Web-Based Data Mining for Quenching Analysis

Aparna S. Varde, Makiko Takahashi, Mohammed Maniruzzaman and Richard D. Sisson Jr.

Center for Heat Treating Excellence (CHTE), Worcester Polytechnic Institute (WPI),
Worcester, MA 01609.
(aparna | tmakiko | maniruzz | sisson) @ wpi.edu

Abstract

A Web-based Data Mining tool called QuenchMiner™ is being developed for the analysis of quenching data obtained from CHTE at WPI. QuenchMiner is incremental to QuenchPAD™, the existing Database System supporting the CHTE Quench Probe System. QuenchPAD™ stores experimental temperature-time data for metal probes quenched in liquid and gas based quenchants. The data is used to compute cooling rates and heat transfer coefficients. QuenchMiner™ is a user-friendly tool for querying and analysis. In addition to providing the features of QuenchPAD™ on the Web for worldwide access, QuenchMiner™ does decision making based on case studies and pragmatic knowledge. It utilizes the principles of Data Mining and Knowledge Discovery in Databases (KDD) for this purpose. It uses information from complex data types like graphs, pictures and tables, in addition to simple relational data types. It builds a Knowledge Base of Association Rules and paths for action. It computes suggested decisions in response to the user's scenarios in quenching. QuenchMiner™ provides at-a-glance information for quick and easy analysis, and serves as a Decision Support System (DSS) in heat treating at CHTE. It sets the stage for an Expert System.

Keywords

Quenching, Data Mining, Web Databases, Heat Treating, Materials, Decision Support System Knowledge Discovery in Databases.

Introduction

Quenching is the process of rapid cooling of a material in a liquid and/or gas medium in order to achieve hardening of the material. It forms the most important step of the *heat treating* operations in the hardening process [1]. There are several media used in quenching like oil, water, molten salts etc. Different *quenchants* have different cooling rates. Within each quenchant, cooling rates and heat transfer coefficients vary with temperature [2]. These variables, along with other quenching information, are used in heat treating analysis. A substantial amount of data is generated during the experiments carried out in quenching heat treatment. This is mostly temperature-time data. Some of it can be captured textually or numerically, while some being in the form of graphs and tables is relatively harder to store and query. There is also background information about experiments and about the quenching process in general.

The Center for Heat Treating and Excellence (CHTE) at Worcester Polytechnic Institute (WPI) has a Database System called QuenchPAD™, the Quenchant Performance Analysis Database [3] to store mostly textual and numerical data in a relational format. This forms the *CHTE Quench Probe Characterization System* [3]. The Database system manages the quenching information keeping it up-to-date with changes, and running the user's queries.

QuenchMiner™ is a tool that makes the features of QuenchPAD™ available on the World Wide Web, and in addition captures graphical, statistical and other complex data in relational formats. Moreover, it also supports decision making. It allows the users to submit certain scenarios and suggests solutions based on current information, history data and domain knowledge. QuenchMiner™ is inspired by Quench Characterization Systems as in [3,4].

Data Mining [5,6] is the process of discovering interesting patterns and trends in large data sets for guiding future decisions. It falls in the realm of *Knowledge Discovery in Databases (KDD)* [6]. Data

Mining techniques are used in our system to build the necessary rules that help make decisions. QuenchMiner™ thus provides a Web-based Data Mining [7] tool for quenching data analysis. It forms a *Decision Support System (DSS)* [8] for heat treating, with the targeted users being CHTE member companies.

Section 1 of this paper introduces the CHTE Quench Probe System and provides the motivation for QuenchMiner™. Section 2 explains how QuenchMiner™ makes the CHTE Quench Probe System accessible through the Web for Query Processing. Section 3 delves into managing the complex data types like graphs and tables. Section 4 describes the Decision Support functionality of QuenchMiner™ from the user's perspective. Section 5 outlines the details of the System Architecture for both the Query Processing and the Decision Support features. Section 6 explains the application of Data Mining principles in heat treating with a focus in quenching. Section 7 presents a detailed case study. Section 8 gives the conclusions and sets future directions for research to enhance QuenchMiner™ into an Expert System.

