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News

Fundamental Research

As energy challenges intensify, numerical modeling and artificial intelligence are becoming essential tools for understanding complex phenomena and designing new systems. This special issue features six scientific briefs that draw on the expertise of researchers from the “Digital Science and Technology” Division, who are developing innovative tools and methods to address the strategic and environmental challenges of the future, working on various scales and using complementary approaches.

The first article concerns numerical models dedicated to air quality, examining phenomena ranging

from the micro-urban level to the regional scale to identify factors that influence air quality and guide local and strategic decision-making. Next under the spotlight is the issue of geological CO_2 storage: simulations, safety concerns, and technical prospects help shed light on the conditions necessary for reliable and responsible deployment. Wind turbine control at IFPEN exemplifies the combination of physics-based control and machine learning, with a focus on reinforcement learning, which promises to optimize wind farm production and sustainability. More broadly, artificial intelligence is being incorporated into closure models for multiscale computational fluid mechanics, providing solutions to reduce approximations and improve the precision of predictions. Electromobility is examined from the perspective of optimal design methodology for charging infrastructure, taking into account optimization, usage, and regional constraints. Finally, generative AI methods for the design of catalytic microstructures demonstrate how the algorithm accelerates the discovery of high-performance materials.
There is a common theme running through all these briefs: the integration of physical models, data, and algorithms to address complex societal challenges. They illustrate how IFPEN researchers, working closely with industry partners and decision-makers, are harnessing digital science and technology to support the energy and ecological transition by deploying innovative solutions.

We hope that you enjoy this issue.

Mongi Ben Gaid, Giovanni De Nunzio, Thibault Faney, Jean-Marc Gratien, Stéphane Jay, Jean-François Lecomte, Jordan Rudloff, Antonio Sciarretta, Delphine Sinoquet, Quang Huy Tran,
The scientific advisor group of the "Digital Sciences and Technologies" Division

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LES BRÈVES

Air pollution remains a major public health issue, particularly in large metropolitan areas, despite the gradual renewal of the vehicle fleet and the development of active mobility solutions, thanks to dedicated urban infrastructure. New European limit values for pollutant concentrations in the air, more closely aligned with WHO recommendations[1], will take effect in 2030. Local authorities therefore need tools capable of assessing pollution levels and sources in order to support pollution reduction scenarios.

Such tools do exist, but they struggle to capture the high variability of pollution at a local level (at the scale of individual streets, for example). The fact is that emissions vary not only with traffic but also with rapidly changing weather conditions. Buildings also alter airflow locally. Therefore, while monitoring stations are essential, they alone cannot capture this variability across an entire metropolitan area.

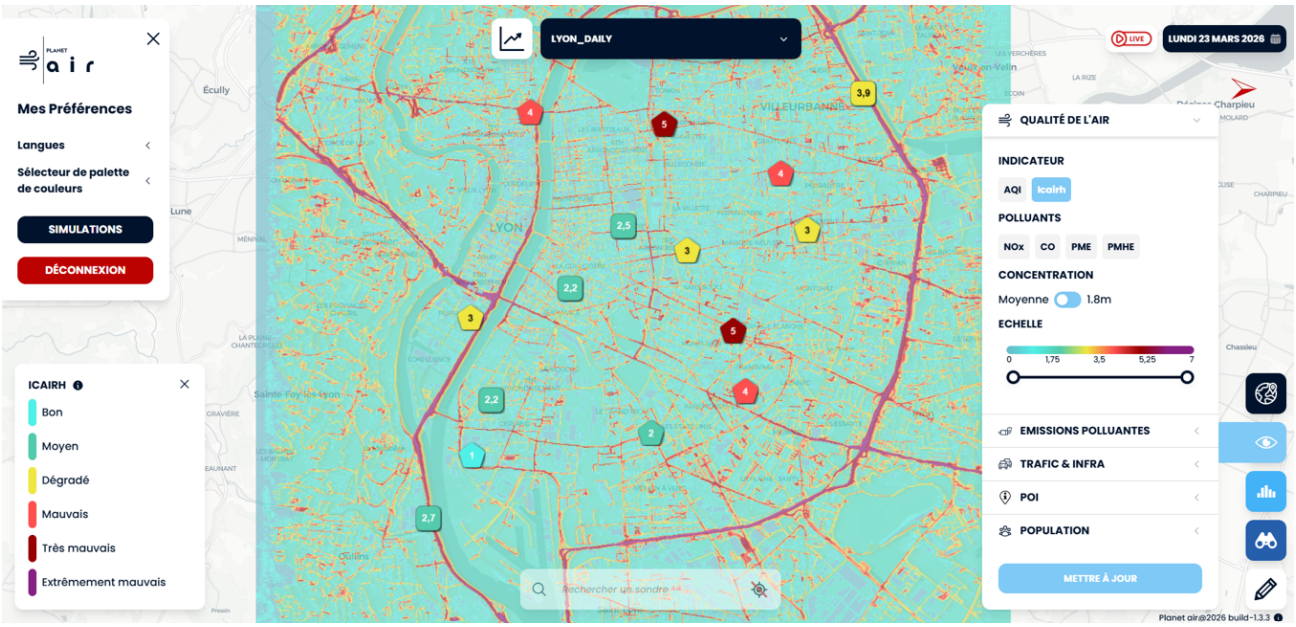

Figure 1: Street-level representation of the air quality index in the Lyon metropolitan area: simulated concentrations using virtual sensors (represented by pentagons) generated by the PLANET'AIR platform and values provided by monitoring stations located throughout the area (represented by squares).

