



# Optimization of wear and cracks in roller contact under different coating and a range of loads and temperature with fixed speed using design expert (DOE) and finite element model

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## Abstract

Superior coating technology and roller materials such as M50 steels (0.8C–4.2Cr–4.3Mo–1V wt. %) and (1.0C–2.0Cr–0.5Mo–1.0Mn–0.5Si wt. %) are well recognized in modern technology. The aim is to present all the external and internal parameters that affect the rolling system by taking into consideration the microstructure importance in identifying the service life of such rolling technique. The most dangerous defects are the cracks and wear under high loading contact and temperature formed during the rolling process. Finite elements method was used to simulate rolling and to calculate the extensive wear in order to use DOE to optimize several conditions from coating to load and temperature. The analysis involved here used the steel rollers with and without coatings, which include titanium nitride (TiN), zirconium nitride (ZrN), and tungsten carbide (WC) under different temperature and loading conditions. Results showed that cracks propagation were limited to extreme load when using coating technology. Design Expert optimization confirmed that TiN and WC coatings would enhance the lifetime of rollers and inhibit cracks initiations and extensive wear that could results in severe plastic deformation.

**Keywords:** Roller Contact; Wear; Cracks under Extreme Load; Temperature; Design of Experiment (DOE).

## 1. Introduction

Rolling is one of the oldest industrial applications; first, it was used to bring water from the well through rollers and pulleys. Cracking and damage, which lead to extensive wear and failure, is the main purpose of his study to determine the rolling fatigue. Previous researchers showed that steel rollers and high-speed steel tools could be greatly improved when using metal carbide and metal nitrite coating or deep cryogenic treatment [1–4]. Rollers are widely used and factors such as loading, materials, and speed will affect their performances, since cracks and wear can lead to their failure and short-term liability and thus increase the cost on the industry (Figure 1). Crack initiation and propagation are sensitive to the microstructure, and coating will play an important role in resisting wear and cracks. Yet coating implimentation required substantial testing to validate the reliability of the materials used. Extreme pressure loadings and its contribution to friction, wear and failure using ball on cylinder tests and 4 ball wear tests were investigated earlier and found that tribofilm like coating adhering on the contact surfaces will protect the material from further deterioration and increase service life [5].

In this study we will determine the relative rolling contact performance of M50 (0.8C–4.2Cr–4.3Mo–1V wt. %) and (1.0C–2.0Cr–0.5Mo–1.0Mn–0.5Si wt. %) steels as a function of different materials and coating combinations using finite element model (FEM). Crack propagation, wear and displacement were investigated earlier by Monzer and Nehme and found that at certain loading contact coats such as WC (tungsten carbide) and TiN (titanium nitride) will protect the rollers from further deterioration and failure by minimizing the crack initiation and serve as buffer zone from further propagation. As a results wear was at minimum especially at lower loads between 1 and 2 kN and a temperature not exceeding 100°C. In order to address this complex problem, crack propagation and initiation, wear, and diaplacement will be investigated under different loading and temperature conditions by comparing extreme stresses with and without coating technology [6–7]. Afterward Design Expert (DOE) is used to optimize all factors presented in Table 1 in order to extrapolate the load and temperature until we see failure and high wear rate.

Design of Experiments in Product Design and Optimization is in contrast to the traditional approach that involves changing the characteristics of one factor at a time (OFAT) and examining the outcome. The limitation of this approach is the large number of experiments that are needed to evaluate a product and its inability to quantify two and multifactor interactions that may be both synergistic and antagonistic. Using a factorial design approach, all the variables are varied simultaneously in a predetermined fashion where it is possible to de-

termine how one factor influences the outcome when two or more of the other variables are varied at the same time. In addition, it is possible to determine the interaction between several factors simultaneously. This outcome would be impossible in an OFAT approach.

