Fraunhofer Center for High Temperature Materials and Design HTL

# Digital tools for the development of sustainable heating processes

Report on the project DiMaWert



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## 1 Executive summary

### F. Raether

Process heat accounts for by far the largest share of energy consumption in the manufacturing industry. In Germany, this share is 68%. These days, three quarters of process heat is generated from fossil fuels resulting in a very high  $CO_2$  footprint .<sup>1</sup> On the other hand, climate change requires efficient strategies to reduce overall energy requirement and  $CO_2$  emissions—not only in Germany but worldwide.

Digital methods, benefitting from increasing computing power, broad availability of artificial intelligence algorithms and large amounts of material data, provide numerous powerful tools for the development of heating processes with reduced carbon footprint. The present report describes such digital methods. They are embedded in a broader approach combining experimental and computational tools being based on Integrated Computational Materials Engineering (ICME).<sup>2</sup> The methods were developed within the project Di-MaWert<sup>3</sup> which was performed between May 2020 and April 2024 at Fraunhofer Center for High Temperature Material and Design (HTL) in Bayreuth (Germany).<sup>4</sup>

Figure 1.1 shows a survey of methods which are used at HTL to optimize industrial heating processes. The so-called digital furnace twin is of crucial importance for this task. It is mostly used for a systematic optimization of setting plans and temperature cycles. If required, the composition and flow of the oven atmosphere can also be optimized. Significant improvements of existing heating processes have been achieved. Due to the strong interaction of parameters, customary optimization tools are often less efficient in industrial heating processes. Using the methodology shown in Fig. 1.1, energy consumption and  $CO_2$  emissions are drastically reduced. Moreover, throughput can be increased or flexibly adapted to production needs. A special feature of our digital furnace twin is the interaction of the thermal management within the usable volume with the response of the charge (see Fig. 1.1). The reaction kinetics and thermodynamics of the charge are coupled to the local heat and gas transfer with the furnace, allowing proper consideration of gradients. This coupling significantly improves the validity of the simulation. It enables a prediction of product quality and the significant reduction of scrap rates.

To achieve the required accuracy, the digital furnace twin uses numerous input data from the industrial kiln, from the refractory materials and the charge. Furnace data can be complemented by mobile furnace testing equipment including an autonomous sensor module (ASM) (see Fig. 1.1).<sup>5</sup> Within the project DiMaWert, special sensors for harsh operating environments were developed for structural health monitoring<sup>6</sup>, key hole

<sup>&</sup>lt;sup>1</sup> Data from 2022: https://ag-energiebilanzen.de/

<sup>&</sup>lt;sup>2</sup> Olson, G.B.: Computational Design of Hierarchically Structured Materials, Science, 277 (1997) 1237 – 1242

<sup>&</sup>lt;sup>3</sup> https://www.htl.fraunhofer.de/en/funded\_projects/dimawert.html

<sup>&</sup>lt;sup>4</sup> https://www.htl.fraunhofer.de/en.html

<sup>&</sup>lt;sup>5</sup> https://www.htl.fraunhofer.de/en/ResearchAreas/thermal-processes/sensor-development.html

<sup>&</sup>lt;sup>6</sup> https://www.htl.fraunhofer.de/en/funded\_projects/dimawert/structural-health-monitoring.html

diagnostics<sup>7</sup> and temperature or gas analysis<sup>8</sup>. Material data are either obtained from data bases or from high temperature measurements on the considered materials. The latter are usually more accurate and more costly. Since many data are required for a realistic simulation, the number of high temperature measurements have to be limited. This is done by sensitivity analyses with the digital furnace twin. Sensitivity analyses make it possible to identify those material properties that have a significant impact on the results and are worth to be measured. A further reduction in measuring effort is obtained by an adequate—preferentially physical—parametrization of the material data. This parametrization enables an accurate interpolation and compensates random errors between individual data points (see Fig. 1.1).

The material data of the charge are obtained by special in situ measuring methods. These so-called thermooptical methods (TOM) were developed to measure reaction kinetics and other important properties during the heat treatment (see Fig. 1.1). Special lab furnaces have been constructed to reproduce exactly the atmospheres of the industrial furnaces. For debinding, sintering and melt infiltration processes sophisticated in-situ measuring methods and reaction models were designed. Other heat treatments like drying and graphitization are addressed in follow-up projects of DiMaWert.

The benefit of the digital furnace twin is closely coupled to the reliability of the simulations. Therefore, we attached great importance to the validation of the models. The reaction and the thermodynamic models were validated using the TOM furnaces. New test rigs have been constructed within the project DiMaWert enabling validations for the three mechanism of heat transfer: heat conduction, radiation and convection (see Fig. 1.1). The digital furnace twin was validated using various batch and continuous furnaces.

Thanks to the generous funding of the project DiMaWert (7 Mio.  $\in$  <sup>9</sup>), the dedicated commitment of numerous colleagues and the high level of optimization methods for industrial heating processes which had been already achieved before, HTL is excellently prepared for the improvement of many thermal processes. Numerous follow-up projects have already been started together with industrial partners. A great advantage of our methods for efficiency optimization is that they provide the probably fastest way to reduce manufacturing costs and CO<sub>2</sub> footprint of the energy-intensive industry without the need for any previous investment in kiln equipment. Thus, we are looking forward to assist the energy-intensive industry in strengthening its competitiveness on the world market by further applications of our methods. The digital furnace twin will be used in future projects also for a more precise control of heating power during operation of the furnaces and for the design of novel furnaces with minimal CO<sub>2</sub> footprint. Regarding the fluctuating energy supply by renewable energy, it enables the implementation of demand side management (DSM) in industrial heating processes without deteriorating the quality of the products.

<sup>&</sup>lt;sup>7</sup> https://www.htl.fraunhofer.de/en/funded\_projects/dimawert/optische-sensorik.html

<sup>&</sup>lt;sup>8</sup> https://www.htl.fraunhofer.de/en/funded\_projects/dimawert/autonomer-sensormodul.html

<sup>&</sup>lt;sup>9</sup> Compare chapter 6: Acknowledgements



Fig. 1.1 Interaction of methods for a high-quality digital furnace twin

Besides the furnace, refractories have a large impact on the  $CO_2$  footprint of heating processes. On the one hand, their production requires a lot of energy. So, their lifetime should be extended. On the other hand, their properties affect energy consumption during their use—especially heat capacity, thermal conductivity and emissivity. Within the project DiMaWert also methods were developed to assess existing and to design new refractories in terms of life time and thermal material properties. Applications are—among others—more efficient thermal insulations, lightweight kiln furniture and flexible resistance heaters.

The technical content of this report is structured as follows: The simulation and validation methods for the digital furnace twin are described in chapter 2. The reaction and thermodynamic models for the charge are presented in chapter 3. Chapter 4 discusses numerous methods for providing high temperature material data. Methods for the design of refractories are described in chapter 5.

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