

REVIEW


Cite this: *RSC Adv.*, 2025, 15, 15408

Thermal analysis as a tool for the environmental assessment of agricultural chemical residues: a systematic review

Tahereh Gholami,^{ID} ^{ab} Meghdad Pirsaeheb,^{*ab} Hooman Seifi,^{ID} ^{ab} Forat H. Alsultany^c and Masoud Salavati-Niasari^{ID} ^{*d}

This review investigates the use of thermal analysis (TA) methods for the assessment of agricultural chemical residues. It also focuses on the use of differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and differential TA (DTA) to evaluate the thermal characteristics and degradation products of such residues. An extensive literature review was conducted in scientific databases such as Scopus, PubMed, and Web of Science to identify relevant studies published between 2000 and 2023. This review also highlights the success of TA in the detection of residue composition and stability as well as the potential hazards posed to the environment. The findings of this review demonstrate that TA methods offer valuable information on the thermal stability and degradation profiles of several agricultural chemicals and are therefore useful in assessing the long-term environmental impact of such chemicals. The discussion majorly revolves around the advantages of thermal techniques over conventional chemical techniques, such as their ability to analyze complex mixtures with minimal sample preparation. Overall, this review finds that TA is a valuable tool for environmental monitoring to help improve sustainable agricultural practices through better management and understanding of chemical residues in the environment.

Received 18th February 2025
Accepted 7th April 2025

DOI: 10.1039/d5ra01170a

rsc.li/rsc-advances

1. Introduction

Agriculture has long relied on the use of chemical inputs such as pesticides, herbicides, and fertilizers to increase yields or protect crops from damage. It is worth appreciating the significant role these chemicals play in food security while noting that they are also the cause of soil, water, and air pollution. If not properly managed, residues of these chemicals can have detrimental effects on ecosystems and human health. Owing to the complexity and variability of these chemical residues, they are difficult to analyze and the qualitative methods used to assess their environmental impacts are sensitive.^{1,2} Among the available techniques, thermal analysis (TA) methods, including TGA, DSC, and DTA, have emerged as powerful analytical methods for providing insights into the thermal characteristics and degradation behaviors of these residues. However, their application in environmental assessments, particularly for

agricultural chemical residues, remains underexplored, warranting a review of their capabilities and efficiency.

The following are some of the challenges that are encountered while analyzing agricultural chemical residues in the environment. Many of these chemicals are present in complex mixtures, making it difficult to identify individual substances. While conventional techniques such as chromatography and mass spectrometry (MS) are valuable under some circumstances, they may not provide sufficient details concerning the thermal stability, degradation pathways, or persistence of these residues in the environment. Furthermore, the low concentrations of these chemicals in environmental samples make their detection difficult, leading to an underestimation of their impacts. Another essential problem is the transformation of such chemicals into secondary products during environmental processes, which turn out to be more hazardous than the primary compounds. These factors highlight the need for advanced analytical techniques to counter these shortcomings and aid in the understanding of the behavior of agricultural chemical residues in the environment.^{3–5}

TA techniques offer unique advantages in the study of agricultural chemical residues. By applying heat in the form of energy to a sample in some of these techniques, information on the thermal stability, decomposition temperatures and phase transitions of chemical residues can be obtained. These data are important for comparing these residues under various

^aResearch Center for Environmental Determinants of Health (RCEDH), Health Institute, Kermanshah University of Medical Sciences, Kermanshah, Iran. E-mail: mpirsaeheb@yahoo.com; Fax: +98 315 5913201; Tel: +98 315 5912383

^bDepartment of Environmental Health Engineering, Faculty of Health, Kermanshah University of Medical Sciences, Kermanshah, Iran

^cDepartment of Medical Physics, College of Sciences, Al-Mustaqbal University, 51001, Babylon, Iraq

^dInstitute of Nano Science and Nano Technology, University of Kashan, Kashan, P. O. Box. 87317-51167, Islamic Republic of Iran. E-mail: salavati@kashanu.ac.ir



environmental conditions, including temperature fluctuations and light exposure. Moreover, TA allows for the analysis of complex mixtures and the study of individual chemical species' behavior, making it a powerful tool for assessing the environmental fate and potential risks of agrochemicals. Furthermore, the non-destructiveness of TA makes it possible to preserve samples for further analysis, making TA an efficient and useful method for environmental monitoring.^{6–8}

The goal of this systematic review is to summarize current knowledge regarding the applications and effectiveness of TA methods in evaluating the environmental consequences of utilizing agricultural chemicals. The review aims to discuss the papers available on the application of TGA, DSC and DTA in this respect, highlighting the strengths and limitations of these techniques. Specifically, this review aims to address the following questions. (1) Which thermal properties of agricultural chemical residues are critical to understanding their environmental behavior? (2) How well do TA techniques identify and characterize complex mixtures of chemical residues? (3) How do TA methods perform in comparison with conventional analytical methods in residue assessment? (4) What recommendations can be made for future research on and the broader application of TA in environmental studies? Through this review, the authors demonstrate the usefulness of TA as an essential tool in mitigating the negative environmental impact of agricultural activities.

