EMERGE
Emerging Printed Electronics Research Infrastructure

D5.5 1st Interim report on modelling and simulation of processes, devices and systems FLAPEP connected

WP5 – TA1: Access to design, modelling and simulation

The EMERGE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement Nº 101008701

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List of abbreviations

3D – Three-dimensional
EU – European Union
FLAPEP – Flexible large-area printed electronics and photonics
FZJ – Forschungszentrum Jülich
JOR – Joanneum Research
RISE – Research Institutes of Sweden AB
SME – Small-medium enterprise
TA – Transnational access activity
WUT – Warsaw University of Technology

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1. Executive Summary

Deliverable **D5.5 "1st Interim report on modelling and simulation of processes, devices and systems FLAPEP connected" (M24)** provides an overview of the incoming projects that required modelling and simulation activities offered by the EMERGE consortium. The different tools proposed by the WP5 partners are listed and briefly described in previous deliverables **D5.1 (M6)** and **D5.2 (M15)**.

2. Overview of user-projects on modeling and simulation

During the reporting period, from July 2022 to June 2023, a total of four open calls were organized, resulting in an impressive submission of 63 projects. The collaborative efforts of 11 European partners have brought together a vibrant community of 88 participants from 26 nationalities. This multicultural and multidisciplinary approach has fueled invaluable knowledge exchange and fostered a dynamic environment within the EMERGE project.

The strong interest and involvement of research institutions in the European Union (EU) is evident, with 43 projects submitted by participants working in institutes located in EU countries. Equally remarkable is the fruitful contribution of 20 projects from industry, start-ups, and small-medium enterprises (SMEs), ensuring that the projects developed under EMERGE are both relevant and applicable in real-world contexts.

Although EMERGE has been receiving increased interest from external users as successive calls are open, only four proposals requested access to modelling and simulation activities. As identified in **Table 1**, three of these user-projects were submitted during the 2nd open call and have been successfully completed, whereas the fourth one has been submitted during the fourth call and is still under revision.

The evaluation of transnational access activity TA1 projects have shown to be the most challenging to evaluate, taking more than 90 days to collect reviewer's feedback. A possible reason for this lies in the level of specificity of the topics covered in the TA1 projects, which leads to successive refusals of evaluation by the reviewers. The turnaround time for proposal evaluation is expected to decrease with the reinforcement of the evaluation panel experts in TA1. A simplified "evaluation form" template, specific for TA1 projects, may also be prepared to address this issue.

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Table 1- Projects requesting access to modelling and simulation tools.

Projects	User's gender/ nationality	Institute	Selected installations	Selected institution	Installations used
2nd Call – 3829: Uniformity in visual appearance of individual cells in laminated OPV devices	Male/ Austria	SME, Sweden	TA1: Modelling & simulation TA4: Device metrology & characterization	Joanneum Research (JOR)	Completed
2nd Call – 3832: High-throughout exploration of amorphous multicomponent phase diagram space for the accelerated design of organic thin films	Female/ Poland	University, United States	TA1: Modelling & simulation	Forschungszentrum Jülich (FZJ)	Completed
2nd Call – 3833: High-throughout exploration of crystaline phase diagram space for the accelerated design of organic thin films	Female/ Poland	University, United States	TA1: Modelling & simulation	FZJ	Completed
4th Call – 4749: Patient-specific numerical modelling in palliative solutions for infants with ductal-dependent pulmonary blood flow	Female/ Albania Male/ Syria	University, Turkey	TA1: Modelling & simulation TA3: Functional 2D & 3D printing	Warsaw University of Technology (WUT) or Research Institutes of Sweden AB (RISE)	Under evaluation

The following section offers a comprehensive analysis of the project proposals concerning modelling and simulation.

2.1. Analysis of the stakeholder's engagement

During the course of the four open calls, a total of four projects were submitted to the EMERGE program. The current number of TA1-related projects is not enough to identify a clear trend in the stakeholders interested in modelling and simulation tools. More projects are needed to gain a comprehensive understanding of their diverse needs and interests

In detail, these projects involved the participation of four individuals (50% female), with one participant, affiliated with an academic institution in the United States, contributing to two

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related projects (projects 3832 and 3833). The remaining two projects were submitted by participants from European institutions, whereas one is from a SME. This not only reflects the active involvement and valuable contributions from the European research community but also showcases the program's commitment to fostering collaboration between academia and industry.

