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INFLUENCE OF VEGETATION MOISTURE ON COMBUSTION OF PYROLYSIS GASES IN WILDLAND FIRES[1]

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ABSTRACT

Since wildland fires occur in living vegetation, the fuel moisture content must be considered in order to correctly predict the behavior of the fire. One facet of combustion of pyrolysis gases that has not been considered in previous research is the effect of moisture on the combustion process. This effect is investigated by using CHEMKIN software to study an opposed diffusion flame model for three pyrolysis fuels relevant to wildfires. The effect of moisture on flame structure is investigated by varying the mole fraction of water vapor in the fuels, with air as oxidizer. In all cases, the flame extinguishes when the water mole fraction is between 0.55 and 0.65. O_2 and H are the only components that exhibit a significant change in concentration under these conditions.

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NOMENCLATURE

A	pre-exponential factor
E_a	energy of reaction [cal/mole]
k	rate constant [cm^3/mole/sec]
R	gas constant [cal/mole/K]
T	temperature [K]

INTRODUCTION

Wildland fires can threaten life, property, and natural resources or can perform necessary ecological functions in many North American ecosystems. Therefore, it is important to develop combustion models to predict the behavior of wildfires especially under rapid transition events. The majority of crown fires and other large fires in the United States occur in live fuels that contain significant moisture, and thus the influence of moisture on fire behavior is of interest.

One of the integral parts of wildland fires is the flame, which is fueled by gases that are released during pyrolysis of cellulose and hemicelluloses. A number of studies have been

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Table 1. Skeletal reaction mechanism for pyrolysis gas combustion

No.	Reaction	A	B	E_a
1	$H+O_2=OH+O$	5.13E+16	-0.816	16507
2	$O+H_2=OH+H$	1.80E+10	1	8826
3	$OH+H_2=H_2O+H$	1.17E+09	1.3	3626
4	$2OH=O+H_2O$	6.00E+08	1.3	0
5	$H+O_2+M=>HO_2+M$	3.61E+17	-0.72	0
6	$H+HO_2=>2OH$	1.40E+14	0	1073
7	$H+HO_2=>H_2+O_2$	1.25E+13	0	0
8	$OH+HO_2=>H_2O+O_2$	7.50E+12	0	0
9	$H+OH+M=>H_2O+M$	1.60E+22	-2	0
10	$CO+OH=CO_2+H$	1.51E+07	1.3	-758
11	$CH_4+H=>CH_3+H_2$	2.20E+04	3	8750
12	$CH_4+O=>CH_3+OH$	1.60E+06	2.36	7400
13	$CH_4+OH=>CH_3+H_2O$	1.60E+06	2.1	2460
14	$CH_3+O=>CH_2O+H$	6.80E+13	0	0
15	$CH_3+OH=>CH_2O+H_2$	1.00E+12	0	0
16	$CH_3+H+M=>CH_4+M$	8.00E+26	-3	0
17	$CH_2O+H=>HCO+H_2$	2.19E+08	1.77	3000
18	$CH_2O+OH=>HCO+H_2O$	3.43E+09	1.18	-447
19	$HCO+H=>CO+H_2$	4.00E+13	0	0
20	$HCO+OH=>CO+H_2O$	5.00E+12	0	0
21	$HCO+O_2=>HO_2+CO$	3.30E+13	-0.4	0
22	$HCO+M=>H+CO+M$	1.60E+14	0	14700

Note: Skeletal mechanism is by Zhou and Mahalingam [1] with updated values of parameters available in most recent version of CHEMKIN.

performed that focus on the modeling of fires using full, skeletal or reduced mechanisms for combustion of pyrolysis fuel gases [1, 2]; however, the influence of moisture on the gaseous mixture that results from pyrolysis and its effect on flame structure have not been quantitatively studied. Moist fuel affects the rate and direction in which wildland fires spread. Moisture content is believed to slow the burning rate since energy released from the flame first evaporates some moisture from the fuel particle before ignition occurs [3]. Previous studies [4,5] show the effect of moisture in live vegetation during combustion; however, in the current study we specifically deal with the gaseous combustion fueled from pyrolysis of wood. The evaporated moisture alters the chemical make-up of the air and the gaseous fuel by increasing the level of H_2O present in the gaseous state.

In this research, focusing on a non-premixed flame, we investigate how increased moisture in the pyrolysis fuel gas will affect the gaseous flames in an effort to better predict the behavior of wildland fires. Several mechanisms have been studied for non-premixed flames such as GRI mechanism [6]. In the current study, the skeletal reaction mechanism reported by Zhou and Mahalingam [1] is used, which is created based on an updated mechanism included in GRI-Mechanism 3.0 [6]. The specific aim of current study is to explore how addition of H_2O vapor to the pyrolyzate gas affects the temperature distribution and species profiles within an opposed diffusion flame.