1. Motivation for QuenchMiner

The various components of the CHTE Quench Probe System are shown in Fig. 1. The QuenchPAD™ system that stores the CHTE quenching data is built using the commercial package MS Access[1]. The targeted users of the CHTE Quench Probe System may not always have the software tools used in CHTE, WPI. Security and protection issues related to the distribution of QuenchPAD™ are also concerns here. Moreover keeping the system up-to-date with the changes made by different users becomes harder since all the users are not accessing one central repository, but rather different copies of the software. Making the existing Database available in one Integrated Store accessible through the Web would solve these problems. This would also provide the required information at any place and any time.

Vast amounts of data are scattered all over the place in different formats. Experimental results, background data, and other information may exist somewhere, but may not be quickly and easily accessible. For example the user may inquire whether "*a polymer solution suitable for quenching of cast iron*" is available. The time spent in simply gathering this information from various sources could be effectively utilized for more productive tasks. Thus we need at-a-glance retrieval of data. This requires an Integrated Store and efficient querying techniques.

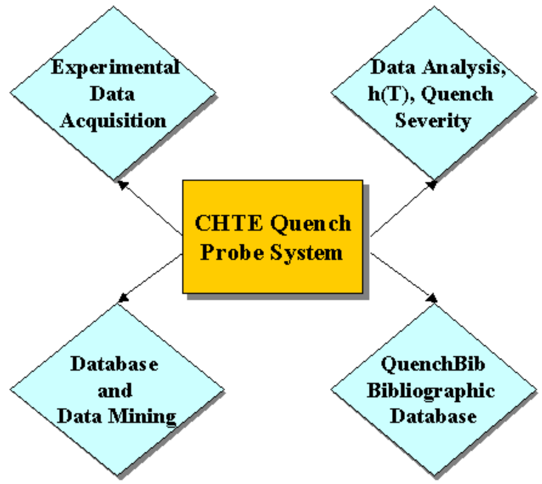


Figure 1: CHTE Quench Probe System

Certain types of data such as "the graph showing the cooling rate curve of a particular mineral oil based on the average of some experiments", or "a statistical table showing the standard deviation for a molten salt quenchant at a given temperature", may not even have been stored in a Database format. It could be raw data. It is helpful to have a customized repository of integrated information catered to the needs of the user. QuenchMiner™ provides this repository.

The users are likely to make decisions and plan for the future based on current performance. This brings us to the realm of Business Intelligence [9]. Consider the following scenario. "Distortion occurs during quenching and the user wants to make the appropriate decision(s) to solve the problem". QuenchMiner™ aims to automate the decision making facility by providing the user with a sample set of alternatives and the best strategy to adopt. In this scenario, the system would prompt the user for detailed input about the case, analyze the situation and suggest a solution e.g. "use a better quenchant or part alloy or carry out the quenching at a different temperature". The system would also give reasons for the suggested decisions.

[1] MS Access is a Microsoft product that serves as a Relational DataBase Management System (RDBMS) to store and query data.

2. Query Processing Feature

QuenchMiner™ makes the existing Database system available on the Web for worldwide access. An example of a QuenchMiner™ screen is shown in Fig. 2. The screen shown here allows the user to search experiments on quenchants, based on criteria like the name of the quenchant, the manufacturing company, the probe used in the experiment, the agitation of the quenchant, the oxidation on the probe, the cooling rate range etc. The user selects the search criteria through the form interface on the Web.

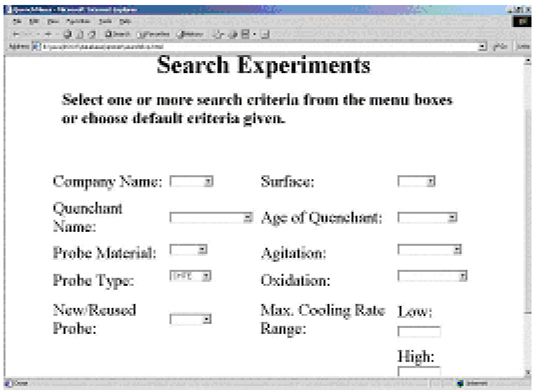


Figure 2: Search Screen in QuenchMiner

Results of the search are displayed to the user in tabular form. The user gets "Details" by further navigation from this screen. Details include the graphs plotted during the experiment showing cooling rate curves, heat transfer coefficients and other temperature-time data. They also show more information about the quenchant and the probe, and provide parameters useful for analysis. For details on the Query Processing functionality of QuenchMiner™, authorized users may refer to the MPI (Metal Processing Institute) Website (http://mpi.wpi.edu) to see a demo of its *alpha version* [2].

