Digital Twin Deployment for AMC Filter Life Cycle Prediction

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ABSTRACT

Chemical filters to remove Airborne Molecular Contamination (AMC) play a pivotal role in removing harmful AMC and provide ultrapure air quality in SEMI cleanrooms, which is a key requirement for manufacturing high quality devices. Filters are expected to have long lifetime and their design optimization plays a central role to provide that. Predicting filter removal efficiency and life cycle are key design parameters. However, it is challenging to obtain these parameters experimentally, particularly at very low gas concentrations, due to long test times, high experimentation costs and technical limitations.

Although computational modeling is an efficient means to generate predictive models, long computational lead time and the inability to capture live failure mode engineering analysis (FMEA) leads to a bottleneck in solving various challenges in filter optimization.

This study is a novel effort in successfully developing and deploying digital twin technology for the AMC filter optimization process. The digital twin approach is a machine learning model and a virtual representation of real word entities and processes, synchronized at a specified frequency and fidelity. It can track the past, provide insights into the present and predict and influence future system behavior and can offer live, system level simulations with real data inputs.

It also offers a unique opportunity to study virtual and physical system either separately or together. Moreover, digital twin models provide profound impacts on industrial product development and businesses with better decision-making ability through human and artificial intelligence by accelerating holistic understanding of the systems of interest. This study successfully developed a complete digital twin for air filtration system and subsequent twin model for a real-life filtration system. By studying the digital twin of AMC filters under actual working conditions, we explored the product in action, over time, when subjected to the physical environment. This deployment allowed the product development team to close the loop on its initial simulations.

INTRODUCTION

Airborne Molecular Contamination (AMC) is a critical issue for numerous state-of-the-art manufacturing processes. These contaminants pose a serious threat in the modern semiconductor industry where feature size continues to shrink. Since AMC can significantly damage semiconductor cleanroom environments, it is crucial to adopt effective means to remove AMC from upstream gases to maintain a high yielding process (J. M. Lobert, 2018) (A. Chakraborty J. L., 2023).

Among the different processes, adsorption and ion exchange systems are efficiently employed to remove AMC (Ruthven, 1984) (Suzuki, 1990). With the miniaturization of semiconductor features to less than 100 nm, AMC was recognized as critical sources of yield reduction and performance deterioration in semiconductor devices (D. Kinkead, 1995) (T. Ogata, 1998) (H. Kitajima, 1997). AMC, unlike particles, is in the gas-phase form and has dimensions of 0.3 – 0.6 nm. At these dimensions, AMC easily moves through high performance particulate filters and negatively impacts yield (S.N. Li, 2007) (Saga, 2006). The effect of contamination on wafer surfaces only grows more serious as feature sizes approach the same order of magnitude of contaminant molecules.

Several different removal processes have been employed to remove AMC, such as adsorption, ion exchange, and photocatalytic oxidation. However, AMC chemical pleated filters play a pivotal role in removing harmful contaminants and result in purified air quality in SEMI cleanrooms, which is a key requirement in generating quality products (A. Subrenat, 2003).

To maximize filter performance while minimizing cost of ownership, it is desirable to optimize filter design to increase both removal efficiency and filter lifetime. This filter optimization requires an understanding of the relationship between design inputs and key outputs. However, it is challenging to obtain all the necessary relationships experimentally, particularly at very low gas concentrations, because of long test times, high experimental cost, and technical limitations. Although computational modeling is an efficient means for developing predictive models, it, too, has long computational lead times and an inability to capture live failure mode engineering analysis (FMEA). This leads to a bottleneck in solving key challenges in filter optimization. Digital twins can complement all these issues efficiently.

Digital Twin Fundamentals

Digital twins are a state-of-the-art machine learning models, which are a virtual representation of real word entities and processes, synchronized at a specified frequency and fidelity. It can track the past, provide insights into the present and predict and influence future behavior and can offer live, system level simulated predictions with real data inputs. It offers a unique opportunity to study virtual and physical systems either separately or together. Moreover, digital twins provide profound impacts on industrial product development where businesses can get better decision-making abilities through human and artificial intelligence by accelerating holistic understanding of the systems of interest. The technology applied here enables the ability to see products in action virtually, which allows engineers faster interactions in the initial design phase. It further entitles true predictive maintenance digitally which drives down costly interruptions and repairs through accurate visualization of maintenance needs. Most importantly, digital twins uniquely offer critical solutions to avoid lost production time and costly investments. (Ansys, 2020) (Migliori, 2021) (M.A.N. DeAndrade, 2021) (T. Y. Lin, 2021).

Reduced Order Model (ROM)

Development of digital twins is dependent on a reduced order model (ROM). Model order reduction is a machine learning system to reduce the complexities of mathematical models in numerical solutions. Benefits of employing ROM are reduced simulation time, reduced storage size, and reusability of complex 3D models. ROM can be classified as static and dynamic. Static ROM are mainly useful where the inlet parameters are fairly steady over time whereas dynamic ROM is useful in capturing the sensitivity of fluctuating unsteady inlet parameters. Development and deployment of specific ROM is dependent on type of applications.

Static ROM

Static ROM is mainly utilized for steady state applications and it generates parametric ROM for the field data governed by the following equation (Ansys, 2020)

$$(x,\theta) = ROM\,(x,\theta) = \sum_{m=1}^{M} \phi_m(x) a_m(\theta)$$

Where

- X is the vector of target variable in sample size of M
- θ is the predictor
- ϕ_m is the regression co-efficient

Dynamic ROM

Dynamic ROM builder uses deep learning technique to build dynamic ROM for any transient simulation data. The governing equation is: (Ansys, 2020)

$$\frac{dx}{dt} = F\big(X(t)\big), B(t) \text{ with } X(t=0) = X_0$$

Where

- The solution vector X is a vector (function of time) of size n_{output}
- B is a vector (function of time) of size $n_{excitation}$
- F is anon linear function of X and B
- X_0 is a vector of size n_{output}, which represents the initial conditions of the solution

Figure 1 represents the different forms of ROM workflow and its development cycle. (Ansys, Ansys Twin Builder Getting Started: Static Rom Builder, 2020).

