Digital Twin Concept for a Novel Aerosol-on-Demand Jet-Printing System

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Abstract: In this article, we present the concept and architecture of a digital twin (DT) used for the development and subsequent control and operation of a novel aerosol-on-demand (AoD) jet-printing system. Since the process of aerosol generation used in the AoD printing process has many complex interactions that can hardly be described by established theories, this paper develops an architecture that enables the digital image to learn from its physical counterpart. Conventional DT architectures only allow the use of digital twins if they can mimic their physical counterpart accurately. Our approach overcomes this limitation by enabling the digital twin to learn empirically and thereby improve its models by using a data loop.

1 INTRODUCTION

Digital twin (DT) technology is commonly described in both academia and industry as a combination of a physical entity, a virtual counterpart, and a data link between the two. In this context, the digital twin is a digital representation of a system in operation, consisting of its main characteristics, attributes and behaviors. (Stark & Damerau, 2019). Digital twins have many definitions depending on the context they are used in (Glaessgen & Stargel, 2012; Grieves, 2014; Grieves & Vickers, 2017; Rosen et al., 2015; Tao et al., 2018; Kritzinger et al., 2018; Autiosalo et al., 2020). DT is of great importance in the production context as it offers the possibility to improve production processes, adjust production processes to other, new means of production, confirm settings and find new operating points and simulate situations to predict performance (Roy et al., 2020).

The development of printed electronics is based increasingly on the functional printing of novel nanomaterials (Das & He, 2021; Suganuma, 2014; Wu, 2017; Choi et al., 2015, Magdassi & Kamyshny, 2017), as the use of inks with special chemical, physical, or optical properties enables the production of novel functional structures (Sirringhaus & Shimoda, 2003; Sieber et al., 2020; Sieber et al., 2021; Magdassi, 2010). Printed functional elements such as conductive tracks or electronic components like resistors and transistors require high quality in terms of line width, edges, and layer thickness to ensure reproducible electrical properties (Subramanian et al., 2008). One promising concept in this context is aerosol jet printing, where functional ink is atomized into a fine spray and then transformed into a stable and over several millimeters well-collimated aerosol jet through hydrodynamic focusing by a sheath gas flow (Ganz et al., 2016, Gupta et al., 2016). Due to this collimation range, the distance between the substrate and the print head can be varied without significantly changing the line width. This is also why aerosol-based printing processes, unlike inkjet printing, are suitable for printing on 2.5D and 3D components (Neotech, 2025).

Recently, the authors presented a new principle for aerosol-jet-on-demand printing, the core of which is an atomization unit integrated directly inside the printhead (Ungerer et al., 2023a). This enables a compact system design, printing operation in all spatial directions, widely tunable distance between printhead and substrate, as well as jet-on demand mode of operation (Sieber et al., 2022). This new

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method of achieving an AoD printing process exhibits many complex interactions that are difficult to describe with conventional theory. Insights into the function of atomization require physical tests on the laboratory setup. These are difficult to perform and interpret due to the complex flow conditions in the AoD printhead. Previous attempts to measure the aerosol flow field using Particle Shadow Velocimetry (PSV) have shown that the small droplet size combined with a highly complex velocity field makes the measurements inaccurate (Pöppe, 2023; Ungerer et al., 2022).
This paper aims to describe the concept and architecture for a DT of the AoD, as well as to present and discuss approaches to model reduction and shows which subsystems are necessary in the DT and how they interact.

The structure of this paper is: Section 2 presents the patented AoD jet-printhead as well as the current lab setup, acting as part of the physical layer, Section 3 deals with the models describing the functioning of the printhead as well as approaches to model reduction. In Section 4 the DT is presented. Here the concept as well as the specific architecture are shown. Section 5 closes the paper with conclusions and gives an outlook over further planned work.

