### **David Breitenmoser**

# Towards Monte Carlo based Full Spectrum Modeling of Airborne Gamma-Ray Spectrometry Systems

- Extended Summary -



Version This extended summary version is based on the doctoral dissertation "Towards Monte Carlo based Full Spectrum Modeling of Airborne Gamma-Ray Spectrometry Systems" by David Breitenmoser, completed at ETH Zurich and the Paul Scherrer Institute (Diss. ETH No. 30551) [1]. This document provides a condensed but comprehensive overview of the key objectives, methodologies, and results of the dissertation, prepared for submission to the ENS PhD Award 2025 call.

Typesetting This document was typeset with LATEX by adopting the MikTeX distribution in combination with the memoir class. Writing and compilation was performed with the Visual Studio Code (VSC) using the following extensions: LaTeX Workshop, GitHub Copilot and Grammarly Figures were created using MATLAB together with Adobe Illustrator.

Cover information The the front and back cover display the angular dispersion of the Swiss AGRS system's detector response in the full spectrum band at a photon energy of 1618 keV using the Cassini projection (linear color encoding with a maximum response of 1945 cm<sup>2</sup>).

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## **Extended Summary**

Building on decades of scientific and engineering advancements, nuclear technologies have become integral to modern society. Today, they support a wide range of applications, from fundamental research and energy production to medical diagnostics, cancer therapy, industrial quality control, and product sterilization. However, as with any technology, nuclear technologies also come with inherent risks and challenges. The nuclear weapon detonations in Hiroshima and Nagasaki, as well as severe nuclear accidents such as those in Chernobyl and Fukushima, have demonstrated the devastating consequences of large-scale radioactive contamination, posing serious health risks to affected populations [2]. In response to such radiological emergencies, decision-makers must implement effective measures to protect the afflicted population. Yet actions like evacuations can have profound public health, social, and economic repercussions [3]. Therefore, to effectively minimize harm to the population, the protective actions must be carefully aligned with the radiological risk. To reach that goal, authorities require a fast and reliable assessment of the radiological situation.

The method of choice for this purpose is Airborne Gamma-Ray Spectrometry (AGRS), which enables the localization, identification, and quantification of terrestrial gamma-ray sources across  $\mathcal{O}(10^8)\,\mathrm{m}^2$  within  $\mathcal{O}(10^2)\,\mathrm{min}$  using large-volume gamma-ray spectrometers mounted on aircraft. This unique capability makes AGRS not only essential for emergency response but also for a wide range of other applications, including nuclear security, nuclear non-proliferation, geological mapping, mineral exploration, and environmental monitoring [4–6]. The accuracy and sensitivity of AGRS systems rely heavily on the adopted calibration and data evaluation protocols. The International Atomic Energy Agency (IAEA) has standardized these methods in two technical reports [7, 8], which combine simplified physics models with empirical calibration.

While effective, these methods have critical limitations. Current empirical calibration methods are restricted to only a few radionuclide sources. Comprehensive calibration can require up to 5 d to cover all relevant source-detector configurations and often involves high costs for source preparation and decommissioning [9–11]. Additionally, these methods are subject to significant systematic uncertainties, primarily originating from varying radiation backgrounds and necessary analytical corrections. The underlying physics models, on the other hand, are reliable only for photon energies  $\gtrsim 400 \, \mathrm{keV}$ , further limiting the radionuclide sources

that can be calibrated [7, 8]. Moreover, these models are restricted to narrow spectral bands, which greatly reduces the AGRS sensitivity by excluding much of the available information encoded in the pulse-height spectra [12, 13].

These limitations in current AGRS calibration and data evaluation protocols significantly compromise the quality and reliability of radiological assessments in emergency response scenarios. This became particularly evident in the Fukushima accident, where the current restrictions in AGRS severely hindered accurate risk assessment and effective response [14]. This in turn led to unintended negative health effects for the public, such as loss of life during evacuations and increased mortality during long-term displacements among the most vulnerable individuals. Improving the current calibration and data evaluation protocols in AGRS to address the discussed limitations in the capabilities of AGRS systems is therefore of immediate relevance and importance for public safety.

**SCOPE** The main scope of this dissertation was to overcome the limitations of the calibration and data evaluation methods currently employed in AGRS to allow the quantification of any gamma-ray emitting radionuclides relevant in radiological emergencies. This was achieved by developing and validating a novel Monte Carlo based full spectrum methodology for AGRS. This methodology features four key innovations:

