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Digital Twins applied to the implementation of Safe-by-Design strategies in nano-processes for the reduction of airborne emission and occupational exposure to nano-forms

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Abstract. Digital Twins (DTs) are one of the most promising enabling technologies for the deployment of the factory of the future and the Industry 4.0 framework. DTs could be labelled as an inherently Safe-by-Design (SbD) strategy and can be applied at different stages in the life cycle of a process. The EU-funded project ASINA has the ambition to promote coherent, applicable and scientifically sound SbD nano-practices. In particular, in the field of nanomanufacturing, ASINA intends to deliver innovative SbD solutions applied to process (P-SbD). In this context, ASINA will investigate the use of DTs as a disruptive digital technology for the prevention, prediction and control of nano-forms airborne emission and worker exposure. This paper introduces the concept of DT in the field of nano-processes SbD and outlines the preliminary architecture of ASINA-DT, that will be developed and implemented by ASINA in one industrial scenario.

1. Introduction and motivation

Manufacturing processes and systems consume significant amounts of material resources, water, and energy, and, in parallel, produce significant amounts of polluting emissions and wastes. Companies face the challenge of reducing resources and energy consumption and minimizing environmental impacts, while guaranteeing productivity and profits.

European industry is already undergoing a significant transformation towards greener industry while remaining competitive on the global stage, where digitalization plays an essential role [1]. Evolving manufacturing more sustainable is essential part of environmental and human health protection [2,3,4,5]. Nanotechnological products and processes although emerging, cannot be foreign to these twin environmental and digital transitions.

In this new industrial context, digital technologies can play an important role in greening manufacturing processes, towards the creation of a more competitive and sustainable European industry

[6]. The current digital revolution is providing the manufacturing sector with innovative technological capabilities to enable smart manufacturing [5]. The combination of sustainability with smart manufacturing to reach sustainable smart manufacturing, is the perfect lever to achieve a more sustainable, digital and competitive European industry [4,7,8,9]. In this context, the SbD concept fits as a decisive strategy for the design of inherently safe manufacturing processes.

Digital Twins (DTs) is an emerging digital technology, considered as one of the most promising enabling technologies to deploy the sustainable smart manufacturing framework [7,8,10]. DTs have been considered by the advisory firm Gartner as one of the ”Top 10 Strategic Technology Trends” between 2017 and 2019 [11]. Recently, Markets and Markets (2020) values the global DT market at USD 3,1 billion in 2020 and predicts to reach USD 48,2 billion by 2026. The increasing demand for DTs in the healthcare and pharmaceutical industries due to the COVID-19 pandemic is one of the key factors driving the massive growth of DTs market [12].

Currently, the availability and accessibility at an affordable cost of computing, modelling, interconnectivity and sensor infrastructures, predicts a wide deployment of DTs technology in manufacturing processes across industries, for applications such as real-time monitoring and control, off-line analytics, process prediction and optimization, engineering design, business models, and data-driven decision making in real time.

The EU-funded project ASINA [13] has the ambition to promote consistent, applicable and scientifically sound SbD nano-practices. In the field of nano-processes, ASINA will investigate the use of DTs as a disruptive digital technology for the prevention, prediction and control of airborne emission of nano-forms in process, and worker exposure by inhalation. The project will develop and validate a technology readiness level (TRL) 5/6 demonstrator (ASINA-DT) in one industrial scenario. The ultimate goal is to implement SbD concept applied to processes, achieving more sustainable and digital nano-processes through this technology.

2. Digital Twin concept and applications

DT concept was coined in 2003 by Prof. Grieves at the University of Michigan [14] and a wide variety of definitions are employed across industry and academia [2,3,7 8, 9,10,15,16,17,18)].

In simple words, a DT is a digital replica of an existing physical entity [10,19]. More specifically and focusing on its functionalities, a DT could be defined as a high-fidelity digital replica of an existing physical asset (e.g. a machine or a process in manufacturing), with real-time bi-directional communication enabled between the virtual and physical worlds (closed-loop), synchronized thanks to digital enabling technologies [3,8,10,19].

Recently, the fist standardized definition has been provided by ISO/DIS 23247-1 [20], on automation systems and integration, that defines DT as *a fit for purpose digital representation of some realized thing or process, with a means to enable convergence between the realised instance and digital instance at an appropriate rate of synchronisation*.