FLAME DESCRIPTION

An opposed diffusion flame [7], which is a one-dimensional configuration with a planar diffusion flame between two opposed nozzles, is simulated with the OPPDIF software available in the CHEMKIN-Pro[1] software package [8]. The program is based on similarity transformation to reduce the three-dimensional flow field to a one-dimensional problem. The opposed-flow geometry makes an attractive experimental

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configuration, because the flames are flat, allowing for detailed study of the flame chemistry and structure.

At the considered opposed diffusion flame, the fuel enters from the left nozzle (boundary) located at $x = 0$ cm while the oxidizer enters from the right boundary at $x = 1$ cm. All simulations are carried out at atmospheric pressure with an initial temperature of 298 K. Both fuel and oxidizer stream velocities are set to 50 cm/s. In all cases, the oxidizer stream is comprised of standard ambient air.

Skeletal reaction mechanism of Zhou and Mahalingam [1] is used in the current study with reactions tabulated in Table 1. A and E_a variables are from the most recent version of CHEMKIN-Pro. In addition to four main pyrolysis gases of H_2, CH_4, CO_2, and CO considered by Zhou and Mahalingam [1], H_2O gas is considered as an initial component to investigate the moisture effect. The simulations are conducted for three different woods of aspen (*Populus tremuloides*, type A), beech (*Fagus americana*, type B) and larch (*Larix sp.*, type C). These fuel types are composed of four main pyrolysis gases with their mole fractions tabulated in Table 2. [9]. In this table, the fuel is assumed dry, i.e., X_{H2O} = 0. To include the moisture effect we scale the dry fuel species mole fractions tabulated tin Table 2 according to the considered value of X_{H2O}. Since the mole fraction of the fuel stream sums to 1.0, for instance, when 10% of H_2O gas is added to the fuel, the mole fractions of the fuel species are multiplied by 0.9 in order to account for the addition of H_2O.

Table 2. Mole fraction (X_i) of four gases released during pyrolysis of three different woods.

	X_{H2}	X_{CO}	X_{CH4}	X_{CO2}
A (Aspen)	0.41	0.256	0.077	0.257
B (Beech)	0.253	0.307	0.112	0.328
C (Larch)	0.398	0.264	0.112	0.226

Sensitivity analysis for the diffusion flame is performed using Chemkin-Pro in order to determine the chemical reactions that are more significantly responsible for the change in temperature when moisture is increased. The sensitivity of temperature to the Arrhenius pre-exponential factors (A-factors) of the various reaction-rate constants and species heats of formation is investigated. The Arrhenius equation describes the relationship between the rate constant (k) of a chemical reaction, the activation energy (E_a) of the reaction and absolute temperature (T)

$$k = AT^B \exp\left(-\frac{E_a}{RT}\right) \tag{1}$$

where R is the gas constant, A is the pre-exponential factor or A-factor, and B is the temperature exponent [8]. The A-factor is specific to each reaction and represents how many collisions occur between reactants when all concentrations are 1 mol/L and the molecules are properly oriented when they collide. The temperature sensitivity of the heat of formation uses the difference in the thermo-chemical property change in the products and the reactants related to the A-factor.

RESULTS

The spatial distribution of temperature within the opposed diffusion flame is plotted in Fig. 1 for various moisture mole fractions. For all three types of fuel displayed in Fig. 1(a-c), it is observed that at X_{H2O} = 0.65, the temperature curve is flat indicating that the flame is not sustained at this mole fraction. This observation implies that at a moisture mole fraction between X_{H2O} = 0.60 and 0.65 the flame is extinguished. Also, it is seen that in the case of Aspen and Larch shown in Fig. 1(a) and (c), respectively, there is a significant drop in temperature as X_{H2O} increases from 0.55 to 0.60, with the flame extinguishing at X_{H2O} of 0.65, whereas in the case of Beech, extinction occurs for X_{H2O} of 0.60 as can be seen in Fig. 1(b).

Variations of mole fractions of multiple major chemical components including CH_4, CO_2, CO, H_2, H, O_2, and H_2O have been examined in detail. A significant change in the mole fractions

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of O_2 and H is observed between X_{H2O} of 0.55 and 0.65. They are the only components that show significant changes.

