Skräddarsydd värmebehandling genom digitaliserad processkedja -Digi3Gas

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Background

- A large amount of process data is generated during heat treatment.
  - Used to control the process
  - Not put together into a whole
- Digitalization has potential to result in better process control and lower consumption

- We wanted to demonstrate the potential of digital tools, methods, data management and machine learning algorithms based on production data from carburizing and neutral hardening.

About the project Digi3Gas

- Two-year project 2019-2021
- Financing: Vinnova, Strategiska innovationsprogrammet Processindustriell IT och Automation (PiiA)
- Participants
  - Bodycote, Sandvik, Epiroc, Calormet
  - Swerim, RISE, KTH

Processes

- Carburizing (Sandvik)
  - Tighter tolerance on case depths depth through better control and optimization of the process.
- Neutral hardening (Bodycote)
  - More even quality with respect to carburizing, decarburizing, and internal oxidation.

- Processes with carbon-bearing atmospheres
  - Control of atmosphere with oxygen probe

- Measurement of CO, CO_2, CH_4 (IR)

- A few hundred heat treatments were documented in each case

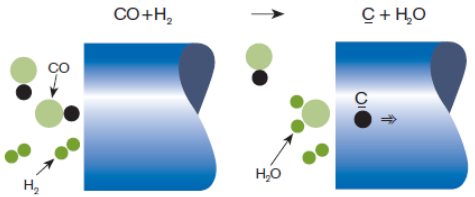
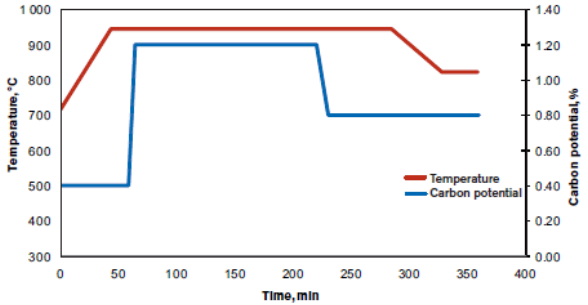


Figure 8.4.8 Principal reactions during case hardening.

Bild från ”Steel and its Heat Treatment – a handbook”

Data collection



- The furnace cycles were documented through available data from the control systems and production controls
- This included:
  - **Time series,** temperatures, Cp, %CO, $\%CO_2$, $\%CH_4$. Cp verified with dedicated samples
  - **Hardening response** (case depth, carbon profile, microstructure, internal oxidation, carburizing and decarburizing)

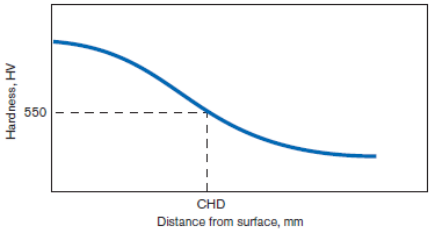


Figure 8.4.1 Definition of case hardening depth, CHD, according to ISO 2639.

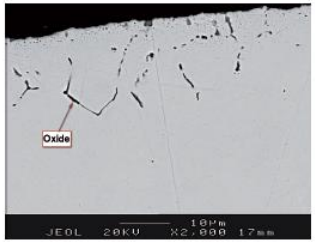


Figure 8.4.27 Internal oxidation. Backscatter SEM image of a polished sample.

Bilder från ”Steel and its Heat Treatment – a handbook”

Machine learning, tsfresh, manually selected features

- Collected data consists primarily of time series
- *Recurrent neural networks* and *Deep neural networks* could handle these directly
  - Very large amount of training data is required for these methods → not suitable
- Our datasets consists of only a few hundred individual heat treatments
- Solution: Represent the time series with a fixed number of **features** describing the **relevant characteristics** of the time series.
  - Manually selected featured based on domain knowledge, ~30-40 features
  - Large collection of standard featured produced by the python package
  - "**tsfresh**", ~6000-7000 features
  - approximation of the time series with polynomials

Examples of manually selected features

- During heating:
  - time to reach set-point
  - time to an extreme point (eg. temperature dip while charging)
  - the value in the extreme point
  - accumulated values of the difference to set-point.
- Holding time:
  - Time
  - Average
  - Variance
  - accumulated value above and below setpoint.
- This is done for temperature, Cp, %CO, %CO2, %CH4

