OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

S. B. Ludwig
Nuclear Science & Technology Division
P.O. Box 2008
Oak Ridge, TN 37831-6472
(865) 574-7916 Fax: (865) 574-3431
Internet Address: ludwigsb@ornl.gov

Date: May 23, 2002

To: Jennie Manneschmidt

From: S. B. Ludwig and A. G. Croff

Subject: **Revision to ORIGEN2 – Version 2.2**

This note transmits ORIGEN2 V2.2 to the ORNL RSICC for distribution. This is the first update to ORIGEN2 in nearly 10 years, and was stimulated by a user discovering a discrepancy in the mass of fission products calculated using ORIGEN2 V2.1. The problem, diagnosis and solutions employed, results, and issues arising are discussed below.

Problem: The user's problem involved irradiating a mixture of 40% Pu and 60% minor actinides (Np, Am, Cm) for about 1300 days at a high power level to reach a burnup of 350 MWd/kg. The total mass of fission products was under-predicted by nearly 10%, and a fact that was readily detected because the total mass of fission products and actinides should remain constant.

Diagnosis: There were two causes of the discrepancy.

1. ORIGEN2 accounts for fission products produced by fissioning minor actinides that do not have an explicit fission product yield library (e.g., Np, Am, and Cm-244) by adjusting the fission product yields of a nearby actinide that does have fission product yield library (e.g., Pu-239) (called "nearest connected actinide") based on the relative total fission rate of all the fissioning minor actinides and the actinide having a fission product yield library. The logic in the algorithm that calculates the total fission rate of the minor actinides was flawed so that this total fission rate for the minor actinides was prematurely terminated, thus resulting in under-prediction of the fission product mass. This error was previously not discovered as most problem cases involved fuel compositions that were composed primarily of uranium and/or plutonium.
2. As a result of the relatively small amount of Pu (in relation to the large fraction of fissioning minor actinides), use of long time steps (up to 400 days), and high specific power in the problem case, a majority of total fissions in the minor actinides and the actinide having a fission product yield library increases significantly during a time step. The adjustment of the fission product yields takes place using the actinide composition (and total fission rate) at the beginning of the time step. As a result, the adjustment factor is too low at the end of the time step, which leads to under prediction of the fission product mass. This can be fixed by simply decreasing the duration of the time step.

Results: Code modifications, as well as reducing the irradiation time step to no more than 100 days/step reduced the discrepancy from ~10% to 0.16%.

Issues Arising:

A. The bug described in Diagnosis 1 above does not noticeably affect the fission product mass in typical ORIGEN2 calculations involving reactor fuels because essentially all of the fissions come from actinides that have explicit fission product yield libraries. Thus, most previous ORIGEN2 calculations that were otherwise set up properly should not be affected.
B. Similarly, the use of excessively long time steps during irradiation is not likely to have adversely affected previous calculations of the fission product mass because the calculated adjustment factor is very small and changes very slowly in typical cases due to relative paucity of minor actinides composition in the fuel matrix.
C. The fission product mass in previous calculations involving high concentrations of minor actinides may have been under-predicted to a noticeable extent.
D. There are certain cases for which ORIGEN2 predictions of fission product mass would still be substantially under-predicted. These cases would involve irradiation of minor actinides exclusively (i.e., in which the concentration of U-233 plus U-235 plus Pu-239, which have fission product yield libraries, is essentially zero) should not be undertaken. In this case it is impossible for ORIGEN2 to adjust the fission product production rate without major modifications to ORIGEN2, which is not likely in the foreseeable future. The suggested work-around is a separate calculation to irradiate an actinide having a fission product yield library to the same burnup as the minor actinides to better estimate the resulting fission product composition.

Other notes:

ORIGEN2 continues to be successfully run on PCs under all versions of the Windows operating system, at least through Windows 2000.