3. Managing Complex Types

There are graphs and tables built during experiments that depict important behavioral trends of quenchants. Figure 3 shows the cooling rate curve for a quenchant. Currently, this would be simply cut-and-paste into QuenchPAD™ or stored separately as an image file in a format like JPEG, or not stored at all.

[2] The alpha version is the first implemented version of a system with real data, i.e. a sample working system, subject to changes.

Figure 4 shows a table comparing the properties of different quenching oils. This, if stored, would be in the format of the software used to build the table e.g. MS Excel. Hence, the queries executed on the Database would not be able to directly access the information in the graphs and tables.

QuenchMiner™ aims to store the paths of these graphs and tables directly in the Database in one common server, to enable seamless querying using an Open Source Database like MySQL[10], speeding up and simplifying data retrieval. It also aims to allow users to automatically plot graphs by entering values of constants required in the respective equations.

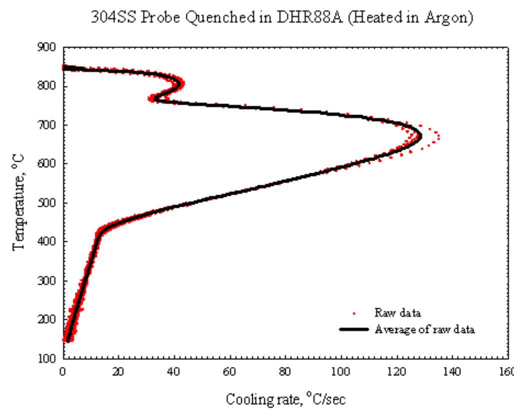
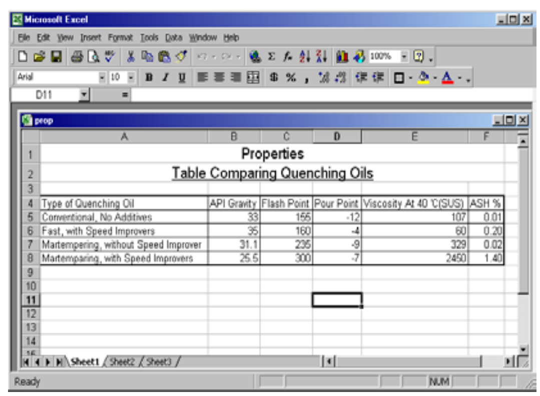


Figure 3: Cooling rate graph of a quenchant



Properties

Table Comparing Quenching Oils

Type of Quenching Oil	API Gravity	Flash Point	Pour Point	Viscosity At 40 °C(SUS)	ASH %
Conventional, No Additives	33	155	-12	107	0.01
Fast, with Speed Improvers	35	160	-4	60	0.20
Martempering, without Speed Improver	31.1	235	-9	329	0.02
Martemparing, with Speed Improvers	25.5	300	-7	2450	1.40

Figure 4: Table of quenching oil properties

4. Decision Support System

There are certain situations in which the user needs help in making decisions. Figure 5 shows an example of a Scenario Screen in the Decision Support System. This allows the user to select the case(s) for analysis. For example, we have a "distortion case", a "maximum heat transfer limit case" and a "quenchant type case". These form a very small subset of the numerous scenarios that can occur in heat treating.