IFPEN has developed a comprehensive methodology that integrates modeling of atmospheric pollutant dispersion with real-world data, including meteorological measurements, road traffic emissions, and urban morphology. The model's results were then compared with observational air quality data. The resulting tool is deployed via a SaaS platform: PLANET'AIR [1]. This tool generates high-resolution hourly maps of air pollution and allows users to determine concentrations at any location using "virtual sensors," while also enabling comparisons betweenvarious mobility or land-use scenarios.

This approach was thoroughly evaluated in the Lyon metropolitan area (figure 1), with validation against data from various monitoring stations, over several days and covering a range of weather and traffic conditions. The results confirm the benefits of this approach, which allows for precise estimates

of population exposure levels, underlining the importance of taking into account:
- emissions data with high spatial and temporal resolution [2];
- local weather conditions;
- the geometric complexity of buildings, which can either channel or obstruct airflow.

PLANET'AIR paves the way for a more precise assessment of population exposure. By helping to identify the factors that influence air quality, the platform provides local stakeholders with quantitative data to prioritize their prevention and mitigation efforts.

These developments have been supported by several publicly funded collaborative projects:
OLGA — Horizon 2020 Program / European Green Deal
MAGPIE — Horizon 2020 Program / European Green Deal
SPARC — ADEME – ADEIP
RTAMS — ANR – PREMAT
AMELIA — DIAT / Caisse des Dépôts et Consignations (CDC)

[1] European air quality directive UE2024/2881

References:

[2] Sabiron, G., Jay, S., Agelas, L., Speirs, E., Feng, G., and Bussod, S., "***From Road Traffic to Virtual Air Quality Sensors: PLANET'AIR - An Integrated Mesoscopic Modelling Framework***", in Proceedings of TAP 2025 (Transport and Air Pollution), 2025.

[2] Bussod S., and Sabiron G., ***"Deep learning-based method for an assessment of road traffic pollutant estimation from predicted driving behaviors»***, IEEE International Conference on Machine Learning and Applications (ICMLA), Miami, FL, USA, 2024, pp. 658-663,
>> DOI : https://doi.org/10.1109/ICMLA61862.2024.00095

Scientific contact: Guillaume Sabiron

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Air quality around the street corner: the contribution of numerical models

The SPE11 benchmark study, conducted under the auspices of the Society of Petroleum Engineers (SPE), brought together teams of researchers from universities, research organizations, and companies specializing in geological CO? storage [1]. The purpose of the project was to compare the performance of numerical simulators designed for this particular application. Based on test cases with common input data and evaluation criteria, the study analyzed the ability of calculation codes to reproduce the main physical processes at play in the injection and migration of CO? in geological reservoirs. The primary goal of the initiative was to build confidence in the simulators used to design and evaluate storage projects by assessing the discrepancies between the results obtained.

For the codes included in the benchmark, the main challenges lie as much in the physics, with the simulation of multiphase flows in highly heterogeneous media and the coupling of multiple phenomena (capillarity, gravity, CO? dissolution, etc.), as in the numerical field, with challenges related to the stability of computational schemes, the convergence of solvers, and the representation of phase interfaces.

Figure 1 shows, firstly, the heterogeneities of the reservoir under study as well as the locations of the two CO? injection wells and, secondly, the final distribution of CO? dissolved in water, revealing the presence of gravity-induced finger-like structures associated with the transfer of CO? into the aqueous phase.

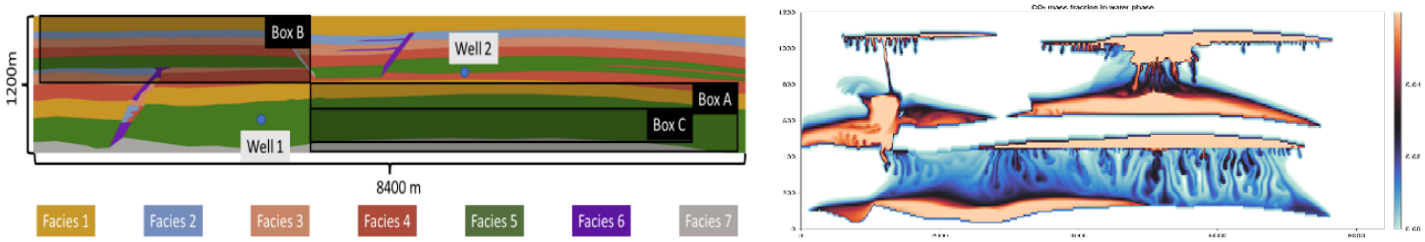

Figure 1: Distribution of lithological facies in the reservoir and locations of injection wells Well1 and Well2 (left), final distribution of CO_2 dissolved in water as calculated by the IFPEN simulator: Geoxim (right)

A total of 45 research groups from academia and industry signed up to the initiative. The simulators were compared on the basis of both their physical results (mass of CO2 in the reservoir, amount of CO2 dissolved in water, temperatures, etc.) and their numerical performance (time step sizes, cumulative number of iterations of the nonlinear solver and the linear solver). Of these teams, only 18 - including IFPEN with the Geoxim simulator - ultimately contributed results to the comparative study [2]. IFPEN thus distinguished itself by presenting results that were cited on several occasions as benchmarks, notably as median results for one of the three cases studied.

