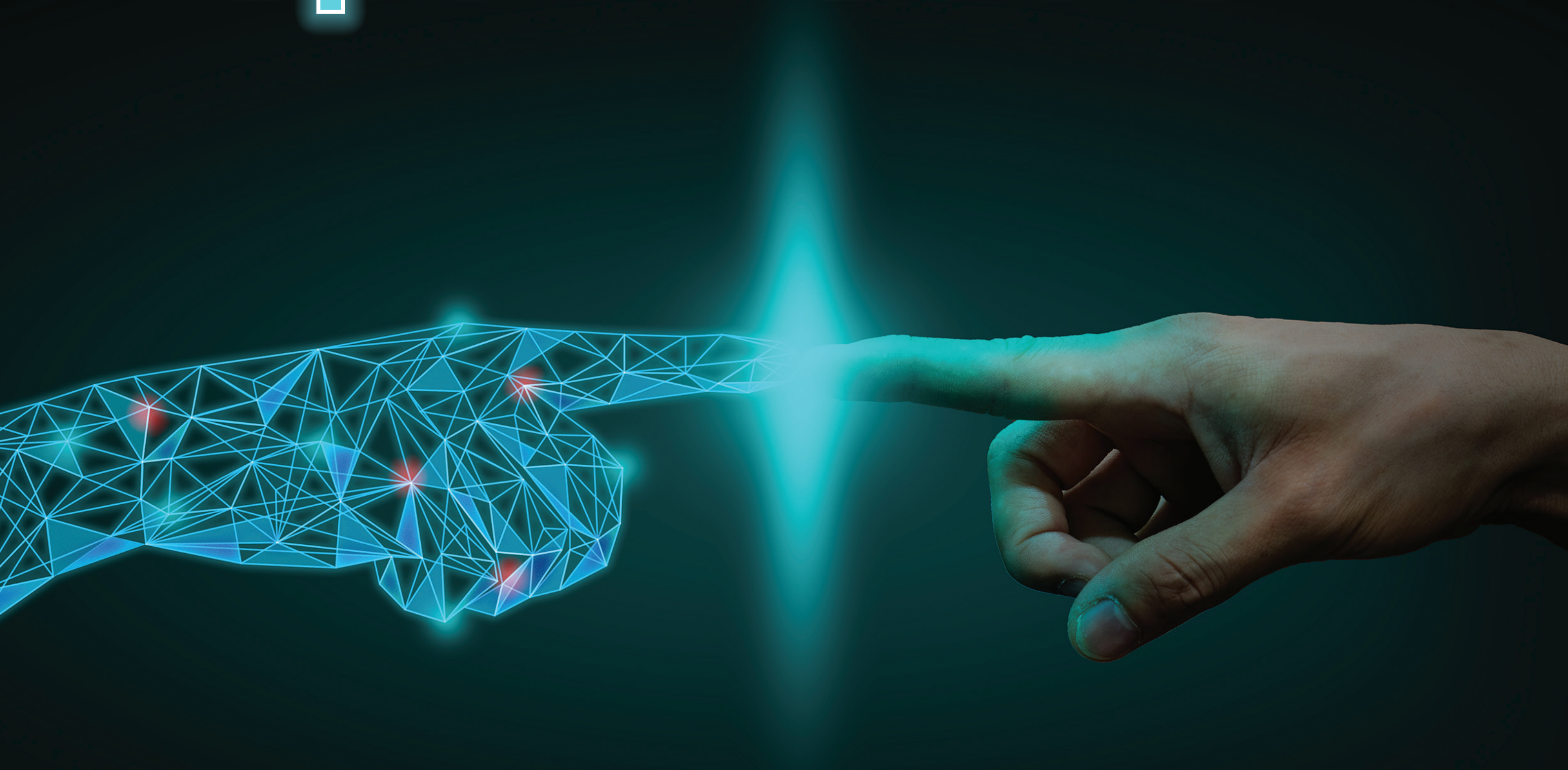
Digital twin optimisation



Svenja Blechmann, Steinmüller Engineering, Germany, discusses the use of digital twins for monitoring and optimising the performance of ammonia waste heat boilers in nitric acid production.

Digital twins of complex plants or plant components have become well-established tools for process monitoring and optimisation.

In the architecture of such digital twins, a distinction is made between online and offline, and between remote and on-site installation. This results in four possible combinations of how such a digital twin is designed and used.

In the following, the added value of a digital twin of an ammonia (NH_3) waste heat boiler will be highlighted.

Such waste heat boilers are critical equipment in nitric acid HNO_3 production. Their performance is crucial for the overall performance of the fertilizer production.

Digital twin

The digital twin operates in parallel to the actual plant and simulates its production process. Comparison between the actual performance values and the simulation results of the digital twin enables various assistance services.

The digital twin is designed to evaluate and monitor operating conditions and to detect deviations from regular performance.

A digital twin can be developed on the basis of a DimBo® model for the thermodynamic simulation of the associated steam generator. The model is designed for the simulation of steam generators in steady-state operation. It is capable of handling complex systems of components for heat exchange and medium conversion.