2 SETUP OF THE AoD JET-PRINTING SYSTEM

2.1 The AoD Jet-Printhead

The primary feature of the novel concept of the AoD-jet printhead is the integration of the atomization process into the printhead (Ungerer et al., 2023a). This enables a compact system design, printing operation in all spatial directions, widely tunable distance between printhead and substrate, as well as jet-on demand mode of operation (Sieber et al., 2022). Fig. 1 shows a schematic of the printhead with all its main components. Aerosol generation takes place by excitation of a fluid inside a glass capillary (2) by means of a piezo actuator (3). The aerosol spray flows into the mixing chamber (1) where it is aerodynamically focused by an inflowing sheath gas and the nozzle (4). The sheath gas flows into the mixing chamber by four inlets which are arranged equidistantly around the circumference. The four inlet channels, from which only two are depicted in Figure 1, have a meandering structure (5). The deflection in the channel bends causes additional mixing so that the velocity profiles of the sheath gas are homogenised within the mixing chamber (Sieber et al., 2022).

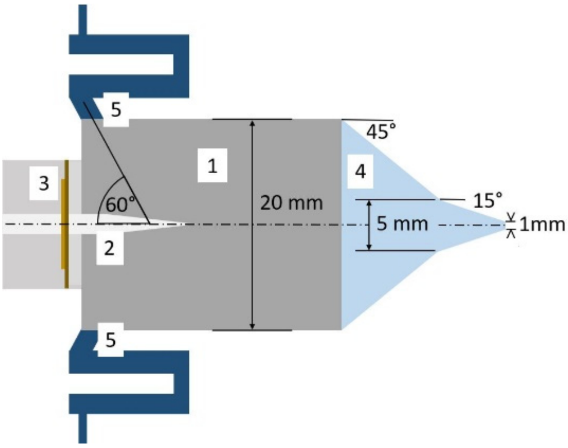

Figure 1: Schematic of the principle design of the AoD-jet print head.

2.2 Lab Setup of the AoD Jet-Printing System

The existing laboratory setup is still under development, its current implementation is shown in Figure 2. It consists of the printhead with atomization unit and nozzle, a frequency generator, an ink reservoir with pressure control and mass flow sensor, a high-power LED, and a high-speed camera. Pressure control of the ink reservoir is carried out by an Ultimus II dispenser from Nordson, while the mass flow of the ink during operation of the printhead is measured between the reservoir and the printhead by a mass flow sensor (SLG-0150, Sensirion, Switzerland). The printhead is connected to a frequency generator (SDG2000X, Siglent Technologies CO) to provide the required frequency for atomization. The piezo actuator is directly connected to the capillary. Focusing of the aerosol spray is done by interaction of the inner contour of the nozzle and the mass flow of the sheath gas. The flow rate of the sheath gas is controlled by the mass flow controller (red-y smart controller GSC, Vögtlin). To monitor the quality of the aerosol jet and the droplet distribution, the setup includes a high-speed camera (EoSens 3CXP Mikrotron, SVS-Vistek GmbH) and a light microscope (VHX-7020, Keyence). This allows the monitoring and control of the printing process exclusively by optical methods to ensure the desired quality is achieved.

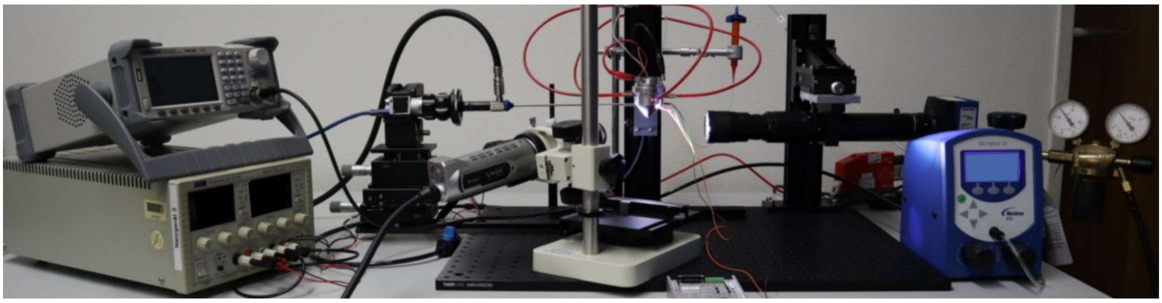

Figure 2: Laboratory setup of the AoD testbed.

