

## An Activation Inventory Estimation Including Spallation Reactions by Modification of FISPACT 2010 Code

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### 1. Introduction

For the radiation safety evaluation in high energy accelerators, the material activation analysis is an important estimation field on the design, operation and disposal. FISPACT [1-3] is a useful inventory code for particle induced activation calculations. It uses activation libraries to obtain the reaction rates. However, the activation libraries were not produced by considering all of the reactions from the induced high energy particles. To overcome the limitation, FISPACT 2003 [1] was modified to SP-FISPACT 2003 by ENEA (Italian National Agency for New Technologies, Energy and Sustainable Economic Development). In the SP-FISPACT 2003 code, the specific reaction rates, which are obtained from MCNPX [4] intermediate energy physics model, can be utilized for the activation analyses.

Recently, FISPACT 2010 [3] was released by Culham Centre for Fusion Energy (CCFE). The EAF-2010 [5] library, which has energy range  $10^{-5}$  eV – 60 MeV, can be used in FISPACT 2010 code. FISPACT 2010 cannot treat some specific reactions for high energy particles. In this study, FISPACT 2010 was modified (Called as modified FISPACT 2010 in this study) to obtain the specific reaction rate from intermediate energy physics model from MCNPX code. For the verification, the results calculated by modified FISPACT 2010 were compared with experimental data and those calculated by CINDER'90 [6] and SP-FISPACT 2003.

### 2. Methods and Results

#### 2.1 Process of Inventory Calculation Using Modified FISPACT 2010

It is noted that FISPACT 2010 code cannot treat the elastic collision (elast), residual nuclei after collision (resid), and gas product (gas) [3]. Therefore, in the code modifications, the reaction treat module was added in the FISPACT 2010 source code. Fig. 1 shows the process of the inventory calculation with the modified FISPACT 2010 in this study. There are mainly two steps for the modified code. In the first step, the neutron

spectrum and spallation production rates from physics model are calculated by MCNPX 2.7 code using HISTP option. The HISTP files are converted by HTAPE3X module to three files. From the conversion module, the 'elast', 'resid', and 'gas' files are produced. In the second step, the one group cross section is collapsed from neutron spectrum and information files of spallation production. The collapsed results are stored in the COLLAPX file. The condensed library data (ARRAYX) is produced by using COLLAPX and decay data library. Then, radionuclide inventories of each time step were calculated by FISPACT 2010 using ARRAYX.

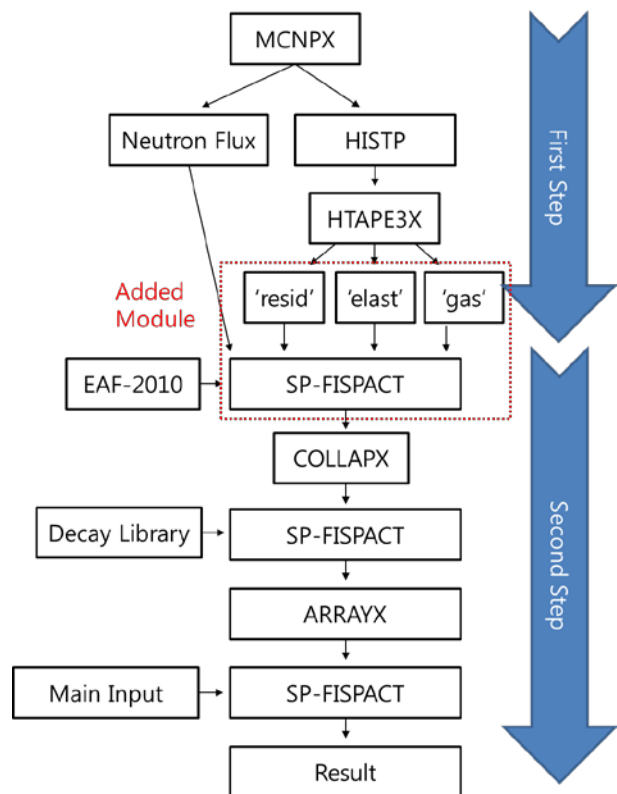


Fig. 1. Diagram of Activation Process using Modified FISPACT 2010

#### 2.2 Condition of Benchmark Problem

For the verification of the modified FISPACT 2010, the activation calculations were performed that

accelerated protons are induced into a cylindrical lead target having 30.9 cm long and 8 cm diameter. The proton beam energy is 660 MeV, and it was irradiated for 530 minutes. The average current of proton beam is set to 1.13 nA. For the first step calculation, Bertini intranuclear cascade and RAL fission evaporation model were applied to get the spallation reaction rates. The decay time steps for the calculation of the long lived radionuclide inventories are 1 day, 30 day, 219 day and 1 year. For the inter-comparison of the activation results, the estimation results from a previous study [7] were used in this study.