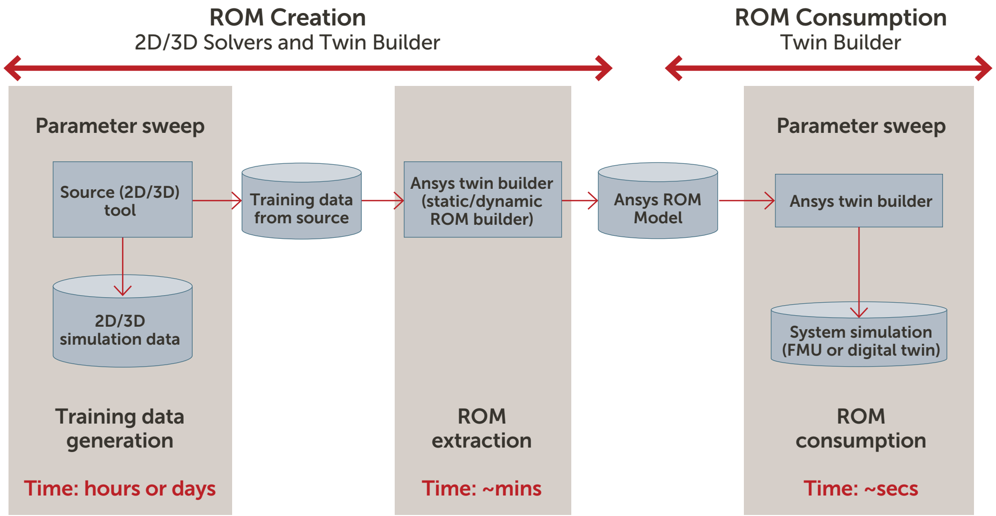


Figure 1. ROM creation workflow.

The current study is a pioneering effort in developing and deploying digital twin technology in AMC air filtration system. By studying a digital twin under actual filter conditions with real time input data, it was possible to see filters in action over time though its connected virtual representation.

Moreover, deployment of a digital twin for an air filtration system enabled momentary true predictive performance evaluation as well as true predictive maintenance by its live FMEA tracking features. Further, through its unique feature of "Virtual Sensors", it was possible to conduct the live FMEA and RCA (root cause analysis) instantly, which helped to avoid costly downtime and repairs. The ability of instant performance prediction further empowers the clear understanding of filter replacement time – thereby bolstered the future filter optimization process. By implementing a digital twin, businesses can have significant cost and time saving techniques in developing a holistic plan of future smart filtration techniques. That said, the technology can be critical from the aspect of superior product development along with significant economic advantages. The objective is to provide real-time response and to predict product lifetime momentarily.

METHODOLOGY

The digital twin technology employed here is based on a neural network machine learning method, which needs substantial amounts of data to train the model. The data can be derived from experimentation, but data can also be generated synthetically in the absence of test data. The current study considered a specific AMC pleated filter system that is utilized to remove ultra-low concentration (5 – 100 ppb) of AMC using adsorption technology. Due to long test times and resource consumption, it was difficult to obtain the required amount of test data to feed into the twin model development. A solution to this challenge was developed for the current effort by utilizing the power of CFD techniques to generate the necessary training data set synthetically. A baseline validated CFD model was first developed before using it to generate the training data.

Baseline CFD model: A prerequisite for model-based digital twins

Initially, a CFD model of a pleated AMC filter was developed. Figure 2 shows a single layer, pleated filter with specific pleat numbers, pleat width, and pleat depth. Activated carbon was chosen as the adsorbent media. The amount of carbon is dependent upon specific adsorbent media loading for any one application. Toluene was chosen as the organic contaminant in the flow path with initial upstream concentration of 1 parts per million (ppm), 100 parts per billion (ppb) and 10 ppb, respectively. Based on the pleat design, the flow of contaminated air was allowed to pass through the adsorbent filter media. Due to the symmetric nature of the filter geometry, a 2D representative CFD model was developed.

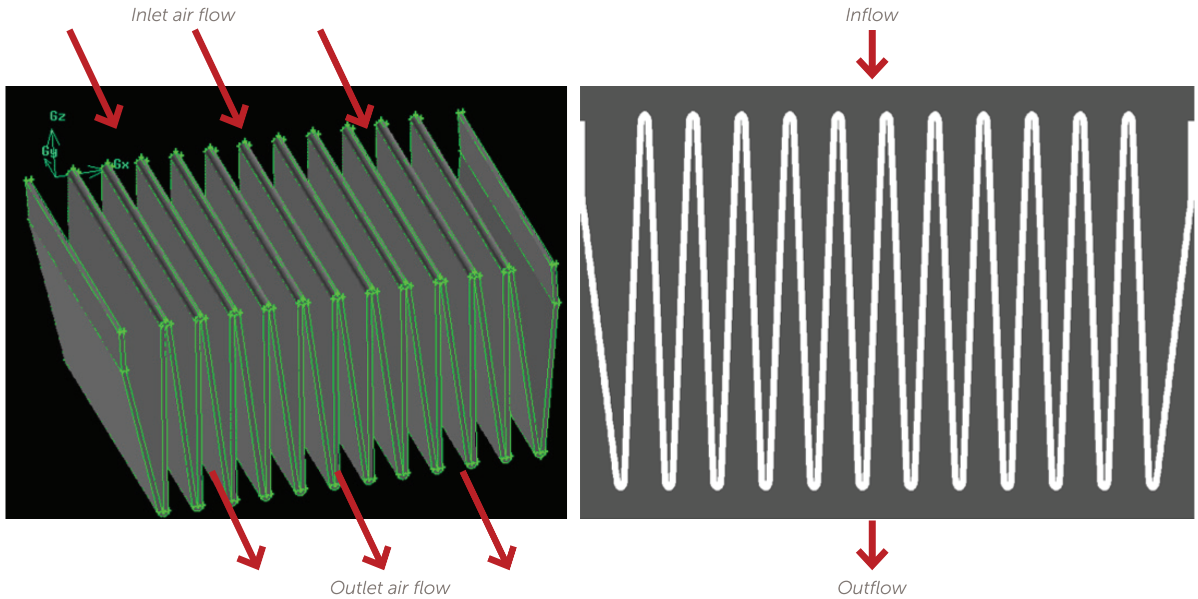


Figure 2. Pleated filter geometry and CFD domain.