3 MODELLING

In order to develop and design the patented concept of the AoD printhead, a CFD model of the printhead is implemented and used for design optimization of the printhead with respect to its manufacturability in our in-house workshop (Ungerer et al., 2023b). Simulation results not only lead to the design but also gives preliminary operation parameters. Ansys Fluent in its versions R19.3, R20.1, and 2024 R2 is used for fluid dynamic calculations. When modelling the ink, the Euler-Lagrange model is used, which includes a particle-based approach to the discrete phase (Sieber et al., 2022).

The generated aerosol is modelled in Fluent using a cone model, which means that the generated aerosol is described by its origin, the cone axis, the cone angle, the radius, the diameter of the droplets, the diameter distribution, the exit velocity of the droplets and the aerosol mass flow rate (Ungerer et al., 2023c). The mesh used for the CFD calculations was optimised using a mesh independence study resulting in $2.1 \cdot 10^6$ elements (Ungerer et al., 2023c). Since the Euler-Lagrange model used is a particle-based consideration of the discrete phase, it must be ensured that a particle can, in principle, be completely contained within a mesh element. To increase the resolution in the atomization zone, i.e., in the area between the capillary and the nozzle outlet, while maintaining this condition with a droplet diameter of approximately 20 µm, an element size of 33 µm is used (see Fig. 3) (Ungerer et al., 2024)

Due to the complexity of the model, the CFD simulations require many hours to a few days for calculation (the CFD simulations are carried out on a workstation equipped with AMD Ryzen Threadripper 3970X processor with 32 cores, 64 threads @ 3.7 GHz, 128 GB RAM, and an Nvidia Titan RTX graphics processor with 24 GB). One goal of the DT is to provide the user with recommendations for optimal settings. This must be done based on simulations. For this reason, a computationally efficient model is required that can represent all relevant aspects of the underlying CFD model. Since the DT regularly updates its CFD models when new data becomes available over the course of the printer's lifecycle the algorithm must also be able to autonomously reduce the models every time they are updated. For this purpose, various approaches to model reduction are investigated, namely polynomial regression (Pfannenstiel et al., 2024a) and the Gaussian method (Pfannenstiel et al., 2024b), with the aim of autonomously determining properties of the aerosol jet solely through its initial injection parameters. The goal of this ongoing work is to autonomously create a reduced model that comes as close as possible to the computationally intensive CFD simulation and can be used inline by the DT.

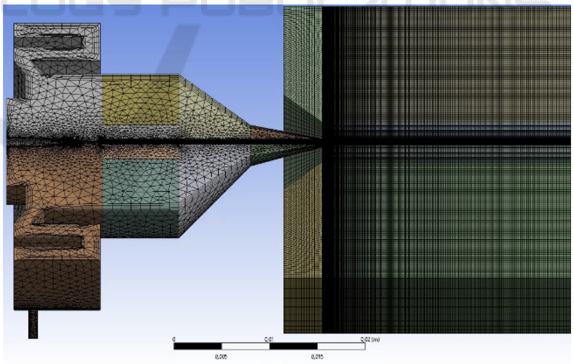

Figure 3: Meshed geometry model of the printhead and a free space area (Ungerer et al., 2023c).

4 DIGITAL TWIN

4.1 Digital Twin Concept

Essential for putting the newly developed concept of the aerosol printhead into operation is the determination of the control parameters and an