**Table 1:** Design Expert Table for Four Factors Representing Temperature, Materials, Coating, and Load and Three Output Responses Shown Below

STD TEST	RUN	Factor 1 A: Temperature 25-100 degree C	Factor 2 B: Materials: M50-100CrMnMo8	Factor 3 C: coatings: TiN-ZrN-WC	Factor 4 D: Load 2-4 kN	Response 1 Displacement mm	Response 2 Crack Length mm	Response 3 Wear Rate mm <sup>3</sup> /m
15	1	25.00	100CrMnMo8	WC: 8 μm (micrometer)	2.00	0.0944	0	7.35E-07
1	2	25.00	M50	No Coat	2.00	0.0511	0	0.012
25	3	25.00	M50	ZrN: 8 μm	4.00	5.02E-05	2.924	0.00092
32	4	100.00	100CrMnMo8	WC: 8 μm	4.00	8.332	0.0113	0.00438
22	5	100.00	M50	TiN: 8 μm	4.00	0.092	0.0233	0.00014
23	6	25.00	100CrMnMo8	TiN: 8 μm	4.00	5.29E-07	0	0.0645
9	7	25.00	M50	ZrN: 8 μm	2.00	4.30E-06	1.023	4.50E-06
14	8	100.00	M50	WC: 8 μm	2.00	0.61	0	3.77E-07
24	9	100.00	100CrMnMo8	TiN: 8 μm	4.00	5.29E-07	0	0.7182
30	10	100.00	M50	WC: 8 μm	4.00	3.15	0.023	0.000438
31	11	25.00	100CrMnMo8	WC: 8 μm	4.00	0.111	0	0.000492
4	12	100.00	100CrMnMo8	No Coat	2.00	0.101	0	0.019
21	13	25.00	M50	TiN: 8 μm	4.00	4.30E-05	0	2.04E-05
6	14	100.00	M50	TiN: 8 μm	2.00	0.0516	0	4.32E-06
20	15	100.00	100CrMnMo8	No Coat	4.00	0.929	0.098	1.012
12	16	100.00	100CrMnMo8	ZrN: 8 μm	2.00	0.01223	1.992	0.00334
19	17	25.00	100CrMnMo8	No Coat	4.00	0.201	0.075	1.14
3	18	25.00	100CrMnMo8	No Coat	2.00	0.00501	0	0.089
11	19	25.00	100CrMnMo8	ZrN: 8 μm	2.00	3.33E-06	0	1.47E-05
10	20	100.00	M50	ZrN: 8 μm	2.00	0.0196	1.933	0.000911
17	21	25.00	M50	No Coat	4.00	0.1022	0.0932	1.32
2	22	100.00	M50	No Coat	2.00	1.92	0	0.432
29	23	25.00	M50	WC: 8 μm	4.00	0.0433	0	0.00242
16	24	100.00	100CrMnMo8	WC: 8 μm	2.00	3.244	0.0022	3.77E-06
27	25	25.00	100CrMnMo8	ZrN: 8 μm	4.00	0.00422	4.335	0.00932
7	26	25.00	100CrMnMo8	TiN: 8 μm	2.00	1.13E-10	0	0.00166
13	27	25.00	M50	WC: 8 μm	2.00	5.32E-05	0	6.72E-06
8	28	100.00	100CrMnMo8	TiN: 8 μm	2.00	1.13E-10	0	0.0205
18	29	100.00	M50	No Coat	4.00	5.22	0.126	14.2
28	30	100.00	100CrMnMo8	ZrN: 8 μm	4.00	0.411	6.443	2.44
26	31	100.00	M50	ZrN: 8 μm	4.00	0.122	3.244	0.0123
5	32	25.00	M50	TiN: 8 μm	2.00	3.34E-07	0	8.21E-07

The efficiency of a factorial design approach is even more apparent as the number of variables increase. For example, a two level factorial design with four variables requires 16 experiments in a full factorial design. If replicates are needed 32 experiments have to be performed. However, in many cases fractional factorial designs can be developed to yield interactions with significantly fewer experiments. For examples, a half-factorial design for a two level with four variables requires 8 experiments. A factorial design is usually set up by first identifying the variables that need to be studied and the ranges over which these variables need to be studied. The choice of variables and their ranges is a critical factor in developing a good factorial design and eventual development of an optimized product. Each variable is assigned either a categorical or a numerical range. In cases where one of the variables is a type of material, it would be classified as a categorical variable and the two types of materials would be the variables used, in this case, the outcome will provide insight into one factor and multifactor interaction with this variable. In a numerical variable, the amount of a particular material is changed over a range of concentration and the outcome will provide insight on how the concentration of the variable influences the outcome as both a single factor as well as its interaction with other factors [8–9].