A number of different digital technologies are being used in the creation and operation of DTs, such as Artificial Intelligence (AI), Cloud computing (CC), Industrial Internet of Things (IIoT), Augmented (AR) and Virtual Reality (VR), Blockchain, etc.

DT is built with data analytics and AI, bi-directionally connected to the process through IIoT, powered by data captured in real time from sensors embedded in the process and other company data sources, and can make informed decisions through real-time communication and collaboration with humans.

Grieves [14] originally described a DT consisting of three layers: the digital asset (virtual part), the real physical asset, and the bi-directional connection between them. ISO/DIS 23247-1 [20] has expanded the DT structure, including a fourth layer of service (Table 3, Figure 2).

DT technology has experienced rapid growth over the past five years, both in academia and industry [2,7,15,17,18]. Current literature is limited, with few studies applying the use of DT to production systems and manufacturing environments [21]. Most of the existing research on the DT is conceptual work and the development of practical DT applications is still at an early stage [17,19]. The main areas of interest of DTs are manufacturing and smart cities, with some healthcare related. Manufacturing industry started using DT around 2012 [10,18] and leads the research, with particular growth in machine health and predictive maintenance areas [2,7,8,9,15,17,19].

Applications of DTs in manufacturing include digital design and simulation, real-time monitoring, production process simulation, evaluation and optimization; digital production line, equipment status monitoring, product fault warning and predictive maintenance, and production index optimization, amongst others [8,9,15]. Most of these applications have been developed to provide monitoring, prediction and optimization functions and can be considered as decision support applications (open loop), because very few of them complete the automatic self-readjustment of the process (closed loop) [2,19].

To the best of our knowledge, there is no systematic research on the application of DTs for the prevention and reduction of airborne emission and occupational exposure of nano-forms, at the aim to improve sustainability of nanomanufacturing processes.

The implementation of DTs in the design and re-design of nano-processes, can be labelled as an inherently safe design strategy [22] and matches very well with SbD concept and expectations. At ASINA, DT is aimed to prevent and reduce the risks resulting from nano-forms emission and exposure. The expected optimization of the nano-process by the DT, will lead to a direct reduction of nano-forms emission at the source.

The introduction of DTs in the design/re-design of nano-processes (new sensors, modelling, IIoT, embedded IA applications) should be considered in the risk assessment stage of the process, in particular AI-machine learning applications [23].

3. Modelling emissions and exposures

Model is the core of DT. Simulation allows the digital model to interact with the physical asset bi-directionally in real time. Models used in DTs comprise three categories [15,25]: 1) Physical models/first-principle models [24], 2) Data-driven models (DDMs), and finally, 3) the combination of both, Hybrid models (HMs). Table 1, elaborated on the basis of references [15,25], summarizes the main characteristics of these models. The hybridization of existing physical models with data captured online (DDMs) is one of the main challenges of ASINA.

Regarding the modelling of emissions and exposures, mechanistic mass balance models describe the impact of an emission source to the exposure level after dispersion and dilution [25]. They are based on a general dynamic equation [27], which describes the time rate of change of an indoor pollutant concentration by including sources, sinks (deposition, filtration), room-to-room air flows (interzonal airflows), air exchange with the outdoors, and transformation processes. Physical and chemical processes can be combined with the mass balance, such as e.g. evaporation of low volatile substances [28], re-suspension [29], ambient air pollution [26,30], portable indoor air purifiers [31], or photoactive surfaces [32].

State of the art exposure modelling approach includes the relevant physical and chemical processes, and all sensitive (i.e. relevant) exposure determinants that are quantified with measurements. The model predictability is tested separately for the dispersion model and the personal exposure assessment. The exposure model parametrization should be based on process parameters and production activity rather than fixed parametrization. This makes possible real time exposure assessment where the process parameters can act as the exposure model input parameters. Environmental emissions and e.g. local exhaust ventilation (LEV) or general ventilation filter loading can be estimated by using the exposure model mass flow analysis.