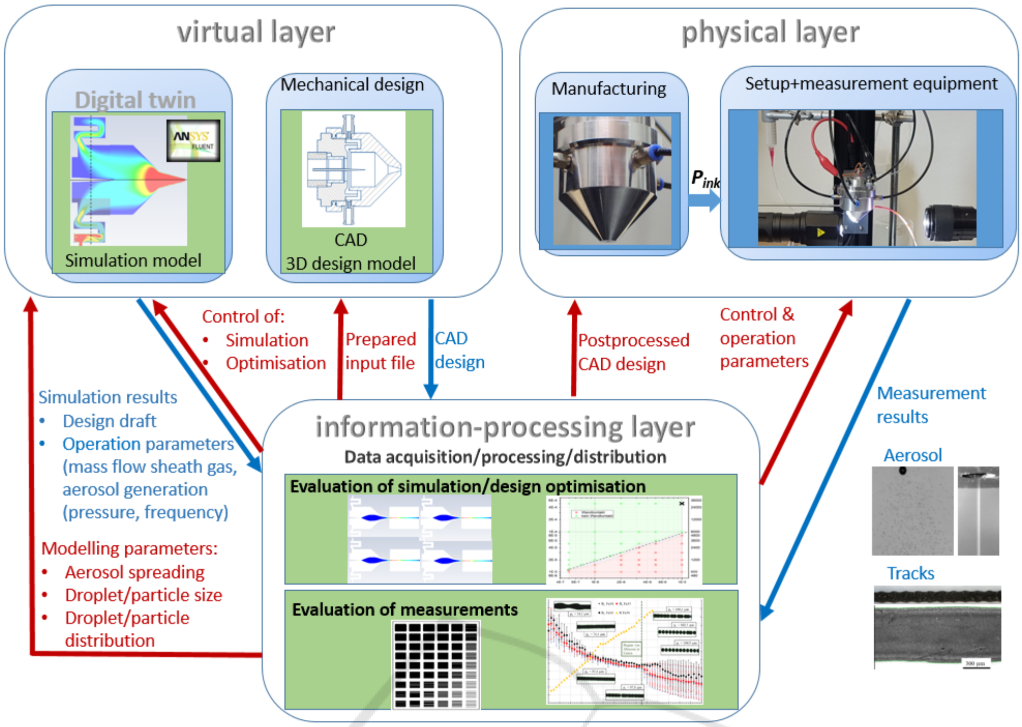

Figure 4: Three-layer concept of the Digital Twin.

adapted chamber design for a proper function. A problem herein is the contamination of the inner walls of the manufactured printhead with ink due to non-optimal control parameters or non-optimal geometry of the chamber design of the printhead, both leading to wall contact of the ink spray (Sieber et al., 2022). Such contaminations would lead to difficult and time-consuming cleaning processes on the real component. Determination of ink-specific operation parameters as well as an adaptation of the chamber design to specific ink formulations is one task of our digital twin concept, which is based on a three-layer design. The virtual layer (VL) is linked to the physical layer (PL) by an information-processing layer (IPL) (see Fig. 1). The bidirectional mapping and interoperability of the physical and the virtual space are realized through data interaction (Zheng et al., 2019).

The VL consists of a simulation model of the printhead, which is implemented using computational fluid dynamic (CFD) and a 3D CAD (computer-aided design)-model. The manufacturing of the printhead as well as the laboratory setup and the measurement equipment is located in the PL. Mapping of virtual and physical layer is conducted by the IPL by means of data analysis, derivation of control parameters for the digital and the physical twin, as well as a quality control. Input of the VL to the IPL are the ink-specific simulation results like e.g. operation parameters, design parameters, and control parameters. Analysis and evaluation of the simulation results take place in the IPL with respect to the defined criteria, like, e.g. non-wetting condition of the inner walls of the printhead, avoidance of turbulences by limiting the Reynolds number to below 1200 (which is controlled by the mass flow of the sheath gas used for aerodynamical focusing), a stable, focused and collimated aerosol jet, and design rules of the manufacturing processes used. Based on the analysis and evaluation results design optimization is controlled. Once the optimized design together with the respective control and operation parameters are achieved, a preprocessed file of the initial design-for-manufacture of an aerosol-on-demand printhead, designed for one specific ink formulation is generated as input to the CAD tool in the VL. Here the final CAD 3D model is constructed, send to the IPL where postprocessing is conducted. The postprocessed file is digital input to the part manufacture in the PL. Up to this transfer, the printhead is entirely described digitally. After the manufacturing process, a real part of the ink specific printhead P_{ink} exists. The manufactured printhead is installed in a laboratory and measurement setup and set into operation with the (in the IPL derived) control and operation parameters. In-operation measurements were carried out with respect to aerosol generation and by inspection of the printed tracks. The resulting data of the measurement again are digital descriptions and input into the IPL. Measurement data are used in two ways:

1. To control the quality of the printed structures (and, hence, validate the simulation model).
2. To derive model parameters of the discrete phase.

