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THERMAL AND MICROSTRUCTURAL ANALYSIS OF QUENCHING PROCESS IN AN CYLINDRICAL BAR OF AISI 1045 STEEL USING THE CLASSICAL INTEGRAL TRANSFORM TECHNIQUE

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Abstract. *Given the importance of the steel market in Brazil and its impacts on the local economy, the simulation of a steel quenching process and stipulation of its microstructures becomes relevant. Thus, it was considered a long cylinder of a specified radius R and length L, where L>>R, made of AISI 1045 steel. To determine the temperature distribution in this cylinder in any point and time instant, it was necessary to solve the heat diffusion equation in cylindrical coordinates. The mathematical method used to solve this problem is the Classical Integral Transformation Technique (CITT), which provides an analytical solution to the transient diffusive problem that represents the cooling process. The results were also compared with numerical data obtained for the same problem from simulations with software ANSYS®, widely used in engineering. Thus, the microstructure profiles were obtained and analyzed through the Continuous Cooling Transformation diagram (CCT). The material will be subjected to a temperature of 860ºC and cooled to 25ºC, using several parameters of cooling. Therefore, the predominant microstructure of the specimen could be stipulated.*

Keywords: *CITT, CCT, Microstructure, Cooling*

1. INTRODUCTION

The process industry applies different means to achieve a certain mechanical strength during the steelmaking process. One such means is quenching, a heat treatment that consists in heating the sample of steel at a high temperature (austenization process) for a certain period of time, and then rapidly cooling it to room temperature. Depending on the cooling rate imposed, different microstructures may form in different regions, which will directly impact the mechanical properties of the sample, such predictions are fundamental in the industrial usage for each material, subjected to different cooling rates according to with its specific application in industry. The original problem involves coupling the transient heat transfer problem with the phase transformation problem in steels, implying a complex problem to solve. (Hömberg, 1996).

In a more simplified way, it is possible to approach the general problem by analyzing it uncoupled, calculating or measuring the transient temperature field and using the Constant Cooling Transformation (CCT) diagrams to determine the percentage of each microstructure of the steel in a specific region of a sample. According to Voort (1991), the use of these diagrams is able to provide good results, although it also has its limitations. Nunura et al. (2015) aimed to develop an empirical method that correlates the cooling rates with the microstructures and hardness at specific points of a sample subjected to a Jominy end-quench test. The experimental data obtained were then confronted with the CCT diagrams, indicating a good agreement between them.

In order to calculate the transient temperature field, the Classical Integral Transform Technique (CITT) was considered as the mathematical method for solving the diffusion heat transfer equation. The technique basically consists in defining an integral transform pair that, when applied to the partial differential equation, transforms it into a decoupled system of ordinary differential equations, which has an analytical solution. The result is then applied to the inverse function of the transformed pair, providing the solution of the temperature field by means of an expansion of eigenfunctions (Mikhailov and Özisik, 1984; Özisik,1993).

Therefore, the present work aims to determine the transient temperature field in a long cylinder made of steel with different convective coefficients in the external boundary condition and estimate the microstructure through its radius by analyzing the steel CCT diagrams. The temperature solution was also compared with a numerical solution obtained through the commercial software ANSYS®.

2. PROBLEM FORMULATION AND SOLUTION METHODOLOGY

Consider a cylinder of a specified radius R and length L, where L >> R. In this case, it is safe to state that, by the theory heat transfer is considered only in the radial direction, for cylinders with L >> R, the axial heat transfer is negligible. It will be considered that the specimen has passed through an austenization process, so the initial temperature can be considered as $T_0 = 860$ °C. The cylinder external wall is subjected to a boundary condition of the third type (Robin boundary condition), with room temperature at $T_\infty = 25$ °C and constant convective heat transfer coefficient (h), although h is dependent on the external wall temperature (Hasan et la., 2011; Çakir and Özsoy, 2011).