This benchmark made it possible to evaluate Geoxim's performance, both in terms of the quality of the solutions obtained and in terms of numerical efficiency, for both linear and nonlinear solvers. Now widely adopted by the scientific community, the SPE11 benchmark serves as a standard tool for validating our code developments. It allows us to evaluate the robustness and precision of our new numerical schemes [3], as well as the quality of our meshing algorithms and modeling choices [4].

References:

[1] Nordbotten, J. M., et al. (2024). ***The 11th Society of Petroleum Engineers Comparative Solution Project: Problem Definition***. SPE Journal, 29(5), 2507–2524.
>> DOI : https://doi.org/10.2118/218015-PA

[2] Nordbotten, J. M., et al. (2025). ***Benchmarking CO? Storage Simulations: Results from the 11th Society of Petroleum Engineers Comparative Solution Project.*** International Journal of Greenhouse Gas Control, 148, 104519.
>> DOI : https://doi.org/10.1016/j.ijggc.2025.104519

[3] ***Application of Convergent Finite-Volume Methods on Polyhedral Grids for CO_2 Injection Simulation in Deep Saline Aquifers***, L. Astart, S. de Chaisemartin, C. Delage, G. Enchéry, I. Faille; IFPEN. ECMOR 2026, 8-11 September 2026, Porto, Portugal.

[4] ***Modeling of Hydrate Formation in CO_2 Geological Storage - Application to The 11th SPE Comparative Solution Project,*** E. Flauraud, D. Ding, A. Michel, IFPEN. SPE Reservoir Simulation Conference , Galveston, Texas, USA, March 2025.
>> DOI : https://doi.org/10.2118/223858-MS

Scientific contacts: Eric Flauraud, Anthony Michel, Guillaume Enchery

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Geological storage of CO?: Geoxim compares favorably with other numerical simulators

To maximize energy production and streamline operations, operators are designing wind farms that incorporate an increasing number of turbines. However, under certain wind conditions, wind turbines frequently interact through what is known as the wake effect. The wake is created behind the rotor as it intercepts the wind's kinetic energy to convert it into electricity. Due to the conservation of energy, a zone of low wind speed develops, accompanied by increased turbulence. Each wake, the length of which is tens of times the diameter of the rotor that generates it, can then disrupt the operation of other wind turbines located downstream, as shown in Figure 1, where exceptional atmospheric conditions made it possible to observe the phenomenon. These wakes result in significant production losses as well as increased mechanical stress.

Figure 1: Aerial photo of visible wake effects at the Horns Rev 1 offshore wind farm - copyright Vattenfall.

To minimize these effects as much as possible, IFPEN is working on several methods:

- The first approach, applied from the outset of the design phase, involves taking into account all expected wind conditions over the wind farm’s lifetime in order to select the locations of the wind turbines in a way that minimizes their mutual interference [1].
- The second approach, applied during operation, involves independently controlling each wind turbine based on wind conditions. To do so, it is possible to redirect the wake by adjusting the yaw angle of the nacelle, as shown in Figure 2.

