Controlled Diffusion:

Quality and Process Optimization of the Heat Treatment

Summary of the innovative and adaptive control technology for the automatic creation of optimized treatment programs for diffusion processes.

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1. Introduction

Through case hardening, the structure of metal is changed to obtain certain characteristics. Due to the number of process parameters to be regarded in this process, it only can be realized with an innovative control technology. This technology saves time and expensive tests for the optimization of the heat treatment process.

demig Prozessautomatisierung GmbH offers a special program for the online diffusion calculation in the control system DE-VR 4008. The tasks of this expert system are as follows:
- automatic generation of optimal treatment programs
- adaption to the current treatment program during the process.
The recorded data are used in the proofing of material damages and for quality assurance according to DIN ISO 9000ff. This document describes the expert system.
It is possible to implement a simulation of the diffusion process in the supervisory system prosys/2. By means of this simulation, treatment programs for the control system may be created and their course may be simulated in advance. It gives a view into the result of the heat treatment. After the simulation, there is also the possibility of doing manual modifications in the automatically created program in order to influence the treatment process. A new simulation is possible at any time. After having obtained the demanded treatment process and the demanded result, the program data are transmitted to the control system. If the expert system exists in the control system, it undertakes the adaptive "online" regulation of the process. Otherwise, the process created in the supervisory system will be worked on statically by the control system.

1.1. Heat Treatment

For the different applications of metallic materials, certain mechanical characteristics that signalize their hardness, tensile strength, yield point, notched-bar test toughness or corrosion resistance, are essential. Special heat treatment processes change the material until the desired structure is reached. Knowledge about the structure in the balanced state (cooled down), the thermal conditioned processes and reactions that lead to a structure modification, are prerequisites to performing this process. In order to obtain a surface that is wear and corrosion resistant, with corresponding notched-bar test toughness, the surface just needs to be heat-treated. One of the most often used processes is case hardening. During the carburization phase of the process, carbon atoms are concentrated in the surface of the material (diffusion) after quenching to the required degree of hardness, without changing the original characteristics of the core.

1.2. Process Knowledge

The exact knowledge and reproducibility of this diffusion process are necessary to obtain the best material qualities. Several parameters (e.g. carburization temperature, duration and atmosphere (C-level)), in combination with the alloy components, the affinity with the diffusion medium, the specialties of the installation and the material geometry, are important for the result of the process. This complex process can only be realized with an innovative control technology. So-called “expert systems”, based on many years of experience, enable not only the input of all known information for the automatic program generation (process analysis), but they also adapt to the process during the process course. The recording and analysis after the treatment enable quality control, and are stored as additional experience for following programs.
Fig. 1: Description of the complete process

- **Conditions**
  (Analysis of the product characteristics, material composition and geometry)

- **Process Calculation**
  (Automatic generation of a treatment program, simulation of the C-profile (only with prosys/2))

- **Process Control**
  (Control of the process values, specification of the quality status due to the calculated C-level profile)

- **Manual Process Manipulation**
  (Manual Mode)

- **"Online" Adaptive Process Control**
  (Automatic adaptation of the treatment program by modifying the duration in the)

- **"Online" Process Monitoring**
  (Graphical and numerical presentation of the process values and the treatment characteristics)

- **Process Recording**
  (Preparation of the process values and the C-profile incl. storage in a data file)

- **Process Documentation**
  (Saved process data for quality proof)

- **Analysis of the modification and evaluation**
  (Method of treatment, system)
2. Description

The fundamental idea behind this expert system was to reach a high quality level with simplified treatment cycles, favorably priced technologies with high rationalization potential, and optimized utilization rates. It was important to find a procedure concept that would avoid long and expensive test series with different treatment programs, but which would also be able to constantly adapt to different conditions.

2.1. Before the Heat Treatment

2.1.1. Conditions

In the program creation for carburization and hardening of the material, the given data are to be analyzed first. In the example “Heat Treatment of Gears“, the task and its basic problems are explained in detail. The shown parameters are fixed in the corresponding program parameters of the process program, as the alloy components of the material to be hardened differ from material to material.

