Inverse Modelling as a Tool for the Optimization of Steel Production Processes

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ABSTRACT: Inverse process modelling is exemplified by the prediction of optimum cooling technology for sheet materials. The inverse modelling approach is discussed exemplary for the determination of optimized set values inside a spray cooling section. For steel grades requiring accurate temperature control, cooling section technology has to deliver prescribed cooling rates while fulfilling specific constraints, e.g. on the minimum surface temperature. The heat transfer coefficient (HTC) depending on the parameters water impact density V_s and the temperature difference ΔT was measured in the Laboratory while the desired final material properties determine temperature control and cooling rate. This information is used to predict the optimum cooling section set values for a specific cooling task. The inverse modelling calculations use a simple cooling section process model. Illustrative examples for optimum cooling of strip or sheet material using water spray cooling demonstrate the approach. Additionally, the specific problems of inverse modelling procedures (ill posed problems, computational complexity ...) are addressed.

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1. INTRODUCTION

parameters boundary conditions equations	(forward) model	results (field variables) measureable quantities
(design) parameters boundary conditions statistics	inverse model	measurement data model (to be validated) desired quantities

Fig. 1: Definition of inverse modelling.

Modelling in general and in particular metallurgical process modelling [23] deals with the definition and solution of a well defined mathematical problem. Inverse modelling may be associated with finding the problem definition for a specific or optimum solution (Fig. 1). Historically the term comes from the inverse heat conduction problem (IHCP [3]). Inverse process modelling has the following applications:

- Inverse measurement problems like tomography or parameter estimation [1], e.g. the calculation of parameter values minimizing the mean deviation between calculated and measured process outputs.
- Inverse design problems, e.g. the optimization of boundary conditions, geometry or process set values (as demonstrated in this paper).

A number of problems or properties are commonly related to inverse modelling:

- The problem is ill-posed, i.e. the assumption of a unique solution depending continuously on the data is wrong.
- The parameters to be determined are correlated or the sensitivity matrix is ill conditioned.
- Instability, i.e. details in the boundary conditions are smoothed out in the forward model (e.g. heat conduction), thus the inverse model amplifies small measurement errors to large artefacts.
- Missing robustness of the inverse modelling algorithms.

There are a number of methods to deal with these problems [22]. By the application of additional constraints biasing the solution the problem is regularized. The usage of an L1-norm reduces the effect of outliers in the data. Additionally, nonlinear inverse modelling may require multiple initial parameter sets for non convex problems and global optimization strategies.

As a conclusion, inverse modelling is best demonstrated by a specific example. The hypothetic optimization of an industrial spray water strip cooling section is chosen, because it is relatively simple and demonstrates the route from laboratory research to optimized plant set values.

In industrial steel strip cooling sections (see e.g. [6,12]) intend high cooling rates *CR* as well as some degree of temperature control. Due to the complexity of all water cooling processes - the realized heat transfer depends in a nonlinear way on surface temperature and cooling technology set values (i.e. the spraying intensity) – the application and set value determination is done experimentally by measuring the surface temperatures before and after cooling. The alternative approach of this paper is to make independent laboratory measurements of the heat transfer coefficients for a specific cooling technology and to use this data for cooling section process simulations. Such a numerical prediction of the set values required for a specific cooling task is demonstrated in this paper. For thick materials (shipbuilding- or offshore-plate and pipeline material), the surface and centreline temperatures differ significantly. As a result, this computational procedure can solve principal problems of the trial and error approach and address the requirements of modern steel grades [2,4,10]. The results allow cooling with locally well defined rates optimized for the desired microstructure [15,16].

Initially, summarized in the next section, the water spray cooling technology was investigated in the laboratory [24]. The result, the measured heat transfer coefficient (HTC) α is defined by the surface heat flux $q = \alpha \Delta T$. It is a function of water impact density V_S and the difference between surface and water temperature $\Delta T = T_S - T_W$. In the following section, these values are used for a cooling section process model. An inverse process model is presented and the physical limitations due to heat conduction and limited HTC will be discussed. The results demonstrate the numerical predictability of optimum cooling section set values as well as its physical limitations. The variation of the real cooling rates inside the material will be discussed. Finally, the approach is summarized together with some conclusions.

