EFFECT OF VEGETABLE OIL OXIDATION ON THE ABILITY TO HARDEN AISI 1045 and 4140 STEEL[1]

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Abstract

There is a continuing and increasing interest in identifying more biodegradable and less toxic alternatives to petroleum oil as quenchants for steel. Two possible candidates where Brazil has a fundament position with respect to production are soybean oil and castor oil. Earlier papers have described the use of these oils as *quenchants* in *heat treating* operations. In this paper, *computational simulation* will be used to estimate the potential capability of soybean and castor oil, both fresh and unoxidized and after oxidation to harden AISI 1045 and 4140 steel. This discussion will include a description of the computational process of starting with INCONEL 600 cooling curve data and calculation of the hardness of the desired steel alloy. The results of this work will not only illustrate the potential applicability of soybean oil and castor oil as quenchants but also, the enormous potential benefit of *computational simulation*, even for problems such as this, will be illustrated.

Key-words: Heat treatment; Quenchant; Vegetable oils; Computational simulation.

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INTRODUCTION

There have been many investigations of the use of both animal and vegetable oils and fats as quenchants. One of the earliest studies was conducted by Tagaya and Tamura in 1954 [1]. Although this study did correlate quench severity with fluid source and viscosity in addition to oxidative stability for various naturally derived fluids, the data is in a different form than commonly reported today. However, the data reported did suggest that although the Grossman Quench Severities factors were comparable for both castor oil (H = 0.199) vs. soybean oil (H = 0.200), the cooling times from 700-300°C was significantly faster for castor oil (1.8 s) than soybean oil (1.42 s) using a JIS K 2242 silver probe test.

To date, the most commonly cited vegetable oil base stocks used for quenchant formulation are canola oil, and soybean oil derivatives [1]. Recently, a crambe oil based fluid has been reported as a potential quenchant [2]. However, in none of these papers was any correlation of quenching performance, including oxidative stability with oil structure reported.

Totten, et. al., Prabhu and Prasad studied the heat flux properties of soybean oils, crude, partially hydrogenated soybean and coconut, sunflower and groundnut oils respectively [1, 3]]. Although quench severities comparable to a conventional, non-accelerated mineral oil were obtained, correlations between vegetable oil structure vs. oxidative stability with corresponding changes in quench severity as a result of the change in molecular structure of the vegetable oil has not been reported in any previous study.

The effect of vegetable oil stability on their use as quenchants for heat treatments of Inconel 600 (Wolfson) probes is studied in this paper by computational modeling, using the Finite Element Software **HT-Mod** (Heat Treating modeling) and the general purpose Finite Element System Analysis **ABAQUS**.

Fresh and oxidized sample of castor oil, soybean oil and a mineral oil [4] are considered as quenchants using the Inconel 600 probe described in ISO 9950. This procedure is based on cooling curve (*T*-*t*) data obtained using a Type K thermocouple inserted to the geometric center of the 12.5 mm dia x 60 mm cylindrical probe. Interfacial temperatures at the cooling metal – liquid quenchant interface and heat transfer coefficients are obtained with HT-Mod.

DISCUSSION

Experimental

The vegetable oils used for this work included: a pale-pressed castor oil which was obtained from Dissoltex Indústria Química Ltda and a refined soybean oil sent by Shell Brasil (it is not a Shell commercial product). A conventional mineral oil, designated as MC1 from Castrol Brasil, was used as the mineral oil for comparison to vegetable oil performance.

An accelerated laboratory aging system was built according the apparatus and procedure used by Bashford & Mills in their earlier study of the effect of quench oil oxidation on cooling curve performance. The apparatus is described in detail in Reference 5.

Chemical structure and fluid oxidation of the fluids used in this work was characterized by fluid viscosity, titration for unsaturation using Wijs reagent, FT-IR and NMR spectroscopy, and thermal analysis. A detailed description of these analyses procedures and results are provided in Reference 4.

Modeling Approach, Results and Software

HT-Mod (**Heat Treating Modeling**)[6-13] is a program that can be used to simulate a wide variety of heat treatment processes, having plane and axi-symmetrical geometries. It may also be used to ascertain heat transfer coefficients as a function of time, provided a record of temperatures at different positions in the component is available to solve an inverse problem. The model is based on a numerical optimization algorithm which includes a finite element module for calculating with respect to time and space the temperature distribution and its coupled micro-structural evolution. The transformation from austenite to ferrite, perlite and martensite is governed by the appropriate CCT or TTT curves and by Avrami's approximation.