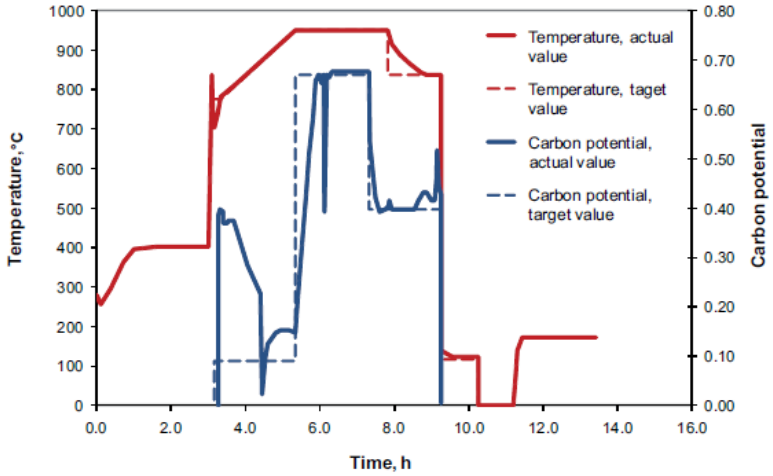
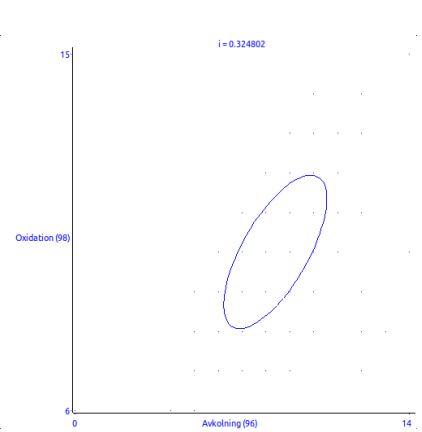


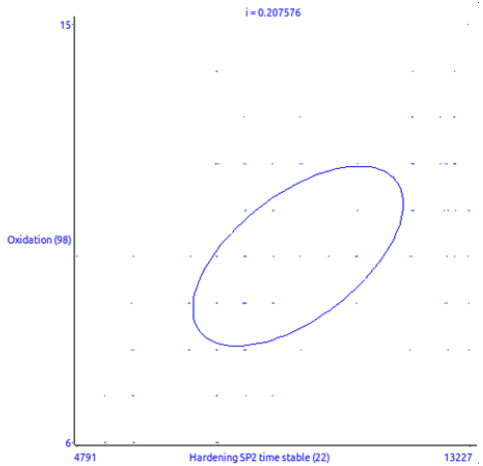
Figure 8.4.61 Registered process from preheating to washing. The red curve indicates temperature and the blue curve carbon potential. The set-points are the broken lines and the actual values are the solid lines.

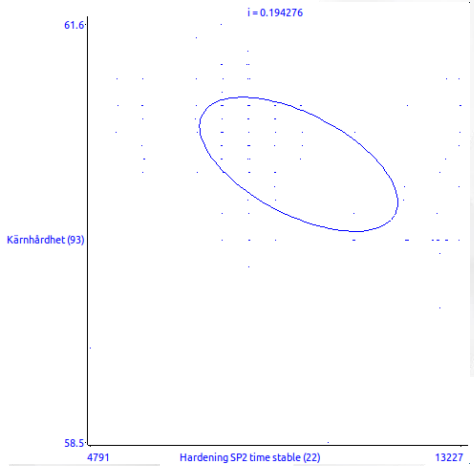
Bild från ”Steel and its Heat Treatment – a handbook”

Correlations, neutral hardening

Variabel 1	Variable 2	Mutual information	Correlation coefficient
Decarburication	Internal oxidation	0.3248	0.6912
Internal oxidation	HT time at stable phase	0.2076	0.5829
Core hardness	HT time at stable phase	0.1943	-0.5674

