J. King Saud Univ., Vol. 21, *Science* (Special Issue), pp. 199-202, Riyadh (2009/1430H.)

Response Calibration of a PGNAA Setup Utilizing Silica Fume Cement Concrete Specimens

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Keywords: PGNAA, 2.8 MeV neutrons, Silica fume cement concrete specimen, Monte Carlo simulations

Abstract. Monte Carlo simulations were conducted to calibrate the response of an accelerator-based PGNAA setup for determining the silicon concentration using silica fume cement concrete specimens. The prompt gamma-ray yield was initially calculated as a function of the specimen dimension to determine its optimum radius and length. It was then calculated from cement concrete specimens containing 0 to 20% silica fume, by weight of Portland cement. The results of the calculations show a linear response of gamma-ray for silicon with increasing concentration of silica fume in the concrete specimens.

Introduction

Prompt Gamma Neutron Activation Analysis (PGNAA) technique is a powerful multi-element analysis method that can be utilized to determine the concentrations of Ca, Si, Al, and Fe in bulk samples [Khelifi R.,et. Al.,1999; Lim C. S., et. Al., 2001; Naqvi A. A., et. al., 2006a; Naqvi A. A., et. al., 2006b; Olivera C., et. al. 1997; Saleh H. H. and Livingston, R. A. 2000; Tickner J. 2000]. It has been successfully utilized in cement manufacturing plants to monitor the concentration of lime, silicon dioxide, alumina, and iron oxide in raw materials [Olivera C., et. al. 1997]. Silica fume contains mainly silica (SiO_2) and thus it can be used to calibrate the response of a PGNAA setup to determine the silicon concentration. An accelerator-based PGNAA setup was developed at the 350 keV accelerator laboratory at King Fahd University of Petroleum and Minerals (KFUPM) for the analysis of cement and concrete samples [Naqvi A. A., et. al., 2006a; Naqvi A. A., et. al., 2006b]. In the reported study, Monte Carlo simulations were conducted to calibrate the response of the PGNAA setup for determining the concentration of silicon in the silica fume cement concrete specimens.

The accelerator-based PGNAA facility at KFUPM is a thermal neutron capture-based setup. It utilizes a rectangular moderator, which can be used to analyze 12 to 14 cm long cylindrical specimens with a diameter of up to 25 cm [Naqvi A. A., et. al., 2006a]. The optimum size of the sample that can be used with the moderator depends upon its material and can be calculated using Monte Carlo simulations [Naqvi A. A., et. al., 2006b]. In this study, the optimum size of the silica fume concrete specimen was determined from the prompt gamma-ray yield calculations, as a function of its radius and length. The prompt gamma-ray yield was then calculated as a function of silicon concentration.

Materials and Methods

Calculation of Prompt Gamma-Ray Yield using Monte Carlo Simulation

The optimum size of the silica fume concrete specimen was determined through gamma-ray yield utilizing Monte Carlo simulations along with code MCNP4B2. These calculations were carried out following the procedures described elsewhere [Naqvi A. A., *et. al.*, 2006a]. Figure 1 is a schematic representation of the PGNAA setup with the rectangular moderator [Naqvi A. A., et. al., 2006b]. The elemental composition of the six silica fume concrete specimens were calculated utilizing the information provided in Tables 1 and 2 [Maslehuddin M., et. al., 1996].

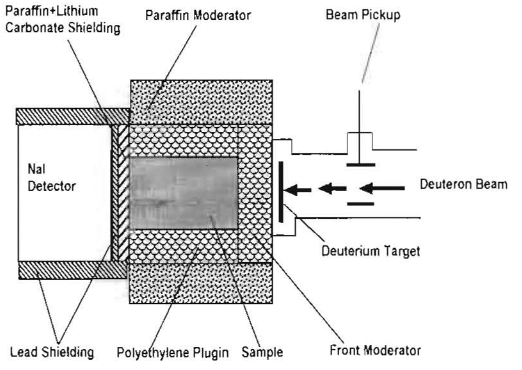

Fig. 1. Schematic representation of the PGNAA setup.

