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Deconvolution and Mass Spectroscopy: an Analysis of Theses and Dissertations in the Nuclear Field

Deconvolução e Espectroscopia de Massas: uma Análise de Teses e Dissertações na Área Nuclear

Deconvolución y Espectroscopía de Masas: un Análisis de Tesis y Disertaciones en el Área Nuclear

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Resumo

A deconvolução tem sido utilizada em diversas áreas do conhecimento, entre elas, na área nuclear, principalmente em processos nos quais são necessários modelos matemáticos para análise de sinais e, nesse cenário, destaca-se a aplicação da espectrometria gama. Com o intuito de demonstrar a relação entre deconvolução e espectrometria na área nuclear, este artigo teve como objetivo realizar uma revisão bibliográfica por meio do Banco de Teses e Dissertações (BTD) da Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) de trabalhos realizados sobre o tema. Constatou-se que, embora tenham sido identificados poucos trabalhos na área nuclear, a grande maioria que utilizou deconvolução envolve espectrometria de massas, em diversas áreas, como no estudo de algoritmos genéticos, coincidência pico-soma, coincidências íon-íon, detectores OSL e termoluminescentes, bem como espectrometria de nêutrons, por exemplo. Compreende-se, portanto, a relevância da gestão do conhecimento científico para o reconhecimento da deconvolução como uma ferramenta importante na análise de sinais na área nuclear, especialmente em processos que utilizam espectrometria gama.

Palavras-chave: deconvolução; espectroscopia de massa; Brasil; CAPES; CNEN.

Abstract

Deconvolution has been used in several areas of knowledge, such as in the nuclear area, mainly in processes in which the modeling of mathematical models for signal analysis is necessary. And one of these applications is related to gamma spectrometry. In order to demonstrate the relationship between deconvolution and spectrometry in the nuclear area, this article aimed to carry out a bibliographical review through the Theses and Dissertations Bank (BTD) of the Coordination of Higher Education Personnel (CAPES) of works carried out on the theme. It was found that although few works were identified in the nuclear area, the vast majority of works that used deconvolution are related to works that involve mass spectrometry, in several areas, such as the study of Genetic Algorithms, Coincidence peak-sum, Ion-ion coincidences, OSL and thermo-luminescent detectors and Neutron spectrometry, for example. It is understood, therefore, the relevance of scientific knowledge management for the recognition of deconvolution as an important tool in the analysis of signals in the nuclear area, especially in processes that use gamma spectrometry.

Palavras-chave: *deconvolution; mass spectroscopy; Brazil; CAPES; CNEN*

Resumen

La deconvolución ha sido utilizada en diversas áreas del conocimiento, como en el ámbito nuclear, principalmente en procesos en los cuales es necesaria la modelización mediante modelos matemáticos para el análisis de señales. Una de estas aplicaciones está relacionada con la espectrometría gamma. Con el propósito de evidenciar la relación entre la deconvolución y la espectrometría en el área nuclear, el presente artículo tuvo como objetivo realizar una revisión bibliográfica a través del Banco de

Teses y Disertaciones (BTD) de la Coordinación de Perfeccionamiento de Personal de Nivel Superior (CAPES), considerando trabajos desarrollados sobre el tema. Se constató que, aunque se identificaron pocos estudios en el ámbito nuclear, la gran mayoría de los trabajos que emplearon deconvolución están vinculados a investigaciones que involucran espectrometría de masas en diversas áreas, tales como el estudio de Algoritmos Genéticos, Coincidencia pico-suma, Coincidencias ión-ión, Detectores OSL y termoluminiscentes, y Espectrometría de Neutrones, por ejemplo. Se entiende, por tanto, la relevancia de la gestión del conocimiento científico para el reconocimiento de la deconvolución como una herramienta importante en el análisis de señales en el área nuclear, especialmente en procesos que utilizan espectrometría gamma.

Palabras clave: *deconvolución; espectroscopía de masas; Brasil; CAPES; CNEN.*

1 Introduction

Nuclear Metrology is an area of measurement science that has several analysis methods, with several study models, in which the correct extraction of data becomes an essential problem in the construction of the solution of the chosen method, the option being considered a factor that directly influences the traceability of these results to those already established (Tauhata et al., 2013; Van Rieken; Markowicz, 1992; VIM, 2012).

