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A metadata schema to standardize non-thermal plasma decontamination parameters in food-related applications

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Non-thermal plasma research has gained significant attention as a promising technology for food-related decontamination. However, the lack of standardization in reporting key parameters restricts the applicability and reusability of results in this field. To address this, the present study introduces a metadata schema (MDS) that standardizes critical parameters and provides operational details for non-thermal plasma microbial inactivation in food-related applications. The metadata schema is implemented as an extension to Plasma-MDS, a metadata schema for plasma science, and aims to apply the FAIR (findable, accessible, interoperable, and reusable) data principles to food-related applications. The framework highlights relevant parameters related to the plasma source, the medium in which the plasma is ignited, the target (food-, and microbial-related parameters) treated with the plasma, and the diagnostic methods used to investigate these properties. Concrete examples of accurate metadata descriptions of all relevant parameter categories are provided in a human and machine-readable format to simplify adoption and dissemination. The introduced metadata schema strives to improve the comparability, reproducibility, and reuse of non-thermal plasma research data for food-related applications, paving the way for more generalizable insights to legal authorities and the food industry.

Introduction

Non-thermal plasma is a partially ionized gas with a broad range of practical applications. It has received much attention in a wide variety of food-related applications including microbial inactivation on food and food processing surfaces[1] or their simulants, enzyme inactivation, seed germination, and physicochemical modifications of food products[2]. This is mainly due to its gentle and mild character, low temperature, antimicrobial efficacy, integrability, and upscaling possibilities in existing food processing chains[3]. For microbial inactivation purposes, there are three main fields of research interest: (i) the decontamination of food product surfaces (including spore inactivation); (ii) the antimicrobial treatment of fresh products using plasma-treated water, and (iii) the decontamination of abiotic surfaces such as packaging materials and food processing surfaces, including the inactivation of biofilms[4,5]. This research interest led to the production of a vast amount of experimental data related to non-thermal plasma microbial inactivation. However, in multiple research articles published in the literature, various non-thermal plasma processing conditions crucial for understanding the experimental setup are not indicated precisely[6]. One explanation for this issue could be that many studies lack multidisciplinary teams with expertise in multiple scientific fields such as plasma physics, chemistry, and microbiology.

The importance of well-reported scientific data and the resulting data quality has received more attention in recent years[7,8]. Frameworks for assessing data quality have become established, particularly in the area of big data[9,10]. To improve reproducibility and replicability, standard research practices must be improved. In addition to improving study design and data analysis, it is also important to provide relevant experimental details that

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are needed to increase transparency in research and therefore reproducibility and reuse[11]. For novel technologies, there can be challenges to accurate descriptions of the processing conditions. For example, with Pulsed Electric Fields (PEF), inconsistencies in reporting crucial parameters led to the establishment of guidelines by the International Society for Electroporation-Based Technologies and Treatments[12].

Plasma classification remains challenging because by definition it is an inherently broad term and multiple categorization methods for plasmas and their applications do exist in the literature. Briefly, plasma can be categorized as thermal and non-thermal based on the thermodynamic equilibrium status. The plasma is categorized as thermal when the electron temperature matches the temperature of heavy particles in the gas, while in non-thermal plasmas the temperature of electrons is significantly higher than the gas temperature[4,13]. Non-thermal plasma categorization is often based on the mode of treatment (direct, indirect), the type of the device used for generating the plasma (e.g., dielectric barrier discharge (DBD)), the voltage frequency to generate the plasma (e.g., microwave plasma source (MPS), radio-frequency (RF)), the operating pressure level, and the discharge type (e.g., filamentary, diffuse)[8,14]. These options are just an excerpt as one type of device can be combined with a different one in the same setup, but also the different power supplies and operating pressures can form new categories.

In recent years, efforts have been started to develop a scheme for the categorization and structured description of plasma studies, including the adoption of the FAIR data principles[15] in plasma-related research. This has led to the creation of the metadata schema for plasma (Plasma-MDS), which is an extension of generic metadata schemata to cover all plasma applications[14]. Additionally, a data platform has been developed to serve as a repository for the stored data[16].

In the current study, Plasma-MDS was tailored specifically to non-thermal plasma decontamination data and metadata for food-related applications, covering (i) the decontamination of food product surfaces and their simulants (including spore inactivation); (ii) the antimicrobial treatment of food products and their simulants using plasma-treated liquids, and (iii) the decontamination of abiotic surfaces such as packaging materials and food processing surfaces, including the inactivation of biofilms. This extension includes recommendations for specific data and metadata descriptions and examples of which processing, microbial, and food-related parameters are critical, in a machine-readable format that adheres to the FAIR data principles. This aims at helping researchers in the field to better describe the key parameters, making results in the literature more comparable and reusable. Additionally, it forms the foundation for providing more generalized insights into the feasibility and decontamination efficacy of non-thermal plasmas for legal authorities and the food industry.

Current standards and missing gaps

The challenge to provide understandable, reproducible, and interoperable data of non-thermal plasma sources, diagnostics (physical and chemical), and application properties are among the largest hurdles to improving the communication of scientific outcomes and supporting the industry to implement non-thermal plasma into their value chains. Recently, the standards needed for plasma sources and their process parameters, diagnostics, and properties have been discussed by Alves *et al.*[17]. Based on the experience obtained at the Gaseous Electronics Conference (GEC) Reference Cell (GECRC) and the Cooperation in Science and Technology (COST) Jet, the authors have recommended developing new standards which include best practices and available standards as well as new inventions to come to shared practices in reporting data sets to enhance the exchange between researchers and industry, to increase the reproducibility and reuse of experiments and models, to strengthen the transparency of methods and data, and to increase the reliability of models and digital data. With better alignment of scientists on reporting practices within the plasma physics community, the fundamental findings within research may be transferred more efficiently to practice[17].

Standardization of parameters in plasma medicine. Nowadays, the use of non-thermal plasma at atmospheric pressure in medical therapy is widely accepted and partly co-financed by health insurance companies. In 2022, the first guideline on the therapeutic use of cold physical plasma in the medical field in Germany was published[18]. However, over 15 years ago, when research in the field of plasma medicine began, the requirements from physical, chemical, and biological points of view had not yet been defined[19]. Therefore, during this time frame, the necessary knowledge and understanding of mechanisms of action were investigated by researchers and physicians[20]. During this time, physical properties like plasma temperature, UV radiation, and electromagnetic fields were characterized, as well as the toxicological aspects of the plasma effluents for patients and therapists, given that direct contact was the preferred application in medical therapies. Additionally, the antimicrobial and *in vitro* / *in vivo* cell biological effects and their mode of action were analyzed. Some of these investigation requirements resulted in national standards like DIN SPEC 91315 (DIN SPEC 91315:2014-06 General requirements for plasma sources in medicine: https://doi.org/10.31030/2141389, accessed 29.07.2024)[21,22]. However, as the therapeutical application of plasma in the field of plasma medicine is dependent on national guidelines, challenges in harmonization across different countries still exist.