To solve this heat transfer problem, we used the CITT methodology, as mentioned above, and in order to facilitate the mathematical procedure, we set homogeneous boundary conditions by applying a filtering scheme as part of the solution, such as:

$$T(r,t) = \bar{T}(r,t) + T_F(r,t) \tag{1.a}$$

$$\rho C_P \frac{\partial T(r,t)}{\partial t} = \frac{k}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T(r,t)}{\partial r}\right), \qquad 0 < r < R, \qquad t > 0 \tag{1.b}$$

$$\left.\frac{\partial T(r,t)}{\partial r}\right|_{r=0} = 0\,; \;\; k\left.\frac{\partial T(r,t)}{\partial r}\right|_{r=R} + hT(R,t) = hT_\infty\,; \;\; T(r,0) = T_0\,; \tag{1.c-e}$$

Given the equations above, is easy to prove that the filter expression is $T_F(r,t) = T_\infty$, ensuring a new set of PDE completely homogeneous for $\bar{T}(r,t)$, that way simplifying the CITT method. Then, once we have the filter equation and the expression for $\bar{T}(r,t)$, we are able to determine the temperature field $T(r,t)$ of the problem.

In this work, the thermal properties of the steel will be considered constant and obtained through the bulk temperature ($T_b = 442.5$ °C). Thus, the density, specific heat and the conductivity coefficient were respectively considered as: $\rho = 7665.29$ kg/m³, $C_P = 632.45$ J/kg.K and $k = 32.04\ W/m.K$. In a case where the thermal properties vary with the temperature a non-linear problem is obtained, and the CITT methodology is no longer valid. In that case, the Generalized Integral Transform Technique (GITT) is the only way to solve such problems (Cotta, 1990 and 1993), which will be considered in future work.

The CITT solution procedure can be readily employed by first defining the inverse and transform formulae that shall be used:

$$\text{Transform:}\quad \bar{T}_i(t) = \int_0^R \tilde{\psi}_i(r) T(r,t)dr; \qquad \text{Inverse:}\quad \bar{T}(r,t) = \sum_{i=1}^{\infty} \tilde{\psi}_i(r)\,\bar{T}_i(t) \tag{2.a,b}$$

where $\tilde{\psi}_i$ are the normalized eigenfunctions and N_i the normalization integrals, defined as:

$$\tilde{\psi}_i(r) = \frac{\psi_i(r)}{\sqrt{N_i}}; \qquad N_i = \int_0^R r\,\psi_i(r)\psi_i(r)dr\,; \tag{3.a,b}$$

To solve Eq. (1) the simplest eigenvalue problem proposed, obtained through Variable Separation Method, and its boundary conditions will be considered as follows:

$$\frac{k}{\rho C_P}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \psi_i(r)}{\partial r}\right) + \mu^2\psi_i(r) = 0 \tag{4.a}$$

$$\left.\frac{\partial \psi_i(r)}{\partial r}\right|_{r=0} = 0\,; \qquad k\left.\frac{\partial \psi_i(r)}{\partial r}\right|_{r=R} + h\psi_i(r) = 0\,; \tag{4.b,c}$$

The resulting eigenfunction obtained is:

$$\psi_i(r) = J_0\left(\mu_i r\sqrt{\frac{\rho C_P}{k}}\right) \tag{5}$$

where J_0 is the Bessel function of the first kind. The eigenvalues can be then calculated employing Eq. (5) in Eq. (4.c).

Operating on Eq. (1) with $\int_0^R r(.)\tilde{\psi}_i(r)dr$ and making use of the inverse formulae given by Eq. (2.b), the following transformed problem with the transformed initial condition is obtained:

$$\frac{\partial \bar{T}_i(t)}{\partial t} = -\mu_i^2 \bar{T}_i(t)\,; \qquad \bar{T}_i(0) = (T_0 - T_\infty)\int_0^R \frac{r}{\alpha}\tilde{\psi}_i(r)dr \tag{6}$$

which analytical solution can be described as:

$$\bar{T}_i(t) = \bar{T}_i(0)e^{-\mu_i^2 t} \tag{7}$$

Finally, to recover the desired temperature field the transformed potentials obtained in Eq. (7) are employed into the inverse problem (Eq. (2.b)), and the expansion is truncated at a specific value N that guarantee a proper convergence.