The goal was to adsorb AMC contaminants (toluene in this case) into the filter media and thereby to produce ultra-pure air. The flow was laminar, and the model was based on governing equations for mass, momentum, and energy balance for gas adsorption processes in a porous adsorbent bed (A. Chakraborty J. C., 2019). The model was developed and solved in a Finite Volume Method through ANSYS Fluent CFD software. The process was governed by the Linear Driving Force model. An adsorption isotherm and gas diffusion model (pore diffusion and film diffusion) were developed by User Defined Functions (UDF) and resolved using ANSYS Fluent solver. Based on experimental data, the Langmuir isotherm model was best suited in this application. The mesh and time step optimizations were performed for each model to obtain the solution convergence. The models were utilized to predict and validate filter adsorption capacity for three different contaminations cases of 1,000 ppb, 100 ppb, and 10 ppb (Figure 3) respectively. The plots exhibited the removal efficiencies (%) as a function of filter capacity (ppb-h). It was evident that the models were well compared to experimental data at all three concentrations, indicating the extent of the accuracy and robustness of the model in predicting filter performance, at even very low concentrations.

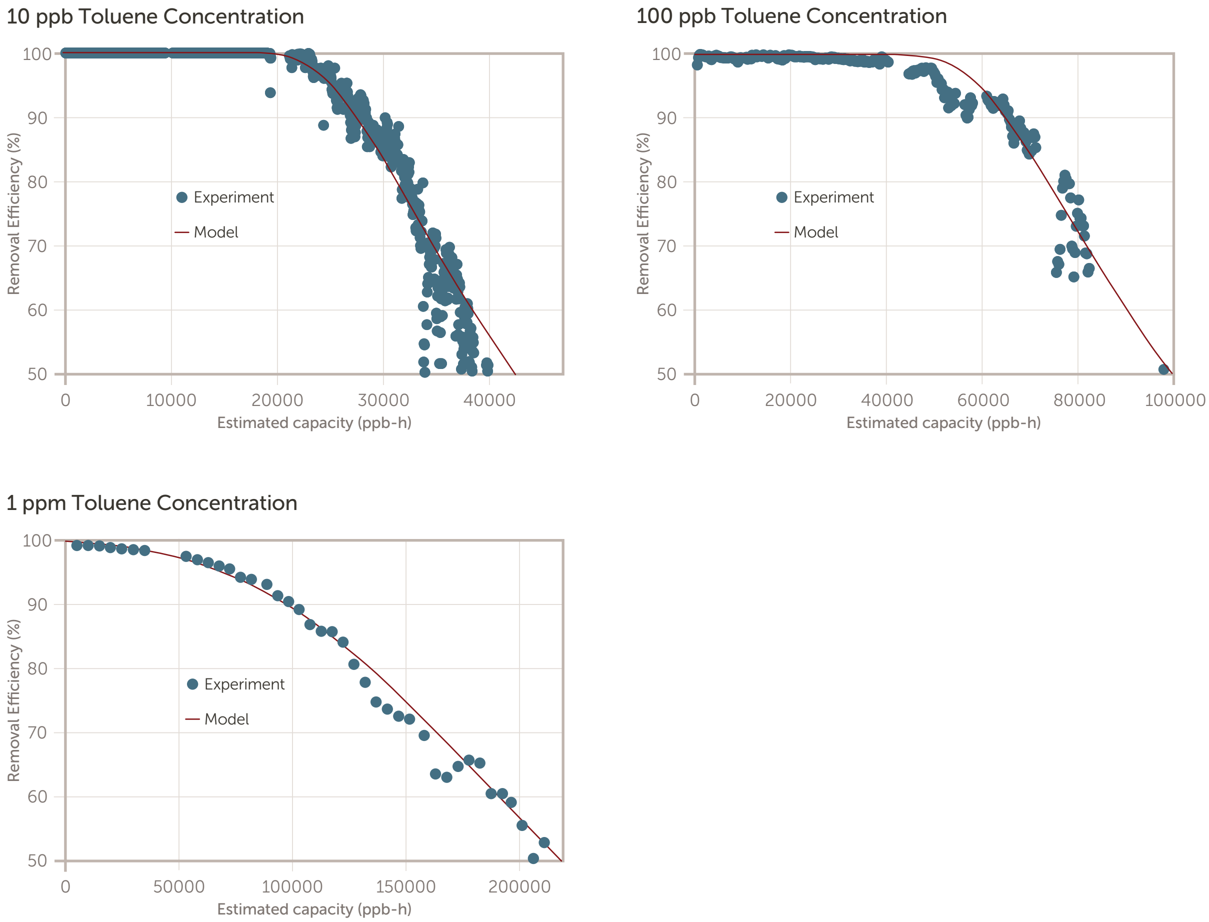


Figure 3. Base model validation.

CFD model utilization to generate training data for ROM creation

The digital twin model, in this effort, was developed over wide ranges of input parameters such as contaminant concentration and air flow rate with a goal to predict filter lifetime, removal efficiencies and to enable live FMEA analysis. The contaminant concentration was varied from 10 ppb to 100 ppb and the flow rate was varied from 0.4 m/s (78 cfm) to 3 m/s (591 cfm). Both the input variables resembled the real time fab conditions.

The key step was to generate sufficient training data to develop ROM over the ranges of input variables stated above. To do so, as a first step, a detailed DOE (design of engineering) was performed in ANSYS workbench tool by altering contaminant concentrations and flow rates, shown in Table 1. Based on DOE, 20 specific CFD models were developed thereafter with distinct combination of concentrations and flow rates. The models were developed based on a validated baseline CFD model. The model outputs were able to generate sufficient training data.