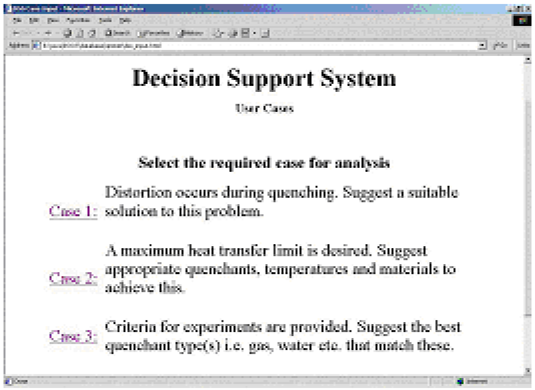


Figure 5: DSS Scenario Screen

QuenchMiner™ prompts the user for input on the selected case through an Analysis Screen. For example, in the "distortion case", it may ask for information about the quenchant and the part such as "quenchant agitation", "part orientation" etc. It uses Analytical Processing, Data Mining and Decision Support techniques [6,11] to break the given problem into sub-problems, use the appropriate rules and paths, consider the various permutations and combinations, and suggest the suitable solution(s). Knowledge Discovery in Databases (KDD) is extremely important here.

QuenchMiner™ gives its response through a Decision Screen. This shows the suggested decision(s) made by the system along with reasons. *The user may accept or ignore the decision(s)*. For example, in the "distortion case", the system may suggest, "choose another quenchant with slower cooling characteristics, because this would lead to more uniform cooling, thus minimizing distortion."

Authorized users may refer to the MPI Website (http://mpi.wpi.edu) for a demo of the *prototype*[3] of the QuenchMiner™ DSS.

5. System Architecture

5.1 Phase I

The first phase of QuenchMiner™ implements the Query Processing functionality. This involves seamless querying over simple and complex data types [10], including the features of QuenchPAD™ and more. Figure 6 shows the system architecture of the first phase.

The user submits a query through the Web Interface. This is transformed to the relational format "SQL" by the Conversion Unit, and sent to the Query Processor.

This interacts with the Integrated Store, a centralized RDBMS (Relational DataBase Management System) drawing information from multiple sources like QuenchPAD™, flat files, complex data types and raw data involved in quenching.

The Query Processor computes the result of the SQL query using data from the Integrated Store, and produces a result in SQL format. This in turn is modified to the format required by the user through the Conversion Unit.

The final output is displayed to the user via the Web Interface.

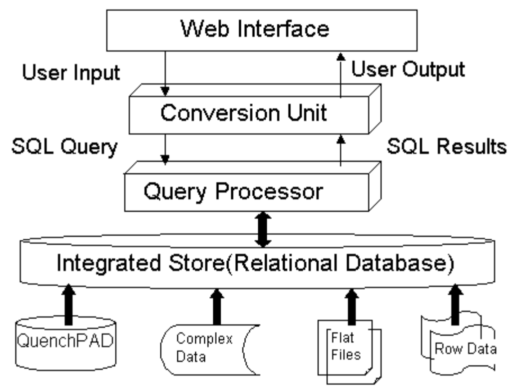


Figure 6: Architecture for Query Processing

5.2 Phase II

The second phase of the system is the one that provides the Decision Support [8,11] functionality. This includes three major components, a Decision Maker, a Data Miner and a Semantic Analyzer. The architecture for the second phase appears in Fig. 7. This architecture is subject to revision.

The user submits a scenario through the Web Interface. This is a plain-text description of the case. The system needs to understand the semantics of the information provided by the user based on the domain [12,13] and convert this into an appropriate form for analysis. This is the responsibility of the Semantic Analyzer. Its output is fed into the Decision Maker that interacts with the underlying RDBMS and Knowledge Base to obtain a sample set of decisions. The output of the Decision Maker is then sent to the

[3] A prototype is a working model of the system built with dummy data, to give the users an idea of what the system will finally look like.

Semantic Analyzer to get the Web output in plain text as needed by the user.