In this sense, knowledge of energy spectra of incident or scattered ionizing radiation is important in the areas of nuclear physics, radiation physics and medical physics, for example. Thus, spectrometry[1] is a proven efficient and non-destructive technique. However, for radionuclides whose decays are more complex, analysis methods are needed that allow the discrimination of close energies or entanglements of statistical data inherent to nuclear phenomena. Generally speaking, a mass spectrometer consists of three main parts: (1) ion source, (2) m/z filter, and (3) detector. The first part is responsible for the generation of ions in the gas phase from the samples. In the m/z filter, the ions generated in the source are separated according to their mass/charge ratios. The detector is responsible for quantifying the ions that pass through the m/z filter. The most natural application of mass spectrometry, and the one that is also linked to its very creation, is the separation and analysis of isotopes (Neto, 2003).

The non-destructive process of investigating materials, known as gamma spectrometry[2], is based on understanding the role that each decay (Alpha and Gamma) plays in all radionuclide emissions, identifying them through a correct measurement of their parameters, being very useful due to a modest amount of core data (Gilmore, 2008).

The changes that occur inside massive nuclei, which have modes and arrangements adjusted to nuclear energies, obey the balance equations in which the mass of the product or products is smaller than the original nuclide. In summary, there is a decrease in the total energy of the system referring to the nuclear bonds, which release energy when they are “broken”, which is in agreement with equation $\Delta E = \Delta m.c^2$, formulated by Einstein. For a given number of nucleons, there is an energy level that is as low as possible. When an atomic nucleus does not remain at this lowest level, it is in an unsAnnex state and has a tendency to emit some type of radiation (Gilmore, 2008).

The document that summarizes this complex chain of events is the spectrogram, producing estimates of the counts of photon emitting sources, as a function of the energies distributed in hundreds of channels in semiconductor detectors. The modeling of this spectrum is done through adjustments of experimental data and non-linear regressions, which can lead to a solution with a reduced number of parameters, thus having the

[1] In general, spectroscopy is the science of studying (theoretical part) the interaction between matter and radiated energy, while spectrometry is the method (practical part) used to acquire a quantitative measure of the spectrum; that is, spectrometry is the measurement of radiation intensity using an electronic device.

[2] In general, gamma spectroscopy is the study of the energy spectra of gamma-ray sources, where spectrometers are devices designed to measure the power spectral distribution of a source. The incident radiation generates a signal that allows to determine the energy of the incident particle. This is because most radioactive sources produce gamma rays, which are of various energies and intensities. they are often accompanied by the emission of alpha and beta radiation, so that when these emissions are detected and analyzed with a spectroscopy system, a spec-trum of gamma-ray energy can be produced.

observer, a doubtful limit in the confidence of this signal. It is at this point that the deconvolution of the spectrum comes in as a differentiated method, as there are very close energy lines or superimposed peaks composing the spectrum (Van Rieken; Markowicz, 1992).

Most spectrograms of unsAnnex radionuclides have been analyzed and revised in recent years for various photon emitters. In the search for improvements in the decay parameters of this alpha emitter, the adjustment and deconvolution methods applied to the geometries of semiconductor detectors, which are present in gamma spectrometry, are used. The processes involving radioactive decays have a random character, and any measurement that is based on information from the emitted radiation is based on some degree of fluctuation, which leads to an ineviAnnex uncertainty (Van Rieken; Markowicz, 1992).