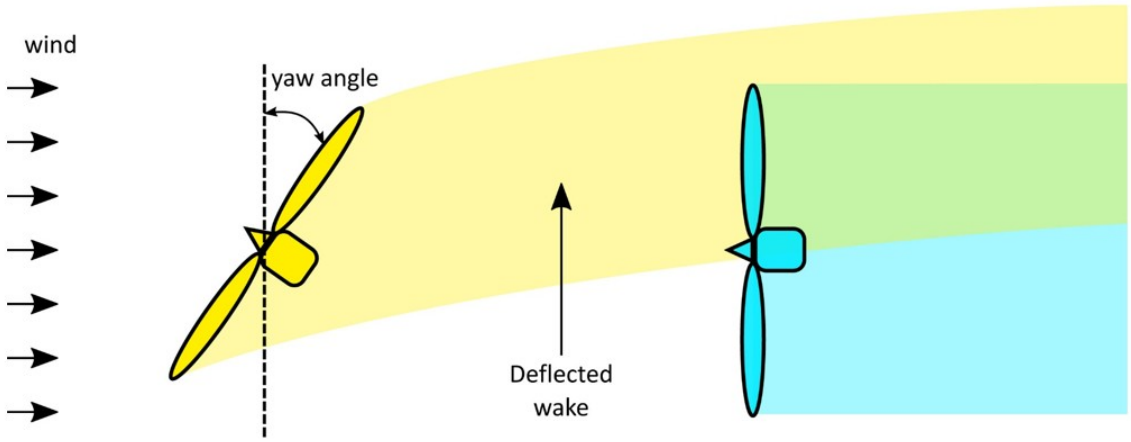
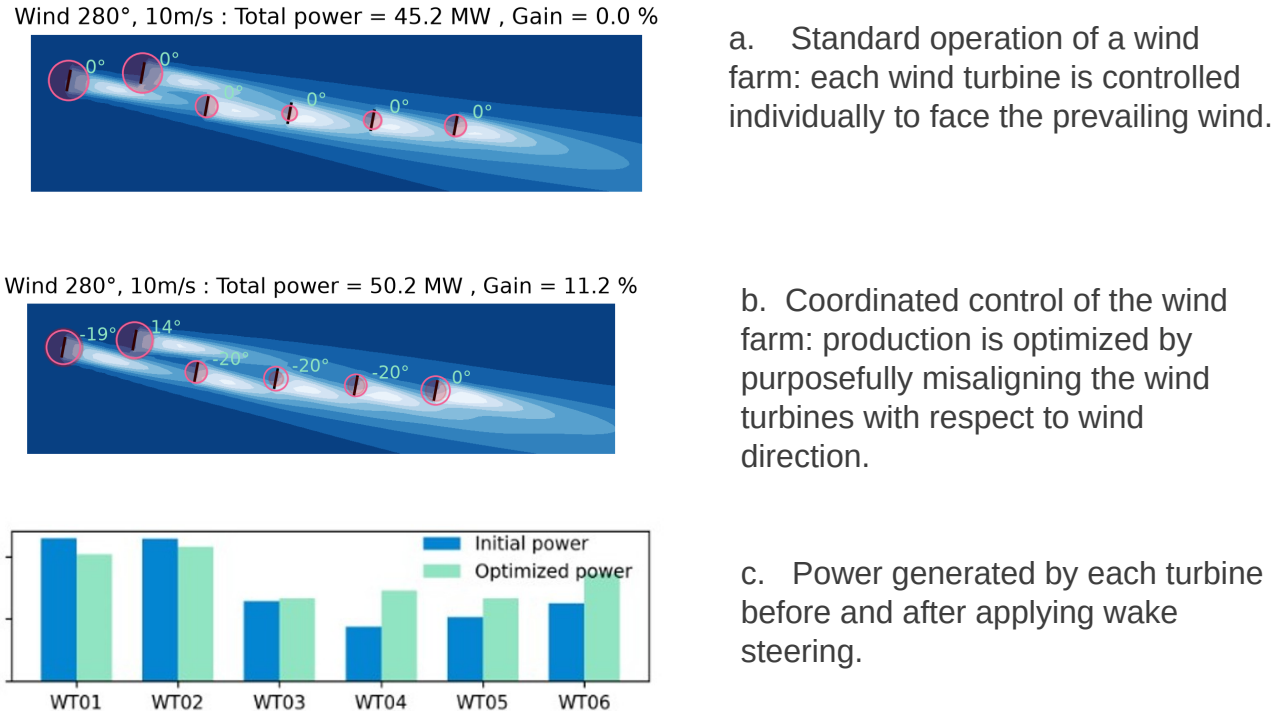


Figure 2: Wake realignment with yaw control

Changing the yaw angle (which is initially zero so that the wind turbine faces the wind) will result in a decrease in production from that particular wind turbine. Therefore, there is an optimal range of angles to be determined that reduces the power output of some wind turbines while increasing that of others, resulting in maximized overall power output (Figure 3).



a. Standard operation of a wind farm: each wind turbine is controlled individually to face the prevailing wind.

b. Coordinated control of the wind farm: production is optimized by purposefully misaligning the wind turbines with respect to wind direction.

c. Power generated by each turbine before and after applying wake steering.

Figure 3: Wake steering increases the total output of a wind farm (the size of the red circle is proportional to the turbine's output).

Calculating these angles is no easy feat, as aerodynamic phenomena are notoriously difficult to model. In addition, optimizing electricity production in real time requires models that are both reliable and fast in terms of computation time. Such models are implemented in the FarmShadow software suite, developed by IFPEN, to predict wind farm output based on given wind conditions and yaw angles. Intensive use of these models and the “cost function” created with FarmShadow makes it

possible to determine the yaw angles that maximize overall electricity production while ensuring that the mechanical stress on the wind turbines remains at an acceptable level in terms of their operational lifespan [2]. In addition, estimation algorithms make it possible to evaluate certain parameters based on observations made by sensors located throughout the farm [3,4] and thus to adapt the model.
All of these numerical model-based monitoring and estimation solutions were developed as part of the CAP project (Contrôle Avancé de Parc or Advanced Farm Monitoring), funded by ADEME[1].
They complement other methods, based solely on data (i.e., they involve no prior modeling), already presented in a previous article and for which reinforcement learning algorithms were used to maximize the farm output [5].
Finally, IFPEN is actively contributing to other research projects that take into account these wake effects in order to better integrate wind power into the power grid [6] and to help ensure its stability. Adjusting the total power output of a wind farm, as required by grid operators, can be achieved using algorithms designed to determine how to distribute this total power among the various turbines in a way that optimizes certain criteria, such as mechanical resistance.
The CAP project also aims to implement and test these control solutions in real operating conditions.

[1] Within the framework of the France 2030 investment plan

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[1] Malisani, P., Bartement, T., & Bozonnet, P. (2025). ***Offshore wind farm layout optimization with alignment constraints.*** Wind Energy Science, 10(8), 1611-1623.

[2] Gharbia, I. B, et al. (2026). ***Wake steering optimization under multiple cumulative fatigue load constraints.*** In Journal of Physics: Conference Series (Vol. 3224, No. 3, p. 032086). IOP Publishing.

[3] Dubuc, D., & Tona, P. (2025). ***LiDAR-assisted closed-loop control of a wind farm.*** In Journal of Physics: Conference Series (Vol. 3016, No. 1, p. 012023). IOP Publishing.

[4] Collet, D., & Tona, P. (2025). ***Design and evaluation of EnKF-based estimators for steady-state-model-based wind farm control.*** In 2025 American Control Conference (ACC) (pp. 2862-2869). IEEE.