Table 1. DOE for process conditions for CFD models

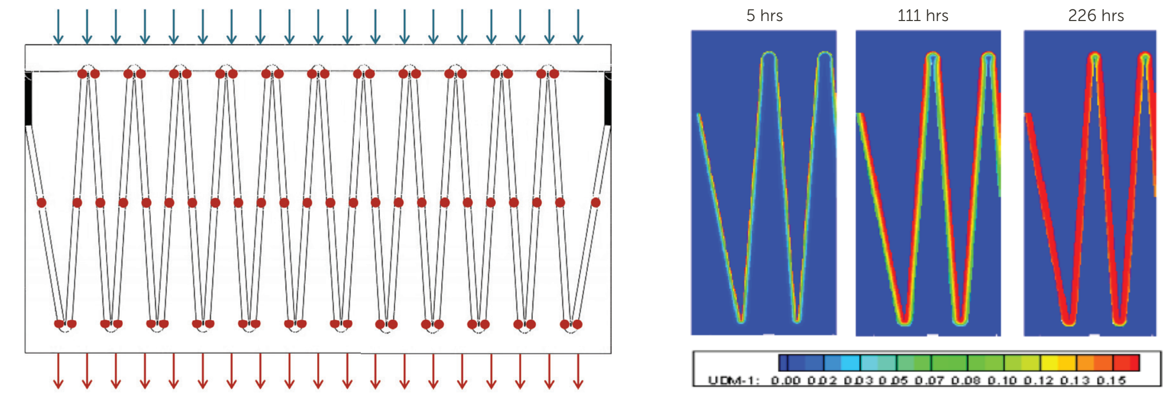
Case	Contaminant concentration	Flow rate
1	52.75 (ppb)	0.985 (m/s)
2	57.25 (ppb)	1.635 (m/s)
3	70.75 (ppb)	2.285 (m/s)
4	97.75 (ppb)	1.375 (m/s)
5	16.75 (ppb)	2.415 (m/s)
6	75.25 (ppb)	1.115 (m/s)
7	61.75 (ppb)	2.935 (m/s)
8	79.75 (ppb)	1.765 (m/s)
9	48.25 (ppb)	2.545 (m/s)
10	21.25 (ppb)	0.855 (m/s)

Case	Contaminant concentration	Flow rate
11	84.25 (ppb)	2.675 (m/s)
12	43.75 (ppb)	2.025 (m/s)
13	39.25 (ppb)	0.465 (m/s)
14	34.75 (ppb)	1.245 (m/s)
15	66.25 (ppb)	0.595 (m/s)
16	88.75 (ppb)	0.725 (m/s)
17	30.25 (ppb)	2.805 (m/s)
18	12.25 (ppb)	1.505 (m/s)
19	93.25 (ppb)	2.155 (m/s)
20	25.75 (ppb)	1.895 (m/s)

Development of virtual sensors

Key features of digital twin were to offer predictive and prescriptive maintenance and troubleshooting of a live, in-service product, i.e. AMC filter in this study. This can be accomplished by generating multiple virtual sensors which can be mounted anywhere in the filter. Capability in developing virtual sensors is a state-of-the-art feature of a twin model. By embodying the unrestricted virtual sensors, for the first time, it is possible to track any irregularities or potential flaws in a live system which can't be obtained by physical sensors due to the limitation of mounting it elsewhere in the system. Figure 4 indicates the development of virtual sensors in an AMC filter. The purpose of the sensors was to capture the local contaminant concentration and flow rate which are critical parameters in filter design. For example, the toluene adsorption over time is shown in Figure 4b. The model predicted the filter adsorption performance in ideal condition – however, in real life, the local concentration can vary at different locations of the filter which might have serious impact on filter performance. The virtual sensors (Figure 4a) were able to track the anomaly of the performance (if any) and can prescribe the much-needed solutions.

To generate the sensors, initially 72 points were chosen at different pleat locations of the filter (top, middle and bottom). Next, a transient CFD model was developed to understand the flow and concentration profiles at 72 specific points. The purpose was to disregard the multiple redundant points with minimum concentration and velocity changes. Results indicated that 72 sensor points can be reduced to 16 where the values can be changed significantly. The 16 virtual sensors were able to translate the local physical behavior of the entire filter. Next step was to develop ROM which included 16 virtual sensors and filter outlet point to predict the filter performances and to conduct live FMEA analysis.



a) b)

Figure 4. Development of virtual sensors in an AMC filter and toluene adsorption (in kg/kg).

DIGITAL TWIN MODEL DEVELOPMENT

Development and deployment of digital twin can provide critical insights to real-life in-service products and directions to new design specification by offering the following key benefits:

a. Live system level simulation with real inputs

b. Momentary prediction of removal efficiency and pollutant concentration

c. Enable predictive and prescriptive maintenance

d. Live FMEA analysis by virtual sensor deployment

e. Operational optimization of air quality

Figure 5 indicated the usual over all workflow to develop the twin model. The input parameters were inlet contaminant concentration and air flow rates, and the goal was to predict filter lifetime and removal efficiencies instantly. Phase 1 involved creation of static ROM and subsequent response surface function.

A dynamic ROM was developed in Phase 2. Phase 3 and Phase 4 corresponded development of subsequent offline and online twin respectively. Offline twin was useful for momentary prediction of filter lifetime as well as filter performance over time whereas online connected twin is mainly used to capture live filter performance over time with a goal to develop live FMEA solution.

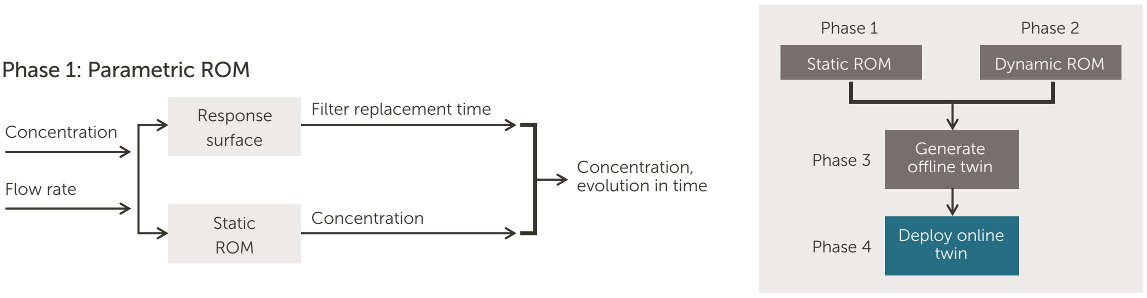


Figure 5. ROM creation workflow.