2. Agricultural chemical residues in the environment

Residues of agricultural chemicals, including pesticides, fertilizers, herbicides, and fungicides, are widely used in most modern farming practices. While these substances play a vital role in enhancing agricultural productivity, they also result in soil, water and air pollution. The persistence and environmental pathways of these residues can adversely affect ecosystems and human health, underscoring the need to thoroughly understand their behavior and impacts.^{9,10}

2.1. Types of agricultural chemicals and their residues

2.1.1. Pesticides. Pesticides, including insecticides and rodenticides, are chemicals designed to protect crops from pests; however, these chemicals can also leave residues in the environment. These residues often persist in soil and water, potentially impacting non-target organisms such as beneficial insects, aquatic organisms and mammals. Pesticides can be a major problem owing to their ability to bioaccumulate within the food chain and thus affect the lives of animals and humans.¹¹

2.1.2. Fertilizers. Among the most commonly used soil treatments are fertilizers, which supply essential nutrients to crops. However, when applied in excess, they leave behind residual chemicals, which contribute to environmental problems. Nitrates and phosphates from fertilizers can easily pollute ground water or surface water through leaching or run-off, respectively. Once introduced into aquatic systems, these

compounds can lead to eutrophication, a process characterized by algal blooms and low oxygen availability, which in turn place stress on aquatic ecosystems and diminish their productivity.¹²

2.1.3. Herbicides and fungicides. Herbicides are applied to control weed growth, while fungicides are used to control fungal infections in crops. However, both can persist in soil and water after application, potentially affecting non-target plant species and microorganisms in the soil. The presence of these chemical residues in the environment can also contribute to the development of resistance in weed and fungal strains, complicating pest management and threatening the long-term sustainability of agricultural practices.¹³

2.2. Environmental pathways and persistence

2.2.1. Soil contamination. Agricultural chemical residues are often deposited in the soil, where they can persist for extended periods depending on the properties of the chemical and prevailing soil conditions. Soil contamination may lead to reduced soil fertility, disruption of microbial activity within the soil, and the transfer of residues to crops grown in contaminated soil. This not only impacts crop yield and quality but also poses potential risks to the food chain through residual contamination.¹⁴

2.2.2. Water contamination. Among the factors contributing to the contamination of water bodies by agricultural chemicals are runoff, leaching and drift during application. In aquatic environments, these residues can persist for extended periods, sometimes remaining in groundwater for decades. The presence of chemical residues in water can be damaging to aquatic life, including fish, amphibians and other aquatic invertebrates. Moreover, the presence of such residues in drinking water sources raises serious health concerns, as some of these chemicals are linked to endocrine disruption and cancer.¹⁵

2.2.3. Airborne residues. Residues of agricultural chemicals applied *via* spraying or volatilization can disperse over large areas. Airborne residues may settle onto soil and water surfaces, thereby causing environmental pollution. Inhalation of these residues poses health risks to humans and animals, particularly in regions with high exposure levels, such as agricultural fields.¹⁶

3. Overview of TA techniques

TA methods are very effective in studying the thermal characteristics and thermal stability of substances, including agricultural chemical residues. These techniques involve heating of a sample under well-defined conditions and studying the changes in its physical and chemical properties to obtain information on decomposition, phase transformation, and thermal stability. In environmental science, TA has been recognized for its applicability to determine the degradation mechanisms and environmental persistence of residues. This section provides an overview of some of the important TA techniques, which include TGA, DSC, and DTA, as well as the advantages of employing combined thermal techniques.

3.1. TGA

TGA is a TA technique used to measure the change in the mass of a sample when heated or cooled under controlled temperature conditions. The sample is placed on a high-precision balance, and its mass is recorded as the surrounding temperature changes within a furnace. Mass loss or gain during heating or cooling is due to processes such as evaporation, decomposition, oxidation, and reduction. TGA provides essential information about a sample's thermal stability and phase composition, enabling the identification of temperatures at which different components degrade or evaporate.^{17,18}

3.2. DSC

DSC is a TA technique that measures the heat flow associated with physical and/or chemical transformations in a sample as it is heated or cooled. By applying the same programmed temperature to both the sample and a reference material, the differences in heat flow between them are recorded. DSC can measure heat changes associated with phase transitions such as melting, crystallization, glass transitions, and reactions. The resulting thermograms provide quantitative data on specific heat capacity and enthalpy changes as well as information on phase transitions.^{19,20}

3.3. DTA

DTA is similar to DSC in that it works on the basis of the temperature difference between a sample and a reference as both are subjected to heating or cooling. However, unlike DSC, DTA does not measure heat flow directly. Instead, it detects endothermic and exothermic events, such as phase transitions and chemical reactions, based on temperature changes. The resulting DTA curve indicates these thermal events relative to temperature. Although DTA provides qualitative insights into a material's thermal behavior, it is often used in conjunction with other TA techniques to give a more comprehensive understanding of the sample's properties.^{21–23}

3.4. EGA

EGA is a TA technique used to study the gases released during the heating of a sample. It provides detailed information about the nature and composition of the evolved gases, enabling the identification of volatile degradation products, reaction mechanisms, and decomposition pathways. This technique is highly valuable for analyzing materials such as pesticides, polymers, and fertilizers as it allows real-time monitoring of volatile substances under controlled thermal conditions.^{24–26}

3.5. Combined thermal techniques

Combining TA techniques, such as TGA-DSC or TGA-DTA, allows for a more comprehensive analysis of agricultural chemical residues. These coupled methods allow for simultaneous measurements of mass change and heat flow or temperature difference, offering detailed insights into the thermal properties and decomposition behavior of the residues. This integrated approach can reveal interactions between

different components, elucidate complex degradation mechanisms, and provide more accurate data on the thermal stability and environmental impact of chemical residues.