3. RESULTS AND DISCUSSIONS

The first case analyzed considered natural convection occurring along the cylinder external wall, with $R = 0.1m$. The convection heat transfer coefficient for this case was calculated using the Rayleigh Number, which returns $h = 192.7W/m^2.K$. The problem was also modeled with a FEM commercial code (ANSYS®) to critically analyze and verify the CITT code. The comparison between both results is presented in Fig. 1 and Table 1, where the transient temperature is analyzed in two distinct points of the cylinder: the center and the external wall. As demonstrated, the results show an excellent agreement, with a deviation below 0.3% throughout the domain, with the inverse problem expansion truncated at $N = 50$. The maximum deviation, 0.53%, where observed at the cylinder surface for very low times, which is intrinsic to the technique applied. So, it becomes evident that the CITT code can be considered verified and others results with different convection coefficient can be obtained through the same code.

Table 1: Deviations between ANSYS and CITT results for different times and locations.

	Center Temperature (°C)		Deviation	Surface Temperature (°C)		Deviation
Time (s)	ANSYS®	CITT	(%)	ANSYS®	CITT	(%)
0.01	859.99	859.99	0.00	859.59	855.07	0.53
1	859.99	859.99	0.00	846.69	846.73	0.00
10	859.99	859.99	0.00	817.59	817.64	0.01
100	839,39	839,25	0,02	719,92	720,05	0,02
1000	376,5	375,89	0,16	318.51	318.22	0.09
2000	160.94	160.53	0.25	138.51	138.25	0.19
4000	45.29	45.21	0.18	41.94	41.89	0.12
6000	27.99	28.01	0.07	27.48	27.52	0.15
7000	26.12	26.16	0.15	25.92	25.97	0.19

So, now it is possible to superimpose the transient temperature curves obtained with CITT into the CCT diagram (Voort, 1991) of the AISI 1045 steel and identify different microstructures formed within the domain, which can be defined as: Martensite (M), Bainite (B), Perlite (P) and Ferrite (F). Three different cases were considered for this analysis. The first one, as mentioned before, consider natural convection as the external boundary condition. The other two cases consider forced convection with a convection heat transfer coefficient of $h = 2000\ W/m^2.K$ and $h = 4000\ W/m^2.K$, respectively. Thus, for these cases, five different regions of microstructures were defined for better visualization of the results and are identified in Table 2.

The results for the first case were superimposed into the CCT diagram and are presented in Fig. 2. The natural convection boundary condition implies a low cooling rate, which guarantees an almost homogeneous microstructure throughout the domain, consisting basically in a combination of perlite and ferrite with different proportions (microstructure M1).

In Table 2 and Table 3, the convergence behavior from the results of the second and third case are presented for different values of time and radius. As can be seen, in both cases, with a truncation order of $N = 50$ it is possible to achieve convergence at the fifth significant digit throughout the whole domain. However, this truncation order is only necessary to converge the results for lower values of time ($t < 1s$). For $t > 1s$, is possible to achieve convergence at the sixth significant digit with a truncation order of $N = 20$ or less.

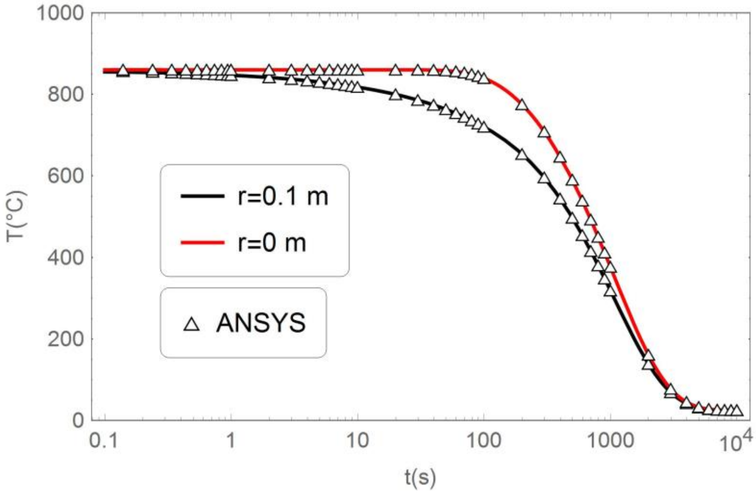

Figure 1: Comparison between the transient temperature obtained with ANSYS® and CITT in the center and in the external wall of the cylinder.