The challenges of standardization in food-related applications. In the agricultural field, Waskow *et al.*, (2022) attempted to standardize the reporting of parameters for plasma treatment of seeds to aid reproducibility and comparison between experiments. They developed a protocol organized into four main parts: (i) plasma device characteristics; (ii) seed pre-treatment; (iii) seed plasma treatment, and (iv) seed post-treatment[23]. For food-related applications, similar to the challenges in plasma medicine, the different plasma sources and application modes make it necessary to define specific requirements for describing the physical and chemical properties of the non-thermal plasma itself as well as the treated target. Differences in applications for food processing involve the consensus of the carrier gas used, which is in most cases atmospheric or compressed air, due to the acceptable consumable costs in the food industry. Another unique aspect is the broad range of

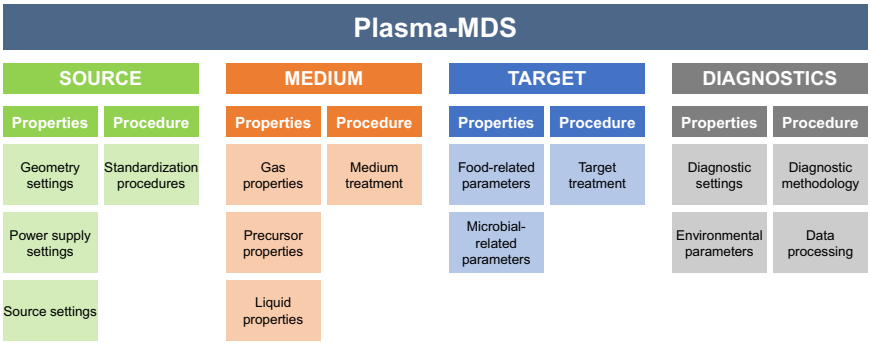

Fig. 1 Extension of the Plasma-MDS core schema elements (solid color) with categories of parameters that are critical in food-related plasma decontamination applications.

applicable temperatures, from sub-zero temperatures (as low as −20 °C) to pasteurization temperatures (up to +70 °C) depending on the application. Therefore, more plasma sources can be used, including DBDs, jets, and microwave discharges[3]. Depending on the energy input, variations in reactive species within the gas composition can be expected. In combination with humidity (originating from the food itself, processing conditions, or intentionally added water) this results in a variety of reactive species forming a bouquet of antimicrobial active components. These components must be understood from a physicochemical and biochemical point of view to understand their mode of action. Further, the impact of plasma treatment on the sensorial aspects of foods, and the toxicological risks need to be assessed to ensure the safety of the technology to the consumers and applicants. In non-thermal plasma applications for food processing and for extending products' shelf life, packaging is also a crucial factor to consider, as the process can impact the material surface properties[24]. The selected plasma parameters must be compatible with the materials and surfaces used in the food industry, including the processing line and packaging materials. This is particularly important for ready-to-eat food products, where the packaging comes into direct contact with the food, which will not undergo further processing before consumption. As most review articles and current guidelines for non-thermal plasma applications in food processing do not provide consistent parameters and terminology for plasma sources, gases, and chemical / biological characterizations, the comparability of the different processes is often lacking, which inhibits the upscaling process and the successful transfer from lab to industry. Inconsistencies in descriptions exist even for the same plasma sources or even for the "same" parameters. A good example of this issue is the term power, where multiple expressions can be found in the literature without being clear about what they represent and how they were estimated, such as applied, forward, reverse, reflected, active, apparent, operating, generating, dissociated, transferred, input, or dissipated power[8]. These inconsistencies undermine the general understanding of stakeholders, potentially leading to less acceptance and realization / applicability within the industry where conventional alternatives are still being used despite their disadvantages. Following the example set by Raso *et al.* (2016) for PEF, where the key information to be reported in microbial inactivation and PEF-assisted processing studies have been outlined[12], a similar approach was applied here for non-thermal plasma applications to improve the comparability of results.

Therefore, this study introduces recommendations and a practical scheme extending Plasma-MDS for standardized documentation of data and metadata that should accompany non-thermal plasma decontamination research in food-related applications. It is worth noting that this also contributes to the implementation of the FAIR data principles in this field of research and development, which is an urgent challenge in many areas. Moreover, explanations and examples are provided through a case study simulation to support the use and dissemination of the suggested metadata schema.

A metadata schema for food-related applications

Extension of Plasma-MDS. In order to extend Plasma-MDS for the description of plasma research studies related to decontamination and food-related applications, the scheme presented in Fig. 1 and detailed in Tables 1, 2, 3, 4, 5, and 6, was developed. Based on this metadata schema, benchmarking examples were also developed, as presented in Tables 7, 8, 9, and 10. These should assist researchers in selecting the critical parameters along with their metadata. Plasma-MDS consists of five main schema elements that should be reported in plasma studies if applicable, namely, (i) "Source" (information about the plasma source, i.e., the device used to generate the plasma); (ii) "Medium" (information about the medium in which the plasma is generated); (iii) "Target" (information about the target treated with the plasma); (iv) "Diagnostics" (information on the diagnostic methods and instruments used to investigate plasma, medium or target properties); and (v) "Resource" (information about the file and data types of the research data belonging to the plasma study)[14]. The suggested metadata schema (Fig. 1) for food-related applications of non-thermal plasmas specifically extends the "Properties" and "Procedure" attributes of the schema elements "Source", "Medium", "Target", and "Diagnostics", while "Resource" remains unchanged since it applies to all metadata documents. Further attributes of the main schema elements, i.e., "source.name", "source.application", "source.specification", "medium.name", "target.name", and "diagnostics.name" also remain unchanged and should be used as intended for general naming and categorization of the data. While for the sake of generality, Plasma-MDS does not further specify the attributes "Properties" and "Procedure" for the different schema elements and considers them free text fields, the metadata schema proposed