4. Applications of TA in environmental and agricultural research

This section highlights the diverse applications of TA techniques in agricultural and environmental research. It emphasizes their role in understanding the properties, degradation behaviors, and environmental impacts of agricultural chemicals, as well as their potential in enhancing safety, sustainability, and waste management through detailed thermal evaluation and process optimization.

4.1. TA in agricultural chemical stability and quality control

TA methods enable the investigation of thermal transitions, decomposition pathways, and reaction kinetics, which are essential for predicting the behavior of agricultural compounds during storage, transport, and application. Table 1 showcases examples of studies that applied TA techniques to analyze these properties. One of the main advantages of using TA in this context is its ability to provide precise and reliable data on thermal stability, enabling manufacturers to optimize formulations and ensure the safe handling of products. For example, TGA can identify decomposition stages and the release of volatile components, which may indicate product instability under specific conditions. Similarly, DSC detects phase transitions, such as melting and crystallization, which are critical for understanding the physical behavior of fertilizers and pesticides.

Gorbovskiy and coworkers provided essential insights into the thermal behavior and stability of complex fertilizers.³⁰ Their study employed TGA and DSC to investigate decomposition stages, reaction pathways, and thermal transitions under controlled heating conditions. These techniques enable precise identification of key thermal events, including weight loss phases, exothermic and endothermic reactions, and gas release, all of which are critical factors for evaluating the safety and efficiency of fertilizers used in agriculture. A key highlight of the study is presented in Fig. 1, which displays a detailed DSC curve capturing multiple thermal events during the decomposition of chloride-containing ammonium nitrate fertilizers. The peaks and troughs on the curve represent distinct reactions, such as melting, decomposition, and phase transitions, offering an in-depth understanding of the material's response to heat. By analyzing these transitions, the study provides valuable information on the safe handling, storage, and application of such fertilizers, particularly in environments prone to temperature fluctuations. This work exemplifies the significant role of TA technique in agricultural chemical research. In addition to stability assessment, the methods help optimize fertilizer formulations and improve environmental safety by minimizing the risks associated with thermal decomposition. These factors underscore the broader applicability of these techniques in

Table 1 Applications of thermal analysis in stability and quality control

Compound/material	Thermal technique used	Purpose of analysis	Key findings	Advantages of thermal analysis	Ref.
Pesticides	TGA, DSC	Stability and decomposition analysis	Multi-stage degradation observed	Precise data on thermal stability	27
Herbicides	TGA, DSC	Phase transition and stability studies	Endothermic peaks detected	Identification of degradation stages	28
Fertilizers	TGA, DSC	Heat sensitivity and decomposition rate	Safe storage conditions determined	Optimization of safe handling	29

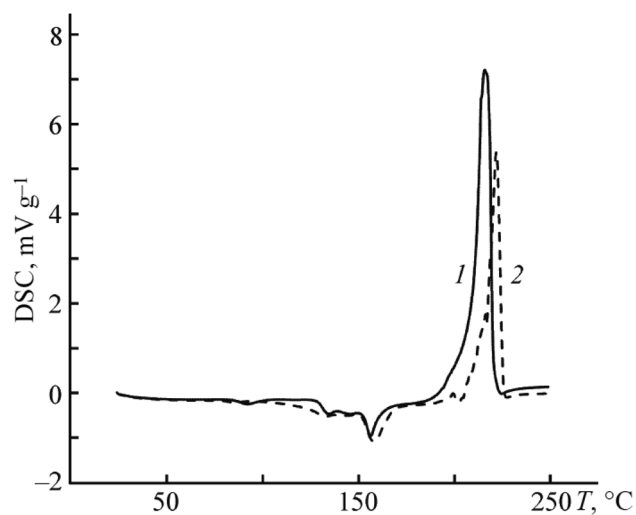


Fig. 1 DSC curves for the samples (1) 1 and (2) 2, obtained at a heating rate of 5 °C min⁻¹. (T) Temperature.³⁰

ensuring the quality and reliability of agricultural inputs, making the study a cornerstone for advancements in sustainable farming practices and safety standards.

Table 1 also highlights the relevance of these techniques in regulatory frameworks. By identifying specific thermal behaviors, TA ensures compliance with safety and environmental standards, minimizing the risks associated with chemical production and use. The studies listed in Table 1 exemplify the utility of TA techniques in agricultural chemical research, underlining their role in quality assurance and risk mitigation.

4.2. Investigating degradation pathways and kinetics with TA

TA provides critical insights into the degradation pathways and kinetic behavior of agricultural chemicals. By calculating kinetic parameters, such as activation energy, reaction order, and decomposition rates, researchers can predict how these compounds behave under varying thermal conditions. Table 2 presents representative studies that leverage TA to understand degradation pathways and assess the environmental and safety implications of agricultural chemicals use. The ability to derive kinetic parameters is a significant advantage of thermal techniques. This information not only enables predictions of shelf life and stability but also informs the development of safer and

more efficient chemical formulations. For instance, studies on thermal decomposition of herbicides often reveal their multi-step degradation processes, where each stage is characterized by distinct thermal behaviors. Such insights are critical for developing strategies to minimize their environmental impact.

As shown in Table 2, thermal methods also enable the identification of degradation intermediates, which can be toxic or environmentally persistent. This knowledge is essential for formulating regulatory compliance and ensuring environmental protection. The studies highlighted in Table 2 emphasize the role of TA in advancing our understanding of chemical stability and degradation mechanisms, providing a robust foundation for safer agricultural practices.