**INNOVATION I** To overcome the limitation in empirical calibration discussed above, the proposed AGRS methodology adopts a numerical approach for system calibration rather than relying on empirical methods. This involves performing high-fidelity Monte Carlo simulations on high-performance computer clusters using the multi-purpose Monte Carlo code FLUKA [15] combined with the graphical interface FLAIR [16]. Unlike previous studies, the Monte Carlo model integrates a detailed mass model of the detector system, aircraft, and environment, enabling, for the first time, the accurate numerical prediction of the full spectrum response of AGRS systems to arbitrarily complex gamma-ray fields across the full solid angle. This was demonstrated through extensive radiation measurements using natural and anthropogenic radionuclide sources (K<sub>nat</sub>, <sup>57</sup>Co, <sup>60</sup>Co, <sup>88</sup>Y, <sup>109</sup>Cd, <sup>137</sup>Cs, <sup>133</sup>Ba, and <sup>152</sup>Eu) with the fully integrated Swiss AGRS system, conducted under a range of laboratory and field conditions [17, 18]. The model predictions demonstrated excellent agreement with the radiation measurements, showing median relative deviations <10 % across the full energy range of the spectrometer from ~50 keV to ~3 MeV. These results highlight that the developed numerical methodology not only effectively addresses the significant deficiencies of previous approaches (reducing relative errors by factor >20, from >200 % to <10 %) [19, 20], but also achieves, for the first time, the accuracy and precision necessary to supersede traditional empirical calibration methods currently in use in AGRS (ten-fold improvement). This marks a major advancement in AGRS. The developed methodology not only allows for the full spectrum numerical calibration of any gamma-ray source with an unprecedented level of accuracy, but also reduces calibration time and costs, minimizes reliance on high-intensity calibration

sources, and eliminates the generation of related radioactive waste.

**INNOVATION II** Most AGRS spectrometers, including the Swiss AGRS system used to validate the numerical calibration framework presented above, rely on large-volume NaI(Tl) inorganic scintillator crystals. For such crystals, the nonproportional scintillation response of NaI(Tl) can introduce systematic spectral biases  $\mathcal{O}(10^4)$  eV, which are inherent in traditional Monte Carlo models [17]. Since the non-proportional scintillation response of each spectrometer is unique [21], we developed a novel empirical method to probe non-proportional scintillation physics in inorganic scintillators by combining gamma-ray spectrometry with Bayesian inference and a custom machine-learning-trained vector-valued polynomial chaos expansion emulator [22]. Applying this new method to NaI(Tl) scintillators provided the first conclusive evidence that the distinct spectral shifts of the Compton edges observed by previous investigators are the result of the scintillation non-proportionality. On a practical level, this new probing technique enables the calibration of non-proportional scintillation physics models (NPSMs) for Monte Carlo simulations, thereby overcoming the systematic spectral biases inherent in traditional Monte Carlo models. This was demonstrated through a series of laboratory-based radiation measurements using radionuclide point sources. Due to the broad applicability of the adopted NPSM, this methodology originally developed for gamma-ray spectrometry—can be adapted to any combination of inorganic scintillators and ionizing radiation fields. This extends its utility to areas such as dark matter research [23, 24], material sciences [25], and total absorption spectroscopy [26]. Moreover, in contrast to existing methods, it does not require any additional measurement equipment and can also be used during detector deployment, which is especially attractive for space missions and remote sensing applications [27, 28]. The originality and broad relevance of this innovation make it a key highlight of this dissertation, as evidenced by its publication in Nature Communications.

**INNOVATION III** While the Monte Carlo based full spectrum modeling approach for AGRS systems has proven superior to traditional empirical methods, its feasibility for integration into routine AGRS spectral analysis pipelines had to be demonstrated, with the associated computational cost posing the primary challenge. To achieve the required precision, a Monte Carlo simulation of a single spectral signature requires a characteristic computation time of  $\Delta t_{\rm MC} = \mathcal{O}(10^4)$  core-hours on a medium-sized computer cluster, such as the one used in this dissertation. Moreover, due to the inherent variability in the source-detector configurations as well as the various changes in the atmospheric and terrestrial properties during a survey flight, spectral signatures need to be predicted for each recorded pulse-height spectrum and each gamma-ray source of interest. As a result, the number of model evaluations necessary for the analysis of a typical AGRS survey flight with  $N_{\rm spec} = \mathcal{O}(10^4)$  recorded spectra and  $N_{\rm src} = \mathcal{O}(10^4)$  gamma-ray sources of interest is in the order of  $N_{\rm src}N_{\rm spec}\Delta t_{\rm MC} = \mathcal{O}(10^9)$  core-hours. Given these numbers, it is evident that

calibrating AGRS systems for extended AGRS surveys using brute-force Monte Carlo simulations becomes computationally prohibitive with the currently available cluster infrastructure. To resolve this limitation in Monte Carlo simulations, this dissertation proposes a surrogate convolution approach, inspired by related applications in astrophysics [29–33] and planetary science [34–36]. By leveraging array programming, this surrogate convolution model accelerates brute-force Monte Carlo simulations by a factor of  $\mathcal{O}(10^6)$ , allowing evaluations on a local workstation in  $\mathcal{O}(1)$ s per spectral signature. When compared with the high-fidelity Monte Carlo model for the Swiss AGRS system across selected source-detector configurations, the surrogate method achieved excellent accuracy, with a median relative deviation <6% over the full energy range of the spectrometer from ~50 keV to ~3 MeV. With this, we have demonstrated that Monte Carlo based full spectrum modeling, accelerated by surrogate convolution models, can achieve not only the required accuracy and precision but also the computational efficiency needed to supersede current empirical-based calibration methods.