The aim of this study is to present all the external and internal parameters that affect the rolling system by taking into consideration the important factors in identifying the service life of such rolling technique. Then optimize the conditions for higher loads and temperature in order to verify the DOE results on MARC (Finite Element) and select the best coating for future rolling technology. Previously, experimental measurement was used to detect friction and non-metallic debris that leads to failure under certain loads [9-10]. Our research will focus on the importance of studying the effects of rolling contact in different industrial application and on increasing their service life by using the appropriate coating technology. Our goal is to present the variables that affect the rolling system in general (Table 1) and taking into consideration the load and temperature of such rolling technique.

## 2. materials and methods

### 2.1. Materials

M50 steels (0.8C–4.2Cr–4.3Mo–1V wt. %) and 100CrMnMo8 steel (1.0C–2.0Cr–0.5Mo–1.0Mn– 0.5Si wt.%) alloys [10] were the materials under investigation with and without coating, with the following properties:

**Table 2:** Roller Materials and Mechanical Properties

Material type	M50	100CrMnMo8
Hardness (HRC)	61	61
Young's modulus(GPa)	190	210
Poisson's ratio	0.28	0.30

Titanium Nitride (TiN) is one of the nanocomposite coating type is widely used in such application even if it is considered expensive material.

**Table 3:** Tin Coating Material and Mechanical Properties

Material coating type	Titanium–Nitride
Elastic Modulus (GPa)	340
Hardness Vickers (MPa)	2500

Zirconium–Nitrite (ZrN) is widely used today as coating layers in many mechanical parts, bolts, rings and medical equipments [9]. It is applied as coating layers on bearing and rollers.

**Table 4:** Zm Coating Material and Mechanical Properties

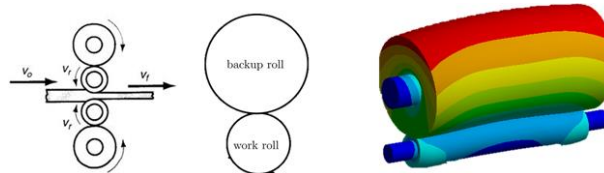
Material coating type	Zirconium–Nitride
Elastic Modulus (GPa)	320
Hardness Vickers (MPa)	1400

Tungsten carbide (WC) is a suitable hard facing material that commonly assigned because of good wettability, high hardness and wear resistance. It traces the good compatibility of tungsten carbide coatings in protecting engineering components that operates in severe environment [3], [11].

**Table 5:** WC Coating Material and Mechanical Properties

Material coating type	Tungsten –Carbide
Elastic Modulus (GPa)	250
Hardness(Vickers) (MPa)	1200

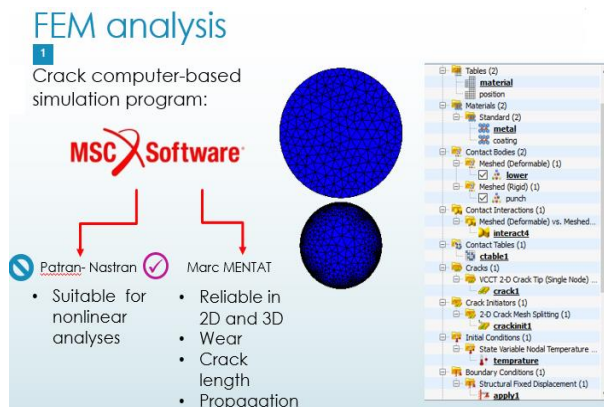
Roller materials with coatings are important to sustain high loads because of other factors such as yield stress and toughness. Coating becomes a leading research in the past 10 years. Cracks and wear resistance are the main factor for the roller failure. The nanocomposite coating layers consist of small grains size that prevent dislocation since the coating microstructure is much smaller than the length of the dislocation. Three different coating will be studied with the specific materials under different loading conditions using finite element simulations.