4.3. TA combined with complementary techniques

The integration of TA with complementary analytical techniques extends its utility and allows researchers to gain deeper insights into the behavior of agricultural chemicals. Table 3 provides examples of studies that combine thermal techniques such as TGA and DSC with advanced methods such as gas chromatography-MS (GC-MS) and isotope analysis. Further discussion on coupled thermal techniques is provided only in Section 4.4 to avoid redundancy. A key advantage of these hybrid approaches is their ability to simultaneously assess thermal behavior and chemical composition. For instance, adsorption/thermal desorption-GC/MS is a powerful method for detecting volatile and semi-volatile compounds generated during thermal degradation, enabling researchers to identify hazardous emissions and degradation products. Similarly, stable isotope analysis provides valuable data on the origin and transformation of carbon-containing compounds during thermal processes.

These combined methods enhance the depth and reliability of analytical results, making them invaluable for environmental monitoring and regulatory purposes. Table 3 highlights studies that demonstrate the effectiveness of integrating TA with complementary tools in addressing complex challenges in agricultural and environmental sciences.

4.4. Identifying toxic by-products using TA

TA is a key tool for identifying toxic by-products released during the thermal degradation of agricultural chemicals. This application is particularly important for assessing the environmental and health risks associated with the production, application,

Table 2 Thermal analysis for degradation pathways and kinetics

Compound/material	Thermal technique used	Purpose of analysis	Key findings	Advantages of thermal analysis	Ref.
Triazine herbicides	TGA, DSC	Degradation mechanism investigation	Multi-step thermal decomposition	Accurate kinetic parameter data	31
Chlorinated pesticides	TGA	Reaction kinetics analysis	High activation energy identified	Understanding reaction pathways	32
Fertilizers	DSC	Oxidative degradation study	Gaseous by-products identified	Safety and risk prediction	30

and disposal of pesticides and fertilizers. Table 4 highlights studies that used thermal techniques, such as TGA and EGA, to detect and characterize harmful emissions. A significant advantage of TA in this context is its ability to simulate real-world thermal conditions, such as combustion or degradation, and monitor the release of volatile or gaseous products. Coupled methods such as TGA-MS and TGA-Fourier-transform infrared spectroscopy (TGA-FTIR) allow researchers to identify specific compounds, including toxic gases such as sulfur dioxide, ammonia, or chlorinated organics.

Giroud and coworkers investigated the thermal decomposition mechanism of the pesticide mancozeb to assess its safety concerns.²⁷ As illustrated in Fig. 2, their study provides a detailed mechanistic view of the thermal decomposition of mancozeb. This figure illustrates key degradation pathways, highlighting the release of gaseous products such as SO₂, CS₂, and COS at specific temperature intervals. The data, derived from TGA and DSC analyses, clearly map critical thermal events, including the breakdown of sulfur-containing bonds and the sequential formation of toxic emissions. Fig. 2 demonstrates the decomposition stages and provides insights into the thermochemical stability of mancozeb under controlled heating conditions. The study uses this figure to establish a connection between temperature profiles and the nature of released products, aiding in the identification of hazardous byproducts that may pose risks to the environment and human health. This mechanistic understanding is crucial for improving pesticide formulations, ensuring safer handling and storage, and mitigating the environmental impact of these chemicals. Compared with empirical data-focused figures, Fig. 2's emphasis on mechanistic pathways offers a broader perspective, making it particularly useful for understanding the fundamental chemical processes underlying thermal decomposition, making it an invaluable addition to discussions of safety and regulatory assessments for pesticides.

Overall, these methods are critical for regulatory compliance, as they provide the data needed to evaluate the environmental

impact of chemical use and disposal. For example, the detection of toxic by-products during pesticide combustion highlights the potential risks associated with waste incineration. Similarly, identifying hazardous emissions from fertilizers ensures safer handling and application practices. Table 4 demonstrates how TA contributes to understanding the environmental consequences of agricultural chemicals, thereby promoting safer and more sustainable practices.

4.5. TA in environmental remediation and waste management

TA plays a crucial role in environmental remediation and waste management, particularly for agricultural chemicals. By analyzing the thermal degradation and combustion behaviors of pesticides and fertilizers, researchers can develop strategies for treating contaminated soil, wastewater, and solid waste. Table 5 presents studies that demonstrate the application of thermal techniques in these areas. One of the significant advantages of TA in this context is its ability to evaluate the efficiency of degradation processes and assess the residual toxicity of by-products. For example, the thermal degradation of pesticides under controlled oxidative conditions can reduce toxicity by transforming them into less harmful compounds. This approach is often combined with biological or chemical remediation techniques to enhance overall efficiency. Additionally, TA assists in evaluating the suitability of agricultural waste for energy recovery, such as through biochar production or combustion in boilers. The studies presented in Table 5, showcase the diverse applications of TA in addressing environmental challenges, from pesticide removal in wastewater to the safe disposal of agricultural residues. These findings underscore the potential of TA as a tool for advancing sustainable agricultural practices.