2. EXPERIMENTAL CHARACTERIZATION OF WATER SPRAY COOLING TECHNOLOGY

Spray water cooling offers a high degree of control and spatial homogeneity. Advantageously, there is only one major control parameter, the water impact density [5]. The large amount of literature on spray water cooling HTC measurements does not include an easy to use correlation for the complete $\alpha(\Delta T, V_S)$ function determined with a sufficient and specified measurement accuracy. The function $\alpha(\Delta T, V_S)$ was thus measured by a laboratory set-up [24]. The HTC measurements were carried out for the horizontal spray position (spraying downwards). In advance, the water impact density as a function of the nozzle-sample distance was determined for different nozzles. The values of V_S are accurate by ±8% ([24] and references therein). Full cone nozzles (Spraying Systems VKE6/60, VKE6/90 and VKE8/60) were used at spraying distances ranging from 62 to 105 mm. Droplet velocity and size distributions where not directly measured but obtained from correlations found in the literature [17]. For the spray parameters used, the average droplet velocity was calculated to be 14±1 m/s and the mean diameter is of the order of 350 ± 50µm. The accuracy of the HTC determination was 11%. We are not in the low HTC mist cooling regime [14,20], i.e. the droplets form a thin water film at the surface.

As a common experience [7], there is a superposition principle for the water impact density from neighbouring nozzles. The dependency of the HTC α on the water impact density V_S and the temperature difference ΔT is therefore sufficient to determine set values for spray water cooling – as exemplified below. The experiments provide the HTC for specific values of V_S as a function of ΔT , as shown in Fig. 2. Using all data from the measurements for the different values of V_S , a fit function $\alpha(V_S, \Delta T)$ was calculated [24]:

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$$\alpha(\Delta T, V_s) = 190 + \tanh\left(\frac{V_s}{8}\right) \cdot \left(140 \cdot V_s \cdot \left[1 - \frac{V_s \cdot \Delta T}{72000} + 3.26 \cdot \Delta T^2 \cdot \left\{1 - \tanh \frac{\Delta T}{128}\right\}\right]\right)$$
(1)



Fig. 2: Heat transfer regimes for spray water cooling (water impact density $V_s=10 \text{ kg/(m^2s)})$.



Fig. 3: Lines of constant HTC α in the ΔT - V_s plane for spray water cooling.

The contour plot of this function (Fig. 3) demonstrates a significant $V_{\rm S}$ dependency in the stable film boiling regime (see Fig. 2) not found in earlier investigations [9]. The nonlinear behaviour of the HTC is therefore described by a simple formula without the need to split the temperature dependency into different regimes. For a detailed discussion of the physical phenomena during cooling, we refer to the literature [24]. As shown in Fig. 2, the nonlinear behaviour implies an amplification of surface temperature inhomogeneities during cooling which are damped inside the material.

3. COOLING SECTION PROCESS MODELLING

The HTC function (1) allows a prediction of the results of a specific cooling procedure by mathematical modelling. Cooling section process modelling (see e.g. [8,21,26,27]) for homogenous cooling technologies like spray water cooling can be reduced to the solution of Fourier's second law in one space dimension, because in high throughput industrial cooling sections, the lateral heat conduction is much smaller than the perpendicular one $(\partial^2 T/\partial x^2 + \partial^2 T/\partial y^2 << \nabla \partial^2 T/\partial z^2)$ in the moving coordinate system). Without loss of generality, a constant temperature conductivity $a = \mathcal{N}(\rho c_p)$ can be assumed. Fourier's law thus reduces to: Proc. of the 3rd STEELSIM Conf., 8-10. Sept. 2009, Leoben, Austria

$$\frac{\partial}{\partial t}T(z,t) = a \cdot \frac{\partial^2}{\partial z^2}T(z,t)$$
⁽²⁾

The boundary conditions are $q = \lambda \nabla T$ specified at the upper and lower surfaces:



Fig. 4: Sketch of the cooling section described by the process model.

For the technological important case of homogenous cooling from both sides, the problem is equivalent to that with the centreline boundary condition q=0 solved for half the original thickness *d*. The basic input data for the process model is shown in Fig. 4: The strip (thickness *d*) enters with homogenous temperature T_{in} and speed v_{in} . In the cooling section, a water impact density $V_S(x)$ is preset. In the boundary condition (3), this is realized by using (1) with $V_S(t=x/v_{in})$. Without loss of generality, the value of $a=4.5 \cdot 10^{-6}$ m²/s is used throughout the calculations ($\lambda=20$ W/(m K), $c_p=560$ J/(kg K), $\rho=7874$ kg/m³). This value is representative for most low alloy steel grades around 700°C. Equation (2) is solved numerically, allowing for a straightforward extension of this work towards material properties depending on temperature and full 3-D calculations.

4. THE INVERSE COOLING SECTION PROCESS MODEL

The process model from the preceding section is able to calculate the temperature T(z,t) for a given set of nozzle parameters, i.e. for a given water impact density distribution $V_S(t=x/v_{in})$ inside the cooling section. The technological optimization task is different: The cooling section should cool down the material from T_{in} to $T_{out,Target}$ with a prescribed centreline cooling rate *CR*, a minimum allowed surface temperature $T_{surface,Min}$ and a maximum homogeneity of the cooling rate ΔCR throughout the sheet thickness coordinate *z*. This requires inverse modelling for the determination of an optimum $V_S(t=x/v_{in})$ -profile in order to reach these optimization targets.