[5] Monroc, C. B. (2024). ***Multi-agent reinforcement learning for dynamic wind farm control*** (Doctoral dissertation, Ecole normale supérieure-PSL).

[6] Corban, B., Buši?, A., Dubuc, D., & Zhu, J. (2026, May). ***Wind farm power tracking using reinforcement learning for secondary frequency regulation.*** In Journal of Physics: Conference Series (Vol. 3224, No. 3, p. 032088). IOP Publishing.

Scientific contacts: Paolino Tona, Donatien Dubuc

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The use of wake-effect modeling to optimize wind farm production

One of the main challenges in computational fluid dynamics is to accurately represent physical phenomena at various scales of time and space. Furthermore, exact numerical resolution at every scale is very cost-intensive in terms of computation time. Obtaining reliable solutions therefore requires simulations performed on a coarse scale but using models capable of describing the effects of physics at a very fine scale. These models are useful, for example, in the study of combustion, where chemical reactions take place in extremely narrow regions called flame fronts, as well as in the study of turbulent phenomena and particulate flows.

There are many models based on physical laws, but their precision is generally limited for such applications because they rely on simplifying assumptions. A recent approach, enabled by advances in artificial intelligence, involves developing more accurate models through direct learning from reference data derived from highly detailed simulations, each carried out on small computational domains [1].

This new approach has been the subject of various studies at IFPEN, beginning in 2022 with the machine learning-based identification of drag force laws for suspended particles. This was followed by a similar approach for turbulence models in fluid mechanics [2].

Very recently, exploratory research was conducted on a simplified case of turbulent combustion. A model based on a convolutional neural network (CNN)[1] was trained using direct numerical simulations (DNS) of the flame and then used to predict the flame's behavior on coarser grids.

The results obtained are encouraging, as shown in Figure 1, which compares the exact reaction rate? (mol/s) with the model's prediction.

This ongoing research is currently the focus of an IFPEN/ONERA PhD thesis launched in 2026 [3].

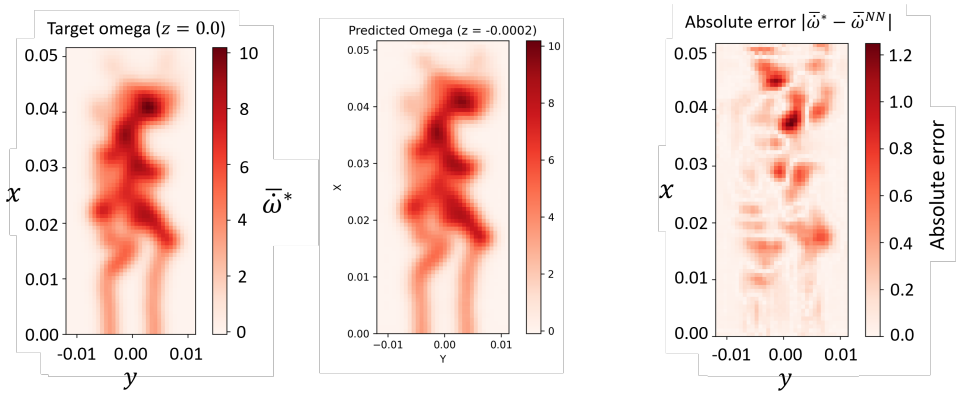

Figure 1: Comparison of the omega hydrogen reaction rate (mol/s) between a reference solution (left) and a field predicted by a CNN (center). The absolute error between the two fields is shown on the right.

[1] Deep learning architecture specialized in processing grid-structured data, such as images

References:

[1] Sanderse, B., Stinis, P., Maulik, R., & Ahmed, S. E. (2025). ***Scientific machine learning for***

closure models in multiscale problems: A review. Foundations of Data Science, 7(1), 298–337.
>> DOI : https://doi.org/10.3934/fods.2024043

[2] Vital, E. et al. (2025), ***Neural Network for Subgrid Turbulence Modeling for Large Eddy Simulations***. Proceedings of ParCFD 2025 conference,
>> DOI : https://arxiv.org/abs/2511.05103.

[3] Flament, C., Thèse ONERA/IFPEN: ***Modélisation du plissement de sous-maille par apprentissage automatique pour les simulations aux grandes échelles de la combustion turbulente prémélangée***. [**Modeling submesh wrinkling using machine learning for large-scale simulations of turbulent premixed combustion**].

Scientific contacts: Cédric Mehl, Thibault Faney

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Artificial Intelligence in Multiscale Computational Fluid Dynamics

The increase in the number of electric vehicles requires the rapid and efficient deployment of EV charging stations (EVCS), since drivers are reluctant to “take the plunge” while the charging network is perceived as being inadequate. At the same time, operators are unwilling to invest without a guaranteed financial return. Yet the widespread adoption of electric vehicles, along with the need to balance energy supply and demand, requires that charging stations be strategically located, particularly along major highways.

The issue is further complicated by the highly interdependent nature of the factors involved: charging needs, route selection, and stations congestion. Consequently, charging demand has a direct impact on queueing times, which in turn alter routes and the distribution of traffic flows. Existing approaches rarely take this interaction into account in a coherent manner, thereby limiting their capacity to effectively determine the network’s requirements in terms of size and distribution of charging stations.