Digital twins can be developed from either static or dynamic ROMs, depending on the process. Figure 6 further indicates the complete structure in which an operational filter can be connected to twin systems by internal network or IoT connections. Based on life inputs, the twin is able to predict filter life cycle and pollutant removal efficiency Instantly and provide continuous live FMEA by newly developed virtual sensors.

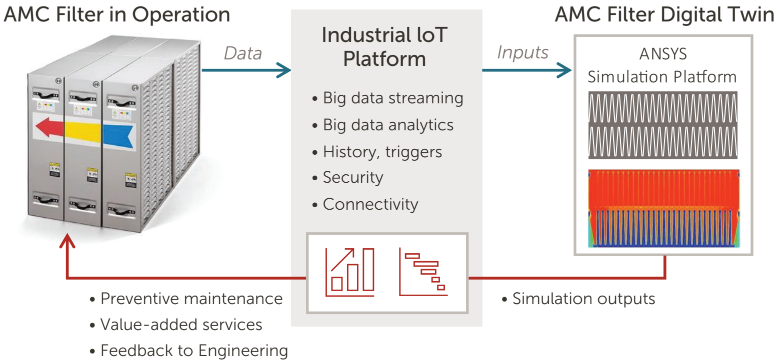


Figure 6. Digital twin structure coupled with filter in operation.

Static ROM development

Static ROM was developed based on the synthetic training data generated by 20 CFD model runs based on 20 different combinations of inlet concentrations and air flow rates as shown in Table 1. ANSYS Twin Builder tool was used to develop static ROM. The workflow of generation of static ROM was as follows:

Training data generation

Synthetic training data was generated by 20 CFD filter model runs. 80% of the training data was used as learning data and the rest was used as validation data.

Learning the ROM

The learning of the ROM was facilitated with data. Figure 7 indicates the snap-shot of the ROM learning process by ANSYS Twin Builder. The figure indicates the model reduction by optimal number of modes of ROM (6 in this case). Once the ROM was learned, the data were passed to the validation part.

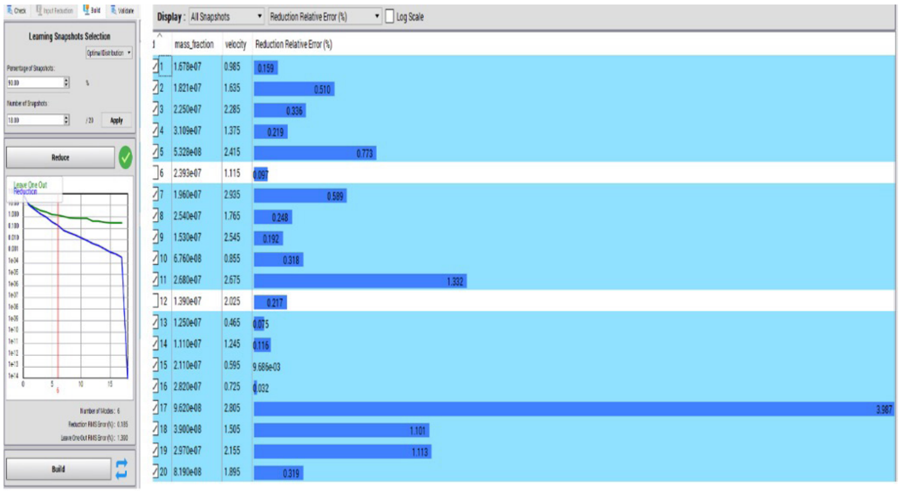


Figure 7. Learning process of ROM.

Validating the ROM

ROM validation was critical for accurate predictions. As stated earlier, 20% of simulated training data were used as validation data and the learned ROM data were compared with the specific validation part. The ROM was continuously trained unless it compared well with the validation data. The validated ROM was then transferred to the Twin builder module.

Dynamic ROM development

Dynamic ROM is applicable when the input parameters fluctuate significantly. A dynamic ROM can capture fluctuations and sensitivities of inlet parameters. Dynamic ROM generation workflow resembles that of static ROM as explained above: training data generation, learning and validating the ROM. Figure 8 shows the workflow of dynamic ROM generation.

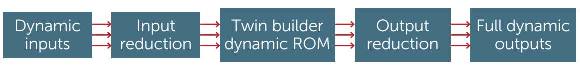


Figure 8. Dynamic ROM generation flow.

RESULTS

Predictions of a digital twin generated by static ROM

Figure 9 shows the filter replacement time and virtual sensor data analysis, which were predicted by the static ROM. Results indicate that the ROM accurately predicted the filter lifetime for 20 design of experiment cases (Figure 9a), each of which was a unique combination of inlet contaminant concentration and air flow rate.

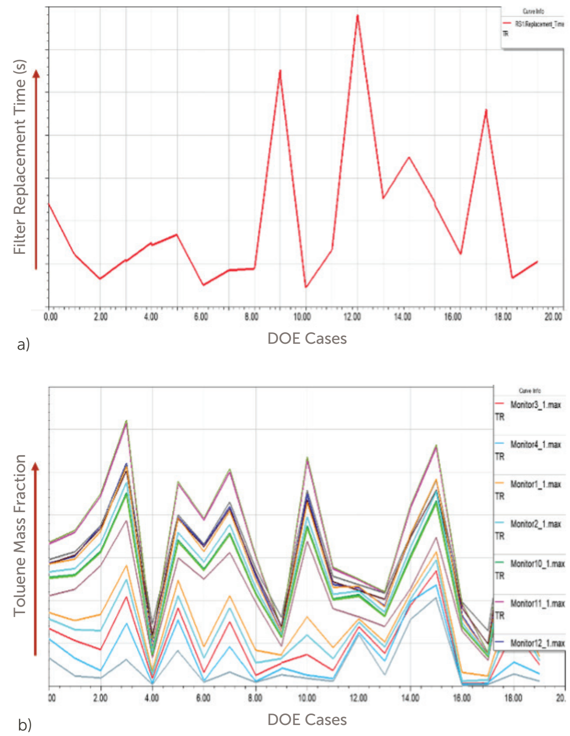


Figure 9. Filter replacement time (a) and virtual sensor prediction (b).