Id	Field name	Description	Field type
1.1.1	**Geometry settings**	**Object including all attributes defining the configuration of the plasma setup such as the type of plasma device used (e.g., DBD, plasma jet, corona discharge, etc.), its physical shape, structure, dimensions, and materials.**	**Object**
1.1.1.1	Geometry description	Free text description of the source geometry and materials.	String
1.1.2	**Power supply settings**	**Object including all attributes defining the electrical power supply used in plasma generation.**	**Object**
1.1.2.1	Power supply [AC, DC]	The electrical power used to generate the plasma.	Enumerated list
1.1.2.2	Waveform [sinusoidal, square, ramp, pulse, arbitrary]	The shape of the electrical signal.	Enumerated list
1.1.2.3	Input power [W]	Total power supplied to the plasma system.	Number
1.1.2.4	Peak-to-peak discharge voltage [kV]	The voltage difference between the highest and lowest points of the discharge.	Number
1.1.2.5	Frequency [kHz]	Frequency of the electrical discharge.	Number
1.1.3	**Source settings**	**Object including all attributes of the plasma source used to generate the desired plasma.**	**Object**
1.1.3.1	Discharge current [A]	Current passing through the plasma discharge.	Number
1.1.3.2	Dissipated power [W]	Power actually used by the plasma discharge, excluding losses.	Number
1.1.3.3	Specific energy input [J/cm^3]	Energy supplied per unit volume of the treated medium.	Number
1.2.1	**Standardization procedures**	**Object including all attributes defining how the plasma source is standardized to ensure consistency across experimental runs.**	**Object**
1.2.1.1	Waiting time [min]	The time needed to reach a stable plasma state before starting the treatment.	Number

Table 1. Minimal set of plasma source-related parameters that are critical in non-thermal plasma research for decontamination purposes.

here specifies and structures the information for the dedicated application field. "Properties" should include specific information and measurable parameters and "Procedure" defines the steps involved, such as those required to stabilize the plasma.

Figure 1 summarizes all relevant categories of parameters that affect the decontamination efficacy of non-thermal plasmas as an extension to the core elements of Plasma-MDS for food-related applications. Those parameters are organized into four levels, which cover the source (i) used in the process, the medium (ii) used for the process, the target (iii) of the process, and possible diagnostics (iv) to mirror the process. The extended metadata schema for all parameters is also publicly available in a machine-readable JSON-schema format[25]. The JSON-schema representation was developed using Adamant: a JSON schema-based metadata editor, allowing the user-friendly collection of standardized metadata in accordance with the given schema[26].

Plasma source-related parameters. Examples of plasma sources, which are about to enter the field of food processing or agriculture are summarized in various reviews[2,3,27–30]. For instance, Misra *et al.*[31] reviewed devices for plasma generation inside sealed packages[31]. In general, DBD is the most frequent setup in food-related applications[8,13,32]. That being said, DBD is not always ideal for food applications particularly those involving matrices with complex 3D shapes. These shapes are difficult to position between two electrodes that require a relatively short distance for effective plasma generation. In these cases, an indirect mode of treatment using plasma-processed gases or plasma-treated liquids, or alternative plasma sources such as plasma jets, or corona discharges may be more suitable.

Plasma source-related parameters are critical in all non-thermal plasma applications and can significantly affect the decontamination efficacy. Additionally, several plasma source properties can serve as substitutes for plasma diagnostics in some applications, as the latter are often complex and difficult to obtain. Specifically, the dissipated power and the estimated dimensions of the generated plasma (e.g., based on the source geometry settings) were used in previous research as an indirect method for summarizing the plasma process intensity for microbial inactivation experiments in the food domain[8]. Table 1 presents the relevant plasma source parameters that are critical in food-related applications. The main properties include the geometry settings, the power supply settings, and the source settings. Source geometry can define the volume and the composition of the generated plasma and thus its decontamination efficacy. Additionally, electrode materials can also play a role, as seen in DBD plasma sources[33]. The power supply specifications are important because as mentioned in the "Introduction" section, different plasma categories can be defined based on them such as RF and MPS, and the chosen settings can lead to different reactive oxygen and nitrogen species in the plasma medium. In addition, non-thermal plasma processes can be categorized based on the operating pressure: (i) low-pressure ($\lesssim 10^3$ Pa); (ii) medium-pressure (10^3 to 10^5 Pa); (iii) atmospheric-pressure ($\approx 10^5$ Pa), and (iv) high-pressure ($\gtrsim 10^5$ Pa), as considered by the "source.specification" attribute of Plasma-MDS. Among these, atmospheric-pressure plasma processes are the most interesting for industrial applications, including food processing, because they do not need any complex vacuum techniques and they are frequently able to ignite plasma in ambient air.

Not only the specifications and the corresponding categorization of the plasma source are important, but also the chosen experimental settings (properties). The power supply settings (Table 1) that can affect the plasma decontamination efficacy, and are therefore critical, include input power[34], peak-to-peak discharge voltage[35],

Id	Field name	Description	Field type
2.1.1	**Gas properties**	**Object including all attributes defining the carrier gas.**	**Object**
2.1.1.1	Gas description	Free text description of the carrier gas.	String
2.1.1.2	Pressure [Pa]	Pressure of the carrier gas during plasma operation.	Number
2.1.1.3	Flow rate [L/min]	The rate at which the gas is supplied to the plasma source.	Number
2.1.1.4	Carrier gas composition	The type and composition of the gas mixture used in the plasma (e.g., 90% N_2, 10% O_2).	String
2.1.1.5	Purity [%]	Purity level of the gases used (e.g., 99.99% purity).	Number
2.1.1.6	Temperature [°C]	Temperature of the gas during plasma operation.	Number
2.1.1.7	Humidity [% RH]	Relative humidity level of the plasma medium.	Number
2.1.2	**Precursor properties (where applicable)**	**Object including all attributes defining the presence of any precursors or added compounds in the plasma medium.**	**Object**
2.1.2.1	Precursor description	Free text description of the precursor added in the carrier gas.	String
2.1.2.2	Amount of precursor added to the medium [ml or g]	Quantity of the precursor added to the plasma medium.	Number
2.1.3	**Liquid properties (where applicable)**	**Object including all attributes defining the plasma-treated liquid.**	**Object**
2.1.3.1	Liquid description	Free text description of the liquid being treated by the plasma.	String
2.1.3.2	Volume [L]	The volume of the liquid being treated.	Number
2.1.3.3	Distance [cm]	The distance between the plasma source and the liquid surface.	Number
2.1.3.4	Stirring [yes, no]	Indicates whether the liquid was stirred during plasma treatment.	Enumerated list
2.1.3.5	pH	The pH level of the liquid before and after treatment.	Number
2.1.3.6	Oxidation-reduction potential [mV]	The oxidation-reduction potential of the liquid.	Number
2.1.3.7	Minimum conductivity [S/m]	The minimum electrical conductivity needed for plasma ignition.	Number
2.1.3.8	Conductivity [S/m]	The electrical conductivity of the liquid.	Number
2.1.3.9	Treatment time [min]	The duration for which the plasma source was applied to treat the liquid, creating a plasma-treated liquid (PTL) intended for subsequent decontamination purposes.	Number
2.1.3.10	Reactive oxygen and nitrogen species	Free text description of the reactive oxygen and nitrogen species measured in the plasma liquid (e.g., hydroxyl radical, hydrogen peroxide, nitric oxide, nitrite, nitrate).	String
2.1.3.11	Temperature [°C]	The temperature of the liquid during plasma treatment.	Number
2.2.1	**Medium treatment**	**Object including all attributes defining the plasma medium.**	**Object**
2.2.1.1	Medium modification (where applicable)	The way the medium was modified before the plasma generation (e.g., humidification of the carrier gas).	String
2.2.1.2	Medium treatment time (where applicable) [min]	The treatment time in which the medium (gas, liquid, or both) is treated by a plasma source that will then be used to treat a target. Only applicable in the indirect mode of treatment.	Number