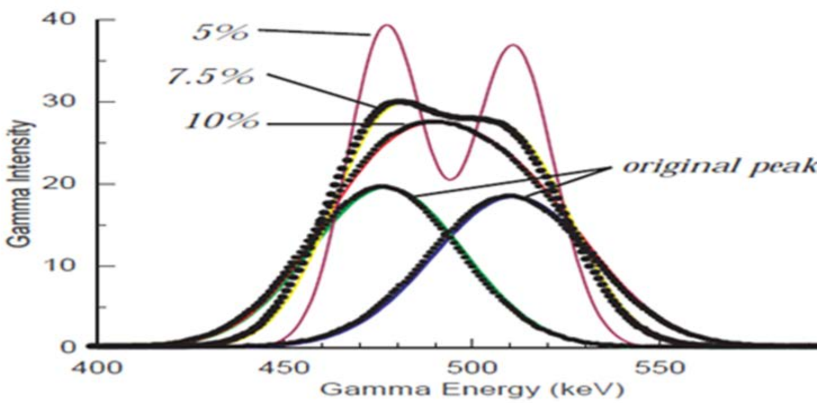
In view of this, improving the reading of these spectrograms means achieving the convergence of these obtained values, to the traceable data of the parameters that involve nuclear decay. For the radionuclide under analysis, the structure of the probabilities related to the decay spectrum can be debugged, comparing methods and software employed and their differences or particularities. Gamma spectrometry is an analytical process that provides the possibility of non-destructive, qualitative or quantitative analysis of the intrinsic properties of radionuclides that emit electromagnetic energies (Gilmore, 2008).

The readings acquired from the emission spectra, which are independent of the impurities in the samples, in different geometries or arrangements, allow calibrations and standardization of the radionuclides taking into account the source-detector distance. The advantage is verified when identifying and quantifying the activities of photon emitters in a sample, without complex chemical separations and simultaneously evaluating several radionuclides (Debertin, 1980; Morhac; Matousek, 2012).

Thus, this method allows determining the number of photons emitted by a given radioactive source, with two types of measurements: absolute and relative. The absolute determine the exact number of particles emitted, while the relative just a fraction of emissions, always taking into account the geometry of the system. Spectrographic analyzes can be influenced by the source-detector geometry, intrinsic efficiency of the material’s active volume, the mode of absorbing radiation and the solid angle, and can be adapted for other types of emissions (Simões, 2018).

In the statistical processes of detection systems, observed fluctuations in peak widths occur. The conversion of gamma energy into electrical or light pulses can lead to very close measurements, such as two identical photons totally absorbed in the detector crystal, which do not produce exactly the same signal as they can have the same energy, but not the same height. The results of these statistical processes are well represented by a normal or Gaussian distribution, which has as resolution the proportion between the width and the centroid value. The finite width of the observed peak implies the difficulty in measuring the centers of two adjacent peaks, with the gamma energies separated by less than the width of these photopeaks, as shown in figure 1 (Venkataramaiah; Sanjeeviah; Sanjeevaiah, 1978).

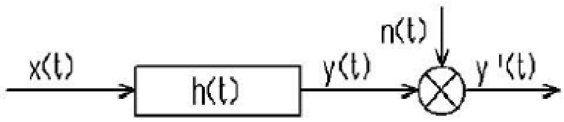
Figure 1 - Overlapping spectra of two equal areas and the percentages of their combinations.



Source: Venkataramaiah; Sanjeeviah; Sanjeevaiah, 1978.

The overlapping spectra above are of two equalarea photopeaks centered at 477 keV and 511 keV. The individual photopeaks are show at 10% resolution underneath the other spectra. The combintion of the two photopeaks is shown for resolutions of 5%, 7.5 and 10%. The quality of the spectrometric data, due to ionizing radiation, is based on the correct identification of the existence of peaks, and a good estimate of the parameters of their positions and intensities (areas). These peaks are the main carriers of information, which are compacted when evaluated in the detectors resolution. Figure 2 shows the signal filtering scheme (Morhac; Matousek, 2011).

Figure 2 - Linear system with added noise.



Source: (Morhac; Matousek, 2011).

The convolution and deconvolution methods represent the most efficient tools to improve this resolution in the data. With the decomposition of the overlapping peaks and the identification of the multiplets, the method is sufficient to improve the determination of the positions and intensities of the energy peaks in the gamma spectra (Delgado; Morel; Etcheverry, 2002; Morhac; Matousek, 2011).

1.1 Materials and Methods

In In this sense, this paper was developed in order to carry out a bibliographic review aiming at scientific knowledge management on the application of deconvolution in studies involving spectrometry in the nuclear area. This is because it can be said that the understanding of scientific knowledge itself, by a teaching and research institution, ends up promoting advances in its activities, helping in the technological innovation of its respective area of activity (Gil, 2009; Razuck; Ferreira, 2025; Gil, 2009).