Instant prediction of filter lifetime is critical and valuable information for the next generation of filter design and is a significant cost saving approach which eliminates costly experimentation and long test time. Further, Figure 9b shows the local concentration profiles at different pleat locations by virtual sensors. This unique performance indicator was able to capture anomalies of filter performance at any filter location. Therefore, it was possible to perform FMEA analysis of a live in-service product digitally. This analysis can offer preventive measures and maintenance, which potentially reduces costly production downtime.

Predictions of a digital twin generated by dynamic ROM

Dynamic ROMs are especially critical for predicting fluctuating inlet parameters. Figure 10 showed the unsteady and fluctuating inlet concentration data in both Figure 10a (10 ppb) and Figure 10b (100 ppb) scenarios, respectively. A digital twin, generated by dynamic ROM, was able to predict filter removal efficiency momentarily and eliminated costly and time-consuming experimentation. Figure 11 further exhibits model validation and local contaminant concentration profiles predicted by virtual sensors. The twin model was able to predict toluene break-through at the filter outlet for both cases (10 ppb and 100 ppb) and compared well to that derived from the previous CFD model. Further, virtual sensors were able to predict local concentration profiles at different filter locations.

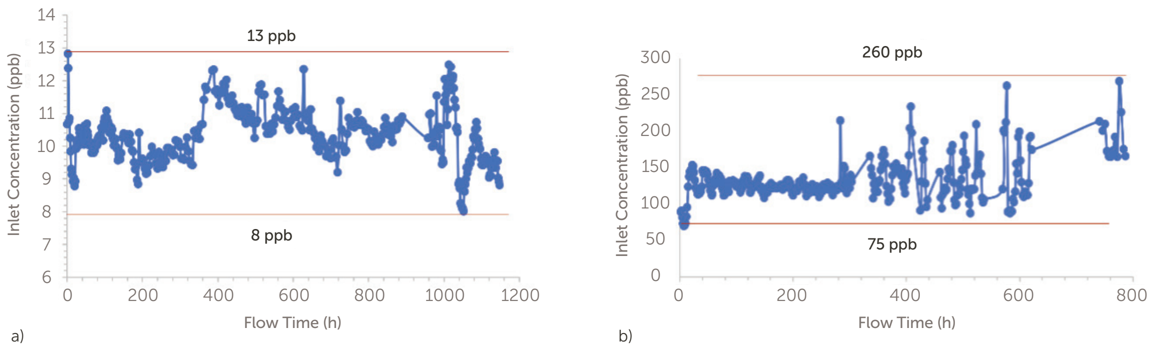


Figure 10. Fluctuating inlet contaminant concentration for 10 ppb (a) and 100 ppb (b).

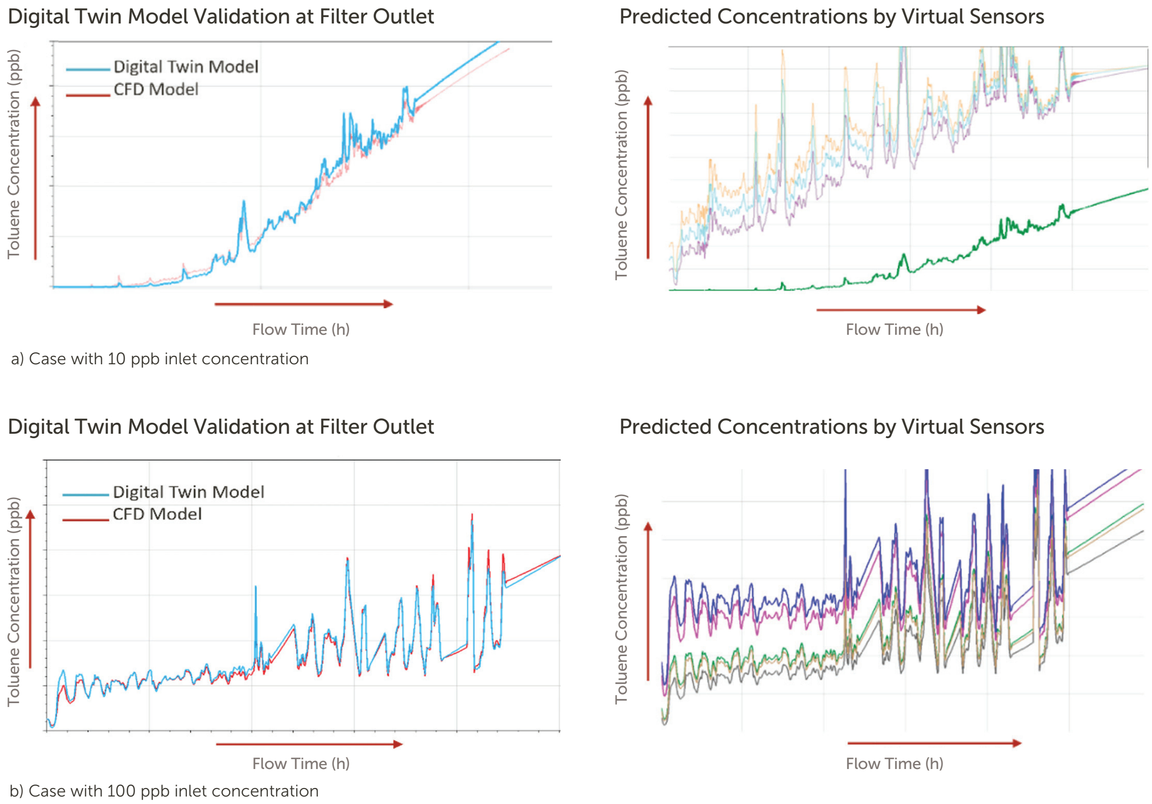


Figure 11. Dynamic ROM model validation.

Digital Twin Development for an Air Filtration System

After developing a digital twin model, the next step was to deploy it for a real-life system. Deployment of the twin carries a high significance in improving, managing, and troubleshooting a complex live, in-service product. This technology offers significant cost and time savings opportunities by attributing key product information. The current study demonstrated a successful twin deployment in an AMC air filtration system. It offered crucial process and product information by instant performance prediction and product monitoring by live FMEA analysis.