Table 2. Minimal set of plasma medium-related parameters that are critical in non-thermal plasma research for decontamination purposes.

Id	Field name	Description	Field type
3.1.1	**Food-related parameters**	**Object including all attributes defining the food matrix, the packaging material, or the food processing surface being treated.**	**Object**
3.1.1.1	Matrix description	Free text description of the matrix being treated.	String
3.1.1.2	Distance to surface [cm]	The distance from the plasma source to the target surface.	Number
3.1.1.3	Surface temperature [°C]	The temperature of the target surface during plasma treatment.	Number
3.1.2	**Microbial-related parameters**	**Object including all attributes defining the microbial properties of the target.**	**Object**
3.2.1	**Target treatment**	**Object including all attributes defining the methodology followed to treat the target.**	**Object**
3.2.1.1	Mode of treatment [direct, indirect]	Specifies whether the plasma treatment was applied to the target in direct (UV / VUV irradiation, plasma particles) or indirect (plasma-processed gas / plasma-treated liquid) way.	Enumerated list
3.2.1.2	Spatial location relative to the plasma source	Free text description of the spatial position of the target with respect to the electrodes or the plasma source geometry (how the target is exposed to the plasma medium (UV / VUV irradiation, plasma particles, plasma-processed gas / plasma-treated liquid)).	String
3.2.1.3	Target treatment time [min]	The duration for which the plasma medium was applied to the target matrix. For direct treatments the medium treatment time and the target treatment time match.	Number

Table 3. Minimal set of plasma target-related parameters that are critical in non-thermal plasma research for decontamination purposes.

and frequency[36]. The source settings that can affect the plasma decontamination efficacy include the discharge current, the dissipated power (the power that goes to plasma generation)[37], and the specific energy input (combination of the dissipated power, time, and volume of the plasma gas).

When it comes to plasma source procedures, the standardization procedures, and especially the waiting time required to achieve a stable plasma, is a critical factor for ensuring comparability between experiments conducted across different laboratories, especially in cases where no plasma diagnostic procedures are implemented.

Treatment matrix	Parameters
Abiotic surface	- Surface material - Surface metrology [roughness, waviness in cm] - Dimensions [e.g., L x W x H or radius, in cm]
Liquid medium	- Type - Volume [L] - Salt content [% w/v] or a_w - Viscosity [Pa·s] - Reflection index [°Brix] - Conductivity [S/m] - Oxidation-reduction potential [mV] - pH - (Commercial brand)
Solid medium	- Type - Weight [g] - Medium shape - Dimensions [e.g., L x W x H or radius, in cm] - Treated surface area [cm^2] - Contact angle (where applicable) [°] - Salt content [% w/v] or a_w - pH - (Commercial brand)
Liquid food	- Volume [L] - Salt content [% w/v] or a_w - Viscosity [Pa·s] - Reflection index [°Brix] - Conductivity [S/m] - Oxidation-reduction potential [mV] - pH - Fat percentage [%] - Protein content [%] - Density [kg/m^3]
Solid food	- Weight [g] - Food shape - Dimensions [e.g., L x W x H or radius in cm] - Treated surface area [cm^2] - Contact angle (where applicable) [°] - Salt content [% w/v] or a_w - pH - Fat percentage [%] - Protein content [%]

Table 4. Minimal set of food-related parameters that are critical in non-thermal plasma research for decontamination purposes.

Microbial forms	Parameters
Vegetative bacteria	- Genus - Species - Serotype - Single- or multi-culture - Strain [ATCC / DSM / NCTC No, or equivalent] - Growth medium before and after treatment - Incubation time before and after treatment [h] - Incubation temperature [°C] - Growth stage [exponential, stationary] - Mode of inoculation [spraying, spotting, spreading, stamping, mixing] - Inoculation procedure - Microbial counts before and after treatment [$\log_{10}$ CFU/(mL, or cm^2, or g)] - Enumeration / quantification procedure
Bacterial cells / spores in biofilms	- Biofilm age [days] - Biofilm formation protocol - Sporulation protocol - All parameters from "Vegetative bacteria"
Yeasts and molds	- Ascospores or endospores [molds] - All parameters from "Vegetative bacteria"

Table 5. Minimal set of microbial-related parameters that are critical in non-thermal plasma research for decontamination purposes.

Where applicable, the parameters reported in Table 1 should also be accompanied by a description of the method used for their estimation in terms of diagnostics to make the parameters of different research studies transparent and traceable.