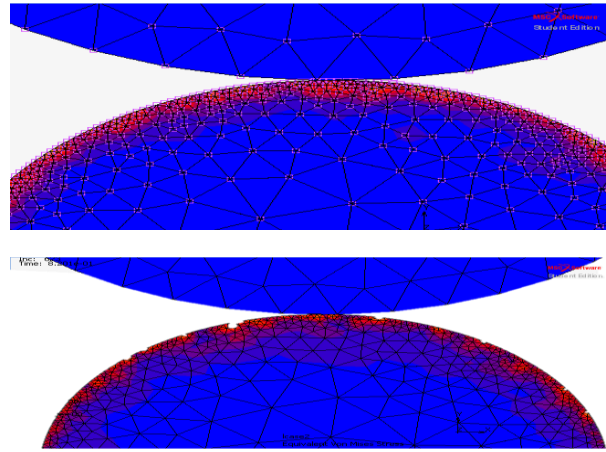
**Fig. 1:** Model Design Roller.

**2.2. Finite element methodology**

Many simulators such as MARC MENTAT represent finite element analysis in these rollers cases. MARC is an MSC software provided by the University of Balamand (Marc was the first commercial nonlinear finite element software developed by Marc Analysis Research Corporation founded in 1971 by Dr. Pedro Marcal). It is based on the analysis of nonlinear elastic study and its main features of cracking and failure [3], [12]. Three and two-dimensional finite element modeling can capture cracks and deformations that were not previously possible with conventional program. Our study focuses on providing a more realistic assessment of inclusion morphology and arbitrary orientations. The scaling of the finite element models has been optimized to capture the coating effectiveness as shown in Figures 2 and 3. To achieve this, two scales of geometric models were developed to provide the results before and after coating. In order to define our model in a appropriate way , we select two rollers with the dimensions ,elements types, and number of nodes shown in Table 6. The constraints were taken as 2 fix displacements applied on the middle nodes of both rollers. The first constraint moves the roller upward with rotation and the second rotates counterclockwise without any translation work. The compression load of the upper roller on the bottom roller varied between 1 and 4 kN.



**Fig. 2:** Flowchart for Finite Element Analysis Using Marc MENTAT for Steel Rollers.



**Fig. 3:** Finite Element Figures for M50 and 100crmmo8 Steel Rollers at Lower Loads (2 Kn) and 100°C with WC Coating.

**Table 6:** Roller Dimensions and Finite Element Nodes and Type

Upper Roller diameter	15 cm
Bottom roller diameter	10 cm
Roller length	20 cm
Number of elements	2700
Number of nodes	2590
Element type	Quadratic
Number of roller	2

### 2.3. DOE Optimization

After conducting several experiments related to the stated variables in Table 1, we used Design Expert to analyze the responses by using the half-normal probability chart and the analysis of variance (ANOVA). Changes were calculated for higher load and temperature and charts that could predict failure for the rollers when using different coating under higher temperature and loads were presented. Once the important variables were identified the interaction between these variables were determined using the Response Surface Method (RSM) method. This method is particularly useful in systems where a curvature is expected in the response, i.e. regions where optimization of the variable can lead to an optimized response. We use both the interaction plot and wireframe plots to show how an outcome is dependent on two variables. Both plots are useful in identifying the optimum numerical or categorical variables to arrive at the desired outcome. Then cracks performances or relative wear resistances of M50 and 100CrMnMo8 materials were reevaluated using FEM model under the optimized higher load and temperature in order to verify the DOE calculation and plot the figures.

## 3. Results and discussion

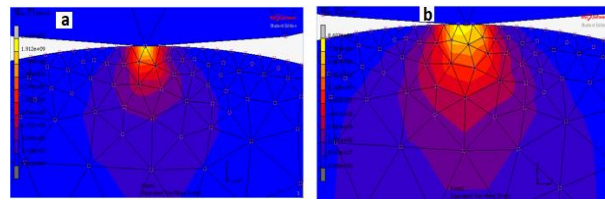
### 3.1. Finite element results before DOE optimization