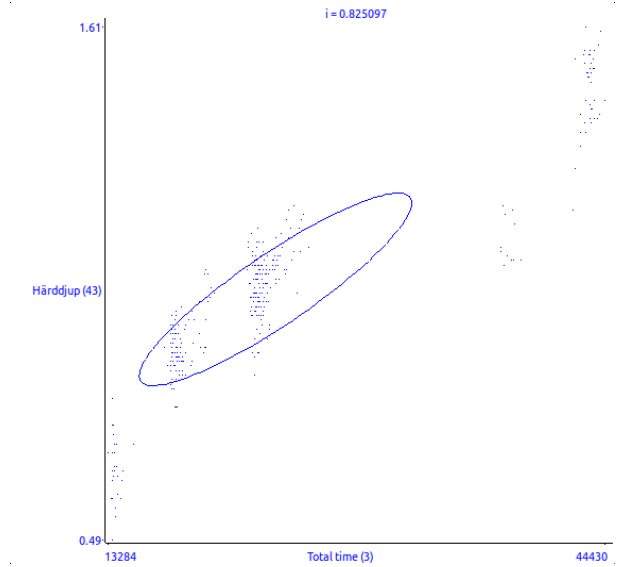


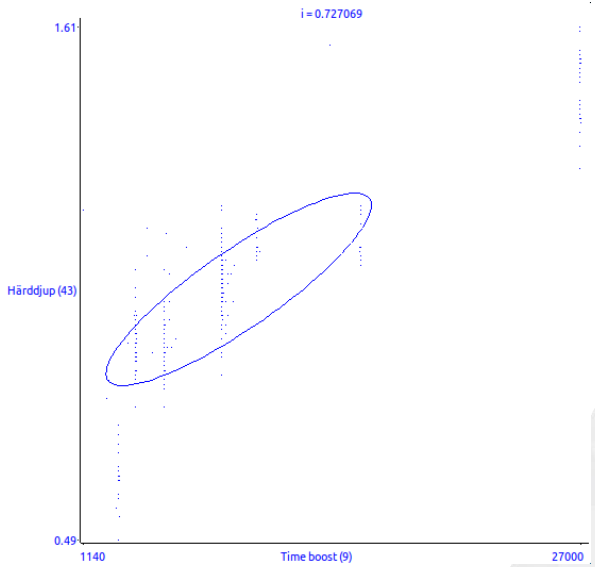




Correlations, carburizing

Variable 1	Variable 2	Mutual information	Correlation coefficient
Case depth	Total time	0.8251	0.8989
Case depth	Boost time	0.7271	0.8755
Case depth	Diffuse time	0.2198	0.5964





Weak connections are not a bad sign in themselves.

May instead mean that the control system is very good at controlling the process

Difficult to predict anything other than case depth in this case

Machine learning

- **Naive Bayes** - statistical machine learning method.
  - Assumes that the contribution of each feature to the case depth is independent of the contributions of the other featured. Continuously-valued featured were modeled with Gauss distributions, and for discrete features with discrete distributions.

- **Random Forest** - ensemble-method based on decision trees.

- **XGBoost** (Extreme Gradient Boosting) - ensemble-method which is based on a variant of decision tree, so-called regression tree, and the training involves “gradient descent” to reduce errors in each iteration.

- **Gaussian Process** is a statistical model based on the assumption that nearby data points probably have similar output values. How much the output value varies is regulated by a core function that one applies to each training example.
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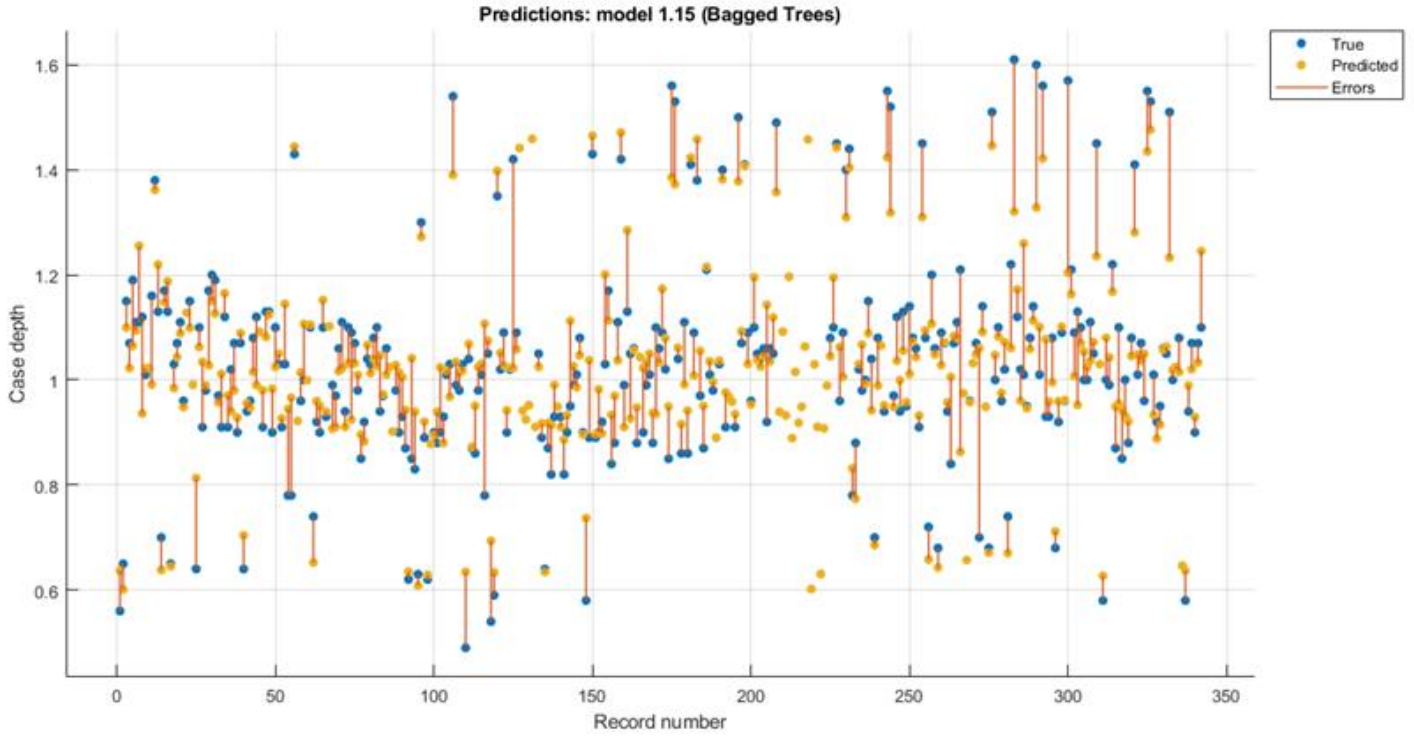
Prediction of case depth, Random Forest