Plasma medium-related parameters. The medium of the process transports the active compounds generated by the source to the site of action (target). Table 2 presents the relevant plasma medium-related parameters that are critical in food-related applications. The measurable properties of the plasma medium include gas properties, precursor properties, and liquid properties (only relevant for plasma-treated liquids). Regarding gas properties (Table 2), the pressure level can affect the decontamination efficacy, especially in low-pressure

Id	Field name	Description	Field type
4.1.1	**Diagnostic settings**	**Object including all attributes defining the diagnostic method used to assess plasma source-, medium-, or target-related properties.**	**Object**
4.1.1.1	Setting description	Free text description of the diagnostic settings (e.g., spectroscopy settings, sensor calibration).	String
4.1.2	**Environmental parameters**	**Object including all attributes defining the conditions in the measurement chamber during diagnostics (e.g., humidity, temperature, pressure).**	**Object**
4.1.2.1	Temperature [°C]	The temperature of the processing environment.	Number
4.1.2.2	Humidity [% RH]	Relative humidity of the processing environment.	Number
4.1.2.3	Pressure [Pa]	The pressure of the processing environment.	Number
4.2.1	**Diagnostic methodology**	**Object including all attributes defining the experimental setup of the diagnostic procedures implemented, such as location, targets, and quantification methods.**	**Object**
4.2.1.1	Methodology description	Free text description of the experimental setup of the diagnostic procedures.	String
4.2.1.2	Location of the diagnostic application	The specific location where the diagnostic method was applied (e.g., on the plasma source, in the plasma medium, on the target).	String
4.2.1.3	Targets of qualitative / quantitative analysis	The specific components being analyzed (e.g., reactive species, target surface properties).	String
4.2.1.4	Quantification method	The technique used for the quantification of the analytes (e.g., simulation with online databases, calibration curves using standards, machine built-in library, sensor direct output). For direct outputs, the limit of detection (LOD) should be provided.	String
4.2.2	**Data processing**	**Object including all attributes defining how raw data were processed and analyzed.**	**Object**
4.2.2.1	Data processing description	Free text description of the data processing and analysis procedures (e.g., spectral deconvolution, data smoothing, software used for data interpretation).	String

Table 6. Minimal set of parameters that should be described in plasma diagnostics procedures taking place in non-thermal plasma research for decontamination purposes.

applications[38]. Plasma can be generated in a static gas environment (enclosed reactor, no gas flow), where the plasma volume is defined by the reactor's size, or in a continuous mode, where the gas flows at a predetermined rate. The flow rate is critical since it affects the gas residence time, which in turn affects the plasma chemistry[23]. The temperature of the gas during plasma operation can also be important, especially if it affects the target's temperature. Additionally, temperature, carrier gas composition, and humidity can all affect the concentration of reactive oxygen and nitrogen species generated in the plasma gas. Moving to the precursor properties, the addition of precursors can create different plasma processes, with the extent of variation dependent on the carrier gas and the amount of added compounds or precursors. For example, Saremnezhad *et al.*[39] observed variations in the efficacy of non-thermal plasma in reducing food allergens and mycotoxins depending on changes in the plasma medium[39]. For decontamination purposes, Majumdar *et al.*[40], Hertwig *et al.*[41], and Patil *et al.*[42] are only a few of the studies that evaluated the effect of the plasma medium (carrier gas) on the decontamination efficacy. Moreover, the influence of added compounds or precursors on a plasma process can be adjusted to achieve the desired target reaction. Numerous studies, for instance, have examined the role of inducer gases with varying oxygen levels, while many contemporary studies continue to employ helium or argon to achieve desired plasma properties[43–45].

In cases where a plasma-treated liquid is used as the medium for decontamination, the properties of the plasma-treated liquid must also be described in addition to the previously mentioned parameters. These properties include the liquid's composition, volume, distance from the plasma source, stirring conditions, pH, oxidation-reduction potential (ORP), minimum conductivity to ignite the plasma, conductivity, treatment time, reactive oxygen and nitrogen species (RONS), and temperature. These parameters are crucial since they can determine the antimicrobial compounds present in the liquid and therefore its decontamination efficacy[46,47]. In addition to these parameters, it is essential to report the actual volume of the plasma medium that was used to treat the target.

As for the plasma medium procedures, the medium treatment consists of two main attributes: (i) medium modification, and (ii) medium treatment time. As discussed in "The challenges of standardization in food-related applications", but also in other studies[42,48], medium modification, such as humidification procedures can result in a variety of different reactive species, and therefore it is crucial to be described. The medium treatment time applies to indirect plasma applications, such as plasma-processed gas or plasma-treated liquid. It refers to the duration during which the plasma source treats the medium (gas, liquid, or both). For these applications, this is distinct from the target treatment time, which refers to the duration the treated medium is applied to the target.

Plasma target-related parameters. The target treated with plasma is the focus of any application whether it is a food product, packaging material, food processing surface, or a simulant of these. As mentioned in "Plasma medium-related parameters", plasma-processed gases or plasma-treated liquids, are considered part of the plasma medium (and not of the target), as they are used to treat a target in an indirect mode of treatment. Table 3 presents the relevant plasma target-related parameters that are critical in food-related applications. In addition to specific food- and microbial-related parameters which will be discussed in detail in the following section, other important properties applicable to all food-related matrices include the distance between the plasma source and the target surface and the surface temperature during treatment.

As for the plasma target procedures, the target treatment consists of three main attributes: (i) the mode of treatment, (ii) the spatial location relative to the plasma source, and (iii) the target treatment time (Table 3). Regarding