Figure 12 shows the full process flow of the twin deployment in a real-life, physical AMC air filtration system. Air flow was allowed to enter from the top of a wind tunnel system in which AMC test filters were placed. The contaminant (toluene in this case) was injected into the air flow. Two tests were performed with different toluene contaminants of 50 ppb and 100 ppb, respectively. The inlet and outlet airflows from the filter with measured contaminants were allowed to pass through an auto sampler and then to a pre-concentrator. The pre-concentrator increases contaminant concentration but reduces its volume, which increases signal to noise ratio and reduces detection limits.

The samples were analyzed by a gas chromatograph with flame ionization detector (GV-FID). The GC-FID provides the sample signal as an analog current at the pico-amp level. This was converted to a digital signal. A calibration curve (from traceable gas standards) was used to convert the digital signal of into a contaminant concentration with ppb unit. The converted digital signal was then passed into the twin system, which was deployed by the ANSYS Twin Deployer tool as a functional mockup unit (FMU).

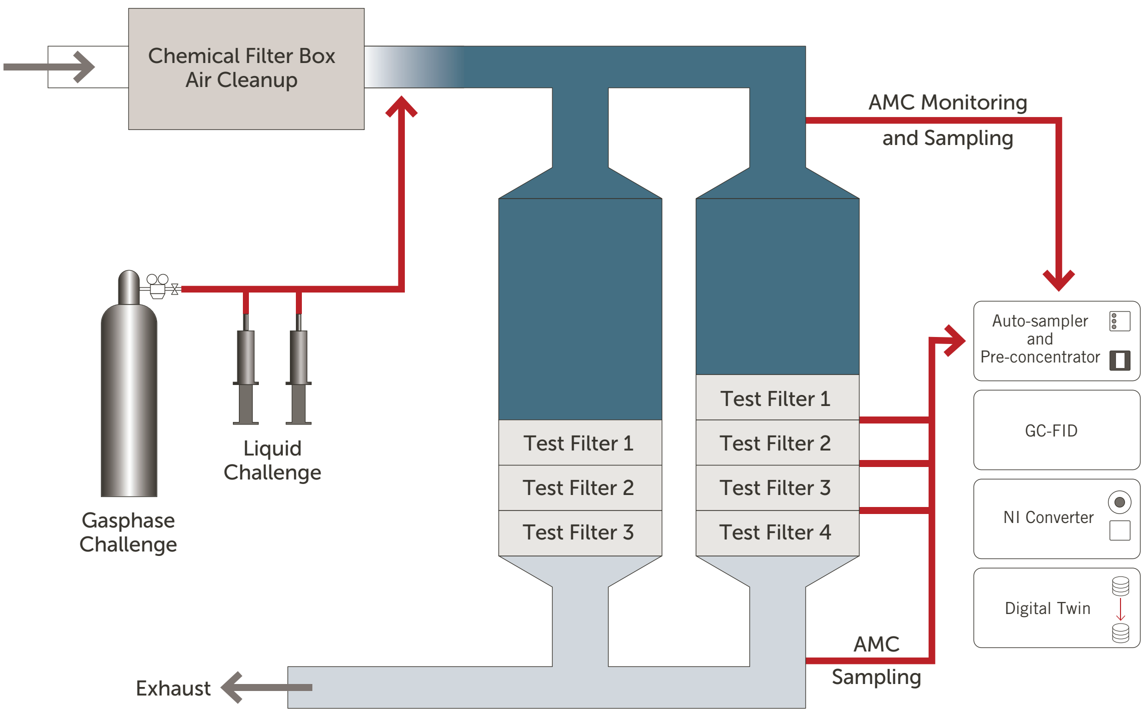
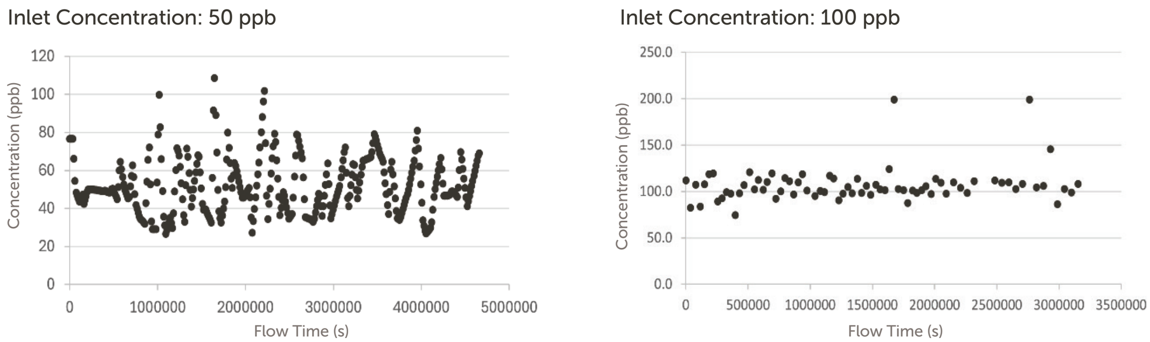
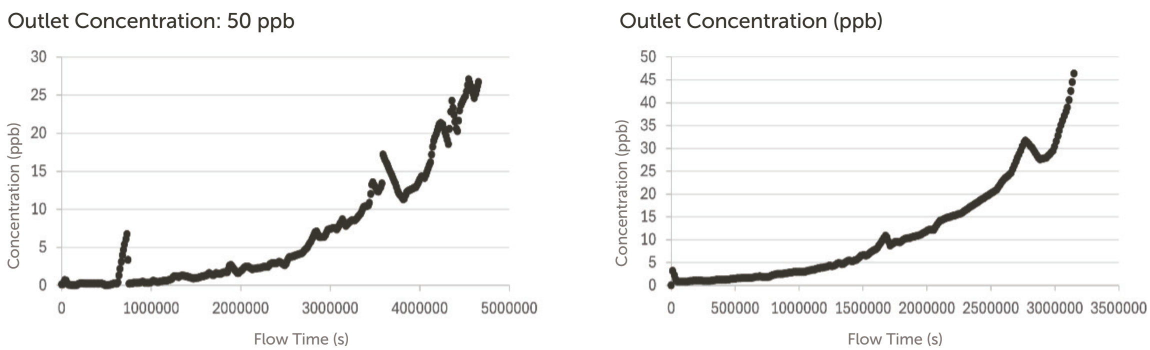


Figure 12. Process flow of twin deployment.