The temperature evolution, as measured by thermocouples at different positions in the component, is used as input for the program. The program calculates the time variation of the heat transfer coefficients, together with the temperature and distribution of phases, and their variation in time throughout the component.

The general purpose finite element system ABAQUS/Standard [14] was used to simulate the distortion and the residual stresses produced in the studied samples, as a consequence of a heat treatment process, with previous calculation of the temperature distribution pattern in each case, based on the heat transfer coefficients obtained with HT-Mod.

Table 1 indicates the thermophysical properties depending of temperature of INCONEL 600, as obtained from ref. 15. On the other hand, mechanical properties of this material used in the present analysis are indicated in Table 2.

Table 1. Thermal conductivity and specific heat as functions of temperature, and constant density used for INCONEL 600 [15].

Thermal conductivity		Specific heat		Density
Temperature [°C]	*k*[W/m.K]	Temperature [°C]	*c* [J/kg.K]	δ [kg/m^3]
50	13.4	50	451	8385.
100	14.2	100	467	
150	15.1	200	491	
200	16.0	300	509	
250	16.9	400	522	
300	17.8	500	533	
350	18.7	600	591	
400	19.7	700	597	
450	20.7	800	602	
500	21.7	900	611	
700	25.9			
900	30.1			

Table 2. Young modulus, coefficient of thermal expansion and the yield stress used for INCONEL 600 as functions of temperature [15].

Temperature		Young modulus		Coefficient of thermal explansion		Yield stress
[°F]	[°C]	[10^6 psi]	MPa	[10^{-6} °F^{-1}]	[10^{-6} °C^{-1}]	MPa
70	21	31.0	213700	6.8	12.2	225.
200	93	30.2	208200	7.5	13.5	202.
300	149	29.8	205500	7.9	14.2	199.
400	204	29.5	203400	8.2	14.8	194.
500	260	29.0	199900	8.4	15.1	191.
600	315	28.7	197900	8.5	15.3	185.
700	371	28.2	194400	8.7	15.7	252.
800	427	27.6	190300	8.8	15.8	81.
900	482	27.0	186200			41.
1000	537	26.4	182000			10.

The simulations performed with HT-Mod Code use a finite element mesh containing 11 nodes along the radial direction and 21 nodes along the longitudinal direction. Most of the microstructural transformations occurs during the first minute, therefore these were the times taken into account for the simulations. For the discretization of the time variable during 50 seconds were chosen 200 time steps.

The total time of each process were divided into a certain quantity of time intervals where the heat transfer coefficient varies linearly. The selection of the initial values for these coefficients and of the quantity and length of the time intervals depended on each sample. The mean square difference between the measured and calculated temperatures obtained after optimization of the heat transfer coefficients was about 1 °C. Table 3, 4 and 5 shows the heat transfer coefficients obtained for each sample for temperatures between about 200 °C and 850 °C. Figure 1 shows the calculated heat transfer coefficients as a function of temperature, comparing the quenching power of the six quenchants studied.