Starting with an initial function $V_S(t=x/v_{in})$ (or $\alpha(t)$), the function sampling points are varied until an optimization target function f_{Min} reaches its minimum. The calculation of the optimization target function uses data from the numerical solution of (2). The simplex optimization algorithm [18,25] is used. The target function f_{Min} is defined as the sum of the scaled square deviations from the desired values for CR, $T_{out, Target}$ and $T_{surface, Min}$ and a measure for ΔCR obtained from the time derivative of the numerical solution T(z,t).

5. RESULTS AND DISCUSSION



Fig. 5: Maximum sheet thickness depending on centre cooling rate for different values of the HTC a (simplified calculation using $\kappa = 5 \cdot 10^{-6} \text{ m}^2/\text{s}$).



Fig. 6: Cooling curve of 30 mm sheet material cooled from both sides with a time dependent water impact density required for a centre cooling rate of 10 K/s (simplified calculation using κ =2.25•10⁻⁶ m²/s).

All calculations were carried out using Mathematica [25]. A general result from cooling section process modelling is shown in Fig. 5. For a specific set of material properties (e.g. $a=5\cdot10^{-6}$ m²/s), the centreline cooling rate depending on sheet thickness can be calculated for a specific value of the HTC α , which is assumed to be constant throughout the cooling section. There is a heat conduction limit, i.e. it is not possible to reach any desired value of the centreline cooling rate *CR* for any specific sheet thickness *d*. As an example, a centreline cooling rate of 50 K/s for a sheet thickness above ~25 mm is not possible for low alloy steel grades. For simplicity, in Fig. 5 the different cooling technologies are interrelated to representative values of the HTC α . Air cooling with $\alpha \approx 1..2$ kW/(m²K) for higher surface temperatures. At lower surface temperatures (near the CHF point in Fig. 2) and in the impingement region of water jets, values above 10 kW/(m²K) are possible [11,13]. Cooling technologies should reach high and homogenous HTC values as well as a high degree of HTC-controllability for a minimum deviation ΔCR throughout the material.



Fig. 7: Local cooling rate as a function of time and depth (surface: z=0, centre: z=15 mm).

Fig. 8: Calculated spray water impact density V_s depending on cooling time (or position in the cooling section at 1m/s sheet velocity) required for the cooling results given in figure 6 (30mm sheet cooled at 10 K/s from 900 to 500°C).

Within these physical limits, the optimum heat transfer coefficient depending on position in the cooling section can be calculated by means of the inverse modelling procedure described above. As an example, the task of cooling d=30 mm low allow steel sheet (a≈2.25·10⁻⁵ m²/s) from 900°C to 500°C at an average cooling rate of 10 K/s, as shown in Fig. 6, is obtained by the water impact density shown in Fig. 8. As shown in Fig. 7, the local cooling rate is always above the desired one near the surface after the start of cooling and below in the centre at the end of cooling. The compromise found by the optimization procedure can be adjusted by fine tuning the optimization target function f_{Min} . Higher cooling rates additionally imply a near surface self tempering at the end of the cooling during

temperature equilibration, i.e. a reheating of the near surface regions. Depending on the number of different cooling tasks to be fulfilled by a specific cooling section, i.e. the number of different V_s functions to be realized, and the number of real control variables (e.g. nozzle position or water mass flow rate), the cooling homogeneity can be optimized.

The minimization of the cooling rate deviation $\triangle CR(z,t)$ has physical limits. As an example, low alloy steel sheet material with 40 mm thickness can be homogeneously cooled at rates from 2-8 K/s. Above a cooling rate of \approx 8 K/s, the heat conduction limits the cooling rates in the centre, finally not allowing centreline cooling rates well above 10 K/s – even when much higher cooling rates at the material surface are reached.

6. SUMMARY AND CONCLUSIONS

This paper demonstrated inverse process modelling by the example of the prediction of optimum cooling technology parameters for steel strip cooling sections. Laboratory measurements of the HTC $\alpha(V_{S}, \Delta T)$ for spray water cooling finally provide cooling system set values $V_{S}(x)$, which can be translated to nozzle positions and water mass fluxes.

While a cooling section process model allows calculation of the temperature course for specific $V_S(x)$, the inverse process model allows the prediction of the optimum set values for a specific cooling task, i.e. hitting exactly the desired temperature course. This approach and the possible cooling rates in general are limited by the heat conduction required towards the surface of the material. The approach can be generalized to complex shaped bodies (e.g. rails or wheels) or continuous casting applications. Compared to conventional trial and error methods, the accuracy controlled laboratory HTC measurement provides the data required to predict cooling system set values for optimum plant configurations and process control.

The inverse modelling approach was exemplified as the link between basic research providing data from laboratory measurements and process models based on physics and the industrial application requiring set values and design parameters for specific applications.

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