The line morphology of the printed lines is examined using image processing methods. With the help of the line width, line density, smoothness of the edges and overspray, statements are made about the quality of the printed lines. Based on the measurement results, a model validation is conducted in the VL in two respects: On the one side the inspection of the printed track is used for quality control and to validate the operation parameter, on the other side, the measurement data of the aerosol spray are used to enhance the model of the discrete phase. This validation step qualifies the CFD model of the aerosol-on-demand printhead for use as a digital twin.

4.2 Digital Twin Architecture

Based on this concept of a digital twin, an architecture for a comprehensive DT is being developed, which clearly defines and structures the individual subsystems and their interactions. This also takes into account the manufacturing tolerances of the individual physical components of the AoD-jet printing system, as well as the autonomously running model reduction, which avoids time-consuming CFD simulations by generating simpler models that estimate the initial printing control parameters from input parameter sets of the CFD models (Ungerer et al. 2024; Pfannenstiel et al., 2024a; Pfannenstiel at al., 2024b).

The architecture of the digital twin proposed in this paper consists of two types of digital twins as a kind of subsystems, following a definition by Grieves (Grieves, 2023). These are the digital twin prototype and the digital twin instance. We apply this concept both to the components that make up the real AoD setup or are used in the printing process and to the printing process itself.

Our new principle of the AoD printing process features many complex interactions that are hardly describable by established theory. Physical tests necessary to gain an understanding of the atomization process have shown to be difficult to perform on the AoD printhead (Pfannenstiel at al., 2024b).

The comprehensive DT architecture is also based on a three-layer architecture consisting of a Physical Layer (PL), a Virtual Layer (VL) and an Information Processing Layer (IPL) (see Fig. 4) and embeds definitions of Grieves who has established the use of DTs in the Product Lifecycle Quality (PLQ) loop where DTs can be used to replace physical tests (Grieves, 2023). Grieves introduces the Digital Twin Prototype (DTP), which contains all information necessary to produce a product. Before a physical product is manufactured, tests can be done on this virtual, idealized version of the product and the Digital Twin Instance (DTI): When a product is manufactured, a DTI is created which is tied to that specific product. The DTI features all the tolerances like e.g. imperfections and differences from the real component to the DTP. It also stores information about the operation of the product it is tied to.

The Physical Layer of our DT architecture contains the printer setup and the user and is connected to the Data Storing Layer. The basic features of the VL are the Part DTP and the Print DTP. In the Part DTP the information of the components of which the AoD printing system consists are stored (e.g. as CAD together with its fabrication requirements, or specific inks defined by there parameters like e.g. viscosity, particle load) and follows very much the definition of Grieves. This looks different with respect to the Print DTP. Because of the high flexibility of digital additive processes, there does not exists one ideal product. Printing results will be dependent on ink parameters, from the interaction of the ink and the substrate and so on. Hence in our architecture, the Print DTP is defined as the ideal model of the manufacturing process. Here all the models describing the AoD printing process are saved. These models include detailed settings for the CFD simulation, a model that describes the atomization as well as the recommendation algorithm.

Combination of this set of initial conditions simulate the specific process and its result. Since the proposed architecture allows for model improvement, the version of the respective model needs to be tracked also. Instantiation of Part and Print DTP takes place by the Part DTI and the Print DTI, respectively. The instances of the parts of the AoD-jet printing system consist of tolerances of the real manufactured part used in the AoD-system and uses the data from the corresponding Part DTP as basis. The result of this DTI is a representation of the real component as detailed as possible. The Print DTI is tied to a specific printed structure and the respective printing process. A Print DTI is created when the user initiates a