2.2. Description of the publicity

As reported in deliverables **D2.4 (M4)** and **D3.1 (M12)**, a communication and dissemination strategy was designed and implemented to publicize all activities involving EMERGE participation. To achieve this, EMERGE utilizes various means of propaganda to effectively promote EMERGE project and engage with a broader audience and build a wide user community network with expertise on flexible large-area printed electronics and photonics (FLAPEP) materials and technologies. This includes active participation in public events, such as conferences, scientific and technological fairs, and workshops, providing valuable opportunities for EMERGE members to directly engage with potential users and establish collaborations. To expand its reach, EMERGE leverages proper online platforms, including the official website, LinkedIn, and online platforms of the EMERGE institutions. Besides, EMERGE partners also explore their internal networks to establish direct contact with potential users of EMERGE infrastructure to encourage the submission of proposals and facilitate collaboration within the project.

Regarding the participants of the projects related to simulation and modelling activities, some projects were proposed after discussions with involved EMERGE partners, while others resulted from direct contacts or conference advertising.

Throughout the EMERGE project, efforts will be carried out to advertise the offer of EMERGE institutions, also aiming to boost engagement of participants working in TA1 activities and increase the number of proposals submitted for virtual access to these facilities.

2.3. Requirements of the submitted projects

In two of the projects (projects 3832 and 3833), the primary focus was on the modelling and simulation activity, while the other two projects combined this installation with experimental activities. In detail, the following modelling/simulation methods have been requested:

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- Project 3829: The in-house optical modelling of optical components offered by JOR;
- Projects 3832 and 3833: The in-house simulation code PFSim-Prost (FZJ) focusing on simulations of process-structure relationships in solution-processed electronics;
- Project 4749: Computational Fluid Dynamics simulations offered by WUT. Note that this project also requests as side activity Computer-Aided Design design for three-dimensional (3D) printing offered by RISE, which corresponds to activity.

Regarding the prefered EMERGE institution selected to develop the project activities, two-related projects were submitted to FZJ (projects 3832 and 3833), one to JOR (proposal 3829), and one was applied to WUT and RISE as prefered insitiutions (proposal 4749). Regarding this last project, which is currently under evaluation, the chosen institutes have no participation in modelling and simulation, and thus they cannot be chosen to carry out the research activities for this specific installation. If the project receives positive feedback from the external viewer, the technical liaison offices will need to allocate the project to a more suitable EMERGE institution (FZJ, UNOVA, JOR) to collaborate in this project or installation.

2.4. Overview of completed projects

In this section, additional details on the concluded user-projects are provided below, including main objectives, relevant results and expected/ achieved outcomes:

Project 3829: Uniformity in visual appearance of individual cells in laminated OPV device (JOR)

- Objectives: In this project, an approach should be developed to use extrinsic measures to reduce the visual differences between cells in an organic solar cell and inhomogeneities on the active area by means of diffusive surfaces and patterns, exploiting also optical effects on a microscopic level but keeping the output power as high as possible. Subsequently, the approach should be validated both theoretically and experimentally. Only approaches that can potentially be scaled up to a cost-effective roll-to-roll production will be considered.
- Results: The main achievements of the theoretical and experimental work were the knowledge that it is possible to change the reflection spectrum of the LEH module by

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inserting a colored foil between the cells and the backsheet. This gives the possibility to change the visual appearance of the LEH modules without losing efficiency. In addition, it is possible to reduce the angle-dependent inhomogeneities with a colored front foil that has high transmission values. This leads to less efficiency losses when using such a front foil.

- Potential use after the project: improvement of the company's products.