In this way, considering the range of applications and the relevance of the gamma spectrometry process, this work aims to evaluate, together with the Theses and Dissertations Bank (BTD) of the Coordination of Support for Higher Education Personnel (CAPES) the production on the use of deconvolution in the nuclear spectrometry process, in view of the lack of a review on the application of this methodology in Brazil (Brasil, 2025a).

By understanding the BTD as an important indicator of bibliographic production, a qualitative-quantitative research was carried out, identifying and classifying the works (qualitative research) and making a quantitative analysis by area of knowledge, using the keyword “deconvolution”. The works whose term was found either in the title, or in the abstract or in the keywords (Brasil, 2025a).

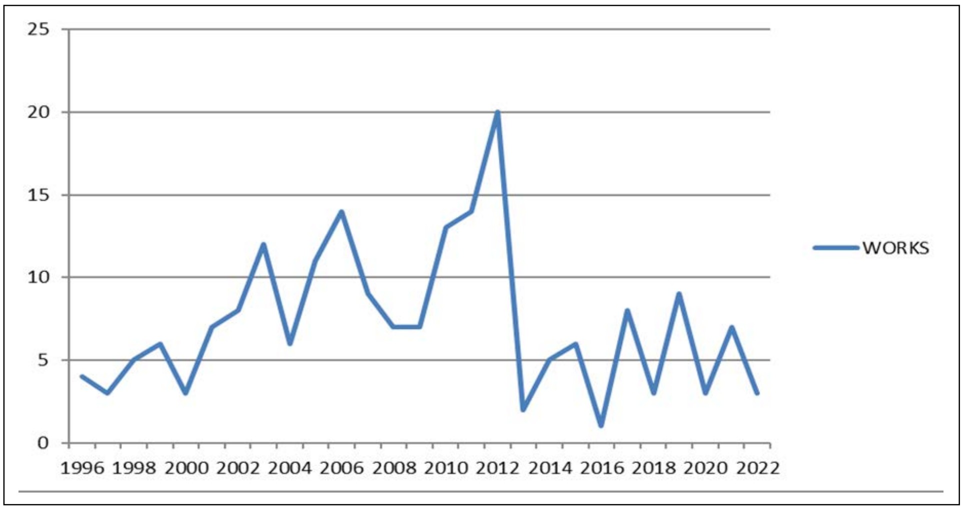
After this search, an individual analysis of those works that used deconvolution in the nuclear area was carried out. For this, a refinement was carried out (work by work) for those who used “spectrometry”, or other related themes, such as “spectrogram”, “spectrum” or “spectrometer”, for example, in the title, in the abstract in the keywords or even in the text. The objective was then to verify the relevance of the theme specifically for the area. At the end, a specific search was carried out for the nuclear area, in the case of Higher Education Institutions (HIEs) linked to the National Nuclear Energy Commission (CNEN) that have stricto sensu graduate programs, namely (Brasil, 2025b):

- Center for the Development of Nuclear Technology (CDTN) – Posgraduate Program in Science and Technology of Radiation, Minerals and Materials;
- Northeast Regional Center for Nuclear Sciences (CRCN) – Posgraduate Program in Energy and Nuclear Technologies;
- Institute of Nuclear Engineering (IEN) – Posgraduate Program in Nuclear Science and Technology;
- Institute for Energy and Nuclear Research (IPEN) – Posgraduate Program in Nuclear Technology; and
- Institute of Radiation Protection and Dosimetry (IRD) – Posgraduate Program in Radiation Protection and Dosimetry.

2 Results and Discussion

A total of 216 works were found when using the keyword “deconvolution”, of which 135 theses (doctorade or Ph.D.) and 81 dissertations (master), between the years 1996 and 2022 (figure 3).

Figure 3 - Evolution of work over the years.

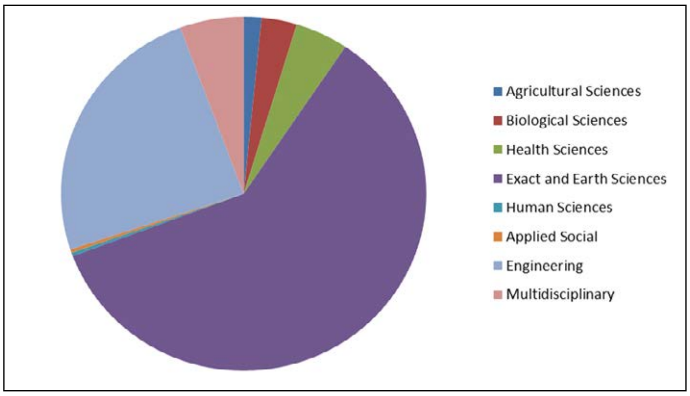


Source: The author.