2.1.1.1. Setting of the Product Characteristics

First, the product characteristics have to be defined. The question is: which areas (tooth root, tooth flank or tooth peak) have the highest mechanical stress? Diffusion calculations are based on a permanent diffusion in plane surfaces. According to Fick’s law, the local concentration gradient (diffusion profile) is proportional to the number of atoms that diffuse in a certain time through a surface vertical to their flow direction. These conditions are valid for the tooth flanks of a gear.

\[
J = \frac{\partial n(x)}{\partial t} = -Dq \left( \frac{\partial c(x)}{\partial x} \right) \quad i = \frac{I}{q} = zF \frac{J}{q} = -zDF \left( \frac{c^0 - c^i}{\delta N} \right)
\]

1. Fick’s law. $J = \frac{\partial n(x)}{\partial t} = -Dq \left( \frac{\partial c(x)}{\partial x} \right)$; $i = \frac{I}{q} = zF \frac{J}{q} = -zDF \left( \frac{c^0 - c^i}{\delta N} \right)$
Here, the diffusion process is easily calculable. However, tooth peaks have large diffusion areas. Therefore, the problem of supercarburization may occur and possibly destroy the material. The tooth root is also a problem. Here, the areas for a permanent diffusion are smaller. It is possible that it will be carburized too little, and that the required wear resistance will not be reached after the quenching.

For a permanent carburization of problematic material, the following information may be entered into the program “online-diffusion calculation”:

a) As a correction factor for the wear criteria "tooth root", the temperature factor, diffusion factor or transfer factor may be needed. Values less than 100% influence the dwell time and the carburization temperatures. The adaptive process optimization uses these values as correction factors for the automatic creation of a treatment program. However, they are also used for the current calculation of the diffusion profile in the work piece (quality characteristic) during the heat treatment.

b) For the wear criteria “tooth peak”, other calculation data e.g. "C-level" as well as the carburization depth, are considered in order to avoid the supercarburization effect. There will be less carbide at a lower C-level content than at a higher C-level content.

2.1.1.2. Material Composition (Alloy Components)
For the diffusion process and its calculation and simulation (prosys/2), it is important to have information about the steel alloy components because they influence, among other things, the activity of the carbon in the steel.

Manganese and chrome, for example, reduce the carbon’s activity. Moreover, chrome decreases the critical cooling rate (increased heat transport in steel due to a smaller heat conduction coefficient $\lambda^2$), therefore reaching a more effective case-depth. Chrome, as well as molybdenum, forwards the formation of carbides. Manganese also increases the effective case-depth, but it does not forward the formation of carbides. The alloy components are indicated in percentages, but may be adopted for different standard steel alloys from a data base.

2.1.1.3. Carburization Temperature
Because of the solubility of carbon and iron, normally only temperatures in the austenite range are to be considered for the carburization temperature because of the “high” crystal structure in this range (cubic face-centered structure). The temperatures for the carburization are usually within the range of 900°C to 950°C. With rising carburization temperature, the diffusion speed increases and influences the growth speed of the layer to be carburized. By means of this procedure, the carburization process may be shortened, therefore saving valuable process time. However, the grain growth of the work piece is negatively influenced. For optimization, it is important to find a mean value.

2.1.1.4. Hardening Temperature
The hardening temperature is the temperature in the hardening procedure at which the quenching begins. Therefore, the temperature of the work pieces is to be cooled down to a lower temperature after the carburization process. The quenching speed of certain steels, starting from the essential higher “carburization temperature”, would be too slow to reach the required hardening process in the material. Moreover, there is the risk of crack formation and/or of stronger deformation in the work piece.