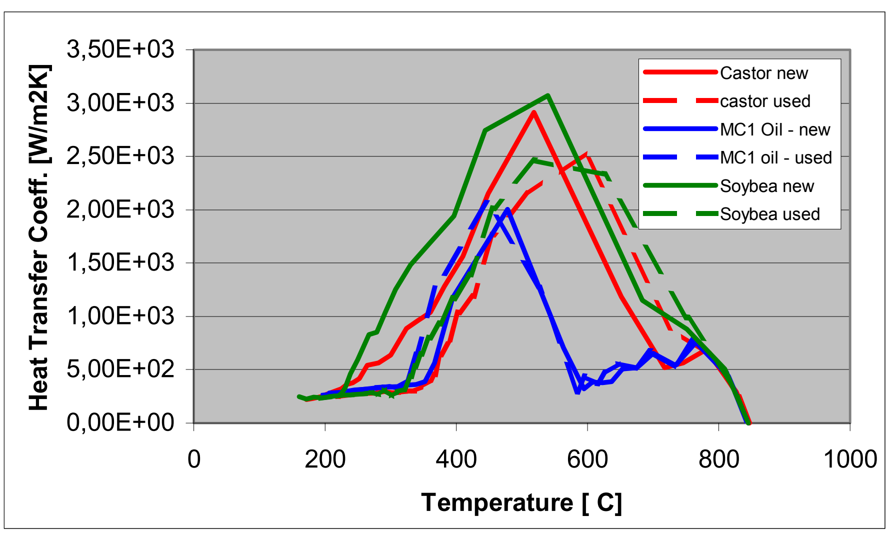

Figure 1. Heat transfer coefficients as depending of temperature determined by HT-Mod for the six quenchants.

Table 3. Heat transfer coefficient calculated for new and used castor oil.

Castor Oil –new.			Castor Oil – used	
Time [s]	Temperature[ºC]	HTC [W/mºC]	Temperature[C]	HTC [W/mºC]
5	826.2	295.2	828.3	282.1
6	780.4	690.4	783.9	648.5
7	746.0	565.3	726.7	887.6
8	717.8	519.6	596.7	2528.3
9	651.5	1185.6	510.3	2148.8
10	518.2	2914.7	455.4	1768.7
11	448.5	2148.8	426.5	1184.0
12	410.2	1564.0	402.5	1040.2
13	381.9	1279.4	387.6	735.0
14	360.5	1038.8	374.9	643.9
15	341.2	961.1	367.4	449.3
16	324.2	886.5	360.2	407.1
18	300.4	639.8	347.0	339.7
20	281.7	566.8	335.5	298.7
22	264.6	539.2	323.9	300.9
24	252.3	416.9	312.7	289.0
26	242.1	379.3	302.1	280.5
28	232.7	360.0	291.2	296.6
30	224.6	321.8	281.0	284.5
35	207.2	282.6	257.8	276.6
40	193.3	246.8	237.5	264.1
45	181.7	229.1	220.4	246.3
50	171.3	220.6	204.2	263.1

Table 4. Heat transfer coefficient calculated for new and used MC1 oil.

MC1 Oil – new			MC1 Oil – used	
Time [s]	Temperature [ºC]	HTC [W/mºC]	Temperature [ºC]	HTC [W/mºC]
5	814,4	441,7	811,4	467,2
6	765,4	755,9	761,7	770,7
7	733,5	542,3	730,8	531,1
8	699,8	655,9	696,6	670,5
9	675,0	518,3	671,7	519,1
10	652,7	506,3	646,9	556,7
11	637,1	391,3	627,6	468,2
12	622,4	376,8	613,5	375,3
13	607,2	384,1	596,6	433,8
14	594,2	324,5	584,0	295,7
15	563,1	705,3	526,7	1278,4
16	478,1	2006,7	446,6	2058,2
18	394,4	1172,8	367,7	1262,6
20	367,1	562,1	339,2	643,3
22	352,2	391,2	325,3	407,1
24	338,3	360,8	313,8	346,4
26	324,2	357,5	302,0	338,1
28	311,5	327,2	290,2	336,4
30	298,5	344,7	278,8	333,6
35	269,5	322,1	253,2	312,0
40	244,8	309,5	231,6	290,9
45	224,1	288,8	213,2	279,0
50	206,2	280,7	197,5	259,6

Table 5. Heat transfer coefficient calculated for new and used soybean oil.

	Soybean new		Soybean used	
Time [s]	Temperature [ºC]	HTC [W/mºC]	Temperature[ºC]	HTC [W/mºC]
5	809,5	509,7	819,9	372,6
6	751,7	882,3	751,4	988,3
7	683,0	1153,5	624,5	2331,8
8	539,5	3073,3	520,5	2463,5
9	444,3	2744,7	456,1	2017,5
10	396,4	1939,6	421,9	1386,7
11	359,4	1690,6	395,1	1165,7
12	329,8	1483,1	375,2	933,1
13	307,7	1251,6	359,0	800,3
14	291,3	1040,4	347,1	643,3
15	279,1	853,8	337,8	539,0
16	266,8	832,3	330,8	434,0
18	249,7	594,2	320,1	318,2
20	238,1	463,2	310,4	291,1
22	230,6	329,6	301,7	256,6
24	224,7	278,1	290,6	318,4
26	219,2	253,2	281,2	264,8
28	213,5	256,2	271,8	286,5
30	208,0	245,8	262,7	275,7
35	194,9	239,8	242,2	266,0
40	182,6	240,7	224,0	259,1
45	171,7	226,7	208,0	248,6
50	161,0	249,0	194,3	232,0