Prediction case depth

RMSE (root mean square error) between predicted and measured value

Training data	Manual features	Automatic features	Polynomial-coefficients
Naive Bayes	0.07152	0.08527	0.16945
Random Forest	0.00965	0.03634	0.05266
XGBoost	0.02143	0.01821	0.02024
Gaussian process	0.05047	0.00408	0.05381

Test data	Manual features	Automatic features	Polynomial-coefficients
Naive Bayes	0.06022	0.06671	0.43510
Random Forest	0.05790	0.05825	0.05778
XGBoost	0.06097	0.07435	0.06738
Gaussian process	0.06196	0.17857	0.07705

- The best results on the test amount are, just below 0.06 mm in RMSE. The measurement precision of the case depth is about 0.05 mm. Thus, getting closer than this precision would only be pure coincidence.
- Random Forest is very good at training amount but shows tendency for overlearning

Alternative to machine learning

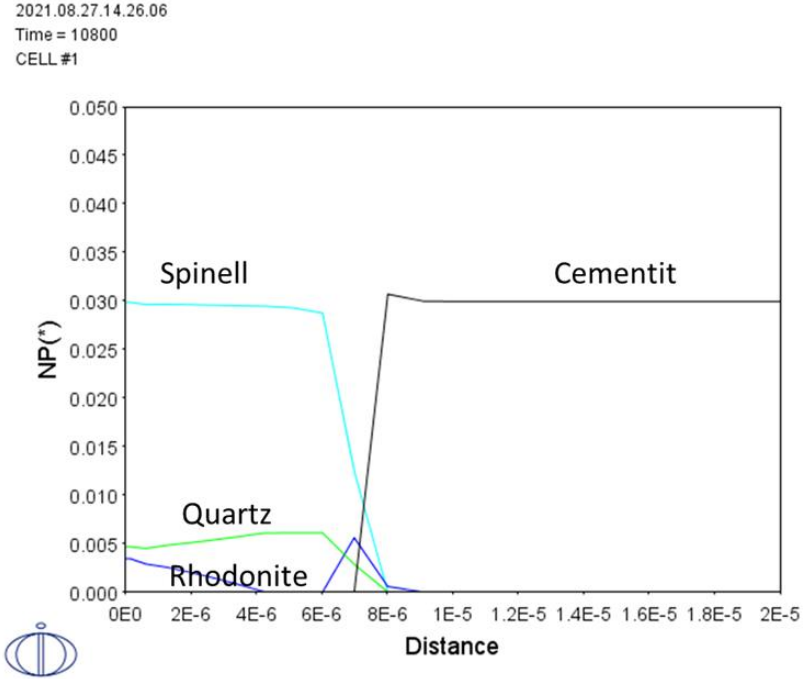
- **Simulate the process**, solve the diffusion equation
- Simulator was correlated against results from Ccalc
- Then used instead of machine learning
- RMSE simulator, test data = 0.0583
- The result is similar to the best of machine learning
- →**Machine learning and simulation can work equally as well to predict the case depth**.