These five sections comprehensively highlight the diverse applications of TA techniques across different facets of agricultural chemical research, environmental remediation, and regulatory compliance. The integration of thermal methods

Table 3 Hybrid methods incorporating thermal analysis

Compound/material	Thermal technique used	Complementary technique	Purpose of analysis	Advantages of thermal analysis	Ref.
Pesticides	TGA, DSC	GC/MS	Emission and residue analysis	Identification of degradation products	33
Fungicides	DSC	Spectroelectrochemistry	Stability and molecular changes	Comprehensive data collection	34

Table 4 Detection of toxic by-products through thermal analysis

Compound/material	Thermal technique used	Purpose of analysis	Key findings	Advantages of thermal analysis	Ref.
Pesticides	TGA-MS	Identification of toxic by-products	Release of sulfur-based compounds	Real-time monitoring of emissions	35
Fungicides	TGA-FTIR	Emission profiling during degradation	Chlorinated compounds detected	Identification of hazardous gases	36
Fertilizers	TGA	Study of decomposition gases	Ammonia and chlorine emissions	Simulates real-world conditions	37

with complementary analytical techniques, coupled with their ability to simulate real-world conditions, underscores their essential role in advancing sustainable agricultural and environmental practices.

5. Gaps in research and future directions

The application of TA techniques in assessing agricultural chemical residues has made significant strides, yet several gaps remain. Addressing these gaps and exploring new methodologies can deepen our understanding of the environmental impact of these residues, leading to more effective mitigation strategies.

5.1. Unexplored areas in the TA of residues

Although TA techniques have proven valuable in studying agricultural chemical residues, there are still unexplored areas that warrant further investigation. One such area is the in-depth analysis of emerging contaminants, such as the newly

developed classes of pesticides and herbicides increasingly used in agriculture. The thermal behavior of these compounds, particularly their decomposition patterns and by-product formation under environmental conditions, remains largely unexplored. Additionally, the interactions of these residues with various environmental matrices, such as soils of varying composition and moisture levels, are not well understood. Research in these unexplored areas could provide critical insights into the environmental fate of these chemicals and their long-term impact on ecosystems and human health.

5.2. Potential for new method development

The field of TA is well-positioned for innovation, particularly in the development of new methods tailored to the unique challenges posed by agricultural chemical residues. One potential area of development is the creation of hybrid techniques that combine TA with advanced imaging or molecular analysis tools. For instance, integrating thermal techniques with mass spectrometry could enable real-time analysis of the decomposition products of residues, offering deeper insight into the chemical

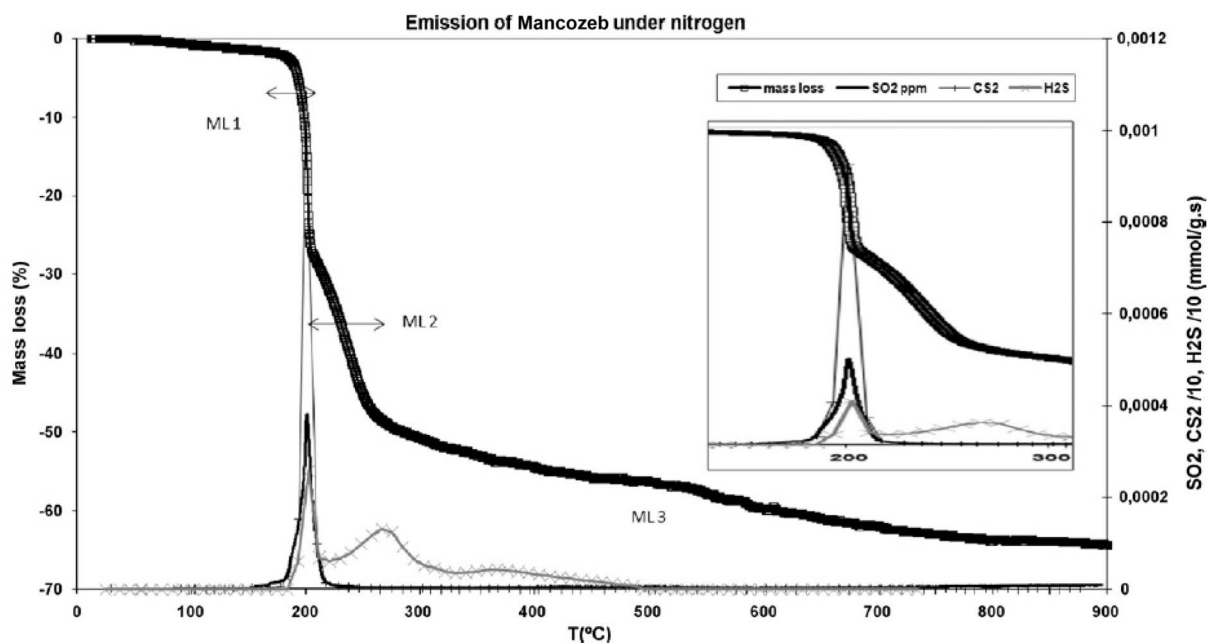


Fig. 2 TG curve and emissions of SO_2 , H_2S and CS_2 per gram of the product during pyrolysis of technical mancozeb (5°C min^{-1}).²⁷

Table 5 Applications of thermal analysis in environmental remediation

Compound/material	Thermal technique used	Purpose of analysis	Key findings	Advantages of thermal analysis	Ref.
Pesticides (<i>e.g.</i> , atrazine)	TGA, DSC	Oxidative degradation	Conversion to less harmful products	Evaluation of remediation efficiency	38
Herbicides	TGA	Soil and wastewater contamination study	Multi-step degradation observed	Residual toxicity assessment	39
Wood pellet residues	TGA, DSC	Analysis of combustion by-products	Pesticide residues detected in char	Combines waste disposal and energy recovery	40

transformations occurring during thermal events. Another promising direction is the development of miniaturized or portable TA instruments, which could be used for on-site environmental monitoring. Such advancements would facilitate real-time assessments of agricultural chemical residues in various environmental settings, thereby more effectively enhancing the detection and mitigation of contamination.