In rolling contact, due to high fatigue cycle leading, the Von-Mises stress surpass the yielding strength of the materials. What differentiates the rolling contact from other fatigue analysis is that it results in high shear stress on the surface level and thus adhesive wear takes over where pulled out materials and cracks will initiate extensive wear in addition to 45-degree tip crack as shown in Figures 4 and 5 especially at 4 kN load. After the tip crack, the propagation of the crack continues to reach certain length in deterioration. In most case, the crack initiation and propagation should not exceed certain length depending on the materials. When the compressive stress on the roller exceed its peak of 4 KN, the molecules become smaller in size and its effects on the dislocation of atoms (which occurs under continuous rolling condition) that could resist external forces will diminish. On the other hand, the material structure inside the body can cause the crack to change its direction easily and progress at approximately 45° that fluctuates depending on the load and the coating condition. Wear was calculated automatically via software using the wear (W) rate equation:

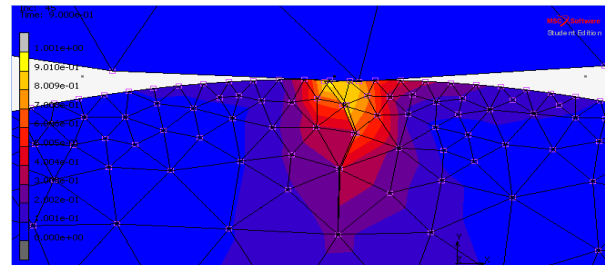
$$W = \frac{KPL}{H} \quad (1)$$

Where: W –wear rate is the total volume of wear per unit length; K– is a dimensionless constant; P– is the total normal load; L– is the sliding distance; H– is the hardness of the softest contacting surfaces [12].

The data in Table 1 indicated higher displacements and larger cracks at extreme load conditions with and without coatings. The performances of the materials with and without coating are related to their mechanical properties features, which were compressed under different conditions in order to understand the observed phenomena. As indicated, carbided and nitrided coatings played different roles in preserving the material structural integrity under higher loads. According to Table 1 and Figures 4 and 5, lowering the compression load promotes less displacement and render cracks negligible especially with titanium nitride and tungsten carbide coatings. Therefore, these phenomena were optimized using Design expert at higher temperature and loads.



**Fig. 4:** Crack Initiation and Propagation at A Load of 2 and 4 Kn Represented by A and B Respectively for An M50 Roller Without Coating Under A Temperature of 100°C.



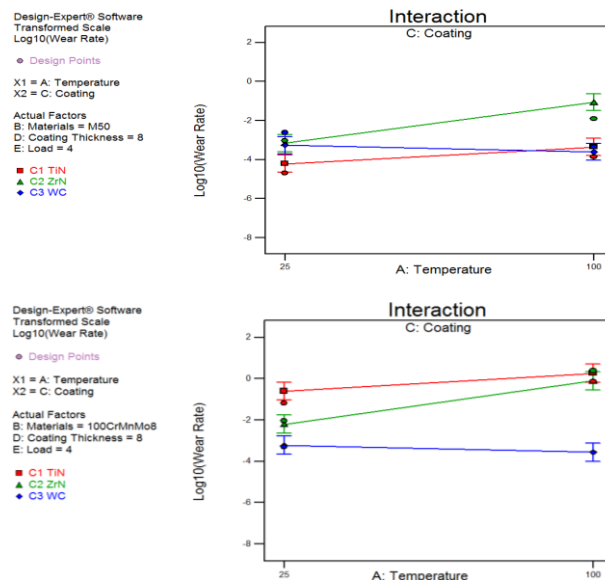
**Fig. 5:** Crack Initiation and Propagation at A Load of 4 Kn for an M50 Roller Coated with WC Under A Temperature Is Kept at 100°C

### 3.2. DOE optimization

DOE 3D plots and factors interactions were used to predict the behavior of materials and coatings under high temperature and extreme loading before failure. Wear rate response Figures were chosen since cracks will be directly affected by higher wear rate. Figure 6 shows two different rollers materials with three different types of coatings. Design Expert optimization showed that there is an increase in wear rate when the temperature goes up to 100°C. DOE analyzes of the data in Table 1 showed some cases of nonlinearity, but it will assume that it is not that important and does not increase the statistical error; therefore, these charts will show the interactions at different level of temperature with respect to the materials used in the analysis.