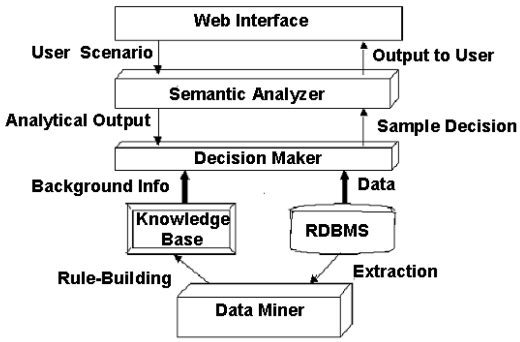


Figure 7: Architecture for Decision Support

6. Data Mining in Heat Treating

Data Mining consists of finding interesting patterns and trends in large data sets in order to guide decisions about future activities [5,6]. It is related to areas of Statistics such as Exploratory Data Analysis and fields of Artificial Intelligence [14,15] such as Knowledge Discovery, Expert Systems [16] and Machine Learning. In fact *Knowledge Discovery in Databases (KDD),* has become a subject by itself. KDD [6] consists of using the information from Databases to derive real world knowledge that is of interest to the user. For example, here KDD helps in the discovery of rules, trends and patterns in the heat treating domain, based on experimental data. KDD involves seven basic steps. These steps and their application in QuenchMiner™ are explained below.

6.1 Steps in KDD

1.Data Cleaning: The Database QuenchPAD™ and other data sources, may have missing entries, redundant tables etc. This needs to be fixed, so that values from all data entries can be used to draw inferences. Blank fields are populated with either null or average values. Cleaning also involves getting rid of duplicate tables, and using normalization [5] wherever necessary.

2. Data Integration: There are several sources of information like QuenchPAD™, picture files, graphs, tables, flat files, raw data etc. It is necessary to integrate the data from all these sources into one central repository.

3. Data Selection: This step identifies only those items that are relevant to the mining task. Applicable columns are selected from the Database, important tables and graphs in the system are chosen, and a decision is made on the best way to represent them.

4. Data Transformation: Irrespective of the form of the underlying sources, the Integrated Store must be an RDBMS (Relational DataBase Management System) [5]. This is a mini Data Warehouse or a Data Mart. Data Mining is easier and more efficient when done over a Data Warehouse/Mart [11].

5. Data Mining: It is very important to understand the relationships between the entities in the system, in order to guide the decision making process. Modeling the data is useful here. E-R (Entity-Relationship) models [5] are built from the Database tables. The Integrated Store is studied in detail to derive rules based on the information there. For example, on studying the quenchant information and experimental graphs, it can be inferred that "an excessively high cooling rate implies a greater potential for distortion'. Likewise, Business Intelligence [9] techniques are use to mine knowledge from the Integrated Store.

6. Pattern Evaluation: The data needs to be filtered after mining to identify patterns based on measures of interest. These measures are user-defined. For example, the relationship between "the agitation during quenching and the hardness of the material" may be of interest to the user, while a relationship between "the quenchant cost and the manufacturer" may be of no interest, depending upon the user's goals.

Among these steps, the most important is the actual Data Mining step. There are several techniques used in Data Mining such as Association Rules, Decision Trees, Clustering, Evolution Analysis, Outlier Analysis and more [6]. We discuss a few of these that we use in QuenchMiner™.

6.2 Data Mining Techniques

1.Association Rules: An Association Rule is a statement of the type, "X => Y" where "X" and "Y" are events or conditions [6]. The Knowledge Base in QuenchMiner™ has Association Rules built using Data Mining techniques. An example of a simple rule in heat treating is, "Non-uniform cooling => Greater distortion". There are more complicated *Conjunctive Association Rrules* [6] involving more clauses, e.g. "A and (B or C or D) and (not F) => X or Y", where each variable again represents an event/condition. These rules would in turn lead to paths that could be represented in the form of Decision Trees [6,17].

2. Decision Trees: A Decision Tree is a structure with a root, nodes, arcs and leaves, designed to represent the possible sequences of action that should be taken, on the occurrence of certain events/conditions [6,17]. A sample Decision Tree is shown in Fig. 8.

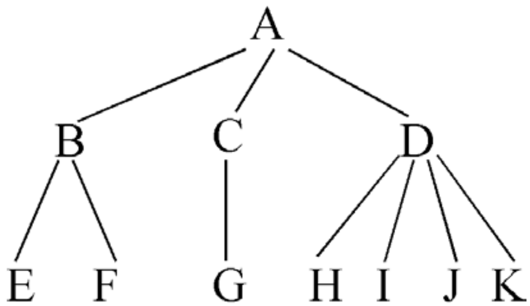


Figure 8: Decision Tree

This can be interpreted as: "if A then B or C or D, if B then E or F " and so on. Here "A" is the root node. This usually represents the problem under study. For example, in a "distortion case", the event "A" could be "the occurrence of distortion". "B", "C" and "D" are non-leaf nodes implying that they lead to further paths. They may represent sub-problems or sequences of action. For example, "B" could state "evaluate the level of agitation". The nodes "E" through "K" represent leaf nodes, i.e. they lead to the outputs of the system. For example, "E" could state, "reduce the agitation during the martensite formation phase". The arcs are the lines that connect the nodes, indicating the paths of action.