5.3. Recommendations for future research

To address the existing gaps and harness the potential of TA in environmental studies, several recommendations for future research can be proposed. First, comprehensive studies examining the thermal behavior of a broader range of agricultural chemicals under diverse environmental conditions are needed. Such studies would provide a more complete understanding of how these residues interact with the environment. Second, interdisciplinary research that combines TA with other analytical techniques, such as spectroscopy or chromatography, should be encouraged. Such collaborative approaches could lead to the development of more robust methods for detecting and characterizing residues. Finally, future research should focus on the standardization of TA protocols for environmental samples. Establishing standardized methods would ensure that data from different studies are comparable, facilitating more accurate assessments of the environmental impact of agricultural chemical residues and supporting informed regulatory decisions.

Additionally, future research should explore the potential of advanced ferrite-based materials in enhancing TA techniques for detecting and characterizing agricultural chemical residues. Notably, studies by Almessiere *et al.*⁴¹ and Slimani *et al.*⁴² highlight the significant impact of Sc^{3+} and In^{3+} co-substitution on the structural, magnetic, and microwave properties of $\text{SrFe}_{12}\text{O}_{19}$ hexaferrites and $\text{Co}_{0.5}\text{Ni}_{0.5}\text{Fe}_2\text{O}_4$ nanospinel ferrites, respectively. These modifications improved electromagnetic performance, making these materials promising candidates for applications in wireless communication, electromagnetic shielding, and sensing technologies. Given their enhanced microwave absorption and optimized magnetic behavior, these materials could be integrated into TA-based sensor systems for agricultural residue detection. TA techniques such as TGA and DSC can be used in combination with these advanced materials, leading to more sensitive and selective detection of pesticides, herbicides, and other chemical residues. Moreover, the

optimization approaches employed in these studies, which systematically adjust dopant concentrations to achieve desired material properties, could be applied to the development of novel sensor materials tailored for residue detection. By leveraging computational modeling and experimental techniques, researchers can refine material compositions to enhance sensitivity, stability, and efficiency in detecting the thermal decomposition patterns of chemical residues. Expanding research in this direction can lead to innovative, high-performance analytical tools for environmental monitoring and food safety assessment, ultimately supporting sustainable agricultural practices.

6. Conclusion

The systematic review of TA techniques for assessing the environmental effects of agricultural chemical residues highlights the capabilities and limitations of these methods. As environmental concerns regarding the persistence and impact of agricultural chemicals continue to grow, the application of these techniques offers significant potential for advancing our understanding and management of these pollutants.

6.1. Summary of findings

This review demonstrated that TA techniques, including TGA, DSC, and DTA, are effective tools for detecting and characterizing agricultural chemical residues. These methods provide detailed insights into the thermal stability, decomposition behavior, and interactions of residues with environmental matrices. The review also identified specific advantages of TA, such as comprehensive data collection and minimal sample preparation, which make these techniques particularly valuable in environmental studies. However, challenges such as the complexity of environmental samples and the interpretation of thermal data were also noted, indicating the need for further methodological advancements.

6.2. Implications for environmental monitoring

The findings of this review have significant implications for environmental monitoring. TA techniques can enhance the detection and characterization of agricultural residues, providing critical data on the persistence and transformation of these chemicals in the environment. This information is crucial for developing effective strategies to mitigate the impact of

agricultural pollutants on ecosystems and human health. The ability of thermal techniques to detect even small changes in the chemical composition of residues makes them particularly valuable in monitoring programs aimed at identifying and quantifying pollutants. By integrating TA with other analytical methods, such as spectroscopic or chromatographic techniques, environmental monitoring efforts can become more robust, leading to more accurate assessments and better-informed regulatory decisions.

6.3. Final remarks on the role of TA

In conclusion, TA techniques play a crucial role in the study of agricultural chemical residues and their environmental impact. While challenges remain, the potential benefits of these techniques in environmental monitoring and assessment are significant. They offer a unique combination of sensitivity, specificity, and versatility, making them indispensable tools in the ongoing effort to protect the environment from the harmful effects of agricultural pollutants. Future research and development in this field should focus on addressing the current limitations and exploring new applications of TA, ensuring that these techniques continue to meaningfully contribute to environmental science. By advancing our understanding of the thermal properties of agricultural residues, we can more effectively manage and mitigate their impact, ultimately promoting a safer and more sustainable environment.

Declaration of AI usage in writing

During the development of this manuscript, the authors utilized ChatGPT to assist with grammar refinement and enhancing the clarity of the text. Following the use of this tool, the authors thoroughly reviewed, revised, and edited the manuscript to ensure accuracy and appropriateness. The authors assume full responsibility for the content and integrity of the final work.

Data availability

No new data were created or analysed in this study. Data sharing is not applicable to this article. All the data discussed and referenced within the paper are available in the original studies cited. For further information, please refer to the respective publications mentioned in the References section.

Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors gratefully acknowledge the Research Council of Kermanshah University of Medical Sciences (Grant Number: 4030476) for their financial support. Professor Masoud Salavati-Niasari and co-authors of the Institute of Nano Science and

Nano Technology, University of Kashan, Iran, are acknowledged for providing access to the analysis facility through grant no. 159271/TG9 from the University of Kashan.