It is possible to verify the presence of works on deconvolution during all years, having its peak between the years 2010 and 2012. In total, works were found in 8 Knowledge Areas (figure 4)[3], distributed as follows:

- Agricultural Sciences (5);
- Biological Sciences (10);
- Health Sciences (15);
- Exact and Earth Sciences (191);
- Human Sciences (1);
- Applied Social Sciences (1);
- Engineering (78);
- Multidisciplinary (18).

Figure 4 - Distribution by Area of Concentration.



Source: The author.

A greater concentration is observed here in the areas of Exact and Earth Sciences, followed by Engineering, which is natural, bearing in mind mathematical applications. However, it is possible to find works in all areas of knowledge (except Linguistics), showing the applicability of the method. Specifically for the nuclear area, 23

[3] According to Capes, there are 9 areas of knowledge: Exact and Earth Sciences; Biological Sciences; Engineering; Health Sciences; Agricultural Sciences; Social and Applied Sciences; Human Sciences; Linguistics, Letters and Arts; and multidisciplinary. In addition, there are a total of 49 Assessment Areas.

(twenty-three) works were found, described below, in Table 1 , in chronological order. According to Table 1, of the 23 works found for deconvolution in the nuclear area, 19 used some paddle related to Spectrum/Spectra (1, 2, 4, 5, 6, 8, 9, 11, 12, 13, 15, 16, 17, 18, 19, 20, 21, 22 and 23), which corresponds to 8.77% of the total on deconvolution and 82.61% of the total on Spectrum/Spectra.

Table 1 – Total of Works found.