It is also confirmed in Figures 6, 7 and 8 that failure happened in both rollers when load is increased to 6 kN and temperature to 160°C. It also show that WC performs better in both rollers under higher loads (Figure 6) where ZrN does not preserve the 100CrMnMo8 roller structural integrity at these loads and temperature (Figure 8). TiN performs better when using M50 steel rollers (Figures 6 and 8). It is also concluded that wear rate will increase tremendously when the load exceed 6 kN but the temperature will not affect the structure much when increased, especially when using WC coating.

The central theme of all these plots are the following: (i) without any coating there is no preservation of the structural integrity of the rollers at extreme loading. (ii) Temperature effects in steel rollers is minimum when compared to increased loads. (iii) There is a synergistic interaction between coating and steel rollers at higher load and temperature and WC provided more protection as shown in the DOE Figures. These results indicate that TiN, ZrN, and WC while good protectors at certain loads their benefits will diminish at increased pressure. The wear is not at all within the limits when using ZrN (Figure 8).



**Fig. 6:** Design Expert Interactions of M50 and 100crmmo8 Steel Rollers for the Wear Rate Response with Different Coating at 4kn Loading and Temperature between 25 and 100°C.

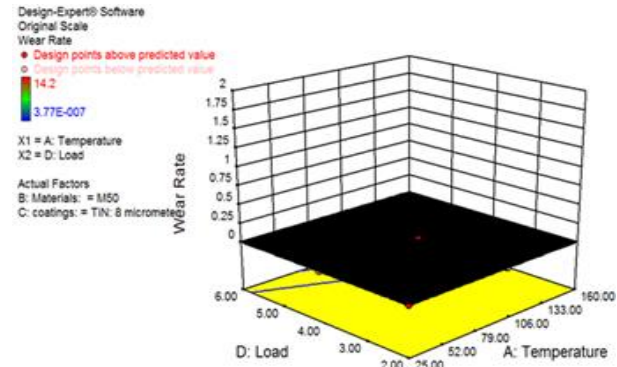
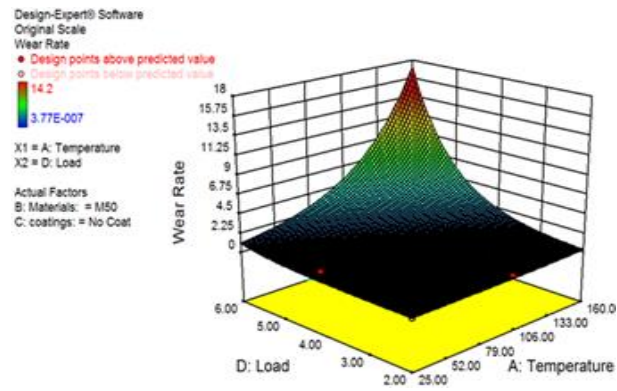


Fig. 7: A) Design Expert Response Surface Diagram of M50 Steel Roller with and Without Coating under A Higher Load and Temperature of 6 KN and 160°C for the Wear Rate Response. They Represent the No Coat Roller, and Tin Roller Respectively.

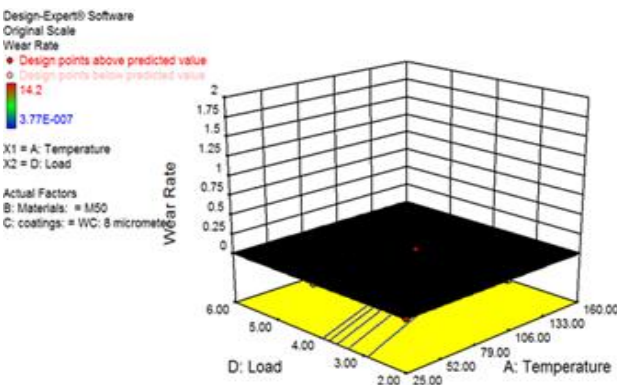
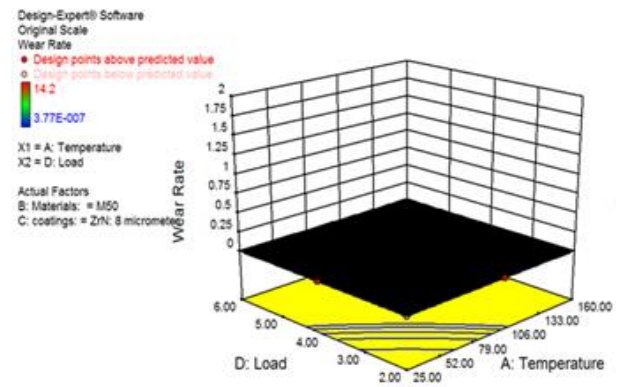