The method proposed by IFPEN [1] introduces a charging demand equilibrium model that makes it possible to estimate the spatial and temporal energy demand of electric vehicles, thereby eliminating the reliance on proprietary data from charging operators. This demand feeds into a queueing model (e.g., M/M/C)[1], the parameters of which are derived from the overall mobility and charging needs across the study area. This tool makes it possible to estimate future queueing times (see example in Figure 1) and to inform decision makers about the optimal sizing and placement of charging infrastructure.

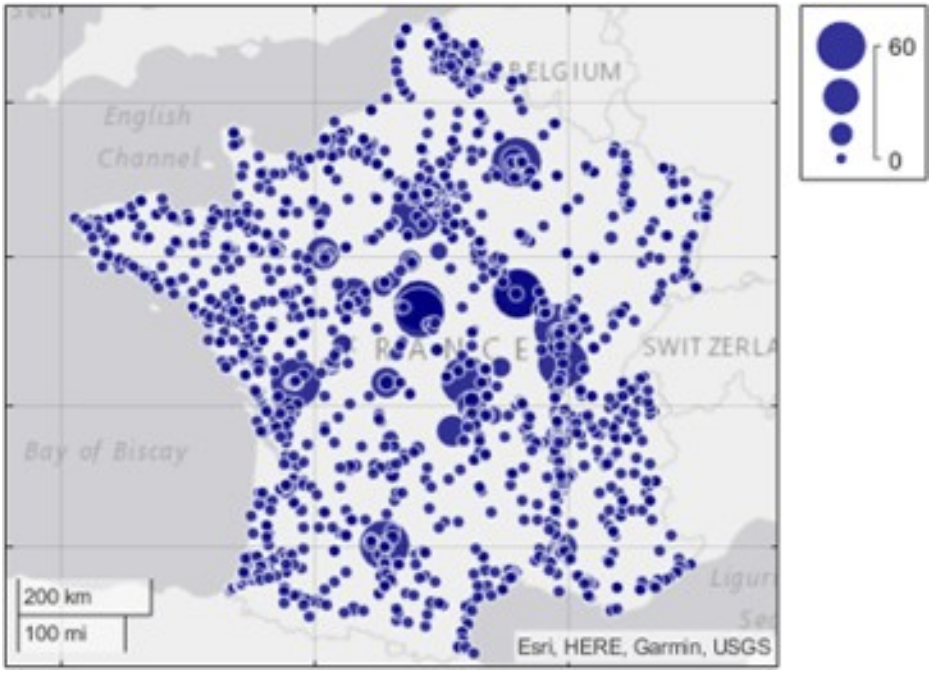

Figure 1 : *Average queueing times (in minutes) during peak periods at electric vehicle charging stations (EVCS data from January 2024, assuming a 2% share of electric vehicles in total vehicle traffic)*

The results for an optimized network (as shown in Figure 2 and discussed in the caption) demonstrate not only greater network resilience in the face of increased demand but also an improvement in total journey time.

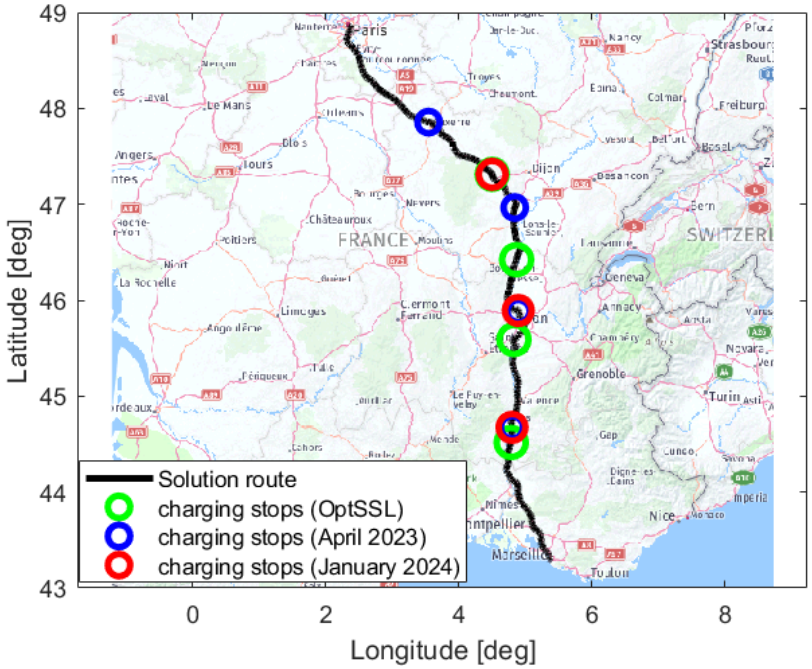

Figure 2: *Optimal route planning for a journey from Paris to Marseille with three EV charging infrastructure configurations: existing infrastructure as of April 2023, existing infrastructure as of January 2024, and optimal infrastructure calculated using our method (OptSSL). For this case study, our optimal solution saves up to 22 hours of total travel time compared to the April 2023 configuration (versus just 6 hours saved by the January 2024 configuration) for an electric vehicle share of 2% of total vehicle traffic.*

This approach provides a decision-making tool for EV charging station planners and operators by enabling them to identify bottlenecks, evaluate various scenarios for the development of electric mobility, and target investments toward the most critical areas.