Calculations of Distortion and Thermal Stress with ABAQUS

The heat transfer coefficients obtained for the six quenchants as described before were used as input for ABAQUS/Standard in order to calculate the thermal field again, as well as the corresponding distribution of thermal stresses depending on time during the heat treating process, solving the corresponding thermal-elastic-plastic problem.

Longitudinal and hoop stresses at nodes in the middle plane calculated for new and used castor oil, new and used MC1 oil, and new and used soybean oil. Calculations showed that in some cases such stresses were high enough to generate residual stresses. Maximum longitudinal and hoop stresses and residual and longitudinal and hoop stresses, are compared in Table 6.

Table 6. Maximum longitudinal and hoop stresses and residual and longitudinal and hoop stresses.

	Castor oil		MC1 oil		Soybean oil	
	New	Used	New	Used	New	Used
Maximum σ_z [MPa]	180	172	180	180	180	180
Maximum σ_θ [MPa]	176	170	183	183	183	175
Residual σ_z [MPa]	-99	-80	$\lvert \sigma_z \rvert < 5$	$\lvert \sigma_z \rvert < 5$	$\lvert \sigma_z \rvert < 5$	-90
Residual σ_θ [MPa]	-123	-104	$\lvert \sigma_\theta \rvert < 5$	$\lvert \sigma_\theta \rvert < 5$	$\lvert \sigma_\theta \rvert < 5$	-111

CONCLUSIONS

Castor oil and soybean oil are among the vegetable oils produced in greatest volumes in the world and Brazil is among the top producers of these oils. Therefore, potential new uses in applications such as quenchants are of fundamental and great interest. Earlier work using molecular structural characterization showed that oxidized vegetable oils exhibit significantly greater variation in cooling performance relative to conventional petroleum oil quenchants relative to their unoxidized condition. Clearly, further work will be necessary to identify effective antioxidants that do not compromise the favorable toxicological and biodegradation properties of these oils if they are to gain substantial use in the heat treating industry.

The results of numerical analysis of the heat transfer properties using HT-MOD of the fresh and used quenchants confirm that oxidation of uninhibited castor oil and soybean oil produces substantially greater impact on the heat transfer properties relative to the petroleum oil quenchant used for comparison. Furthermore, using ABAQUS to compute the comparative residual stress profiles and predicted (of the as-quenched probe) showed that, as expected, fluid oxidation produced a substantial increase in residual stresses and distortion when compared to fresh fluids for both vegetable oils and the petroleum oil quenchant. This work illustrates the enormous insight that numerical analysis of the heat transfer and residual stress properties exhibited by a quenchant can provide relative to the rather limited analysis provided by conventional cooling curve analysis using a procedure such as ASTM D 6200.

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EFEITO DA OXIDAÇÃO DOS ÓLEOS VEGETAIS NA TÊMPERA DOS AÇOS AISI 1045 E 4140

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Resumo

Ultimamente o interesse em identificar alternativas aos óleos minerais, mais biodegradáveis e menos tóxicas, como *meio de têmpera* tem aumentado. Dois potenciais candidatos, onde o Brasil tem papel fundamental como produtor, são os óleos de mamona e soja. Trabalhos recentes descrevem o uso destes óleos como *meios de têmpera* em processos de *tratamento térmico*. Neste artigo, a *simulação computacional* será usada para estimar a capacidade dos óleos de soja e mamona (novos e usados) em endurecer os aços AISI 1045 e 4140. Para tanto será descrito o processo computacional: a aquisição das curvas de resfriamento com uma sonda de Inconel 600 e o cálculo da dureza da liga estudada. Os resultados aqui apresentados não ilustram apenas uma possível aplicação para os óleos de soja e mamona, mas também todas as vantagens que a simulação oferece em problemas como este.

Palavras-chave: Tratamento térmico; Meio de têmpera; Óleos vegetais; Simulação computacional.

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