Fig. 7: B) Design Expert Response Surface Diagram of M50 Steel Roller with and without Coating under A Higher Load and Temperature of 6 Kn and 160°C for the Wear Rate Response. They Represent the Zrn Roller and WC Roller Respectively.

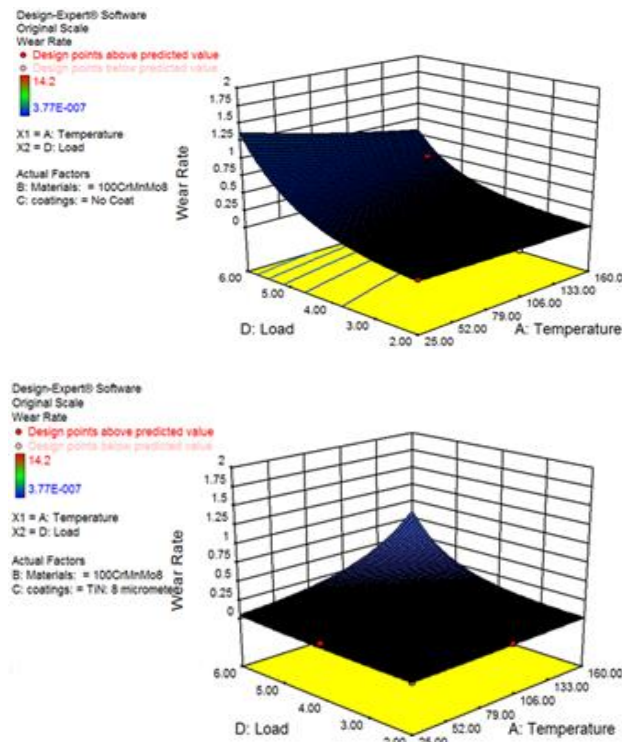


Fig. 8: A) Design Expert Response Surface Diagram of 100crmnmo8 Steel Roller with and Without Coating under A Higher Load and Temperature of 6 KN and 160°C for the Wear Rate Response. They Represent the No Coat Roller, and Tin Roller Respectively.

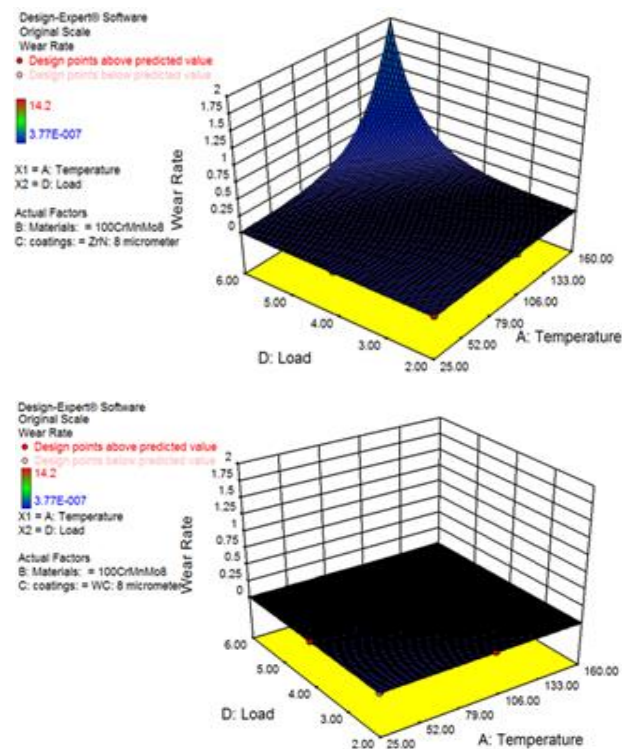
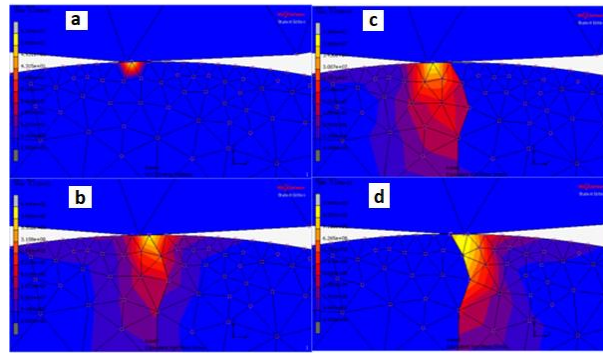