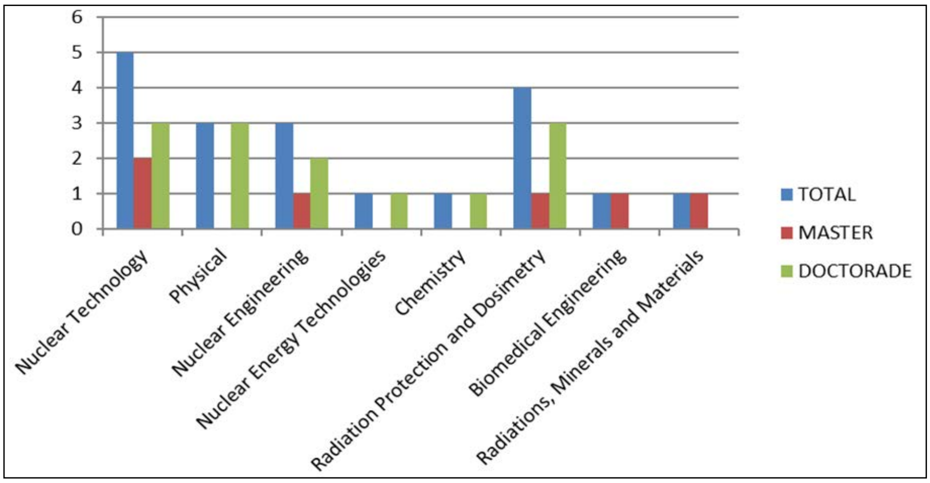
TITLE	AUTHOR	Master (M)/ Doctorade (D)	YEAR	PROGRAM/ HIE
1) Mean cross-section measurements in the U-235 fission spectrum, for some threshold reactions	MAIDANA, N. L.	M	1993	Nuclear Technology/ IPEN
2) Photoproduction of Neutrons in Th-232 and U-238 with Gamma Radiation of Thermal Neutron Capture in the Energy Range between 5.61 to 10.83 meV	LELIS, G. O.	D	1998	Nuclear Technology/ IPEN
3) Applications of quadrupole nuclear resonance in two dimensions	RODRIGUES, H. J. C.	D	1998	Physics / University of São Paulo
4) X and Gamma Emission Probabilities Determined by Spectrometry in Complex Regions	DELGADO, J. U.	D	2000	Nuclear Engineering/IEN
5) Study of Neural Networks for Application in Neutron Spectrometry and Dosimetry	BRAGA, C. C.	D	2001	Nuclear Technology/ IPEN
6) Inverse problems in experimental physics: the photonuclear cross section and electron-positron annihilation radiation	TAKIYA, C.	D	2003	Physics / University of São Paulo
7) Effects of gamma irradiation on b-lactoglobulin: structural changes and aggregation	URREJOLA, L. DEL C. DE LA H.	D	2006	Food and Nutrition/ Campinas State University
8) Measurements of 9Be, 13C and 17O Photoneutron Cross Sections with Thermal Neutron Capture Gamma radiation	SEMMLER, R.	D	2006	Nuclear Technology/ IPEN
9) Unfolding neutron spectra using the Monte Carlo method and neural networks	JUNIOR, R. M. DE L.	D	2009	Nuclear Engineering/IEN
10) Study and evaluation of bubble detectors for neutron field measurements	DANTAS, J. E. R.	M	2010	Nuclear Engineering/IEN
11) Deconvolution of neutron spectra obtained with the EB-TLD system using genetic algorithm	SANTOS, J. A. DE L.	D	2011	Nuclear Energy Technologies/CRCN
12) Synthesis, microstructural and electrical characterization of ceramic compounds based on solid solutions of strontium titanate, calcium titanate and iron oxide	CARMO, J. R. DO	D	2011	Nuclear Technology/ IPEN
13) Applications of the Warren-Averbach method of diffraction profile analysis	ICHIKAWA, R. U.	M	2013	Nuclear Technology/ IPEN
14) Use of multivariate normal functions in the study of the fragmentation of sulfur-containing molecules ionized by electrons and photons	VARAS, L. J. R.	D	2016	Chemistry/UFRJ
15) Studies of Thermoluminescence (TL), Paramagnetic Resonance (EPR) and Optical Absorption (AO) properties for characterization of the mineral Monticelite	QUINA, A. DE J. A. DE	M	2016	Nuclear Technology/ IPEN
16) Primary standardization of complex decay radionuclides by pico-sum coincidence method and photon spectrometry with GeHP detector	SILVA, R. L. DA	D	2017	Radiation Protection and Dosimetry/IRD
17) Absolute standardization of Ra-223 and calibration of LNMRI reference systems	SIMOES, R. F. P.	D	2018	Radiation Protection and Dosimetry/IRD
18) In vivo dosimetry using EPID	SILVEIRA, T. B. DA	D	2018	Radiation Protection and Dosimetry/IRD
19) Artificial bee colony-based algorithm for deconvolution of neutron spectra obtained with Bonner spheres	SILVA, E; R. DA	D	2019	Radiation Protection and Dosimetry/IRD
20) Personal dose equivalent Hp (10) in diagnostic imaging using OSL detectors based on Brazilian fluorite	PAGOTTO, I.	M	2021	Biomedical Engineering/ UFTPR
21) Theoretical study of the spectroscopic and structural properties of LiF, EuF3, AF2 (A = Ca, Sr and Ba) doped with Eu3+	MESQUITA, B. R. DE	D	2021	Physics/UFS
22) Study of Bonner spectrometer responses with spheres of different polymeric materials	MENDES, L. M. M.	M	2021	Science and Technology of Radiation, Minerals and Materials/CDTN
23) Application of spectral deconvolution algorithms to estimate probabilities of Ra-223 photon emission in complex regions	RAMOS, M. DOS S.	M	2021	Radiation Protection and Dosimetry/IRD

Source: The author.

The works were produced between the years, between the years 1993 and 2021, 6 of which were master's and 13 were doctoral, in 8 Graduate Programs from 7 different institutions (figure 5):

- Nuclear Technology - 5 (2M and 3D from the University of São Paulo/Nuclear and Energy Research Institute);
- Physics – 3 (2D from the University of São Paulo and 1D from the Federal University of Sergipe);
- Nuclear Engineering – 3 (1M and 2D from the Federal University of Rio de Janeiro);
- Nuclear Energy Technologies – 1 (1D from the Federal University of Pernambuco);
- Chemistry – 1 (1D at the Federal University of Rio de Janeiro);
- Radiation Protection and Dosimetry – 4 (1M and 3D from the Institute of Radiation Protection and Dosimetry);
- Biomedical Engineering – 1 (1M from the Federal Technological University of Paraná); and
- Science and Technology of Radiation, Minerals and Materials – 1 (1M from the Center for the Development of Nuclear Technology at the Federal University of Minas Gerais).