Table 1 Chemical composition of Portland cement, silica fume, and coarse and fine aggregates [Maslehuddin M., et. al. 1996].

Composition (wt. %)	Portland cement	Silica fume	Coarse aggregate	Fine aggregate
SiO_2	21.96	92.50	4.29	90.70
Al_2O_3	4.53	0.40	0.20	1.40
Fe_2O_3	2.92	0.40	0.23	0.48
MgO	1.74	0.90	0.44	0.26
$CaCO_3$	--	--	93.20	5.62
CaO	65.03	0.50	0	0
Na_2O	0.10	0.10	0.03	0.17
K_2O	0.17	0.40	0.09	0.43
TiO_2	0.05	0	0.05	0.05
SO_3	2.30	0.50	0.40	0.20

Table 2. Mixture composition of six silica fume cement concrete specimens.

Mix. #	Portland cement Wt. %	Coarse aggregate wt. %	Fine aggregate wt. %	Silica fume wt %	Water, wt. %
1	15.97	47.59	29.26	0.00	7.18
2	15.84	47.22	29.02	0.79	7.13
3	15.79	47.07	28.93	1.11	7.11
4	15.71	46.85	28.80	1.57	7.07
5	15.59	46.48	28.57	2.34	7.02
6	15.47	46.12	28.35	3.09	6.96

The bulk density and moisture content of the concrete specimens were assumed to be 2.2 g/cm^3 and 5 wt %, respectively. The energies of the prompt gamma-rays used to analyze the concentration of calcium, aluminum, silicon, and iron in the concrete specimens were assumed to be: Si (3.539 MeV, 68%} and 4.935 MeV , 63%); Ca (1.942 MeV , 73% and 6.420 MeV, 31%); Fe (7.631 MeV , 29% and 7.646 MeV , 24%) and Al (7.724 MeV, 27%) [Naqvi A. A., et. al., 2006a]. The percentage number after each gamma-ray line is the corresponding intensity. It required approximately 35 minutes of computation time to reduce the statistical uncertainty from 1% to 2% in the prompt gamma-ray yield calculations for the most prominent lines from calcium and silicon.

Determination of Optimum Size of Silica fume Cement Concrete Specimen

The size of a cylindrical silica fume concrete specimen was obtained from the gamma-ray yield calculations as a function of its specimen radius and length. Additionally, the front moderator thickness was also optimized to obtain the maximum yield of prompt gamma-rays in a 25 cm x 25 cm (diameter x height) detector. Figure 2 shows the calculated yield of the prompt gamma-rays for calcium and silicon from silica fume concrete specimen as a function of the front moderator thickness of 14 cm and 23 cm diameter.

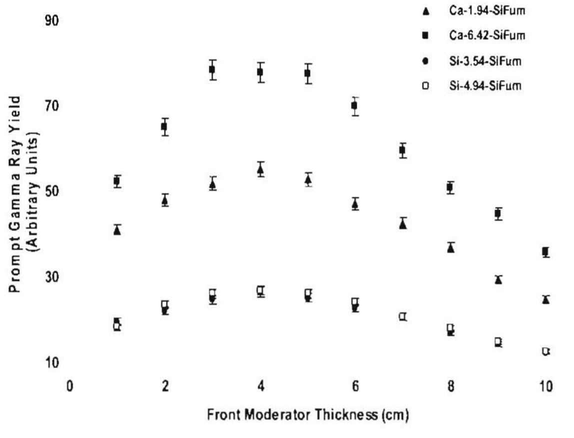

Fig. 2. Yield of gamma-rays from calcium and silicon in the silica fume cement concrete specimen plotted as a function of front moderator thickness.