The depth of a Decision Tree is the number of levels in its longest path. The tree shown here is a very simple one with a depth of only 3. In practice, a tree for each case under study, would be deeper and more complicated, since several sub-problems and actions have to be considered.

3. Clustering: This is a technique used to represent information by maximizing intra-class similarity and minimizing inter-class similarity. Objects are grouped accordingly. For example, quenching experiments could be grouped based on the nature of their results, like the type of graph obtained. This gives the behavioral trends during quenching, thus helping in mining.

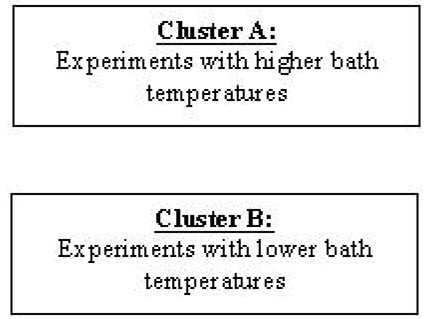


Figure 9: Clustering

Figure 9 shows examples of clusters in the heat treating domain. Here, Cluster A represents those experiments that have higher bath temperatures during quenching, thus lowering the characteristic temperature for heat extraction, and lengthening the vapor blanket stage, while Cluster B represents experiments with lower bath temperatures, thus in effect reducing the vapor blanket stage. This helps make decisions.

7. Case Study: Distortion Case

Distortion is one of the biggest problems encountered during quenching. Understanding its causes and effects presents an important case. A sample case study on distortion is presented here. Its steps include the application of Data Mining principles.

Following the example from section 1, the user's scenario is: "Distortion occurs during quenching. Suggest a suitable solution to the problem." In order to analyze this situation, the user's input is collected. This gives an overview of how the quenching was conducted. For example, information about the quenchant used in the experiment, the material of the work-piece and the quenching conditions is obtained. Once data specific to the given case is available, detailed analysis is performed to find out the exact cause of the problem. Accordingly, decisions are made about a suitable solution. There are various steps in this process. These are being incorporated at different stages in the design of QuenchMiner™.

7.1 E-R Modeling

To perform further analysis, it is necessary to understand the relationships between the entities in the distortion case. For example, consider a sub-case of distortion, namely "Bowing".

Problem: A flat and thin plate bows when it is quenched. Give suggestions to reduce bowing.

- *Suggest alternative alloys*
- *Suggest alternative quenchants*
- *Suggest quenching conditions*

User inputs: Quenchant, Work-piece, Conditions

Figure 10 shows the E-R model for the "Bowing" case. From here the following simple relationships can be inferred.

1. The quenchant cools the work-piece
2. The quenchant uses the quenching conditions
3. The quenching conditions control the quality of the work-piece

These set the stage for more detailed rules that are built later based on the behavioral trends during quenching. The E-R models help in further analysis.