2.1.1.5. C-level at Carburization Depth (CD) and Surface C-Level
The effective case depth (ECD) is the distance from the work piece’s surface to the point where the hardening value of 550 HV (hardening test method according to Vickers) should be reached after

\[ \Delta T = \frac{A(x)}{s} \frac{\Delta T}{dx}, \text{ for balance (time independent: } t \rightarrow \infty) \]
the hardening process. This hardening value with a C-content between 0.3% and 0.5% (standard value 0.35%) is reached when the given quenching time is kept. The carburization depth (CD) is the set point for the depth in a work piece, where a certain C-level has to be reached (C-level at CD). This is in direct connection with the ECD when the hardening process is according to the given data (optimal quenching speed). If this is not the case, the ECD may move to higher limit C-levels. With the "Surface C-level“, the program calculates a diffusion profile under consideration of the already explained inputs. It may generate different diffusion sections within the process program.

2.1.1.6. Atmosphere Composition

The data of the atmospheric composition goes into the calculation of the C-level in the control system, as well as in the program creation. The measured value of the O₂-probe, along with the CO-analyzer, the thermocouples and other atmospheric values that are not measured by sensors, are very important for the C-level calculation. For the simulation of a created process program without sensor-measured process variables, as well as for the “online” diffusion calculation with controller without CO-analyzer, the indication of the atmosphere composition is necessary for the calculation of the carbon transition factor \( \beta \), which indicates the value for the carburization intensity. The composition is indicated in percentages or may be adopted directly from a data bank.

2.1.2. Process Calculation

2.1.2.1. Creation of Process Program

For the creation of a process program, the creation of a handling program is necessary first. This handling program may be created using the symbolic programming (DSP), which is very quick and easy. In the simplest case, three program sections are sufficient. In this example, every program section shows a process phase:

I. Preparation:

First, set the process phase to “prepare the furnace” for example, to heat the furnace to a certain temperature in order to start the carburization process. Set the data according to the
description of the operating instructions for the control system. The possibilities result from the particular configuration of the control system, which is individually created according to the individual furnace.

II. Carburization:
In the next step, the diffusion automatic is activated. Set points like temperature, section time and C-level may be set to 0. These values are automatically calculated from the previously inputted parameters. In case these values are not set to 0, the input values in the program will be selected from the values of the parameters.

III. Hardening and Quenching:
In the last step, the values for the quenching have to be set. These are inputted the same as in the first process phase. However, it is important to activate the diffusion automatic in only one program section - the diffusion section.

The handling program may be programmed as follows:

After the creation of the program, it has to be linked with a parameter set to a process program. This process program may be loaded in the working memory of the control system. The course of the process program may be as follows:
In this illustration, the red line shows the course of the programmed temperature set point, and the blue line shows the course of the C-level set point. All 3 program sections are shown, whereas in the diffusion sections, all set points are set to 0.

After the calculation of the diffusion sections, the set point course in this example is as follows:

This is the complete process program that is used as set point for the process. The example shows that 5 further program sections have been added. Thus in the parameters, a different hardening temperature is set than the carburization temperature. In section 6, you see a falling of the temperature set point down to the hardening temperature. From this temperature, the quenching starts at the end of the process program. This program is called "Program with temperature lowering". This problem has been already described in chapter 2.1.1.4.

If the hardening temperature and the carburization temperature are the same, only three program sections are added by the automatic diffusion calculation. This program is called "Program without temperature lowering". The course of the set points in this example – supposing all other parameters are equal - is as follows:
2.1.2.2. Determination of the Carbide Limit and of the Carbide Regulation

Carbides result from the carburization beyond the carbon saturation of work pieces, especially in the areas where large diffusion surfaces exist (compare example gear). They may destroy materials, and it is only possible to remove them with high heat-treatment efforts. There are different methods to avoid carbides:

a) Regulation of the surface C-level

This method measures the C-level in the work piece’s surface. The user has to set a carbide limit (max. allowed C-level content). That means the work piece is permanently controlled in the endangered range of developing carbides. This method reduces the process time due to the excessive C-level and the resulting accelerated diffusion process.

b) Regulation of the furnace atmosphere C-level

The expert system works with an atmospheric measuring method. That means that the special program with the input of the alloy factor, the hardening and the carburization temperature, and a carbide-factor\(^3\) calculate the work piece’s carbide limit. It also sets this value as C-level set point of the furnace atmosphere for the duration of supercarburization up to the switching point (C-level reduction). Practical experience and a great number of tests using work pieces different in size and alloy, have shown that the carbide-factor and the difference between atmosphere C-level and surface C-level of a work piece – depending on the alloy – keep the process in all cases below the dangerous carbide range. The process time will be calculated from the expert system.