INNOVATION IV Since no data evaluation framework currently exists to incorporate the newly developed surrogate convolution models for AGRS applications, it became apparent that a new data evaluation approach is required to fully exploit the capabilities of the Monte Carlo based full spectrum modeling approach. For that purpose, this dissertation introduces a novel full spectrum analysis methodology to perform accurate quantification of arbitrary gamma-ray fields by AGRS. This methodology integrates the newly developed numerical models discussed above within a Bayesian inference framework. Unlike traditional spectral analysis methods, this new framework allows for the quantification of any type and number of gamma-ray sources, including those with photon energies <400 keV and source vector dimensions >5. Validation with the Swiss AGRS system using a series of field measurements demonstrated excellent accuracy and precision in quantifying the source strengths of deployed radionuclide sources with relative errors < 2 % for a measurement time of 1 s. This represents a ten-fold improvement in accuracy compared to traditional methods. Additionally, leveraging the Monte Carlo based approach, this method extends the capability of AGRS to quantify not only terrestrial gamma-ray sources but also atmospheric ones, including radon and cosmic-ray-induced backgrounds. This was demonstrated in a series of geophysical survey flights conducted in Switzerland and over the North Sea, providing the first comprehensive quantification of the secondary cosmic-ray flux and radon progeny activity concentrations in the lower atmosphere at altitudes ranging from  $\approx 30 \,\mathrm{m}$  to  $\approx 2500 \,\mathrm{m}$ . The flights revealed a potential enhancement of radon levels over the Swiss Alps and indicated that existing best-estimate numerical models tend to increasingly underestimate the secondary cosmic-ray flux at latitudes closer to the poles. This latter finding is particularly important, as it not only advances our understanding in geophysics but also has practical implications for refining aviation dose calculations, which depend on accurate predictions of the secondary cosmic-ray flux in the atmosphere.

CONCLUSION In conclusion, the Monte Carlo based full spectrum modeling approach developed and validated in this dissertation marks a major advancement in AGRS. The presented methodology not only significantly enhances detection accuracy and sensitivity but more importantly also substantially broadens the operational capabilities of AGRS systems in emergency response to radiological incidents like severe nuclear accidents and nuclear weapon detonations. Moreover, these advancements offer promising new capabilities for AGRS applications beyond emergency response, including advancing geophysical research, nuclear security and mineral exploration, among others. The Swiss nuclear regulator has recognized the importance of this innovation, committing funding for its integration into the routine evaluation protocols of the Swiss AGRS system. The ongoing close collaboration with over ten AGRS teams worldwide, alongside the publication of a comprehensive monograph that synthesizes the developed Monte Carlo-based full spectrum modeling approach, ensures that the work presented in this dissertation benefits global AGRS missions. By providing a paradigm shift in calibration and data analysis, this work contributes to the establishment of a new international standard for AGRS, ultimately supporting better-informed protective actions and reducing health risks during radiological emergencies on a global scale.

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This dissertation focuses on improving Airborne Gamma-Ray Spectrometry (AGRS), a critical tool in responding to radiological emergencies such as severe nuclear accidents or nuclear weapon detonations. AGRS systems use large-scale gamma-ray spectrometers mounted on aircraft to rapidly identify and quantify radiation hazards over extensive areas, providing essential data to guide emergency response efforts.

Current AGRS calibration and data evaluation methods struggle to accurately quantify many radioactive materials expected in radiological emergencies, limiting the risk assessment and hence the effectiveness of emergency response actions. The goal of this work is to address these challenges by developing and validating a novel Monte Carlo based full spectrum modeling approach for the Swiss AGRS system.

The methodology features four key innovations: high-fidelity Monte Carlo simulations that integrate detailed geometric representations of the aircraft and detector system; an advanced physics model to characterize the spectrometer's non-proportional scintillation response; a surrogate model that replicates the Monte Carlo simulations with significantly reduced computation time; and a new data evaluation method that leverages the surrogate model within a Bayesian inversion framework, enabling the quantification of any gamma-ray emitting radionuclide involved in radiological emergencies. These models were rigorously validated under various laboratory and field conditions, demonstrating strong agreement between model predictions and radiation measurements.

In conclusion, this dissertation represents a significant advancement in AGRS calibration and data evaluation. The developed methodology not only enhances detection accuracy and sensitivity, but also significantly expands the operational capabilities of AGRS systems during radiological incidents. These innovations lay the groundwork for improving AGRS practices in Switzerland and may contribute to establishing a new global standard for AGRS systems, ultimately supporting better-informed protective actions and reducing health risks during radiological emergencies.