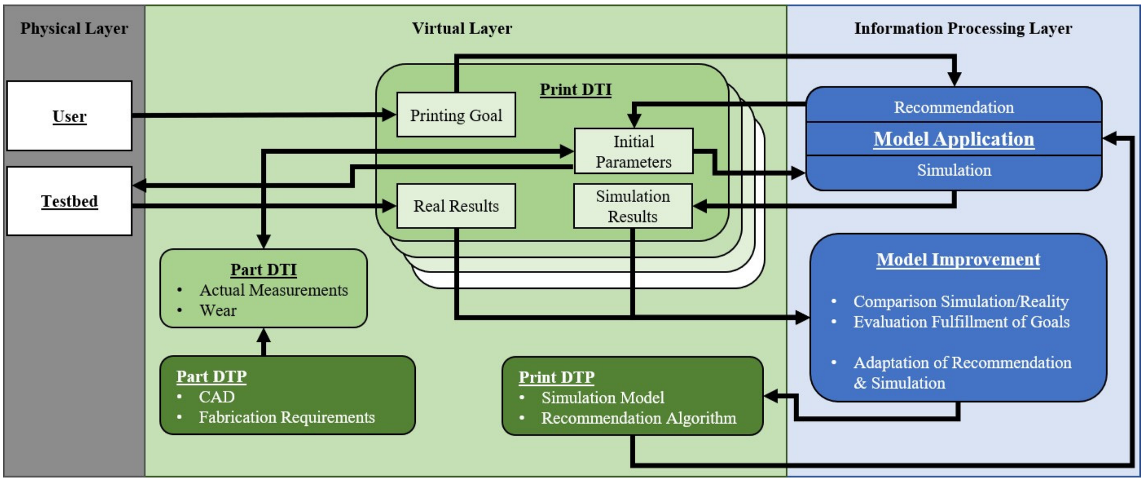

Figure 5: DT architecture to support the AoD printing process including the necessary structure to enable automated improvement (Pfannenstiel et al. 2024b).

printing process by defining the printing goals which are saved as a dataset in the Print DTI. The printing goal then is input into the recommendation algorithm (in the IPL) which deduces on basis of simulations the set of initial parameters. The initial parameters also take deviations of real parts used in the AoD-system resulting from the manufacturing process into account, depicted by the link from the Part DTI in Figure 5, and are input into the AoD-systems control. A simulation on basis of these initial parameter set is carried out which enables a model improvement by a comparison of the simulation results with the printing results. This does not need to happen simultaneously to the physical printing process and can be done when there is computational power available. If the simulation is found to be not accurate enough, an automated method can change model settings in the simulation in certain capacities (Pfannenstiel et al., 2024a). Since initial conditions and results are all saved in a DTI, the simulation can calculate the same case with different model settings and determine which model settings better describe reality. Based on the best simulation model, a model reduction is automatically initiated, on the basis of which a line prediction and control is created. The same approach is used for improving the recommendation algorithm.

5 CONCLUSIONS AND OUTLOOK

In this article, we present a digital twin architecture that uses the DTP and DTI proposed by Grieves as subsystems. We apply this structure both to the components that make up the printing process and to the actual product, the printed structure. Since in the case of highly flexible, digital, additive manufacturing technologies, there is no definition of a SINGLE product, but the printed structure/component depends on a variety of different influencing factors, we use an ideal model here. This model is constantly validated and improved through the implementation of a data loop during the lifetime of the DT. This approach enables the application of this DT architecture to our newly developed AoD-jet printing system, as the actual atomization process is not yet fully understood and therefore cannot be modelled. However, by continuously comparing the printing result with its simulation prediction, a continuous model improvement is made, which increasingly approximates the description of the actual effects.

The possibilities offered by the proposed DT architecture include real-time capability, use in design optimization, and autonomy. To achieve real-time capability for in-line control of the printing process, a transition from computationally intensive CFD models to less computationally demanding models is necessary. The basis of in-line control is that sensor signals are read during the printing process and input into the simplified model, thus adjusting the control variables of the printer during the printing process. Investigations regarding suitable model reduction have already been conducted using regression fitting and the Gaussian process. Future investigations into model reduction will address approaches that proceed more specifically in data collection, such as Bayesian optimization.

Once the models are sufficiently trained through the DT process to provide a detailed description of the AoD printing process for a variety of different applications, the design can be iterated using the DT. This means that design optimization of individual components can be carried out in the virtual layer, and validation can be performed using digital testing. Through the interface to the physical layer, the manufacturing of the optimized component can then be carried out.

In principle, the presented DT architecture also provides autonomous control of the AoD-jet printing process. This requires targeted further development of the AoD-jet printing system. In this case, user interaction would be limited to specifying the printing goal, and the DT would autonomously send the recommended settings to the printing system and carry out the printing.

Additionally, further investigations are being conducted into the model representation of the atomization process to allow for detailed phenomenological modelling.

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