2.2. During the Heat Treatment

2.2.1. Process Monitoring

By starting the process program, the actual values are controlled according to the set points and the program functions (control tracks). The current process variables are permanently prepared for a continuous control of the running process. Depending on the system and on the configuration, you may choose between visualization, numerical display, trend displays and different recorders. Manual interventions in the running process are possible at any time, as long as the user has the proper authorization.

\(^3\) Correction value depending on the alloy factor
Fig. 11: Functioning of the diffusion automatic

Start of the process

Calculation of the Quality Characteristics (diffusion profile)

C-level at CD fulfilled?

yes

Diffusion process will be interrupted

no

Switching point for C-level or temperature reached?

yes

no

Treatment program at the end of a diffusion section?

yes

Prolongation of section if necessary (if the process time is insufficient)

no

Treatment program finished?

yes

Heat treatment procedure is finished

no
2.2.2. "Online" Adaptive Process Control

In contrast to the standard process flow, where the process program may only be changed by manual interventions after the start, the tasks of the control system are extended by the integration of the automatic diffusion calculation. In the program sections that were programmed without diffusion automatic\(^4\), the control system leads the process by realizing section extensions with the help of limit values (bandwidths) and control tracks necessary for a process optimization.

In the sections with diffusion automatic created from the calculation of the process program, the control system calculates the current quality characters (diffusion profile) from the current process variables every minute. The diffusion profile is shown in the diffusion recorder "online" and intervenes adaptively according to the following criteria:

a) **The current calculation shows that the switching point for the reduction of the C-level and of the temperature has been reached.**

The switching points are the points (of time) in which the C-level is reduced in order to decarburize the surface zones, or in which the temperature is reduced in order to reach the hardening temperature. In the automatic program creation, these switching points are calculated from the input parameters. To reach the C-level at the corresponding carburization depth as soon as possible, the carburization takes place with a higher C-level value than needed for the surface C-level. That means that the C-level atmosphere in the furnace has to sink in the further treatment to decarburize the surface C-level to the required value. This switching point is calculated from the diffusion speed, the C-level in the furnace atmosphere and the fact that even after the reduction of the C-level, a diffusion of the carbon in the core of the work piece takes place within a certain limit. Due to disturbances, e.g. excessive temperature or C-level, this (switching) point may be reached ahead of the scheduled time. The control system recognizes this situation and changes the section times of the program. The section with the high C-level is now shortened so much that the program directly changes to the next section (reduced C-level value). The same procedure is done for reaching the switching point of the temperature reduction to the hardening temperature.

b) **The diffusion section of the treatment process is near at its end**

Just before the end of each diffusion section, the expert system again calculates the diffusion sections from the "online" diffusion calculations. System disturbances such as low C-level and temperature values which delay the treatment process, cause an extension of the current diffusion section. This diffusion section is calculated again and the section times are extended automatically. That means that the time section will be extended until the required treatment effect is reached. This procedure will be repeated until the heat treatment is successfully finished and the next step of treatment may follow.

c) **The carburization depth is reached**

If the permanent "online" diffusion calculations show that the optimal carburization depth has been reached because of unforeseen influences, the process will be immediately interrupted, independent from the current program status. At the same time, a treatment program is calculated and activated. Therefore, the heat treatment will be continued with the next step. This avoids exceeding the C-level in the carburization depth which may destroy the work piece.

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\(^4\) Only in the first and the last process phase
2.2.2. "Online" Process Diagram

The user may see the current status of the heat treatment at any time by means of the diffusion and temperature recorder during the running process. Depending on the installation type, the configuration of the control system and the requirements, all process variables and the current plant status are shown graphically and numerically. Therefore, the expert system provides the status of the heat treatment as diffusion profile (in the diffusion recorder) from the calculations that are made every minute.

2.2.3. Process Recording

a) The recording and generation of process variables will be done according to the aspects of process engineering, the requirements of the system and customer, as well as according to quality aspects.