As was observed in earlier studies [Naqvi A. A., et. al., 2006a], the maximum value of the prompt gamma-ray yield has been observed for a 3 to 5 cm thick front moderator. In the present design of the PGNAA setup, the thickness of the front moderator was chosen to be 5 cm. Figure 3 shows the calculated prompt gamma-rays intensity from calcium and silicon as a function of the specimen radius for a length of 14 cm.

For the 1.94 MeV calcium and silicon gamma-rays, the maximum yield of prompt gamma-rays has been observed for a specimen with a radius in excess of 11 cm; but for the 6.42 MeV gamma-rays from

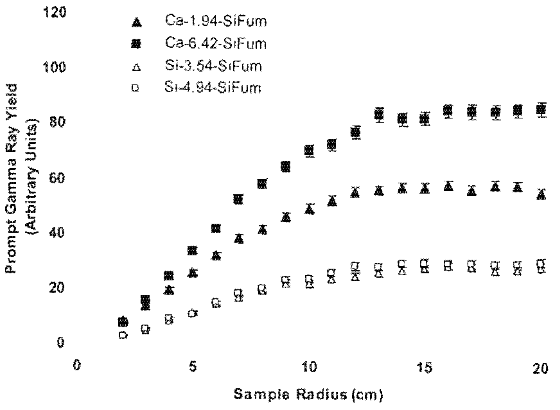

Fig. 3 Yield of gamma-rays from calcium and silicon in the silica fume cement concrete specimen plotted as a function of its radius.

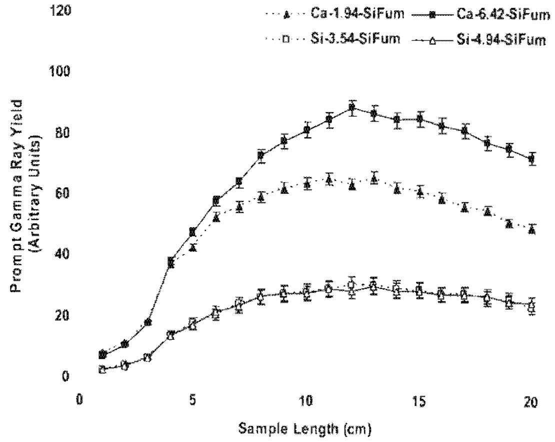

Fig. 4 Yield of gamma rays from calcium and silicon in the concrete specimen plotted as a function of its length.

calcium the maximum radius was observed to be more than 13 cm. Based on the results of the silicon and calcium prompt gamma-ray yield, an average radius of 11.5 cm can be taken. As shown in Figure 4, the maximum yield of calcium and silicon gamma-rays has been observed for a specimen length of 10 to 16 cm. An average length of about 14 cm may be a good choice. The results of these calculations reveal that the optimum radius and length of the specimen are 11.5 and 14 cm, respectively, for a front moderator thickness of 4 to 5 cm.

Results and Discussion

Calibration of the PGNAA setup using Silica Fume Cement Concrete Specimen

The prompt gamma-ray yield was calculated from the six silica fume cement concrete specimens containing 0-20 wt. % silica fume by weight of Portland cement. Since silica fume contains mainly silica, increasing the silica fume concentration in the concrete specimen increases the silicon concentration but the corresponding calcium concentration decreases.

For an addition of 0-20 wt. % of silica fume, by weight of Portland cement, in concrete, it resulted in an increase in the silicon concentration from 14.97 wt. % to 15.84 wt. % while the calcium concentration decreased from 25.85 wt.% to 25.06 wt.%. The calculated yield of prompt gamma-rays from calcium and silicon from these specimens is plotted in Figures 5 through 7. The data in Figures 5 through 7 indicate a linear correlation between the gamma-ray yield and the corresponding compound concentration in the concrete specimen. Figures 5 and 6 show almost similar trends. The slope of the 6.42 MeV prompt gamma-ray is almost 36% more than that of the 1.94 MeV gamma-rays. There is a constant increase in the gamma-ray yield for a corresponding increase in the calcium concentration. Figure 7 also shows a linear increase in the silicon gamma-rays yield for a corresponding increase in the silicon concentration in specimen. The slopes of the yield of the silicon gamma-rays are almost equal; therefore, both the gamma-rays have parallel lines. This study has provided valuable information on the use of silica fume cement concrete for the calibration of a PGNAA setup for the determination of silica. The response was calibrated using six silica fume cement concrete specimens prepared with 0-20 % silica fume by weight of the Portland cement.