The exposure model with main exposure determinants and stationary measurement locations for quantifying the model parametrization is represented in Figure 1. It consists of two compartments, where near field (NF) compromises the source and a worker breathing zone (V_{NF}, m^3) and the far field (FF) volume (V_{FF}, m^3) rest of the room (*i.e.* $V_{tot} = V_{NF} + V_{FF}$). The air exchange is limited between the NF and FF volumes (β, m^3/sec) that causes a concentration gradient. The room is ventilated via FF volume (Q_{OUT}, m^3/min) and three local exhaust ventilation at the coating unit entrance ($Q_{LEV,ent}$, m^3/min), spray chamber (Q_{LEV}, m^3/min), and exit ($Q_{LEV,exit}$, m^3/min). The ventilation replacement air (Q_{IN}, m^3/min) is assumed to be filtered outdoor air which concentration is (C_{IN}, mg/m^3). It is assumed that: 1) all mass entering the model is created by a source *ER* (mg/min) in the NF and the concentrations entering via replacement air $Q_{IN} \cdot C_{IN}$ (mg/min) to the FF, 2) concentrations are fully mixed at all the times both in NF and FF volumes, 3) there are no other losses for the concentrations than the FF ventilation, and 4) there is no significant cross draft. Figure 1 shows the model concept which mathematical description is:

$$V_{NF}\frac{dC_{NF}(t)}{dt} = ER(t) + \beta C_{FF}(t) - (\beta + Q_{LEV})C_{NF}(t) \tag{1}$$

$$V_{FF}\frac{dC_{FF}(t)}{dt} = Q_{IN}C_{IN}(t) + \beta C_{FF}(t) - \left(\beta + Q_{OUT} + Q_{LEV} + Q_{LEV,ent} + Q_{LEV,exit}\right)C_{FF}(t) \tag{2}$$

Exposure determinants and their assignment methods are presented in Table 2. The air flows are assumed to be balanced, i.e. $Q_{IN} = Q_{OUT} + Q_{LEV,ent} + Q_{LEV} + Q_{LEV,exit}$. If emissions occurs from the coating unit entrance or exit those can be implemented as additional sources in the NF volume or as additional compartments.

NPs release form the spray process is product of the nanoparticle feed rate via coating suspension ($\dot{q}_{NP}$, mg/min) and spray process transfer efficiency ε_T (-). The NP tranfer efficiency from the spray nozzle to substrate can be quanitfied by measuring the NP mass flow via local exhaust ventilation ($\dot{m}_{LEV}$, mg/min) and the coating suspension NP mass flow rate as $\varepsilon_T = \dot{m}_{LEV}/\dot{q}_{NP}$ when other NP loss mechanisms are insignificant.

Table 1. Typologies of models for DTs [15,25].

1. Physical models	2. Data-driven models (DDMs)	3. Hybrid models (HMs)
Require comprehensive understanding of the physical properties and their mutual interaction. Quality determined by the availability of knowledge and computational feasibility. Robust extrapolation and low data demand. Expensive to develop and compute. Detailed enough models for application can be challenging.	Do not require a deep understanding of the process. Trained by known inputs and outputs, using AI methods. Highly dependent on the quantity and quality of data used for their development. Poor extrapolation and generalization, due to lack of underlying process knowledge. Can only be as good as the data available to train them. Usually developed to supplement physical models. The most uncertain mechanisms are commonly modelled by DDMs.	Essential for high-fidelity modelling. Combines physical models and DDMs, either in parallel or in series. Performance determined by the quality of sub-models (physical models and DDMs) and the way they are combined. Performance of serial HMs determined by the quality of the physical models. Usually used when the physical model is unable to fully modelling, due to complexity (complex processes, unavailable knowledge, computational solution infeasible) Performance of parallel HMs dependent on the quality of the DDMs.

