system code benchmarks and comparisons have been performed over the last decade, coinciding with the rapid development of new codes due to improvements in computational capabilities, new software platforms, and the need for various institutions to provide technical feedback on potential fuel cycle strategies and policies. Many of these studies (Guérin et al., 2009; Kuijper et al., 2010; OECD/NEA, 2012) were performed within the framework of established international organizations (EC-PUMA, NEA) or organized as an *ad hoc* study with voluntary contributions from participants (MIT). These studies achieved different levels of agreement depending on the scenarios analyzed and values compared, varying from excellent agreement in annual mass flows and inventories to general agreement in terms of trends. Since validation is challenging for these types of codes, these comparison studies helped develop confidence in the results from these forecasting codes. In addition, many of these codes were developed independently with limited feedback due to the lack of a widely-established user base. Therefore, such studies are also great opportunities for the developers and users to calibrate interpretations as well as modify/debug the codes themselves.

The work presented in this paper is a code verification study similar to previous studies but unique in several ways: (1) all participants were working under a common effort funded by the US Department of Energy (DOE) for the development of analysis tools, (2) a strict level of agreement between codes was targeted, and (3) during the verification process, modifications were made to the participating codes in the pursuit of achieving such a high level

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of agreement. The codes involved in this verification study are DYMOND (Yacout et al., 2005), VISION (Jacobson et al., 2010), ORION (Gregg and Grove, 2012), and MARKAL (Shay et al., 2006). Many authors of this paper were also participants in these previous activities; consequently, many of the lessons learned from preceding experiences were applied toward this new collaborative effort.

1.1. Context of work

The present code verification study was conducted in a coordinated effort as part of the Fuel Cycle Options (FCO) Campaign, a multi-laboratory collaborative effort within the US DOE-Nuclear Energy's Office of Fuel Cycle Technologies. The Campaign recently completed a multi-year evaluation and screening of a comprehensive set of nuclear Fuel Cycle Options (Wigeland et al., 2014), assessing the potential for performance improvements compared to the existing once-through cycle in the US across a wide range of criteria with an objective of informing on research and development priorities. It was found that regardless of the relative importance of the benefit criteria, the fuel cycles that consistently scored high overall performance were ones that involved continuous recycling of co-extracted U/Pu or U/TRU in fast spectrum critical reactors. A key feature of the evaluation and screening study was that the performance for each fuel cycle was evaluated assuming a fully-deployed nuclear energy system at equilibrium to properly understand the end-state benefits. Based on the findings from this study, the next step in understanding research and development needs is to assess and inform on the fuel cycle transitions from the current state to these promising future end-states. However, before initiating the time-dependent transition analyses, it was necessary to assess the systems analysis tools and capabilities within the Campaign to (1) ensure that the fuel cycle simulations produce consistent results, (2) identify reasons for differences between code behaviors and analyst interpretations, and (3) identify limitations or advantages of individual codes.

1.2. Objectives

The main objectives of this paper are: (1) to show the consistent agreement among the participating fuel cycle codes for an artificial test scenario involving transition, thereby demonstrating confidence in the code calculations and modeling capabilities, (2) to show the level of effort and iteration required to obtain agreement between codes, and (3) to publish the scenario specifications and results so that other fuel cycle codes can be used to repeat this verification exercise.

First, each of the three fuel cycle codes (DYMOND, ORION, and VISION) and one market analysis code (MARKAL) involved in this verification study will be briefly described. Then, the specifications and methodology for the test transition scenario for this verification exercise will be discussed. As briefly mentioned, part of this verification exercise also involved using external calculations, *i.e.*, spreadsheets, to serve as an additional means of cross-checking. To avoid biasing the presentation of the results toward a particular code solution, the spreadsheet results are first presented in this paper and then a few selected results from each code will be presented to highlight any differences from the spreadsheet solution as well as differences among each of the code results.

2. Code descriptions

Detailed descriptions of system dynamics and fuel cycle systems modeling are not provided in this paper since it is assumed that the reader has a general understanding of these concepts. Only brief descriptions are provided in this section, emphasizing some of the differences that will be pertinent to the results. Additional information on these codes is provided in their respective literature listed in the references. Table 1 summarizes the laboratories that have completed this benchmark and the tools they used (each also produced the same spreadsheet solution).

2.1. DYMOND description

DYMOND (Yacout et al., 2005), the main software tool used at ANL for this study, is a nuclear fuel cycle system dynamics model run within the *iThink* software with Microsoft Excel templates for data input/output. The code was first developed in 2001 at ANL for the Gen IV Fuel Cycle Crosscut Group activities and is a predecessor to several system dynamics codes in wide use today. Since 2012, the code structure and user interface were heavily updated while maintaining its relative simplicity. Like all codes involved in this study, some modifications were made as a result of this study as well as other verification studies that are currently underway.

The major inputs to the code are the reactor and fuel characteristics, the fuel cycle facility properties, the various pathways of each fuel type (enrichment, recycling, storage, *etc.*), and the nuclear power demand as a function of time. The code uses externally-calculated fuel cycle recipes for both the input and output fuel compositions. Currently only described in lumped materials (U, Pu, *etc.*). The major output is the reactor fleet composition (installed capacities of each type of reactor) over time. All other system data including mass flows (mining rates, fabrication rates, reprocessing rates, *etc.*) and inventories (spent fuel inventory, recovered uranium, *etc.*) can be output via an Excel spreadsheet based on the user's selection. Typical run times are less than a minute for scenarios lasting over a century with month-long time steps. The time steps can be varied at the user's discretion.

During the development of the DYMOND code, the ability for the user to easily understand the code's behavior and variables was considered a priority over model sophistication and hidden logic and automation. This allows a higher level of manual control and input flexibility that allows a scenario to fail. For example, when there are insufficient fissile materials for fuel fabrication, the correct amount of existing reactor capacities will go into "idle" mode and the user-specified energy demand will not be met. In addition, a dynamic resource allocation module was implemented to allow prioritization of fissile material allocation to different reactor technologies based on user-specified priorities. One of the original simplifications that has been maintained is that individual isotopes are not tracked; materials are lumped into categories such as fission product (FP), minor actinide (MA), and several types of U and Pu. In addition, radioactive decay is not currently implemented. These approximations were acceptable for the present verification study since only lumped elements were modeled to allow for simple spreadsheet comparisons. Any reactor and fuel types can be modeled so long as the technical details are provided as input, and individual reactors can be simulated to transition from one fuel type to a completely new one within a few cycles.

Table 1
Participants and codes/programs used for fuel cycle modeling verification effort.

Participant	Code/tool used	Code/tool type
Argonne National Laboratory (ANL)	DYMOND	Nuclear fuel cycle
Idaho National Laboratory (INL)	VISION	Nuclear fuel cycle
Oak Ridge National Laboratory (ORNL)	ORION	Nuclear fuel cycle
Brookhaven National Laboratory (BNL)	MARKAL	Energy market