Project 3832: High-throughout exploration of amorphous multicomponent phase diagram space for the accelerated design of organic thin films (FZJ)

- Objectives: To generate the library of phase diagrams that will become the input to machine learning pipeline to (i) illustrate the alternate approach for screening of materials based on the phase diagram characteristics and (ii) to facilitate the discovery of the design rules of material selection for organic thin films, including flexible electronics.
- Results: We generated three libraries with 245 ternary phase diagrams each for amorphous blends consisting of three compounds: polymer, small molecule, and solvent. We screened three configurations: (i) polymer-small molecule-solvent, (ii) small molecule-small molecule-solvent and (iii) small molecule-solvent-solvent. We defined and sampled the design space of interaction parameters to provide the data for the clustering. Data has been generated by group of Oliver Ronsin and Jens Harting from FZJ, and subsequently analyzed by us. As a result, we derived the initial design rules for the amorphous ternary materials systems.
- Potential use after the project: Design rules for the organic blends – this data most likely will lead to the publication.

Project 3833: High-throughout exploration of crystalline phase diagram space for the accelerated design of organic thin films (FZJ)

- Objectives: To generate the library of phase diagrams that will become the input to machine learning pipeline to (i) illustrate the alternate approach for screening of materials based on the phase diagram characteristics and (ii) to facilitate the discovery of the design rules of material selection for organic thin films, including flexible electronics.

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- Results: We generated six libraries with 405 temperature-dependent phase diagrams each for crystalline binary blends. We screened three configurations: (i) polymer-solvent, (ii) polymer-small molecule and (iii) small molecule-solvent. For each configuration two cases were considered, where either the first or the second component crystallizes, while the other is amorhous. In each dataset, we screened five-dimensional input space with the following material properties varied in the range with three sampling levels: interaction parameter between components, the heat of fusion of each component, the melting temperature of each component. Data has been generated by group of Oliver Ronsin and Jens Harting from FZJ, and subsequently analyzed by us. Now we work on learning the design rules for the binary crystalline-amorphous materials systems.
- Potential use after the project: Design rules for the organic blends – this data most likely will lead to the publication.

2.5. Potential difficulties of experiments

For all three projects, the work realized (type of activity accomplished and the resources used) was in-line with expectations. The success rate was evaluated to be 100% without particular difficulties reported. The only exception is for one of the three sub-tasks of project 3829, for which the expected results could be reached to only 75% due to lack of time and technical difficulties.

2.6. User feedbacks

The feedback on how the projects were carried out is excellent, with the participants expressing their intention to recommend access to EMERGE infrastructures to their colleagues. The particiapants are considering follow-up projects, which is a clear indication of their very positive experience. It is worth noting that the participants feel that the project duration offered by the EMERGE consortium could be increased.

Regarding the general EMERGE workflow for project submission, operation, and finalization, as well as the EMERGE tools, such as website and guidelines, the feedback is marked systematically as “excellent” However, there are areas that have received "satisfactory" ratings, indicating room for improvement. These areas include enhancing logistic support at the host institution to facilitate research activities, improving the EMERGE

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website and guidelines to meet all users' needs effectively, and addressing occasional delays in the review process to streamline project evaluation and approval. Addressing these points will lead to a more satisfactory experience for all participants.

3. Final remarks

During the reporting period of this deliverable, a small number of projects (only four) requesting modelling and simulation activities have been submitted, with three already concluded and one currently under evaluation. The low number of project was to be expected in the ramp-up phase of EMERGE, howevere it is particularly low for modelling activities. This risk had also been identified, notably because the scientific community in the FLAPEP field is focused on experimental work. To address this issue, the report suggests active publicity efforts, relaxation of project duration limitations, and the promotion of coupled theoretical-experimental approaches. Most of the TA1 projects that could be implemented would require several weeks of work to meet the scientific objectives. Implementing these recommendations will enhance the attractiveness of EMERGE for potential project owners and foster further engagement in modelling and simulation activities.

Overall, the feedback from the completed projects has been positive, with the results aligning with the expectations. The participants are considering follow-up projects, and a significant impact of the results in terms of product or publication is foreseen. Additionally, the EMERGE workflow has received positive feedback, contributing to an overall excellent user experience.

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