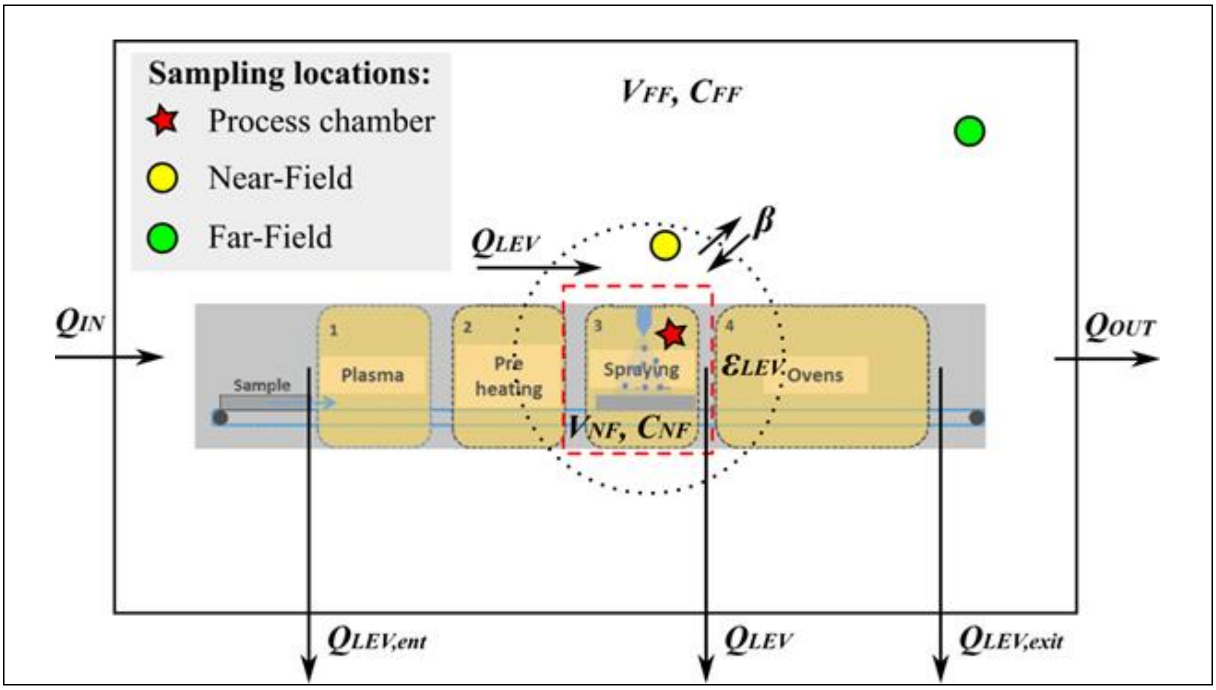

Figure 1. Exposure model with main exposure determinants and stationary measurement locations for quantifying the model parametrization. The coating unit consists of four segments: 1) Plasma neutralizer, 2) Pre-heating zone, 3) Spray chamber and 4) Thermal treatment. Table 2 shows the model exposure determinants. Dotted area illustrates the NF volume.

Table 2. Exposure determinants and their assessment methods. The parameters are probabilistic or deterministic by nature.

Exposure determinant	**Symbol, [units]**	**Assessment method**
Emission rate from coating	S, [μg s^{-1}]	Product of Q_{LEV} and measured concentration. It is assumed that particle losses via deposition on the chamber walls and escape to the room are insignificant and background particle concentrations from the room air are insignificant.
Far-Field volume	V_{FF}, [m^3]	Measured
Near-Field volume	V_{NF}, [m^3]	Assigned: A volume of ~1 m from the spray chamber covering the operator breathing zone.
Air mixing between NF and FF	β, [m^3 s^{-1}]	Measured by using NF/FF concentrations or estimated.
General ventilation	Q_{FF}, [m^3 s^{-1}]	Mechanical ventilation; Set according to the measured flow rate.
Local control efficiency	ε_{LEV}, [-]	Measured with two diffusion chargers from inside and outside of the spray chamber.
Local exhaust ventilation	Q_{LEV}, [m^3 s^{-1}]	Measured
LEV at the entrance of the coating unit	$Q_{LEV,ent}$, [m^3 s^{-1}]	Measured
LEV at the exit of the coating unit	$Q_{LEV,exit}$, [m^3 s^{-1}]	Measured

The NP emission rate to the room air (ER) is defined by the coating chamber emission control efficiency ε_{LEV} (-) as:

$$ER(t) = q_{NP}(t) \cdot (1 - \varepsilon_T) \cdot \varepsilon_{LEV} \quad (3)$$

When transfer efficiency is quantified for different process parameters (e.g. number of nozzles, nozzle pressure, substrate type) the relation can be used to predict NP emission rate from the coating chamber to the room air. LEV mass flow, $\dot{m}_{LEV}$, can be used to estimate the environmental emissions or LEV filter loading by assuming $ER \ll \dot{m}_{LEV}$.