the first attribute, the mode of treatment is considered a plasma target-related parameter because it defines how the plasma source is acting on the target[14]. In this aspect, two main categories can be formed, i.e., (i) direct (including direct and semi-direct), and (ii) indirect treatment. In direct treatments, plasma is in direct contact with the substrate, and the interaction is based on irradiation (UV, VUV), charged molecules, radicals, and reactive species. In semi-direct treatments, the distance between plasma and substrate is larger, and therefore, only irradiation, long-lived radicals, and metastable inhibitory substances reach the target. In this case, the antimicrobial effect is due to irradiation, long-lived radicals as well as metastable and inhibitory substances, but no interactions with charged particles take place[49]. In the food industry and agriculture, products with a resistant matrix are predominantly treated with a direct treatment. Numerous studies have used direct treatment to decontaminate various products including black peppercorn[50], fresh vegetables, fruits, nuts, powdered food samples[51], and sliced cheese[52]. Additionally, direct treatment has been applied to decontaminate food processing surfaces[53,54]. However, direct treatments are predominantly surface treatments that can be applied for treatment goals without any vulnerable surface. Indirect treatments can be applied through irradiation with UV and VUV (where applicable) light (e.g., UV lamps) where plasma is enclosed in a UV / VUV-transparent reactor without any interaction with plasma particles or by using previously generated plasma to process a gas or treat a liquid[49]. The decision between direct and indirect treatment is mainly based on the desired goal and the matrix properties (including geometry) of the target. Vulnerable products are better treated with an indirect plasma-based method, whereas more resistant products with regular surfaces can also be subjected to direct treatment. Schnabel *et al.*[55] described the differences between direct and indirect treatment of food products for decontamination purposes[55]. Indirect treatments are regularly applied for treatment goals with vulnerable surfaces that may change color, texture, or taste. Whichever process type, direct or indirect, is chosen, the effect of such a process is always realized by the chemical components that are generated by an ignited plasma. In contrast to direct treatment, in which the plasma-produced reactive compounds directly act on the treatment target, the reactive compounds used in indirect treatments do not act at their production site. Consequently, processes, designed upon indirect plasma treatments need a carrier for the reactive compounds such as RONS. This carrier can either be a plasma-processed gas (PPG) or a plasma-treated liquid (PTL), as explained in "Plasma medium-related parameters". Among gases, plasma-processed air (PPA) is the most extensively studied category in recent literature, while among liquids, plasma-treated water (PTW) also referred to as plasma-activated water (PAW) or plasma-functionalized water (PFW) is the primary focus. For instance, PTW can be used to improve the microbiological safety of fresh-cut produce (mainly leafy greens)[56–58]. Indirect treatments offer the possibility of mild plasma treatments for vulnerable treatment goals like food products or other sensitive goods. Additionally, indirect treatments are realized on the laboratory scale for water treatments[59]. It should be noted that in most cases indirect treatments involve additional parameters to be described for example the plasma-treated liquid parameters (Table 2). Also, the description of the design of the setup, the definition of the distance of the plasma source, and how plasma is transferred to the target are often more challenging. Clearly defining the spatial location of the target relative to the plasma source (Table 3) is essential for both direct and indirect treatments, as it impacts the treatment uniformity due to variations in plasma source geometry. Additionally, this spatial relationship complements the mode of treatment as it helps clarify whether the target is exposed to UV / VUV irradiation, plasma particles, reactive species within the plasma effluent, or a combination of these factors. The last attribute of the plasma target procedures refers to the target treatment time because as with all processing technologies, the treatment time of the target is essential for determining the decontamination efficacy.

Food-related parameters. Based on the target matrix, important parameters or prerequisites and restrictions may enter the process design. Product properties such as the structure[60], vulnerable ingredients[61,62], or the water content[63] may play a crucial role in the process design since they may alter the whole process chemistry. In Table 4, there is a summary of the food-related parameters that can affect the decontamination efficacy of non-thermal plasma.

It should be noted for clarification purposes that an abiotic surface is different from the other treatment matrices due to the condition of being dry. The surface material (Table 4) refers to the part of the abiotic surface that is contaminated with microorganisms and treated with non-thermal plasma. If more than one material constitutes the abiotic surface then all of them should be described. The matrix category of solid / liquid medium in Table 4 corresponds to those experimental setups where the microorganism is inoculated to a growth medium, a buffer, or water and then treated directly with non-thermal plasma. Solid medium is the category that covers all the experiments conducted in growth media contaminated with microorganisms, either inoculated and mixed before solidification or inoculated as a drop, a spread, a stamp, or a spray after the medium has solidified. In contrast, the liquid medium is the equivalent of an abiotic surface but when treated in a wet mode (e.g., as a droplet on an abiotic surface), and can correspond to a growth medium (e.g., brain heart infusion), or water (e.g., distilled or saline). Additionally, the shape of a solid matrix (food or medium), is critical, as the dimensions can be used to estimate the treated area during a plasma process (Table 4). This aspect is particularly important for direct plasma experiments, where treatment predominantly occurs at the surface. Lastly, for some of the parameters mentioned, it needs to be clear where they were measured (location in the product or the processing environment) and if they were measured before, after treatment, or both (e.g., temperature, conductivity, pH).

Microbial-related parameters. In Table 5, there is a summary of the relevant microbial-related parameters that can affect the decontamination efficacy of non-thermal plasma. These parameters relate to how the microorganism of interest was cultured and inoculated in the matrix before plasma treatment. The importance of these parameters has been demonstrated across various non-thermal processing technologies such as pulsed electric fields (PEF)[12,64,65], high-pressure processing (HPP)[66,67], and non-thermal plasma[68].

Id	Field name	Value
1.1.1	**Geometry settings**	
1.1.1.1	Geometry description	DBD plasma reactor treats the sample between two circular electrodes; a circular dielectric barrier covers the upper electrode. The diameter of the electrodes, as well as the diameter and thickness of the dielectric barrier, were measured.
1.1.1.2	Upper electrode diameter [cm]	5.5
1.1.1.3	Ground electrode diameter [cm]	5.5
1.1.1.4	Dielectric barrier diameter [cm]	7.5
1.1.1.5	Dielectric barrier thickness [cm]	0.1
1.1.1.6	Electrode distance [cm]	0.8
1.1.1.7	Upper electrode material	Stainless steel
1.1.1.8	Ground electrode material	Stainless steel
1.1.1.9	Dielectric material	Glass
1.1.2	**Power supply settings**	
1.1.2.1	Power supply	AC
1.1.2.2	Waveform	sinusoidal
1.1.2.3	Input power [W]	30
1.1.2.4	Peak-to-peak discharge voltage [kV]	9
1.1.2.5	Frequency [kHz]	9
1.1.3	**Source settings**	
1.1.3.1	Discharge current [A]	0.01
1.1.3.2	Dissipated power [W]	25
1.1.3.3	Specific energy input [J/cm^3]	300
1.2.1	**Standardization procedures**	
1.2.1.1	Waiting time [min]	5
2.1.1	**Gas properties**	
2.1.1.1	Gas description	The plasma medium (gas) was ambient air without any further treatment or precursors.
2.1.1.2	Pressure [Pa]	1.01×10^5
2.1.1.3	Flow rate [L/min]	4
2.1.1.4	Carrier gas composition	NA
2.1.1.5	Purity [%]	NA
2.1.1.6	Temperature [°C]	35
2.1.1.7	Humidity [% RH]	40

Table 7. An example of accurately describing the plasma source- and plasma medium-related parameters of non-thermal plasma using a DBD device.

Plasma diagnostics. In food-related applications of plasma decontamination, diagnostics usually refer to the processes that take place to monitor plasma generation and stability throughout processing. Table 6 presents the relevant plasma diagnostics parameters that should be described in food-related applications. The main properties include the diagnostic settings and the environmental parameters, whereas the important procedures involved are the diagnostic methodology and the data processing procedures.