Process control

- The prediction was tested to optimize furnace programs
  - Boost-diffusion cycle with different case depths
- Both ML and simulator worked well at 1 mm case depth (like in the experiments)
- Simulator worked better at lower case depths.
  - ML have a harder time extrapolating
  -
- **A simulator takes longer to construct, and longer time to run, but it can extrapolate outside the optimal range or be used in situations that have never occurred before.**

Decarburization and internal oxidation in neutral hardening

- From correlation analysis: correlation between decarburization and internal oxidation
- DICTRA-simulations for better understanding
- Comparison with measured concentration profiles (GD-OES)



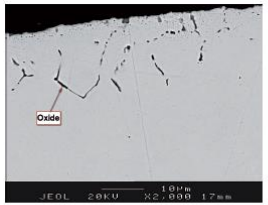
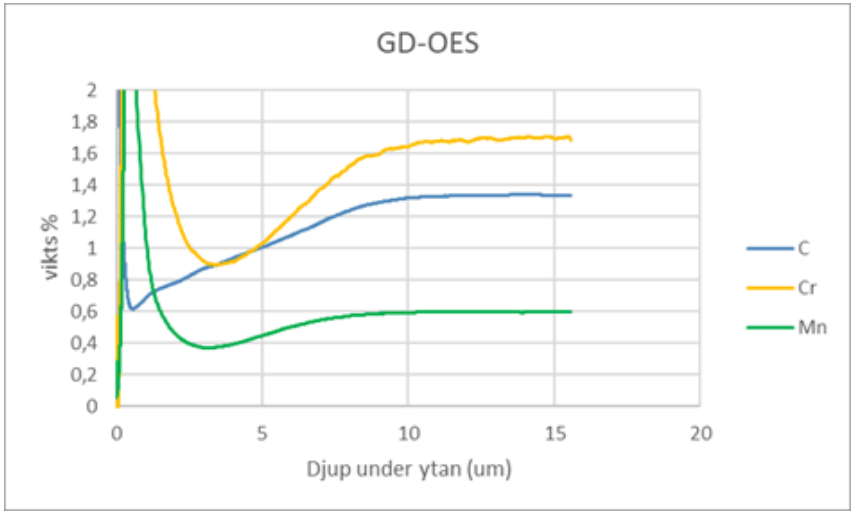
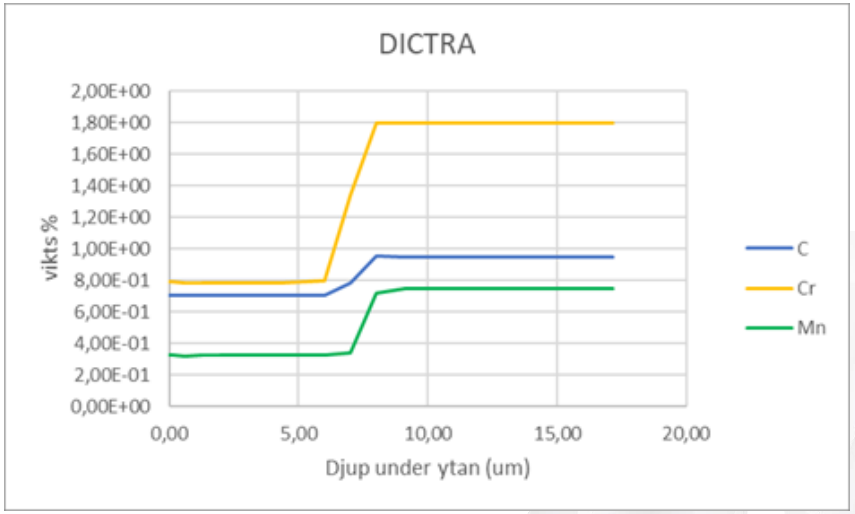


Bild från ”Steel and its Heat Treatment – a handbook”

Figure 8.4.27 Internal oxidation. Backscatter SEM image of a polished sample.

GD-OES compared to DICTRA





- Major similarities in concentration profiles

Conclusions

- **Machine learning** and **simulation work equally well** to predict case depths
  - error of the same order of magnitude as the error in the case depth measurement itself.
- **Simulation** on phenomenological/physical basis remains an important role in investigating, controlling and **predicting outside the known subspace of process data**.
- Only a few correlations could be detected
  - decarburizing - internal oxidation, case hardening depth – furnace time.
- Relatively rough quality measures are used (microstructure at scale 1-4) which is also operator-dependent.
- There are indications that decarburization in neutral hardening, which is observed as the absence of cementite, can be explained by internal oxidation.


SWERIM