References

- 1 A. Alengebawy, S. T. Abdelkhalek, S. R. Qureshi and M.-Q. Wang, Heavy metals and pesticides toxicity in agricultural soil and plants: ecological risks and human health implications, *Toxics*, 2021, **9**(3), 42.
- 2 L. Horrigan, R. S. Lawrence and P. Walker, How sustainable agriculture can address the environmental and human health harms of industrial agriculture, *Environ. Health Perspect.*, 2002, **110**(5), 445–456.
- 3 M. Pirsaeheb, T. Gholami, E. A. Dawi, H. S. Majdi, F. S. Hashim, H. Seifi and M. Salavati-Niasari, Green synthesis and characterization of SnO₂, CuO, Fe₂O₃/activated carbon nanocomposites and their application in electrochemical hydrogen storage, *Int. J. Hydrogen Energy*, 2023, **48**, 23594–23606.
- 4 Ż. Bargańska, D. Lambropoulou and J. Namieśnik, Problems and challenges to determine pesticide residues in bumblebees, *Crit. Rev. Anal. Chem.*, 2018, **48**(6), 447–458.
- 5 J. W. Wong, D. G. Hayward, and K. Zhang, Gas chromatography-mass spectrometry techniques for multiresidue pesticide analysis in agricultural commodities, in *Comprehensive Analytical Chemistry*, Elsevier, 2013, pp. 3–22.
- 6 M. Pirsaeheb, H. Seifi, E. A. Dawi, T. Gholami, S. Q. Badraddin, A. Ryadh and M. Salavati-Niasari, Thermal analysis techniques in herbal medicine: A comprehensive review on unveiling integrity and quality for future perspectives, *J. Anal. Appl. Pyrolysis*, 2023, 106192.
- 7 M. Pirsaeheb, H. Seifi, T. Gholami, S. H. Ganduh, L. S. Jasim, M. A. Mahdi and M. Salavati-Niasari, Thermal analysis techniques for evaluating the thermal stability of battery materials: a comprehensive review, *J. Anal. Appl. Pyrolysis*, 2023, 106136.
- 8 H. Seifi, T. Gholami, S. Seifi, S. M. Ghoreishi and M. Salavati-Niasari, A review on current trends in thermal analysis and hyphenated techniques in the investigation of physical, mechanical and chemical properties of nanomaterials, *J. Anal. Appl. Pyrolysis*, 2020, **149**, 104840.
- 9 F. Sánchez-Bayo, Impacts of agricultural pesticides on terrestrial ecosystems, *Ecological Impacts of Toxic Chemicals*, 2011, pp. 63–87.
- 10 P. Nayak and H. Solanki, Pesticides and Indian agriculture—a review, *Int. J. Res. Granthaalayah*, 2021, **9**(5), 250–263.
- 11 P. Nicolopoulou-Stamati, S. Maipas, C. Kotampasi, P. Stamatis and L. Hens, Chemical pesticides and human health: the urgent need for a new concept in agriculture, *Front. Public Health*, 2016, **4**, 148.
- 12 S. Savci, An agricultural pollutant: chemical fertilizer, *Int. J. Environ. Sci. Dev. Monit*, 2012, **3**(1), 73.
- 13 P. K. Gupta, Herbicides and fungicides, in *Reproductive and Developmental Toxicology*, Elsevier, 2022, p. 665–689.