Figure 13 shows the experimental inlet and outlet concentrations for 50 and 100 ppb cases, respectively. The unsteady and fluctuating nature of inlet concentrations (Figure 13a) necessitated the generation of a dynamic ROM. Figure 13b shows the breakthrough curve at the outlet of the filter of subsequent cases. The twin was developed based on the dynamic ROM. The ROM was trained for a contaminant concentration range of 10 ppb to 100 ppb. The goal was to validate the filter removal efficiency and adsorption breakthrough for 50 ppb and 100 ppb inlet concentrations, derived from the twin with that derived from experiment.



a) Inlet concentrations



b) Onlet concentrations

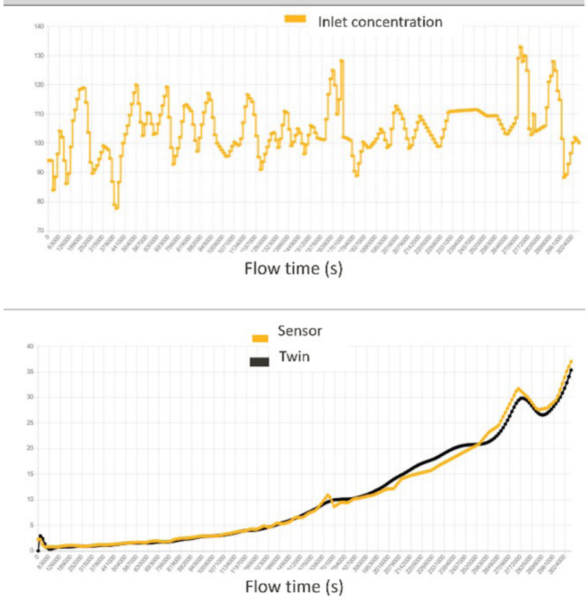
Figure 13. Experimental inlet and outlet concentrations.

For the validation part, a desktop WebApp was developed to capture all possible outcomes from twin models (prediction / maintenance) as shown in Fig. 14. The figure shows a few snapshots of different concentration cases (50 and 100 ppb). The twin model was embedded in a WebApp and the process was integrated by the ANSYS Twin Deployer tool. Both online and offline twins were developed. The online twin was used to monitor filter performance over time and to enable live FMEA analysis.

The offline twin was employed to predict the filter removal efficiency/adsorption breakthrough at filter outlet. The WebApp accurately captured the inlet sensor data, i.e. test data at 50 and 100 ppb inlet concentrations. Figure 14 further shows the accurate validation from sensor (test) and twin model.

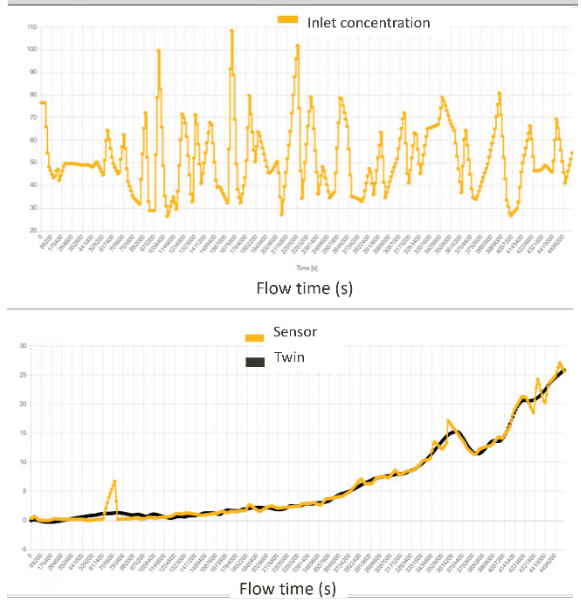
The figure indicates that the breakthrough curve from the twin model followed the experimental data very well, but in a significantly shorter time scale. The twin model was able to generate the data almost instantly (by 10 – 15 seconds), compared to experimental test times of 6 – 8 weeks. This implies that the generated twin was able to predict filter performance and removal efficiencies instantly for any inlet contaminant concentration in the range of 10 to 100 ppb. Instant prediction capability of a twin carries paramount importance in investigating a live process by eliminating costly and lengthy experimentation. It further offers significant values for product development by speeding it up.

Label	Caption	Value	Unit
t	Acquisition time	3.062e+6	[s]
Inlet concentration	Concentration (NI sensor)	100.2	ppb
Outlet concentration	Toluene concentration at outlet (NI sensor)	37.03	ppb



a) Case with 100 ppb inlet concentration

Label	Caption	Value	Unit
t	Acquisition time	4.574e+6	[s]
Inlet concentration	Concentration (NI sensor)	54.39	ppb
Outlet concentration	Toluene concentration at outlet (NI sensor)	25.61	ppb



b) Case with 50 ppb inlet concentration

Figure 14. Twin validation from WebApp.

SUMMARY

The digital twin unlocked a unique potential to transform product maintenance, repair, and performance predictions for every industrial domain where product optimization is difficult or impossible to predict by traditional measures. However, even with obvious prospects of having high economic impact, the technology is still far from being used in most product implementations due to lack of investment or strategy. Twin model technology is still in development and not yet widely adopted.

Among the successful implementations, the current study is an effort to develop and deploy digital twin technology in the filtration industry. It can complement the shortfalls of previous model based/experimental approaches through its ability to predict filter life cycles momentarily, live FMEA analysis. This offers optimization of filter performance and operational cost of ownership.

By studying the digital twin of AMC filters under actual working conditions, we explored the product in action, over time, when subjected to the physical environment. This allows the product development team to close the loop on its initial simulations. Engineers can make more informed choices for future designs and make their simulations even more accurate.

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