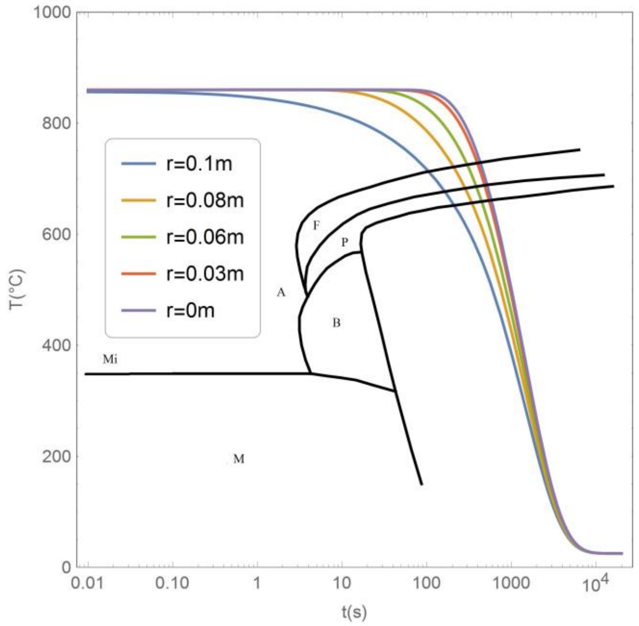

Figure 2: The transient temperature for different radius superimposed the CCT diagram with $h = 192.7\ W/m^2.K$.

Table 2: The five different regions of microstructures identified for this problem.

M1	Perlite (90% ~ 70%) + Ferrite
M2	Perlite (>90%) + Ferrite
M3	Bainite (>40%) + Perlite (>30%) + Ferrite (<4%)
M4	Bainite (40% ~ 20%) + Perlite (30% ~ 10%) + Ferrite (<3%) + Martensite
M5	Martensite (>93%) + Ferrite (<2%) + Bainite + Perlite

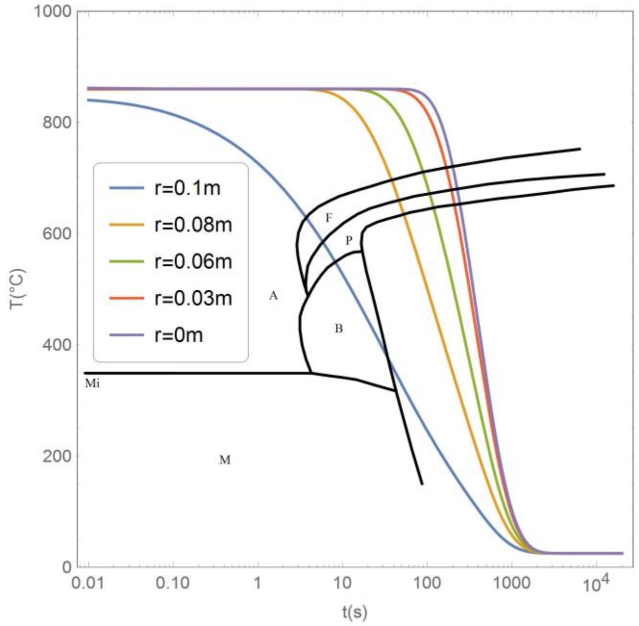

Figure 3: The transient temperature for different radius superimposed the CCT diagram with $h = 2000\ W/m^2.K$.

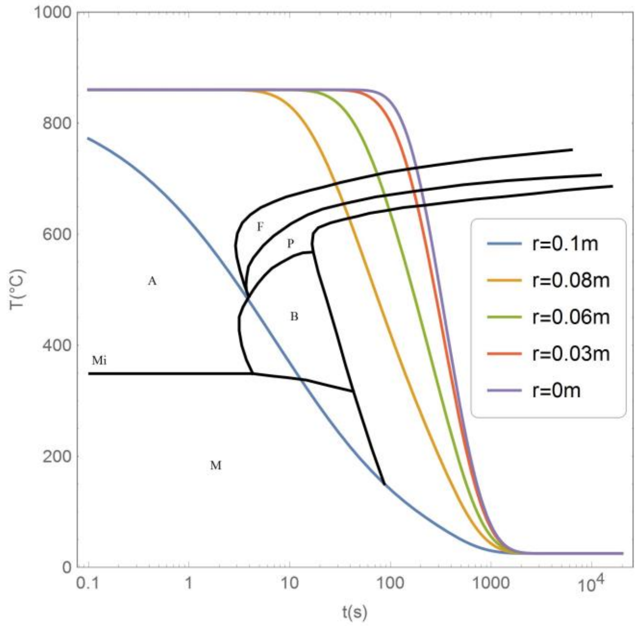

Figure 4: The transient temperature for different radius superimposed the CCT diagram with $h = 4000\ W/m^2.K$.