Subsequent research will be aimed at enhancing the method's operational effectiveness through the use of a dynamic equilibrium model and the provision of real-time monitoring of congestion at stations. The main scientific challenge now lies in the scale of the optimization problem and in the capacity to develop resolution methods that are sufficiently "scalable" to handle national networks and increasingly complex mobility scenarios.

[1] In queueing theory, M/M/c is a multi-server queueing model. It describes a system in which arrivals form a single queue and behave according to a Poisson process, where there are c servers and the task processing times follow an exponential distribution.

Reference:

[1] I. Ben Gharbia and G. De Nunzio, ***"Location Planning of Fast Charging Infrastructure for Electric Vehicles and System Resilience Analysis via a Demand-Based Queueing Model"***, 2024 IEEE 27th International Conference on Intelligent Transportation Systems (ITSC), Edmonton, AB, Canada, 2024, pp. 1606-1613,
>> DOI : 10.1109/ITSC58415.2024.10919557

Contacts scientifiques : Ibtihel Ben Gharbia, Giovanni De Nunzio

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Towards more robust planning of charging infrastructure for electric vehicles

The performance of a catalyst support — whether alumina or zeolite — depends on the properties of its porous microstructure: porosity, specific surface area, and the connectivity of the solid network, which govern the access of reactants to active sites. Designing an optimal support thus amounts to solving an inverse problem, i.e., identifying the microstructure, and then the manufacturing parameters, that satisfy a set of property specifications.

However, the problem here is compounded by the fact that several very different microstructures can exhibit the same macroscopic properties, and that traditional optimization methods - which are costly in terms of computation - will explore only a fraction of them.

Typically, a geometric model starts with manufacturing parameters to simulate a microstructure, and then calculates the resulting properties: this is the forward loop. To solve the reverse problem – tracing back from target properties to a microstructure, and then to its manufacturing parameters – researchers at IFPEN supplemented this forward loop with a reverse loop [1], based on a guided diffusion model, the type of AI used in image generators (Figure 1). Trained on 30,000 virtual microstructures derived from a random geometric model (COX[1] process), the neural network gradually "denoises" an image of random noise until it obtains a microstructure that conforms to the target properties. The target properties guide the neural network at each step, acting like a filter that directs the transformation of noise into a microstructure (Figure 2).

Since the starting point is chosen at random each time the calculation is run, each use of the trained model produces a different but valid microstructure, since it possesses the same target properties, reflecting our physical reality.

Once a satisfactory microstructure has been established, a second convolutional neural network[2] (dedicated to image analysis) then derives the four aggregation parameters of the geometric model, which are directly linked to the manufacturing parameters.

Based on nearly 3,000 test microstructures, these parameters were identified with an average coefficient of determination (R^2) of 0.85 (where a value of 1 corresponds to a perfect prediction). The "round-trip" validation[4] confirms the physical consistency of the properties obtained, all thanks to a calculation that takes just a few seconds, compared to several hours using traditional methods.

Subsequent research steps will focus on the 3D generation of microstructures, the inclusion of additional mass transport descriptors (tortuosity, physisorption), and validation using real materials characterized experimentally.

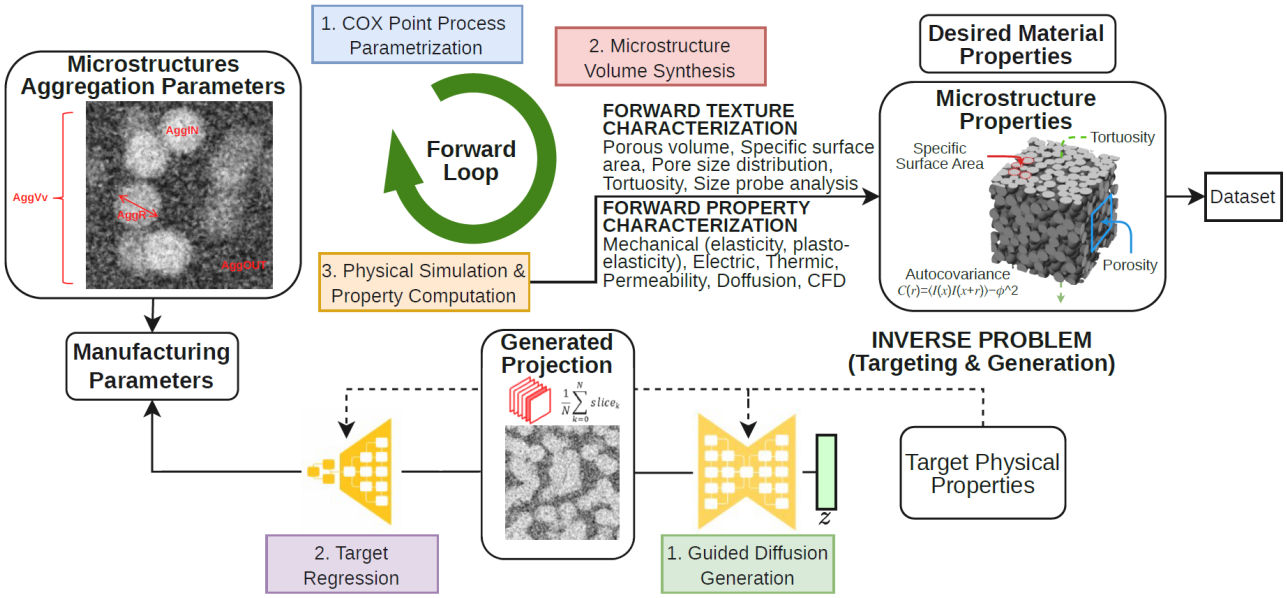

Figure 1 : Microstructure co-design loop: top, forward loop – synthesis of properties from manufacturing parameters; bottom, reverse loop – generation of a microstructure from target properties, then back to the manufacturing parameters.