### 2.3 Result and Validation

Fig. 2 and Table I are the results of selected radionuclides in the whole of the activated lead target. The activities of the selected nuclides give good agreements within 200 % relative error comparing with experiment results. Especially,  $^{102m}\text{Rh}$  nuclide was only calculated by the modified FISPACT 2010. However,  $^{83}\text{Rb}$ ,  $^{88}\text{Y}$ ,  $^{95}\text{Zr}$ ,  $^{102m}\text{Rh}$ ,  $^{110m}\text{Ag}$ , and  $^{121m}\text{Te}$  were relatively underestimated less than 50 %. The results calculated by CINDER'90 and the modified FISPACT 2010 agree well within 16 %. Meanwhile, the results calculated by modified FISPACT 2010 and SP-FISPACT 2003 relatively have differences more than 20 % for  $^{175}\text{Hf}$ ,  $^{183}\text{Re}$ , and  $^{194}\text{Au}$  nuclides.

Table I: Calculated and Measured Activities at 219 Day Decay Time [7]

Nuclide	Experiment (Bq)	CINDER90 (Bq)	SP-FISPACT 2003 (Bq)	M. FISPACT 2010 (Bq)
$^{60}\text{Co}$	1.48E+02	7.66E+01	7.66E+01	8.35E+01
$^{65}\text{Zn}$	2.74E+02	5.13E+02	4.98E+02	5.30E+02
$^{83}\text{Rb}$	3.54E+03	1.51E+03	1.49E+03	1.69E+03
$^{85}\text{Sr}$	1.64E+03	9.12E+02	8.94E+02	9.44E+02
$^{88}\text{Y}$	6.05E+03	2.84E+03	2.72E+03	2.78E+03
$^{95}\text{Zr}$	5.07E+03	1.44E+03	1.26E+03	1.34E+03
$^{102m}\text{Rh}$	9.05E+02	-	-	2.87E+02
$^{110m}\text{Ag}$	3.46E+03	2.50E+02	2.49E+02	2.36E+02
$^{121m}\text{Te}$	1.58E+03	1.65E+02	1.65E+02	1.66E+02
$^{173}\text{Lu}$	6.64E+03	1.25E+04	1.02E+04	1.10E+04
$^{175}\text{Hf}$	1.34E+04	1.77E+04	8.15E+03	1.85E+04
$^{183}\text{Re}$	3.29E+04	5.24E+04	3.86E+04	5.42E+04
$^{185}\text{Os}$	6.38E+04	7.30E+04	6.68E+04	7.31E+04
$^{194}\text{Au}$	4.35E+02	3.33E+02	2.88E+02	3.96E+02
$^{203}\text{Hg}$	4.48E+03	6.13E+03	5.61E+03	5.83E+03
$^{207}\text{Bi}$	8.25E+02	1.20E+03	1.22E+03	1.14E+03

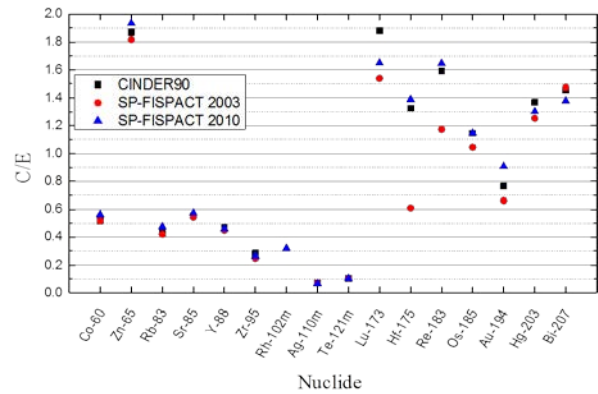


Fig. 2. Calculation/Experiment (C/E) of Activity at 219 Day Decay Time

In the previous paper [7], it is noted that SP-FISPACT 2003 seems to miss some decay channels in the process which is neutron poor-nuclides derived from spallation reaction. To check the problem, twenty radionuclide inventories, which have highest activities, are calculated and compared for 1 day, 30 day, and 1 year decay time. The results are given as shown Table II, III, and IV. It shows that the results estimated by the modified FISPACT 2010 and CINDER'90 agree well within 30% for the selected nuclides except  $^{169}\text{Yb}$ . Thus, it can be analyzed that the modified FISPACT 2010 can effectively solve the decay channel problem.

Table II: Activity Results at 1 Day Decay Time

Nuclide	CINDER90 (MBq)	SP-FISPACT 2003 (MBq)	M. FISPACT 2010 (MBq)
$^{203}\text{Pb}$	5.35E+01	5.33E+01	3.97E+01
$^{200}\text{Tl}$	4.65E+01	4.06E+01	3.90E+01
$^{200}\text{Pb}$	3.78E+01	3.69E+01	3.42E+01
$^{201}\text{Tl}$	3.33E+01	2.99E+01	2.99E+01
$^{193}\text{Au}$	3.33E+01	3.11E+01	3.35E+01
$^{201}\text{Pb}$	3.16E+01	3.18E+01	3.04E+01
$^{199}\text{Tl}$	2.76E+01	2.02E+01	2.32E+01
$^{195}\text{Hg}$	2.63E+01	2.59E+01	2.53E+01
$^{197}\text{Hg}$	2.49E+01	2.32E+01	2.48E+01
$^{187}\text{Ir}$	1.83E+01	1.50E+01	1.70E+01
$^{186}\text{Ir}$	1.77E+01	1.43E+01	1.78E+01
$^{192}\text{Au}$	1.61E+01	1.14E+01	1.43E+01
$^{198}\text{Tl}$	1.57E+01	1.37E+01	1.31E+01
$^{189}\text{Pt}$	1.51E+01	9.97E+00	1.46E+01
$^{185}\text{Ir}$	1.49E+01	1.36E+01	1.44E+01
$^{183}\text{Os}$	1.34E+01	9.71E+00	1.47E+01
$^{191}\text{Pt}$	1.29E+01	1.09E+01	1.14E+01
$^{203}\text{Bi}$	1.17E+01	1.17E+01	1.15E+01
$^{182}\text{Os}$	1.16E+01	9.58E+00	1.19E+01
$^{204}\text{Bi}$	1.07E+01	9.47E+00	9.46E+00