During the recording, all data – directly measured process variables (actual values) and their according set points, as well as the current plant status - are stored on an internal data storage of the control system. These data may be additionally generated and stored by means of calculation algorithms (e.g. average of measured values of different charge thermocouples).

2.3. After the Heat Treatment

2.3.1. Process Documentation

Today, the process reconstruction is one of the most important quality criteria, and is also important for a faultless process run. These documents are important for the customers and for following departments (manufacturing). They serve as, among other things, the proof of material damages and as the possible resulting recourses of the customer. They are also valid for the rejections of lots in the stock receipt. Furthermore, they may be used for quality assurance and for error prevention tools, e.g. FMEA, as well as for quality audits.

Moreover, the results go in the modification analysis and cause - depending on the effort and importance – modifications of the parameter settings, of the process programs and of the composition of the atmosphere, as well as of the system parts like mechanic, measuring systems, control and, if necessary, modernization.
3. Simulation of the Treatment Run (only process supervisory system prosys/2)

In the modern quality assurance, error preventive measures are mostly used in contrast to the former “good/bad method” after the production. Therefore, the process programs generated from the system or manually entered are proofed before the treatment of the work piece starts by means of a computer simulation. This method offers the possibility to influence the process run by modifying the parameters.

After the selection of a process program, or after the combination of a handling program and a parameter file, the simulation of the diffusion may start. With the simulation, the expected diffusion profile is calculated and graphically shown from the parameters and the program data.

The curves are to be interpreted as follows:

- **Blue Curve:** core C-level in the material
- **Yellow Curve:** max. carbon profile in the material with initial supercarburization
- **Purple Curve:** actual carbon profile in the material
- **Red Line (vertical):** set point carburization depth
- **Red Line (horizontal):** C-level at carburization depth / CD C-level/ limit-C-level

Even during the simulation, it is clearly shown how to reach the required C-level content in the carburization depth (CD) – in an optimal (shortened) time – with an increased C-level, and how the C-level is reduced in the last step to decarburize the surface zone to the predefined value.

The simulation shows the course of the diffusion during the C-level superelevation and the course after the treatment with the reduced C-level. Now the expert may analyze the S-profile with the numerical data. In most cases, expensive tests may be avoided. For special work pieces e.g. single-part productions, tests are not possible.
The simulation will be done for an optimal process run. Disturbances, which may influence the heat treatment process, have to be recognized by the system, and they vary the time as well as the set points of the sections.

By means of the simulation, the process program will be extended by 3 and 5 program sections. They may be modified to reach another carburization profile. The modifications in the parameters and in the handling program may be shown graphically by means of a new simulation. After having reached the required result, the process program may be transferred to the control system. The adaptive “online” regulation now takes place as described below. By means of the supervisory system, it is possible to see the current recording data, as well as the program course in the control system.

4. Summary

The special program for the automatic diffusion calculation (optimization):

- **Before the Heat Treatment:**
  It automatically creates the process program by means of parameters, and simulates the diffusion profile of the process program (only process supervisory system prosys/2).

- **During the Heat Treatment:**
  It graphically shows the diffusion profile "online", and ensures the adaptive process control with automatic process program optimization.

- **After the Heat Treatment:**
  It allows the reconstruction of the heat treatment process from the recorded data.
# 5. Glossary