The dispersion model performance will be tested by comparing the predicted NF and FF concentrations with measurements. The worker exposure can be calculated based on the person working practices. Parametrization describing the working practices needs to be developed in situ for different production phases having a potential impact on personal exposure.

4. Methodological approach and preliminary reference architecture for the ASINA-DT

The spraying coating line selected by ASINA for the implementation and validation of the ASINA-DT is owned by WIVA Group Company (Florence, Italy). It manufactures n-TiO_2 coated ceramic and plastic photocatalytic substrates.

The manufacturing line is a multistep process, consisting of four modules (Figure 2): 1) Plasma unit, to activate the substrate and improve the coating spreading, 2) Pre-heating, to maximize the bonding capacity between substrate and coating, 3) Gun spraying chamber, with four movable sprays guns for spraying tunable grammage on the substrate, and 4) Heating, to dry the product, equipped with eight furnaces individually controlled for an improved temperature profile regulation, with a final cooling unit.

The ISO 23247 series provides guidance on how to build up DTs for manufacturing [20]. In particular, ASINA is using ISO/DIS 23247-2 [33] as a reference for the preliminary design of DT (high-level architecture).

According to this reference, DT is structured in four domains or layers: 1) Observable manufacturing domain, 2) Data collection and device control domain, 3) DT domain, and finally 4) DT user domain. The first domain represents the physical world - the manufacturing process and its elements - which connects and synchronizes with the virtual world (third domain) through the communications layer (second domain). The fourth domain is a layer of services where the user can find information.

Table 3 specifies these four domains and provides the preliminary architecture of the ASINA-DT according to the ISO / DIS 23247-2 reference model. Besides Figure 2 shows a conceptual approach on the projected deployment of ASINA-DT in the selected industrial scenario.

Monitor airborne emission and occupational exposure, predict and alert about risk level and optimize process performance to prevent and control potential emission and exposure [through Key Performance Indicators (KPIs)], will be the key functionalities to be deployed by the future ASINA-DT.

The main challenges of the work will focus on deploying a network of sensors to capture on-line data on emissions/exposures to nano-forms, and on hybridizing the existing physical models with the data captured on-line (DDMs).

Finally note that, although the ASINA-DT will be designed for bi-directional operation (closed loop), due to limitations related to process safety (CE marking), the ASINA demonstrator will work in open loop, providing, in this first stage, only outputs for decision-making by using KPIs. Thus, automatic self-readjustment of the process - without human control - is beyond the scope of ASINA.

Table 3. Domain-based DT reference model for manufacturing according to ISO/DIS 23247-2 [33], and proposed architecture for ASINA use. case

	Domain/Layer	**Description** (ISO/DIS 23247-2)	**Proposed architecture for ASINA use case**
4	Digital Twin user domain INTERFACE	A user can be a person, a device, or a system who uses applications and services provided by Digital Twin domain.	This domain will provide the user with a series of functionalities such as: dynamic data visualization, event alerts and optimization KPIs (inputs for decision making), through a friendly and easy to use ASINA interface (e.g. a computer screen).
3	Digital Twin domain INTELLIGENCE	It is responsible for overall operation and management of Digital Twin for manufacturing, including, among other functionalities ad applications: monitoring, digital modelling, analysis, simulation, optimization managing, presentation, synchronization and interoperability.	This domain will be based on a hybrid model (physical models + DDM), and will provide functionalities for data analytics, prediction and optimization. The exposure physical model will be a tailored mass balance model, which uses a probabilistic parametrization based on measured values. The software will be hosted on an ASINA - computer screen, working in local or cloud server mode.
2	Data collection and device control domain DATA COLLECTION	It monitors and collects data from sensors in observable manufacturing domain, and control and actuate devices in observable manufacturing domain. This domain links observable manufacturing elements and digital entities for synchronization.	This domain will monitor and collect data from three main sources: 1) the machine/process data-bus (process parameters, such as e.g. temperature, pressure, fluid velocity, cycle time), 2) the network of particle sensors directly implemented by ASINA, and 3) the enterprise and manufacturing data systems. Different types of low-cost sensors and portable monitors will be explored for particle monitoring. The ASINA demonstrator will work in open loop, providing only outputs for decision-making by utilizing KPIs. Automatic self-readjustment of the process (without human control) is beyond the scope of ASINA.
1	Observable manufacturing domain PROCESS ELEMENTS	It consists of the physical manufacturing resources such as personnel, equipment, material, process, facility, environment and products. This domain is monitored and sensed for data collection and device control in Digital Twin for manufacturing.	At ASINA, this domain consists of an industrial spray coating process. In addition to the process machinery, emissions of particles to the work environment, derived occupational exposures and background levels are identified as relevant elements of the process.