Table III: Activity Results at 30 Day Decay Time

Nuclide	CINDER90 (MBq)	SP-FISPACT 2003 (MBq)	M. FISPACT 2010 (MBq)
<sup>189</sup> Ir	6.51E-01	4.22E-01	6.42E-01
<sup>202</sup> Tl	6.14E-01	5.79E-01	6.22E-01
<sup>188</sup> Ir	6.08E-01	4.16E-01	6.25E-01
<sup>205</sup> Bi	5.33E-01	5.09E-01	5.39E-01
<sup>188</sup> Pt	5.05E-01	3.45E-01	5.19E-01
<sup>195</sup> Au	3.74E-01	3.68E-01	3.75E-01
<sup>183</sup> Re	3.41E-01	2.51E-01	3.52E-01
<sup>185</sup> Os	2.97E-01	2.70E-01	2.95E-01
<sup>178</sup> Ta	2.86E-01	1.18E-01	2.95E-01
<sup>178</sup> W	2.86E-01	1.18E-01	2.95E-01
<sup>181</sup> W	1.62E-01	3.65E-02	1.67E-01
<sup>206</sup> Bi	1.21E-01	1.08E-01	1.23E-01
<sup>175</sup> Hf	1.15E-01	5.31E-02	1.20E-01
<sup>203</sup> Hg	1.02E-01	9.46E-02	9.70E-02
<sup>169</sup> Yb	7.22E-02	4.28E-02	4.57E-02
<sup>171</sup> Lu	6.05E-02	4.62E-02	6.26E-02
<sup>201</sup> Tl	5.08E-02	3.71E-02	4.63E-02
<sup>167</sup> Tm	3.55E-02	2.45E-02	3.36E-02
<sup>3</sup> H	3.50E-02	3.50E-02	3.66E-02
<sup>204</sup> Tl	3.14E-02	3.12E-02	9.46E+00

Table IV: Activity Results at 1 Year Decay Time

Nuclide	CINDER90 (MBq)	SP-FISPACT 2003 (MBq)	M. FISPACT 2010 (MBq)
<sup>195</sup> Au	1.07E-01	1.06E-01	1.08E-01
<sup>3</sup> H	3.33E-02	3.32E-02	3.47E-02
<sup>204</sup> Tl	2.65E-02	2.64E-02	2.70E-02
<sup>185</sup> Os	2.48E-02	2.27E-02	2.48E-02
<sup>181</sup> W	2.38E-02	5.34E-03	2.45E-02
<sup>179</sup> Ta	2.02E-02	7.28E-03	2.22E-02
<sup>183</sup> Re	1.24E-02	9.10E-03	1.28E-02
<sup>173</sup> Lu	1.02E-02	8.30E-03	8.90E-03
<sup>172</sup> Lu	6.34E-03	5.72E-03	6.09E-03
<sup>172</sup> Hf	6.27E-03	5.67E-03	6.03E-03
<sup>175</sup> Hf	4.17E-03	1.92E-03	4.36E-03
<sup>193</sup> Pt	3.29E-03	3.08E-03	3.37E-03
<sup>88</sup> Y	1.41E-03	1.36E-03	1.37E-03
<sup>207</sup> Bi	1.19E-03	1.21E-03	1.13E-03
<sup>106</sup> Rh	1.05E-03	-	7.89E-04
<sup>106</sup> Ru	1.05E-03	7.82E-04	7.89E-04
<sup>109</sup> Ag	7.22E-04	-	7.20E-04
<sup>109</sup> Cd	7.22E-04	7.19E-04	7.20E-04
<sup>203</sup> Hg	7.00E-04	6.40E-04	6.64E-04
<sup>159</sup> Dy	6.86E-04	3.54E-04	7.70E-04

### 3. Conclusions

In this study, the FISPACT 2010 code was modified to consider spallation products for the high energy particle activations. In the modified FISPACT 2010, the 'elast', 'resid', and 'gas' files are automatically collapsed and used as the FISPACT activation data file. The results compared with experiment results give good agreements within 200 %. Also, for the validation, the inter-comparison of the other codes was performed. The analysis shows that the modified FISPACT 2010 code can solve the decay channel problem generated in SP-FISPACT 2003 code analysis. It is expected that the modified FISPACT 2010 can be utilized as an additional tool to pursue activation analyses induced by high energy particles.

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