Table 3: Temperature convergence for different times and radius with $h = 2000\ W/m^2.K$.

$t(s)$	$r(m)$	$N = 10$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
	0.1	709.268	726.032	726.569	726.576	726.577
1	0.05	863.293	859.883	860.002	860.	860.
	0.01	865.874	859.782	860.004	860.	860.
	0.1	526.797	526.809	526.809	526.809	526.809
10	0.05	859.998	859.998	859.998	859.998	859.998
	0.01	860.018	860.	860.	860.	860.
	0.1	245.301	245.301	245.301	245.301	245.301
100	0.05	746.99	746.99	746.99	746.99	746.99
	0.01	841.587	841.587	841.587	841.587	841.587

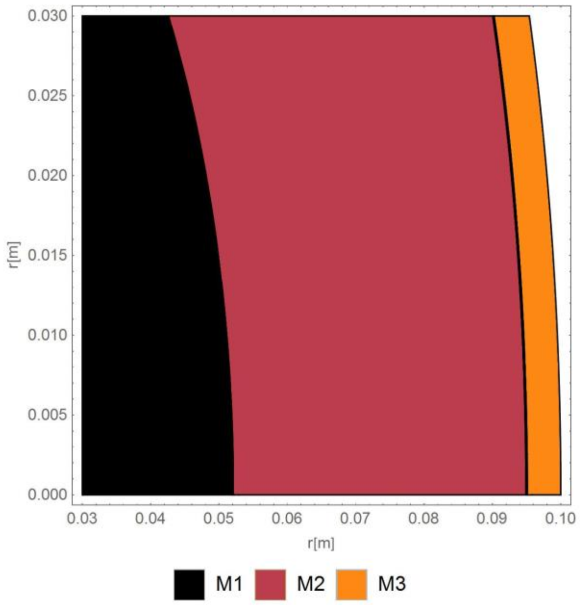

Figure 5: Different regions of microstructures formed throughout the radius with $h = 2000\ W/m^2.K$.

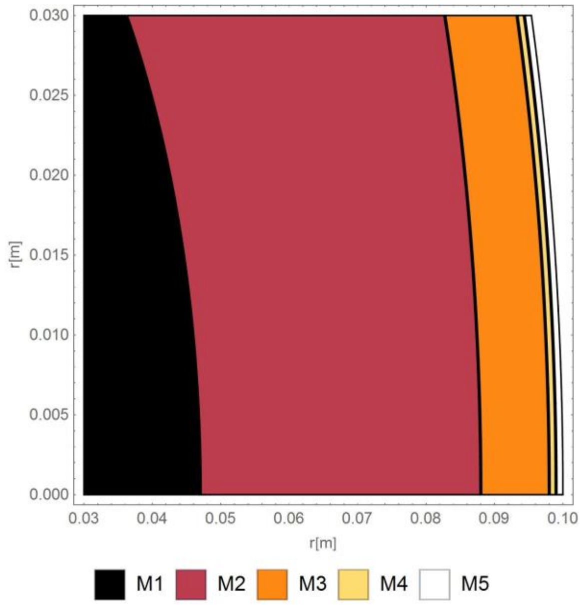

Figure 6: Different regions of microstructures formed throughout the radius with $h = 4000\ W/m^2.K$.

Table 4: Temperature convergence for different times and radius with $h = 4000\ W/m^2.K$.