The most representative application of plasma diagnostics is the processes that take place to monitor the generation of reactive species. In this respect, the key information on reactive oxygen and nitrogen species (RONS) in the plasma gas should be provided not only in relative terms but also as absolute values with clear metric units. Spectrographs, though commonly reported in the literature, are often challenging to compare across studies due to their qualitative nature. Therefore, they should be accompanied by detailed metadata, including the conditions and devices used for sample analysis, as well as the raw data used to create the corresponding graphs. Additionally, the methodology used to identify the reactive species (including the analytical method, specific species measured, and location in the product or the processing environment) as well as environmental conditions (humidity, temperature, pressure) must also be documented.

Examples of data descriptions

To make the schema-based collection of the parameters more accessible to the reader, the aforementioned metadata schema was used to generate a complete, hypothetical non-thermal plasma case study. This case study includes tables for the elements of Plasma-MDS and the corresponding parameters. The scenario involves the decontamination of black peppercorns contaminated with *Salmonella* (plasma target), treated with a DBD device (plasma source) in a direct mode of treatment using ambient air (plasma medium). Plasma diagnostics were also simulated to assess the RONS in the plasma gas. This case study is summarized in Tables 7, 8, 9, and 10, and is also made publicly available in a machine-readable JSON format, generated by completing only the relevant fields of the metadata schema for this example[25]. Again, the "Adamant" tool was used to facilitate this task[26].

Id	Field name	Value
3.1.1	**Food-related parameters**	
3.1.1.1	Matrix description	The target matrix was black peppercorns bought from a local supermarket and sterilized before treatment.
3.1.1.2	Distance to surface [cm]	NA
3.1.1.3	Surface temperature [°C]	30
3.1.1.4	Weight [g]	5
3.1.1.5	Food shape	spherical
3.1.1.6	Dimensions [cm]	~0.5 diameter
3.1.1.7	Treated surface area [cm^2]	NA
3.1.1.8	a_w	0.6
3.1.1.9	pH	5.5
3.1.1.10	Fat percentage [%]	3
3.1.1.11	Protein content [%]	10
3.2.1	**Target treatment**	
3.2.1.1	Mode of treatment [direct, indirect]	direct
3.2.1.2	Spatial location relative to the plasma source	The peppercorns were placed directly between the two electrodes of the DBD device. The product was exposed simultaneously to plasma-generated reactive species, charged particles, and UV irradiation emitted uniformly from the electrode surfaces.
3.2.1.3	Target treatment time [min]	5

Table 8. An example of accurately describing the food-related parameters and the target treatment procedures (plasma target-related parameters) in non-thermal plasma decontamination studies.

Plasma source- and plasma medium-related parameters. In Table 7, an example of plasma source- and plasma medium-related parameters is presented. For this example, a DBD device was simulated, but the same approach could be applied to generate equivalent tables for other plasma sources and devices. Some parameters from Fig. 1 for the plasma medium were not reported in Table 7 (i.e., precursor properties, liquid properties, medium treatment) as they were irrelevant to this scenario (see also: Table 2). If the plasma medium was a plasma-treated liquid (e.g., water), then its properties would also need to be reported (Table 2).

Plasma target-related parameters. *Food-related parameters.* In Table 8, the matrix (solid food)-related parameters and the target treatment procedures are presented, as sub-schemes of the plasma target-related parameters. In this example, a solid food matrix (black peppercorn) that is treated in a direct mode of treatment was simulated, but the table could also be adapted to describe the information of other matrices, for example, an abiotic surface such as a packaging material or a food processing surface (Table 4). The "distance to surface" was reported as "NA" (not applicable) because of the direct treatment scenario where the product is placed between the two electrodes. Also, the treated surface was not quantified in this example due to the complexity of the food product (multiple spheres being treated simultaneously) which would require further diagnostics for precise assessment. This highlights the flexibility of the presented metadata schema, allowing adaptation based on the resources available in each laboratory.

Microbial-related parameters. In Table 9, an example of the microbial-related parameters is presented, as a sub-scheme of the plasma target-related parameters. In this example, a vegetative bacterium i.e., *Salmonella* Typhimurium, is simulated but the table could also be adapted to report the information of other microorganisms, for example, *Listeria* cells in a biofilm or *Bacillus* spores (Table 5). Regardless of the microbial form, ensuring FAIR data in microbial-related parameters requires that preculture conditions are clearly defined and thoroughly discussed. This example was based on the assumption that the product of interest i.e., black peppercorn was sterilized before the inoculation with *Salmonella*, and then treated with non-thermal plasma.

While the example provided is comprehensive, more complex experimental setups would require additional parameters. For instance, if the microbial form were spores, then the sporulation protocol would also need to be reported (Table 5).

Plasma diagnostics-related parameters. In Table 10, an example of the plasma diagnostics-related parameters is presented. In this example, Fourier Transform Infrared Spectroscopy (FTIR) was used to analyze reactive oxygen and nitrogen species (RONS) generated directly in the gas phase within the discharge region, immediately above the peppercorn surface.

It should be noted that although FTIR can characterize the plasma-generated reactive species that were mentioned in Table 10, other plasma-induced effects, such as UV irradiation may require additional diagnostic techniques for a comprehensive assessment.

Id	Field name	Value
3.1.2	**Microbial-related parameters**	
3.1.2.1	Microbial form	Vegetative bacteria
3.1.2.2	Genus	*Salmonella*
3.1.2.3	Species	*enterica*
3.1.2.4	Serotype	Typhimurium
3.1.2.5	Single- or multi-culture	single-culture
3.1.2.6	Strain	LMG 14933
3.1.2.7	Growth medium before and after treatment	From −80 °C, the stock culture was grown in Tryptic Soy Agar (TSA) for 48 h and then a single colony was inoculated to Tryptic Soy Broth (TSB). TSA was used for the enumeration after treatment.
3.1.2.8	Incubation time before treatment [h]	24
3.1.2.9	Incubation temperature [°C]	37
3.1.2.10	Growth stage	stationary
3.1.2.11	Mode of inoculation	mixing
3.1.2.12	Inoculation procedure	1 ml of the initial inoculum of known concentration was mixed with the treatment matrix and let dry for 30 min at room temperature.
3.1.2.13	Microbial counts before treatment [$\log_{10}$ CFU/g]	8.0
3.1.2.14	Enumeration / quantification procedure	Samples were immediately analyzed after treatment through homogenization with physiological salt solution (PPS) followed by serial dilution. A 0.1 ml aliquot of each dilution was plated on TSA, and incubated.
3.1.2.15	Incubation time after treatment [h]	48
3.1.2.16	Microbial counts after treatment [$\log_{10}$ CFU/g]	1.5

Table 9. An example of accurately describing the microbial-related parameters (plasma target-related parameters) in non-thermal plasma decontamination studies.