The steam generator is represented by a mathematical model, a so-called flow schematic. For all of the usual components in steam generator design, the corresponding circuit elements are defined and can be adapted to the desired functions by parameters. The DLL version of DimBo is used in the digital twin to simulate the process.

In a continuous cycle with adjustable time intervals, measurement values are extracted from the control system's database, process calculations are performed, and key performance indicators (KPIs) are returned to the database.

Based on the measurement values, the simulation determines the intermediate and outlet process conditions that can be expected according to the plant's design and control philosophy. KPIs, defined as relations between actual and expected parameters, indicate a malfunction of the plant, if they are found outside of a certain confidence range.

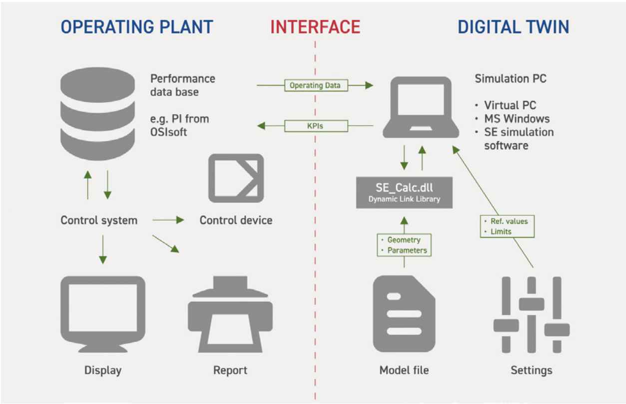


Figure 1. Overview digital twin interface.

Figure 2. NH_3 waste heat boiler during manufacturing.

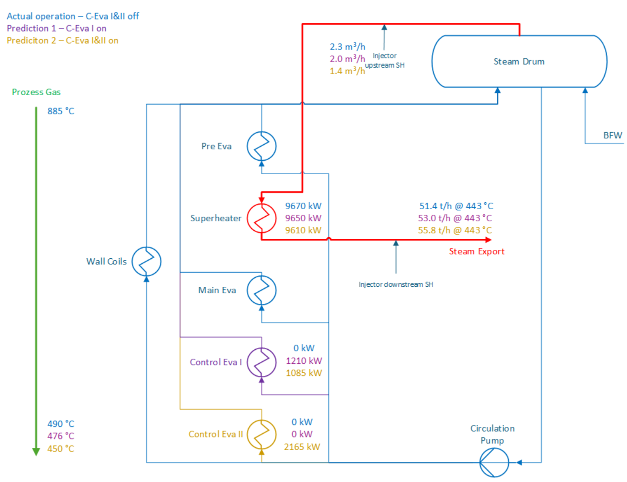


Figure 3. Process data from digital twin for predictive operation.

The deviation between actual measurement values and calculated values can also be defined as KPIs, but it is not limited to that.

KPIs

The KPIs can be set according to the requirements at site and include material temperatures, process gas temperature at different stages of the process, and efficiency of the heating surfaces. Based on the KPIs obtained, data on the database can then be used to trace tendencies, generate reports, and display advice and warnings with escalating severity levels.

Considering material temperatures as KPIs will support operators to determine remaining lifetime of their equipment and to detect severe operating conditions at a very early stage. Also, historical operating data can be re-calculated in the digital twin to obtain information on material temperatures of different heating surface sections to perform a remaining lifetime assessment. In case of failures, the re-calculation of historical data may support the evaluation of root causes at the site.

Setting the mass and energy balance as a KPI will give the operator the opportunity to detect malfunctions in the instrumentation; out-of-range measurements are erroneous when the overall mass and energy balance is in line with design conditions.

The thermal efficiency and, correspondingly, the evaluation factors for all heating surface packages will enable the operator to detect any malfunctions due to increased fouling as well as the occurrence of any leakages since any deviation in efficiency will be directly displayed in the graphical interface.

Linked to the efficiency of heating surfaces, the circulation ratio of each heating surface can be back calculated in the digital twin. In this way, any high steam contents in any evaporator heating surfaces or any low mass flow densities due to changed operating conditions can be avoided and countermeasures can be developed and initiated immediately.

In addition, pressure drop on critical parts such as a steam superheater or the process gas cooler across different sections inside of the waste heat boilers can be calculated by the digital twin, and values for increased or decreased load can be predicted to give more information to the operators.

Operation modes

In the first stage, the digital twin can be developed as an Excel-based provisional solution for testing and tuning in 'offline-remote' mode. If the plant owner wishes to operate the monitoring as a permanent service and use the calculated KPIs for visualisation, report generation, and eventually for operational optimisation, the digital twin can be provided with a user interface (GUI) as an 'online - on-site' solution and be integrated into the IT infrastructure of the plant operator. In this case, there is no data security risk involved as data does not leave the operators environment.