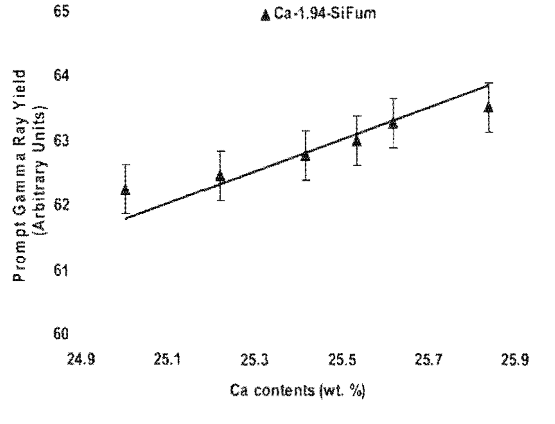

Fig. 5. Yield of 1.94 MeV gamma-rays from calcium plotted as a function of calcium concentration in the six silica fume cement concrete specimens.

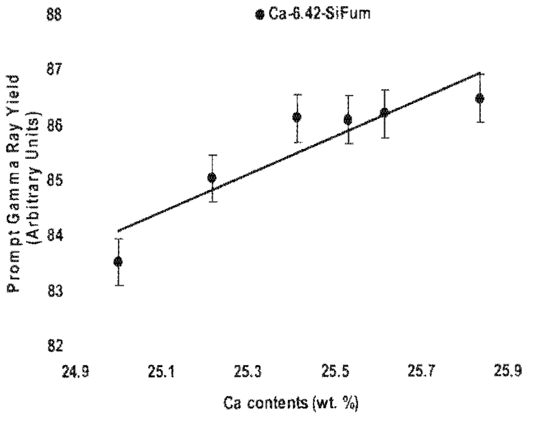

Fig. 6. Yield of 6.42 MeV gamma rays from calcium plotted as a function of calcium concentration in six silica fume cement concrete specimens.

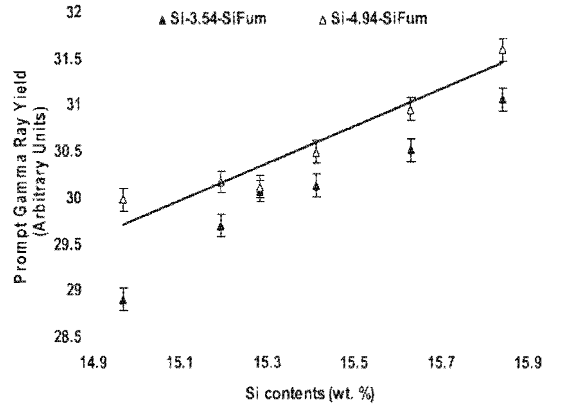

Fig. 7. Yield of 3.54 and 4.94 MeV gamma rays from silicon plotted as a function of silicon concentration in the six silica fume cement concrete specimens.

Conclusions

In this study Monte Carlo simulations were carried out to calibrate the response of the PGNAA setup using silica fume cement concrete specimens for the determination of silicon concentration. The results of the calculations show a linear response of the silicon gamma-rays yield with increasing silica fume concentration in the concrete. This study has shown that silica fume cement concrete specimens can be utilized to calibrate the response of the PGNAA setup for silica measurements.

Acknowledgement. This study is part of KFUPM funded Project No. IN060305. The authors acknowledge the support provided by King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia.

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