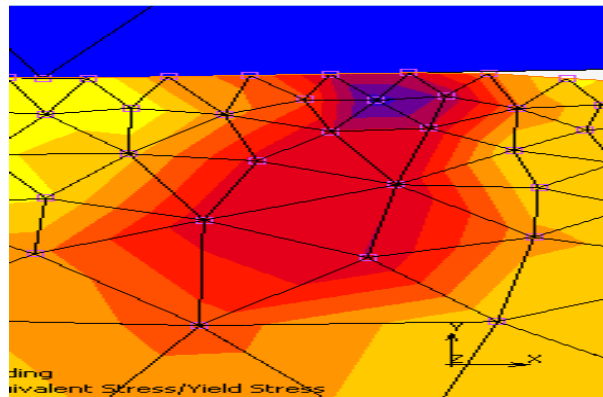
Fig. 8: B) Design Expert Response Surface Diagram of 100crmnmo8 Steel Roller with and Without Coating under A Higher Load and Temperature of 6 KN and 160°C for the Wear Rate Response. They Represent the Zn Roller and WC Roller Respectively.

### 3.3. Finite element results after DOE optimization

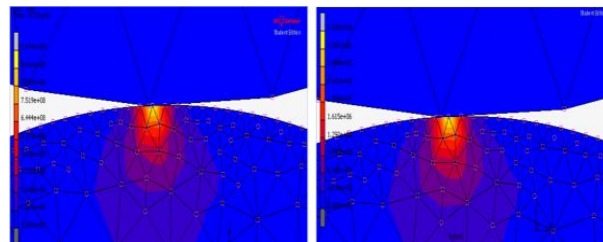
Statistical analysis is a powerful tool to predict the influence of individual variables on the desired outcome. Base on the DOE Figures we used the Finite element tools to verify the Design expert results. Figures 9, 10 and 11 show the stresses and cracks initiation of M50 and 100CrMnMo8 steels rollers coated with TiN and WC at higher load and temperatures. ZrN coating was not shown since failure was imminent when the load is increased. The Figures results were consistent with the DOE results with little difference in M50/WC coated roller. The analysis clearly indicates that steel rollers at higher load should be coated in order to have longer service life.



**Fig. 9:** Crack Initiation and Propagation AT AN Optimized DOE Temperature of 160°C and Various Loads for an M50 Roller Coated with Tin: A Represents A Load of 2kn, B Represents A Load of 4kn, C Represents A Load of 5kn, D Represents A Load of 6 KN.



**Fig. 10:** Crack Initiation and Propagation at A Load of 6 KN for an M50 Roller Coated with WC at an Optimized DOE Temperature of 160°C.



**Fig. 11:** Crack Initiation and Propagation at A Load of 4 Kn and 6 Kn Respectively for 100CrMnMo8 Steel Roller Coated with WC Under A Temperature of 160°C.

## 4. Conclusion

It is evident from the analysis that differences in stresses, displacements and the intensity of cracking on the body are more influenced by loads and type of coating than temperature. TiN and WC are the leading coating types in the industry and are better suited for rollers usage than ZrN. Their effects are clear and illustrated in the previous table and figures. Research showed that the mechanism of cracks propagation and wear rate are related to materials, coating, loading condition and increased compressive stresses. Moreover, DOE figures show some differences between M50 and 100CrMnMo8 steel rollers depending on the type of coat at higher load.

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