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition/Description</th>
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</thead>
<tbody>
<tr>
<td>Program</td>
<td>Program created by the user, which is processed step-by-step from the control system.</td>
</tr>
<tr>
<td>Visualization</td>
<td>Graphical display of the installation, including an overview of the most important</td>
</tr>
<tr>
<td></td>
<td>process values.</td>
</tr>
<tr>
<td>Carburization Depth</td>
<td>Vertical position from the surface of carburized work piece where the carbon content</td>
</tr>
<tr>
<td></td>
<td>reaches a defined limited value.</td>
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<tr>
<td>Treatment Program</td>
<td>see Process Program</td>
</tr>
<tr>
<td>Carbides</td>
<td>They come into being at the supercarburization of work pieces, especially in large</td>
</tr>
<tr>
<td></td>
<td>surfaces. They may destroy the material.</td>
</tr>
<tr>
<td>C-level</td>
<td>A controlled carbonic atmosphere created in the furnace. The C-level is the value for</td>
</tr>
<tr>
<td></td>
<td>the carburization effect of the carburization medium and for the carburization</td>
</tr>
<tr>
<td></td>
<td>atmosphere. It specifies the carburization potential in contrast to pure iron.</td>
</tr>
<tr>
<td>Diffusion Profile</td>
<td>Concentration profile of the carbon diffused in the surface of the material.</td>
</tr>
<tr>
<td>Effective Case Depth (ECD)</td>
<td>Definition of depth of the material to be hardened where the hardness has to be 550HV.</td>
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<tr>
<td>Hardness</td>
<td>The hardness of materials may be measured and defined with different methods. The</td>
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<tr>
<td></td>
<td>most commonly used methods are according to Brinell (HBW), Vickers (HV) and Rockwell</td>
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<td></td>
<td>(HRB, and HRC).</td>
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<tr>
<td>Notch Toughness</td>
<td>The notch toughness is a factor in the capability of material to absorb shocks and</td>
</tr>
<tr>
<td></td>
<td>impacts without breaking.</td>
</tr>
<tr>
<td>Core C-level</td>
<td>Existing carbon through alloy contents in the complete material before the</td>
</tr>
<tr>
<td></td>
<td>carburization.</td>
</tr>
<tr>
<td>Carbon Activity</td>
<td>Potential difference between the carbon concentration in the atmosphere and the</td>
</tr>
<tr>
<td></td>
<td>material to be carburized.</td>
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<tr>
<td>Carbon Transition Factor</td>
<td>Different carburization reactions run with very different speeds. In the description</td>
</tr>
<tr>
<td></td>
<td>of the carburization kinetic, all these reactions are mentioned and described with</td>
</tr>
<tr>
<td></td>
<td>the carbon transition factor $\beta$.</td>
</tr>
<tr>
<td>Carburization Profile</td>
<td>see Diffusion Profile</td>
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<tr>
<td>Manual Interventions</td>
<td>Intended manual modifications of the set point and of the actual value in the running</td>
</tr>
<tr>
<td></td>
<td>process.</td>
</tr>
<tr>
<td>Meta Stable Structure</td>
<td>No permanent structure of steel e.g. austenite. This structure changes after cooling</td>
</tr>
<tr>
<td></td>
<td>e.g. in martensite or bainite.</td>
</tr>
<tr>
<td>Numerical Display</td>
<td>Display of the current process data in numbers.</td>
</tr>
<tr>
<td>Diffusion Automatic</td>
<td>Permanent adoption of the current treatment program to the running process.</td>
</tr>
<tr>
<td>Program Parameter</td>
<td>Material data (among others alloy combination) of the charge and possible bandwidths</td>
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<tr>
<td></td>
<td>for the heat treatment.</td>
</tr>
<tr>
<td>Term</td>
<td>Description</td>
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<tr>
<td>Process Program</td>
<td>Loadable program in the control system. It consists of a handling program and a program parameter.</td>
</tr>
<tr>
<td>Yield Strength</td>
<td>This work piece-specific variable is analyzed in tensile tests.</td>
</tr>
<tr>
<td>Recordings</td>
<td>Graphical display of the recorded values of the current process. After the process, these data are stored and they may be printed out as quality proof or archived.</td>
</tr>
<tr>
<td>System Parameter</td>
<td>Parameters valid in each process program e.g. control parameters and endogas combination.</td>
</tr>
<tr>
<td>Trend Display</td>
<td>Display of the current comparison of the set point and the actual value and display as bar graph.</td>
</tr>
<tr>
<td>Supercarburization</td>
<td>The over-enrichment of carbon, danger of carbides.</td>
</tr>
<tr>
<td>Tensile Strength</td>
<td>The tensile strength of a material is the maximum loadable tensile stress (tensile force/surface), which may be defined by tests.</td>
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