Results and solutions derived from digital twin

In an advanced application, the digital twin is utilised for optimisation of control loops, e.g. condition-based

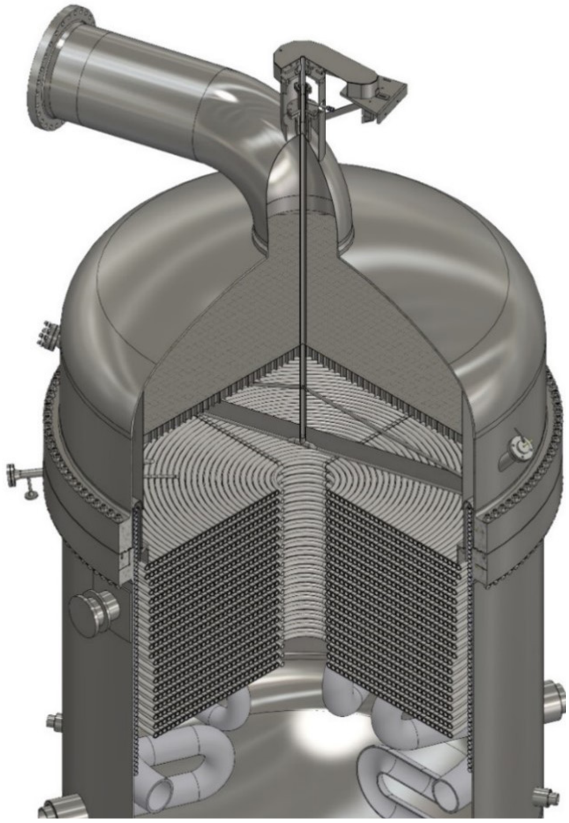


Figure 4. 3D model of NH_3 waste heat boiler.

operation of cleaning devices, to operate the plant at its techno-economical optimum.

Operation conditions for pre-defined operating modes can be predicted by a digital twin and will support the operators to monitor increasing fouling of heating surfaces and to determine maintenance and inspection intervals. It is also possible to predict operation with increased fouling or to predict the performance after cleaning to define the optimum point in time for shut down and cleaning intervals.

Using a digital twin, the operational state of control heating surfaces can be monitored. As a result, plant performance can be predicted for control heating surfaces on/off modes.

Example application

Figure 1 displays the data of a digital twin already installed in a nitric acid plant with two control evaporators.

Control evaporator heating surfaces can be switched into or out of operation to increase or decrease the process gas outlet temperature. Having a digital twin in place will allow the operator to retrieve the impact on plant performance based on the actual fouling of the heating surfaces. In this way, the best time to switch the operation mode of a control evaporator can be determined. The digital twin will not only give the operator information about the process gas outlet temperature but also about the impact on steam generation, steam control loops, and the oxidation rate.

In addition to the impact on the process gas outlet temperature, the impact on steam production will also be calculated for the different prediction cases. The operator will also receive information about the devices which are regulating the steam temperature and about the material temperatures in the steam temperature based on increased or decreased steam flow. Also, the material temperatures of the control evaporators will be monitored and predicted considering the different operational modes and process gas outlet temperatures which will vary over a certain number of campaigns due to increased fouling.

The values at the battery limits of the digital twin can be transferred to an overall plant simulation to get the full set of information on how a decrease in process gas outlet temperature may impact any tertiary nitrous oxide (N_2O) abatement or to evaluate the impact on the economiser due to increased boiler feedwater flow.

Post-oxidation in nitric acid plants

For the first digital twin application in heat recovery boilers of nitric acid plants, the DimBo calculation procedure had to be enhanced. Two different tools were formerly used for the design of such boilers:

- DimBo for the heat transfer calculation between synthesis gas and water/steam.
- OXY for the prediction of nitric oxide (NO) exothermal converted to nitrogen dioxide (NO_2) during the travel time of the synthesis gas from the burner/catalyst through the boiler.

Each calculation has a significant impact on the other calculation and therefore an iteration from one tool to the input of the other tool was necessary until the parameters became stable and a final result was achieved. Since this iteration with different tools and manual transfer of data between the tools is not appropriate for digital twin applications, the calculation of the NO to NO_2 conversion was integrated into DimBo.

This improvement, initially necessary for the digital twin, also provides a benefit for the interactive use of DimBo during the design phase of a corresponding boiler.

Moreover, based on this, it is possible to forward the information about the gas composition for different load cases and different operation modes to any abatement technologies downstream of the waste heat boiler to optimise the abatement by optimising the operational parameters.

Conclusion and outlook

Based on the above-described functions, digital twin technology offers operators the possibility to monitor plant condition, even for parameters which cannot be measured directly, and to identify causes of deviation in the performance at a very early stage. It can also be used for historical data to determine the remaining lifetime of the equipment or to evaluate the root cause of any failure.

This will result in more confidence about plant performance, an early detection of anomalies, longer lifetime, and less wear of the equipment.

There is also huge potential to transfer the technology to other types of plant. All forms of energy recovery from waste (WtE = waste to energy) or chemical plants promise high potential. Steinmüller Engineering is deeply involved in the development of digital twins in these areas. WF