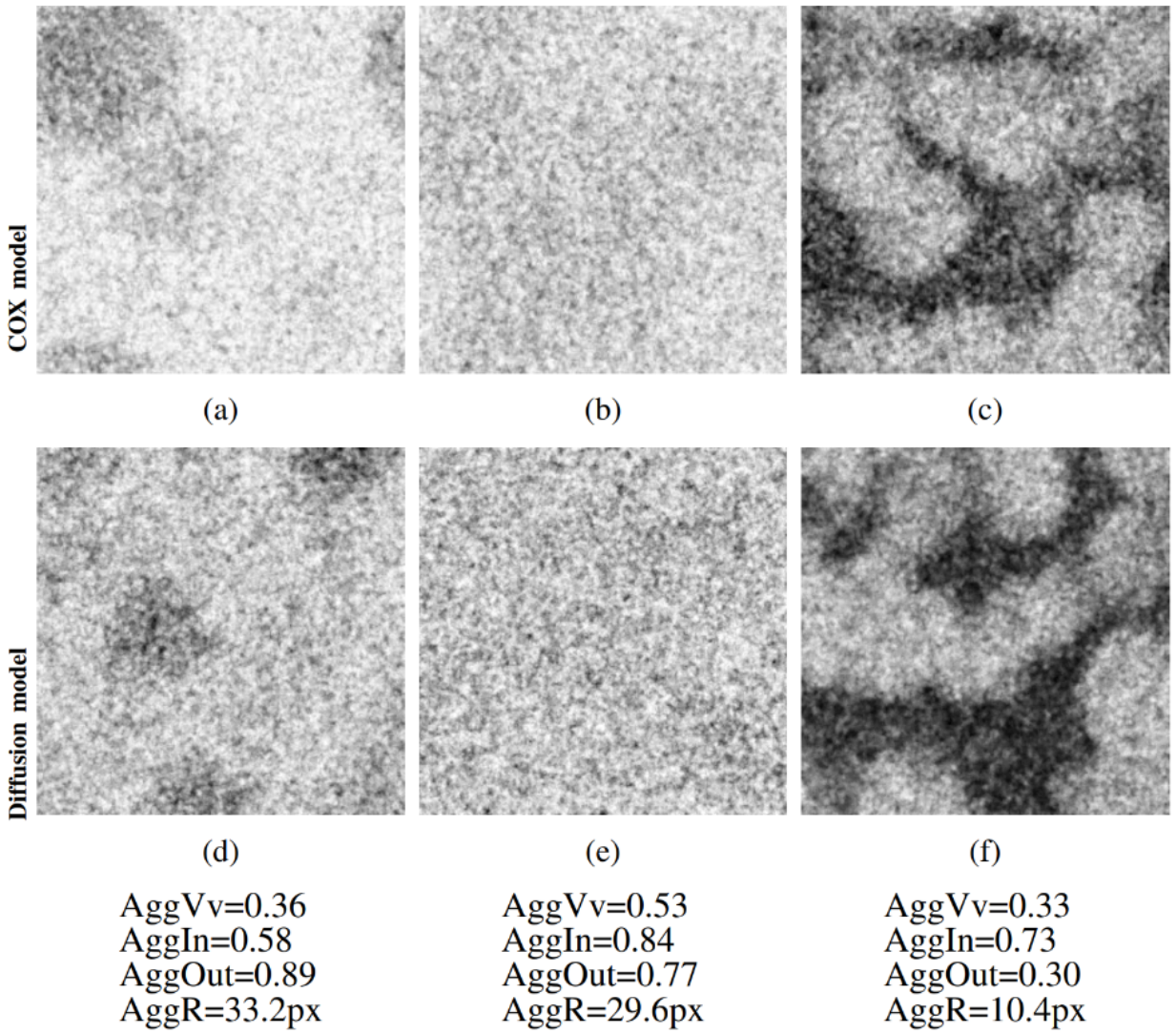

Fig. 1: COX model-generated (a–c) vs. diffusion-generated microstructures (d–f).

Figure 2 : Comparison, based on three microstructure cases with distinct AggVv, AggIn, AggOut, and AggR parameters, between images from the direct geometric model (top) and those generated by the guided diffusion model (bottom).

[1] A probabilistic microstructure generation method that can be used to simulate polycrystalline grain assemblies in 2D or 3D, based on randomly placed nuclei that then grow in regular circles to define the grain boundaries

[2] Deep learning architecture specialized in processing structured data in matrix form

[3] A stochastic model driven by four parameters: AggVv (aggregate volume fraction), AggIn (intra-aggregate fraction), AggOut (extra-aggregate fraction), AggR (average aggregate radius)

[4] Resynthesis of a microstructure from predicted parameters

Reference:

[1] J. Peyrelon, A. Pirayre, L. Sorbier, M. Moreaud, A. Hammoumi, ***Guided Diffusion Model for Microstructure Generation Design***, conference paper, 2026 (DOI pending).

Scientific contact: Julien Peyrelon

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Catalyst supports designed using generative AI

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