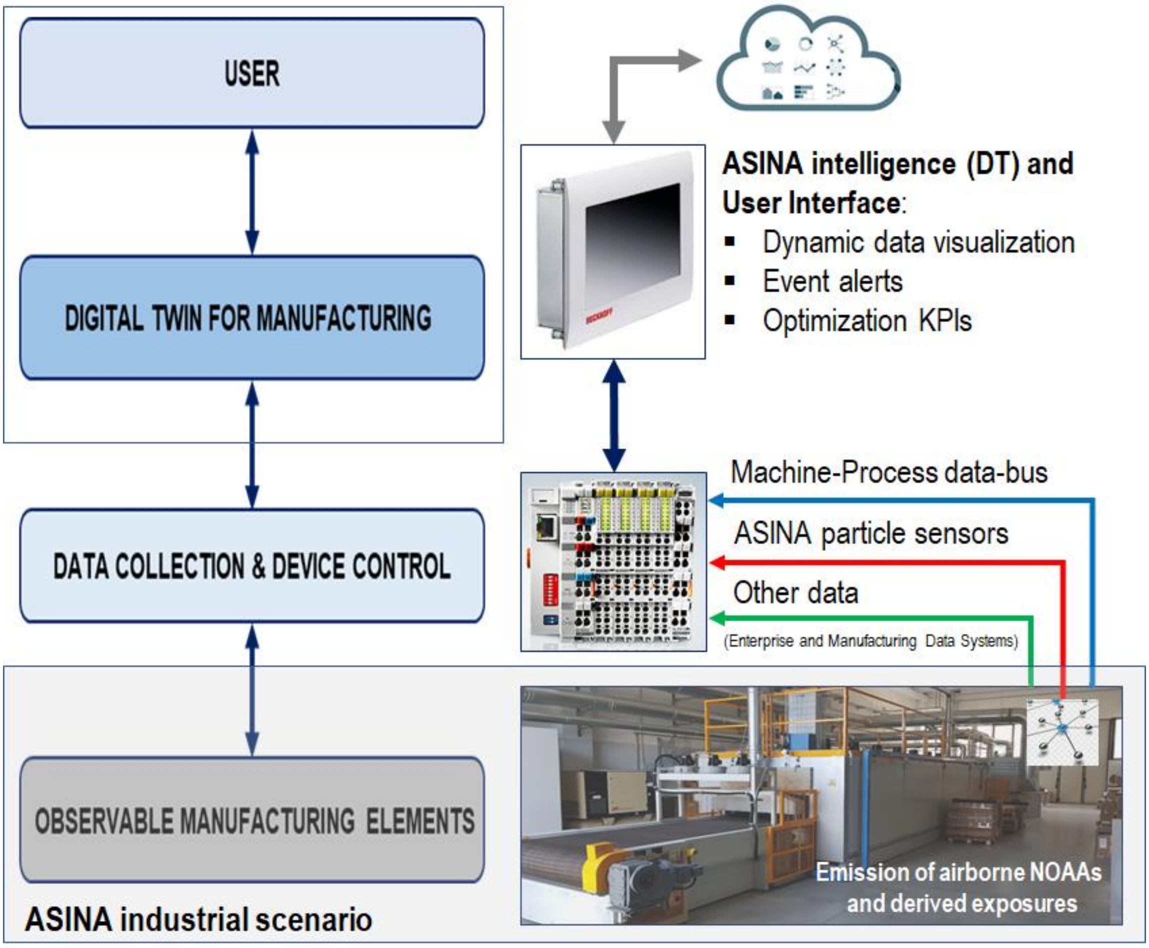

Figure 2. ASINA on premises and ASINA cloud for DT implementation in the industrial use case, conceptualized according to ISO/DIS 23247-2 high-level structure [33].

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