Additional considerations for better data descriptions

Besides the specific challenges related to describing parameters in non-thermal plasma research, as discussed in "The challenges of standardization in food-related applications", it is important to note that the principle of "findable" data can be challenged when authors reference one or more previously published studies to describe certain experimental parameters. Although in general this approach is considered valid to avoid repetition, it can be problematic when one or more experimental parameters are already different when compared to the study of interest because it becomes then unsure if also other parameters have changed over time or not. Therefore, it is advisable for authors to clearly define the reported parameters and specify precisely which aspects remain the same and which differ from previous research.

The parameters discussed in this study can set the basis for researchers to determine which information is critical to document in non-thermal plasma decontamination experiments for food-related applications, and how this information can be effectively described. However, these parameters can be expanded to cover certain applications if needed. A practical way to facilitate and process validation and regulatory approval is to distinguish between parameters that directly affect plasma chemistry and those that are more device-specific. In this view, environmental and operational conditions such as humidity, temperature, and pressure are different from factors such as electrodes' material or geometry that are essential to replicate the setup but are not always directly comparable across different systems. This approach can help identify and quantify the most critical processing conditions (e.g., a "dose") in a standardized manner. Nevertheless, the metadata schema that is presented in this study covers all use cases either when comparing the same or different systems since the relevance of each parameter (and the determination of the "dose") highly depends on the context. The more comprehensively the data are documented, the broader the range of potential reuse scenarios, ultimately bringing non-thermal plasma applications closer to regulatory approval. That being said, we acknowledge that not all parameters, such as plasma diagnostics-related parameters, are equally accessible and can be limited by expensive methods and the need for trained personnel. Therefore, in this study, we provide definitions and guidance on parameters ranging from easily accessible to more complex, to assist researchers in clearly and accurately describing their experimental data, regardless of their laboratory equipment. In this way, parameters that are generally more easily accessible to researchers could be used by other researchers as indirect methods of plasma diagnostics through the estimation of more complex metrics. For example, as mentioned in "Plasma source-related parameters", the dimensions and geometry of the electrodes (e.g., in DBD devices), when clearly defined, can be used to calculate their respective areas, volumes, and other relevant physical properties depending on the shape. These properties can then be combined with the plasma source-related parameters (e.g., the dissipated power and the processing time) and be used as metrics for comparison of the decontamination efficacy[8].

Conclusion

The purpose of this study is to provide a metadata schema to guide the consistent and traceable descriptions of the relevant parameters and aims at improving the interoperability, reproducibility, and reuse within the non-thermal plasma community for food-related applications. This would allow for more accurate overviews, and comparisons of the results in the literature, for example in the context of systematic reviews and meta-analyses. With this study, the Plasma-MDS platform that was previously developed[14] is given

Id	Field name	Value
4.1.1	**Diagnostic settings**	
4.1.1.1	Setting description	RONS in the plasma-processed medium were determined with FTIR spectroscopy with the following settings: absorption path length 0.25 m, resolution 0.6 cm^{-1}, wavenumber range of 4000 – 400 cm^{-1}, 64 scans in each measurement.
4.1.2	**Environmental parameters**	
4.1.2.1	Temperature [°C]	22
4.1.2.2	Humidity [% RH]	40
4.1.2.3	Pressure [Pa]	1.01×10^5
4.2.1	**Diagnostic methodology**	
4.2.1.1	Methodology description	After the plasma discharge had stabilized, FTIR measurements of reactive species were performed in the gas phase adjacent to the peppercorns, placed between the electrodes, using a device (specify brand and model).
4.2.1.2	Location of the diagnostic application	The plasma gas phase was sampled 1 cm above the peppercorn surface, within the discharge region between the two electrodes.
4.2.1.3	Targets of qualitative / quantitative analysis	Hydrogen peroxide (H_2O_2), Ozone (O_3), Nitrate (NO), Nitrite (NO_2). FTIR spectroscopy, specific peak centers: 1400 cm^{-1} and 876 cm^{-1} for H_2O_2; 1050 cm^{-1} for O_3; 1875 cm^{-1} for NO; and 1600 cm^{-1} and 2900 cm^{-1} for NO_2.
4.2.1.4	Quantification method	Calibration curves based on known standards for H_2O_2, O_3, NO, NO_2.
4.2.1.5	H_2O_2 [mol/m^3]	1.6×10^{-4}
4.2.1.6	O_3 [mol/m^3]	2.04×10^{-3}
4.2.1.7	NO [mol/m^3]	1.2×10^{-4}
4.2.1.8	NO_2 [mol/m^3]	4.08×10^{-5}
4.2.2	**Data processing**	
4.2.2.1	Data processing description	Spectral deconvolution and baseline correction using a data analysis software (specify), and Savitzky-Golay smoothing. Peaks were identified via an atomic spectra database (specify).

Table 10. An example of accurately describing the plasma diagnostics-related parameters in non-thermal plasma decontamination studies.

a specific context for decontamination in food-related applications, to become easier to implement. That is because it provides specific guidance with examples regarding what is expected to be reported for each case while still maintaining some flexibility for additional or less information. In this way, researchers without specific expertise in non-thermal plasma can still conduct more reproducible research. Similarly, non-thermal plasma experts can use this metadata schema to accurately describe relevant food- and microbial-related parameters. From a data management perspective, like all schemes, Plasma-MDS will benefit from continuous updates as knowledge advances in the field of non-thermal plasma and new applications emerge. This will ensure its relevance and effectiveness in capturing essential information for future applications. The parameters provided in this study are expected to also be applicable to other non-thermal plasma applications.

Code availability

No custom code or algorithms were used to generate or process the data described in this manuscript.

Data availability

The metadata schema to standardize non-thermal plasma decontamination parameters in food-related applications is publicly available in a machine-readable JSON format on GitHub: https://github.com/gpampoukis/plasma-food-metadata-schema[25]. The repository includes both the complete metadata schema and the case study presented in this manuscript.

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Competing interests

The authors declare no competing interests.

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