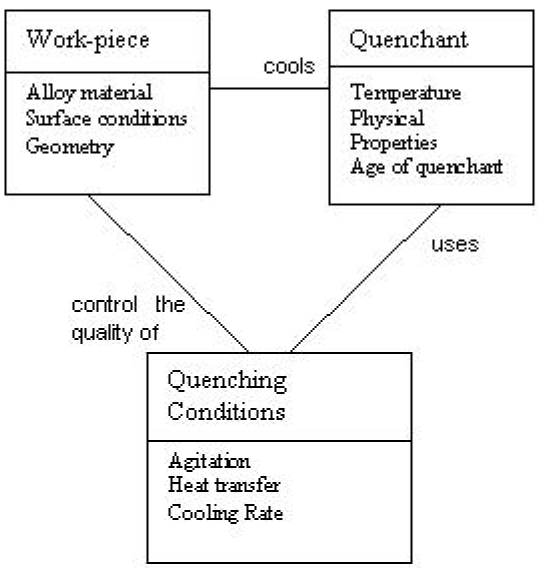


Figure 10: E-R Model for Bowing Case

7.2 Detailed Analysis

On examining the Databases and doing a literature survey in quenching, the causes of distortion are found. One important inference that can be drawn is, "An excessively high cooling rate implies a greater potential for distortion." Likewise, other factors affecting distortion are studied, and the mechanism of distortion is outlined.

Factors used to evaluate quenching conditions (thereby affecting distortion) [18] are listed here.

- Quenched Material: The behavior of the alloy varies depending on its chemical composition.
- Work-piece Design: This affects the uniformity of cooling e.g. the areas of the work-piece with thinner cross-sections cool faster.
- Orientation: The manner of placing the work-piece into the quenchant affects the distribution of heat.
- Quenchant: The characteristics of the quenchant affect the rate of cooling of the work-piece.
- Agitation: Greater agitation causes faster cooling of the work-piece.
- Surface Conditions: The roughness of the work-piece, and the presence of an oxide layer on the surface determine the time of breaking of the vapor blanket thereby affecting cooling rate. A very thick oxide layer however acts as an insulator, causing slower cooling.
- Racking/Fixture: The nature of the racks to store the work-piece affect the uniformity of cooling.

The mechanism of distortion [19] is shown in Fig. 11.

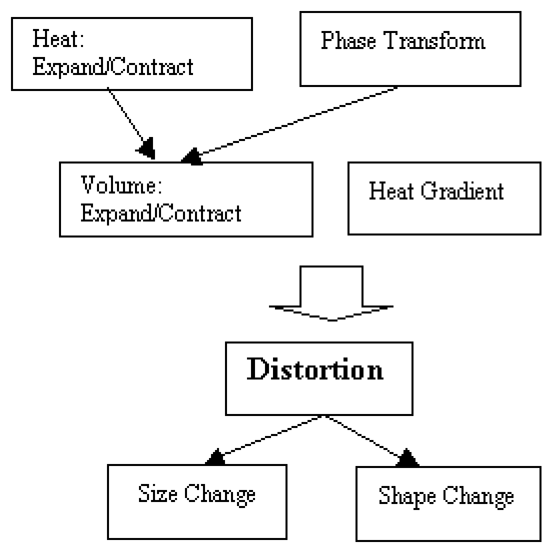


Figure 11: Mechanism of Distortion

The types of distortion in form are:

- Out of Bound
- Out of flat
- Bending
- Buckle
- Taper
- Dishing
- Bowing
- Closing in of bores

Further details on distortion are analyzed, and are used to populate the Knowledge Base with Association Rules and Decisions Trees that serve as the basis for the functioning of QuenchMiner™.

7.3 Populating the Knowledge Base

The Knowledge Base is built by extracting information from the Database. Data Mining principles are applied to understand the behavioral trends in the data. Association Rules are built to predict patterns of behavior. These serve as the basis for building Decision Trees that guide further courses of action.

Listed below are a few Association Rules relevant to the "distortion case." These are represented in the simple "X=>Y" format. They are categorized into rules based on the alloys used in the work-piece, on the agitation of the bath, and on the quenchant in the experiment.

<u>*Association Rules for Distortion*</u>

1.Based on Alloys:

a) *Higher carbon content => Greater potential for distortion*
b) *Greater difference between start and finish temperature of martensite transformation phase => Greater potential for distortion*
c) *Higher martensite transformation temperature => Lower potential for cracking / distortion*

2.Based on Agitation:

a) *Excessive agitation => Excessively high cooling rate*
b) *Insufficient agitation => Non-uniform flow of quenchant*
c) *Low agitation level during martensite transformation phase => Reduced cooling rate*
d) *Use of impellers => Better control over quenchant flow*

3.Based on Quenchant:

a) *Low Quenchant Temperature => Greater tendency for distortion*
b) *Use of water quenchant => Sharper cooling curve*
c) *Lower viscosity => Faster cooling rate*

These are just a small sample among the numerous Association Rules in QuenchMiner™. Association Rules represent tendencies while Decision Trees represent paths of action.