- 14 J. Sun, L. Pan, D. C. Tsang, Y. Zhan, L. Zhu and X. Li, Organic contamination and remediation in the agricultural soils of China: a critical review, *Sci. Total Environ.*, 2018, **615**, 724–740.
- 15 A. Agrawal, R. S. Pandey and B. Sharma, Water pollution with special reference to pesticide contamination in India, *J. Water Resour. Protect.*, 2010, **2**(5), 432–448.
- 16 S. Lee, R. McLaughlin, M. Harnly, R. Gunier and R. Kreutzer, Community exposures to airborne agricultural pesticides in California: ranking of inhalation risks, *Environ. Health Perspect.*, 2002, **110**(12), 1175–1184.
- 17 R. Bottom, Thermogravimetric analysis, *Principles and Applications of Thermal Analysis*, 2008, pp. 87–118.
- 18 B. Lothenbach, P. Durdzinski and K. De Weerd, Thermogravimetric Analysis, *A Practical Guide to Microstructural Analysis of Cementitious Materials*, 2016. vol. 1, pp. 177–211.
- 19 J. D. Menczel, L. Judovits, R. B. Prime, H. E. Bair, M. Reading and S. Swier, Differential Scanning Calorimetry (DSC), *Thermal Analysis of Polymers: Fundamentals and Applications*, 2009, pp. 7–239.
- 20 K. Lukas and P. K. LeMair, Differential Scanning Calorimetry: Fundamental Overview, *Reson. J. Sci. Educ.*, 2009, **14**(8), 807–817.
- 21 S. Yariv, Differential thermal analysis (DTA) of organo-clay complexes, in *Thermal Analysis in the Geosciences*, Springer, 2005, pp. 328–351.
- 22 Z. Zhang, P. Shen and Q. Jiang, Differential thermal analysis (DTA) on the reaction mechanism in Fe–Ti–B4C system, *J. Alloys Compd.*, 2008, **463**(1–2), 498–502.
- 23 F. Sahnoune, M. Heraiz, H. Belhouichet, N. Saheb and D. Redaoui, Thermal Decomposition Kinetics of Algerian Tamazarte Kaolin by Differential Thermal Analysis (DTA), *Acta Phys. Pol. A*, 2017, **131**(3), 382–385.
- 24 D. Schöps, C. Schmidt and K. Heide, Quantitative EGA analysis of H₂O in silicate glasses, *J. Therm. Anal. Calorim.*, 2005, **80**, 749–752.
- 25 M. Beneš, N. Milanov, G. Matuschek, A. Kettrup, V. Pláček and V. Balek, Thermal degradation of PVC cable insulation studied by simultaneous TG-FTIR and TG-EGA methods, *J. Therm. Anal. Calorim.*, 2004, **78**, 621–630.
- 26 M. Demyan, F. Rasche, M. Schütt, N. Smirnova, E. Schulz and G. Cadisch, Combining a coupled FTIR-EGA system and *in situ* DRIFTS for studying soil organic matter in arable soils, *Biogeosciences*, 2013, **10**(5), 2897–2913.
- 27 N. Giroud, S. Dorge and G. Trouvé, Mechanism of thermal decomposition of a pesticide for safety concerns: case of Mancozeb, *J. Hazard. Mater.*, 2010, **184**(1–3), 6–15.
- 28 I. J. Al-Nuaemi, K. F. Abbas, R. M. Jebir Al-Alawy and H. N. Al Ani, Thermal and Biological Degradation of Herbicides to Treat Wastewater and Soil Pollution, *Asian J. Water, Environ. Pollut.*, 2022, **19**(4), 17–23.
- 29 Y. Pelovski, Thermal analysis for control of the properties of mineral fertilizers, *J. Therm. Anal. Calorim.*, 2000, **60**, 53–58.
- 30 K. Gorbovskiy, A. Kazakov, A. Norov, D. Pagaleshkin and A. Mikhaylichenko, Thermal decomposition study of chloride-containing complex ammonium nitrate-based fertilizers by thermogravimetry and differential scanning calorimetry, *Russ. J. Appl. Chem.*, 2016, **89**, 1383–1392.
- 31 A. Książczak, K. Drożdżewska and H. Boniuk, Thermal decomposition of triazine herbicides II. 6-Chloro-N₂-ethyl-N₄-isopropyl-1, 3, 5-triazine-2, 4-diamine (atrazine) and its metabolites, *J. Therm. Anal. Calorim.*, 2001, **65**(2), 473–479.
- 32 F. Rodante, S. Vecchio, G. Catalani and M. Guidotti, Thermal analysis and non-isothermal kinetic study of some pesticides. Part II. Chlorinate derivatives, *J. Therm. Anal. Calorim.*, 2000, **60**, 605–622.
- 33 M. Clément, S. Arzel, B. Le Bot, R. Seux and M. Millet, Adsorption/thermal desorption-GC/MS for the analysis of pesticides in the atmosphere, *Chemosphere*, 2000, **40**(1), 49–56.
- 34 B. Tutunaru, A. Samide, C. Tigae and B. Oprea, Assessment of captan pesticide stability by thermal and spectroelectrochemical analysis, *Int. J. Electrochem. Sci.*, 2024, **19**(5), 100561.
- 35 M. Sankowska, A. Gajek, M. Celiński and K. Sałasińska, Determination of gaseous products of thermal degradation of thiram, *J. Therm. Anal. Calorim.*, 2017, **128**, 1639–1647.
- 36 M. Borucka, M. Celiński, K. Sałasińska and A. Gajek, Identification of volatile and semi-volatile organic compounds emitted during thermal degradation and combustion of triadimenol, *J. Therm. Anal. Calorim.*, 2020, **139**(2), 1493–1506.
- 37 K. Gorbovskiy, A. Kazakov, A. Norov and A. Mikhaylichenko, Effect of Gaseous Products on the Kinetics of Thermal Decomposition of Chloride-Containing Complex Ammonium Nitrate-Based Fertilizers, *Russ. J. Appl. Chem.*, 2020, **93**, 352–361.
- 38 O. Senneca, F. Scherillo and A. Nunziata, Thermal degradation of pesticides under oxidative conditions, *Russ. J. Appl. Chem.*, 2007, **80**(1), 61–76.
- 39 V. Andreu and Y. Picó, Determination of pesticides and their degradation products in soil: critical review and comparison of methods, *TrAC, Trends Anal. Chem.*, 2004, **23**(10–11), 772–789.
- 40 J. Růžicková, H. Raclavská, M. Šafář, M. Kucbel, K. Raclavský, A. Grobelak, B. Švédová and D. Juchelkova, The occurrence of pesticides and their residues in char produced by the combustion of wood pellets in domestic boilers, *Fuel*, 2021, **293**, 120452.
- 41 M. Almessiere, *et al.*, Impact of Sc³⁺/In³⁺ ions co-substitution on structural, magnetic, and microwave features of SrFe₁₂O₁₉ hexaferrites, *J. Alloys Compd.*, 2023, **968**, 172197.
- 42 Y. Slimani, *et al.*, Impact of the Sc³⁺/In³⁺ co-substitution on the structural, magnetic, and microwave characteristics of Co_{0.5}Ni_{0.5}Fe₂O₄ nanospinel ferrites, *Ceram. Int.*, 2024, **50**(5), 7605–7616.