$t(s)$	$r(m)$	$N = 10$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
1	0.1	592.669	623.269	624.307	624.322	624.322
	0.05	866.778	859.758	860.004	860.	860.
	0.01	871.112	859.57	860.008	860.	860.
10	0.1	368.078	368.098	368.098	368.098	368.098
	0.05	860.017	859.996	859.996	859.996	859.996
	0.01	860.031	860.	860.	860.	860.
100	0.1	140.18	140.18	140.18	140.18	140.18
	0.05	712.676	712.676	712.676	712.676	712.676
	0.01	834.383	834.383	834.383	834.383	834.383

It can be seen from Fig. 5 and Fig. 6 that, even doubling the value of h, the microstructure in the central region of the cylinder remains practically unchanged. Thus, the region of greatest interest of study is that one close to the cylinder surface, which will present the largest variety of microstructures along the radius due to the higher temperature gradient at this point. For better visualization of the temperature transient on the cylinder surface, Fig. 7 presents a series of results considering different values for the convection heat transfer coefficient. With that in mind, it is possible to conclude that the bainite microstructure will only be formed for $h > \mathbf{1}000\ W/m^2.K$, whereas the martensite microstructure will only be formed for h> 2000 W / m².K. Knowing the type of microstructure existing in a particular region of the steel it is possible to estimate its hardness. This property, in turn, is of great importance for engineering.

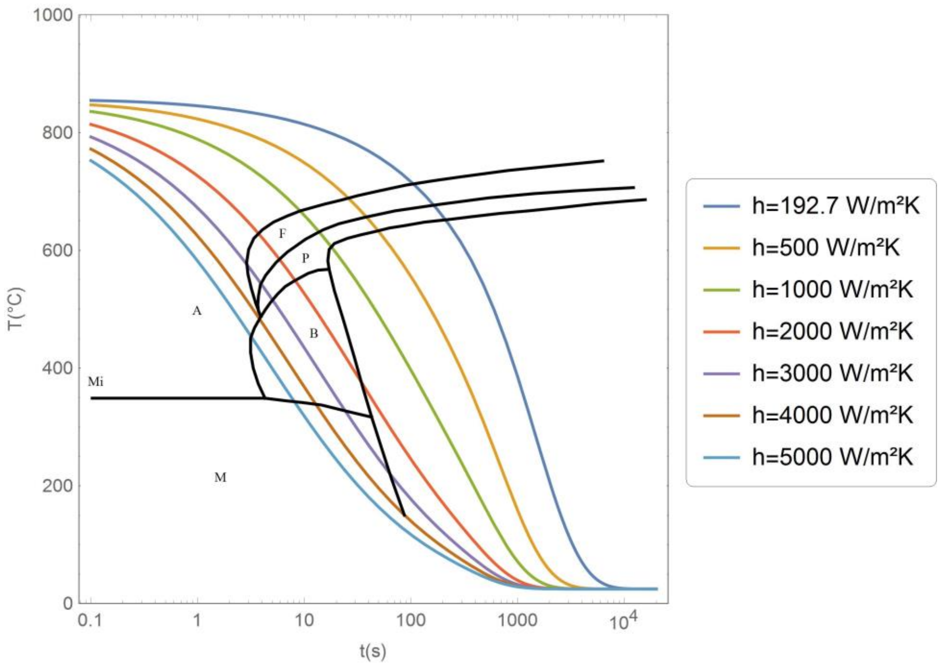

Figure 7: The transient temperature at the cylinder surface for different convection heat transfer coefficient (h).

It is important to note that the data presented herein result from a simplified model where thermal properties are assumed constant and no phase transformation problem was coupled to the thermal problem. In addition, we considered a mean convection heat transfer coefficient for each simulation, when in fact this property will also depend on the external wall temperature. More precise results can be obtained considering such non-linearities in the energy equation, which can be solved through GITT.

Moreover, a comparison with experimental results is very important to evaluate the quality of the results obtained with this simplified model and the real importance of considering a more complex model with a higher computational cost.

4. CONCLUSIONS

The Classical Integral Transform Technique (CITT) is employed herein to simulate a quenching problem of a steel cylinder. This methodology was verified with the commercial software ANSYS®, showing an excellent agreement between both results and illustrating the feasibility of employing the CITT in this type of problem. The transient temperature curves obtained were also superimposed the CCT diagram, allowing the identification of five different types of microstructures throughout the cylinder radius for different boundary conditions. The extension of this problem, considering a non-linear diffusive problem with temperature dependent thermal properties can be readily achieved by means of GITT.

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