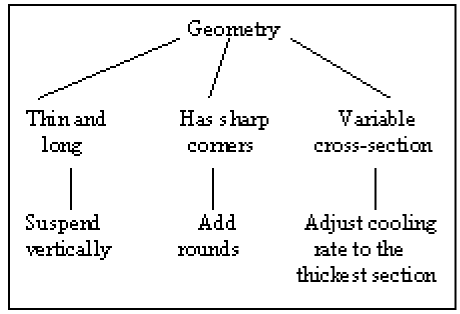


Figure12: Sample Decision Tree for Distortion

Figure 12 shows a small sample Decision Tree used in the "distortion case". The paths of action that can be inferred from this tree are self-explanatory. For example one path would be, "If the geometry of the work-piece is thin and long then suspend it vertically. This helps minimize distortion." Decision Trees and Association Rules are both fed into the Knowledge Base.

7.4 Flowchart for DSS

It is clear that the Knowledge Base provides the foundation for the computer program that runs the Decision Support System. For example, the "if-else" statements and the "switch-case" statements in a programming language like Java [20] would follow the logic of the Association Rules and Decision Trees. A flowchart is presented in Fig. 13 that summarizes the flow of the program for the Decision Support System. This flowchart is applicable only to the "distortion case".

The final output of the flowchart is based on the decision made after considering the conditions of each individual processing module. The whole combination has to be taken into account. For example, if the agitation is insufficient, the surface is rough, and the part geometry has variable cross-sections, then this combination implies non-uniform cooling, which leads to greater distortion. Thus the output suggestions in this situation could be as follows

- Use impeller stirrers for better agitation
- Polish the surface to make it smooth
- Adjust cooling rate to thickest section

Likewise the system would output different sets of suggestions, depending on different combinations of the processing conditions.

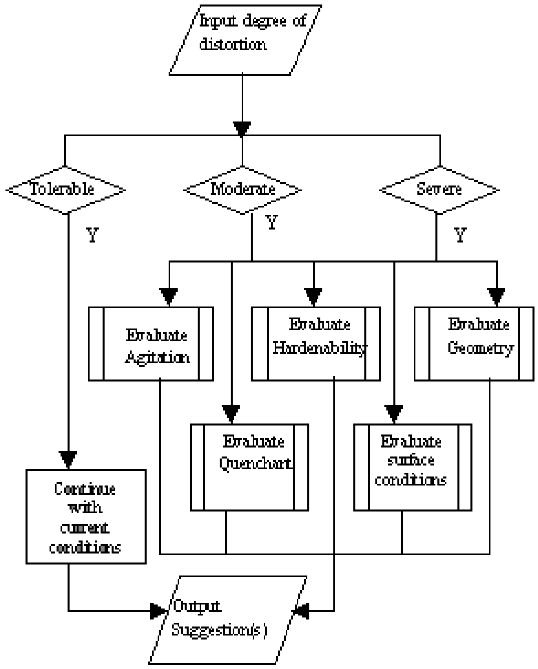


Figure 13: Flowchart for DSS (DistortionCase)

This flowchart represents a subset of the functioning of the Decision Support System in QuenchMiner™. The software for the DSS will be designed on these lines.

Thus, a detailed case study on the "distortion case" has been presented. It shows by example, the various stages of analysis and decision making in QuenchMiner™.

8. Conclusions and Future Issues

QuenchMiner™ is being built to serve as Web-based Data Mining tool. It makes the Quenchant Performance Analysis Database QuenchPAD™ available on the Web in a user-friendly manner, and does analysis and decision making based on the knowledge of the system, using Data Mining techniques. In addition to performing Query Processing over simple and complex data types, QuenchMiner™ also serves as a Decision Support System in heat treating at CHTE. The focus of this system is quenching data analysis.

Future issues include introducing Artificial Intelligence [14,15] features into the system like Neural Networks and Human Computer Interaction and building an Expert System [16]. This would make heat treating analysis at CHTE even more sophisticated.

Acknowledgements

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