Figure 5 - Distribution by Programs in the Nuclear Area.

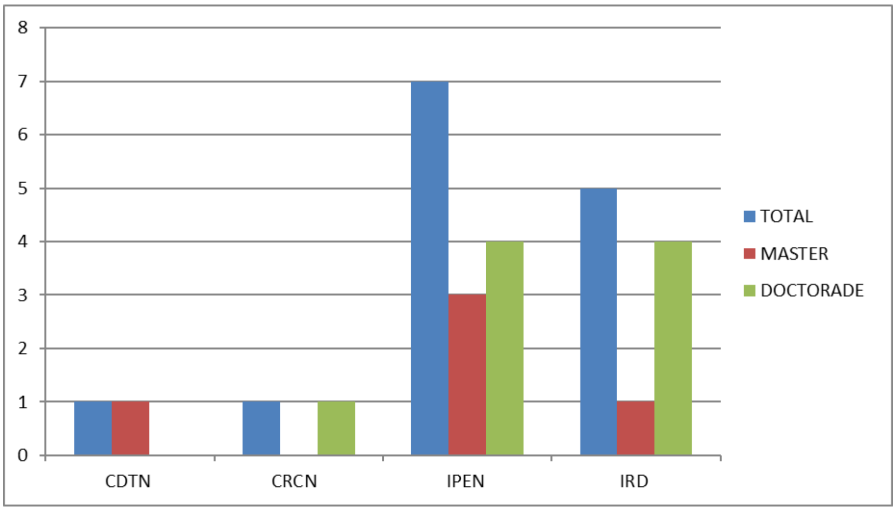


Source: The author.

Thus, the works involved different applications in the nuclear area (according to the keywords), such as the study of: 133Ba; 223Ra; Optical absorption; Genetic algorithms; Activity; Interaction load; Peak-sum coincidence; Ion-ion coincidences; Colony of artificial bees; OSL detectors; Thermo-luminescent detectors; Multivariate normal distribution; Electrons; Bonner spheres; Neutron spectrometry; Gamma spectrometry; Time-of-flight mass spectroscopy; $Eu^{3+;}$ Brazilian natural fluorite; 3D printing; Artificial intelligence; MCNPX; Computational modeling; Individual monitoring; Monticellite; Neutrons; Olivine; Absolute standardization; Primary standardization; PEPIPIC; Probability of photon emission; Radiation protection; Fluoride crystals; Gamma radiation capture; synchrotron radiation; Photonuclear reactions; Photoneutron cross section; Silicate; Symmetry; Crystal field theory; and Thermoluminescence. Specifically with regard to HIEs linked to CNEN, 14 works were found, which corresponds to 6.50% of the total on Deconvolution and 60.87% in the nuclear area. Thus, the distribution of work is as follows (figure 6):

- CDTN - 1 work, 1 dissertation;
- CRCN – 1 work, 1 thesis;
- IPEN – 7 works, 3 dissertations and 4 theses; and
- IRD – 5 works, 1 dissertation and 4 theses.

Figure 6 - Distribution by CNEN HIEs.



Source: The author.

3 Conclusion

Although few works were found that use deconvolution in the nuclear area (23 in total), practically all (19) were applied in relation to mass spectrometry, more especially in gamma. In this sense, it is possible to verify the intrinsic relationship between deconvolution and spectrometry, in several areas of research related to the nuclear area. Specifically regarding the use of deconvolution in the nuclear area, a total of 8.77% of works were found, while about the application of spectrometry would be related to about 82.61% in the nuclear area.

In the future, it is intended to deepen studies on the issue of mathematical models applied to deconvolution. In this sense, it is worth mentioning that one of the main objectives of this work was to carry out a Scientific Knowledge Management on the use of spectrometry in works involving deconvolution in Brazil, since it was not possible to find more data in the national bibliography. Thus, it is understood that this analysis can help in future work on the subject.

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