Figure 2 shows the mole fraction of O_2 in the considered opposed diffusion flame. O_2 is an initial component in the oxidizer stream, which enters from the right boundary. For $X_{H2O} = 0$, the O_2 mole fraction starts to decline at a distance of 0.7 cm and is fully consumed at an approximate distance of 0.45 cm from the fuel nozzle. As the mole fraction of H_2O increases, the start point of decline of O_2 mole fraction shifts to the fuel nozzle.

Figure 3 shows the mole fraction of H in the considered opposed diffusion flame. H is not an initial component in the fuel or oxidizer; however, it is derived from H_2 which is an initial component in the fuel stream. For all three types of fuel, the mole fraction of H is negligible throughout the domain for X_{H2O} greater than 0.65. Furthermore, a significant decline in the amount of H is found between X_{H2O} of 0.55 and 0.65. For the case of Beech seen fig. 3(b), at X_{H2O} of 0.60, the H mole fraction is no longer produced and for the case of fuel types A and C (see Figs. 3(a) and (c)), the mole fraction of H → 0 between X_{H2O} of 0.60 and 0.65 but it is still produced.

Table 2. Reactions associated with the temperature A-factor sensitivity. M is used in the following reactions as a placeholder for multiple chemical species. [10]

Reaction No.	Reaction
1.	$H + O_2 = OH + O$
3.	$OH + H_2 = H_2O + H$
5.	$H + O_2 + M = HO_2 + M$
6.	$H + HO_2 = 2OH$
9.	$H + OH + M = H_2O + M$
11.	$CH_4 + H = CH_3 + H_2$
10.	$CO + OH = CO_2 + H$
14.	$CH_3 + O = CH_2O + H$
15.	$CH_3 + OH = CH_2O + H_2$
16.	$CH_3 + H + M = CH_4 + M$
19.	$HCO + H = CO + H_2$
22.	$HCO + M = H + CO + M$

Further research is performed to better understand the role of specific chemical reactions responsible for the decrease in flame temperature, and its eventual extinction. The sensitivity analysis, performed in CHEMKIN-Pro, shows that temperature variation is more sensitive to the reactions displayed in Table 2. The normalized sensitivity coefficient is displayed against distance in Fig 4 for five reactions to which temperature are most sensitive to. Among all reactions, reaction no. 5, $H+O_2+M=HO_2+M$, has both the most positive and negative sensitivity coefficient values.

CONCLUSIONS

Wildland fires often burn live vegetation that holds a significant amount of moisture, which is released to the gaseous phase as the cellulose and hemicellulose in the vegetation are pyrolyzed. Ignition of pyrolysis gases produces a gaseous flame which is important to model in order to characterize the behavior of the fire. By characterizing the gaseous fire that includes the moisture found in live vegetation, a more accurate mechanism can be developed to better understand the fires behavior.

The moisture found in a gaseous state was found to have an impact on the temperature distribution within an opposed diffusion flame for three types of fuels. The temperature steadily decreased as the moisture content was increased until a significant decrease was observed at mole fraction 0.55. At H_2O mole fraction of 0.65 the flame extinguished for all cases examined.

In order to understand the role of chemistry on flame extinction, the distribution of major gas components were examined. The components that showed dramatic changes were O_2 and H. In addition, a sensitivity analysis was performed to identify reactions that could potentially contribute to the observed reduction in flame temperature, and its eventual extinction.

In the future, we will further investigate how these reactions affect the flame and whether they should be included in a reduced mechanism for use in wildland fire behavior models. The new reduced mechanism will be altered based on reactions, which show

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significant importance to the effect of moisture. Our ultimate goal is to include other test environments such as premixed flames to develop a new reduced mechanism and compare it to that reported in Ref. 1.

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REFERENCES

[1] Zhou, and Mahalingam, 2001. "Evaluation of Reduced Mechanism for Modeling Combustion of Pyrolysis Gas in Wildland Fires." *Combustion Science and Technology*, 171: 39-70.

[2] Leroy, Leoni, and Santoni, 2008. "Reduced mechanism for the combustion of involved gases in forest fires." *Combustion and Flame*, 154: 410-433.

[3] Anderson, 1969. "Heat transfer and fire spread." USDA Forest Service Research Paper INT-69, Intermountain Forest and Range Experiment Station, Ogden, UT.

[4] Morvan, D. and Dupuy, J. L., 2004. "Modeling the propagation of a wildfire through a Mediterranean shrub using a multiphase formulation." Combustion and Flame, 138: 199-210

[5] Manzello, S.L., Maranghides, A. and Mell, W. E., 2007. "Firebrand generation from burning vegetation." *International Journal of Wildland Fire*. 16: 458-462.

[6] Smith, G.P., Gholden, D.M., Frenklack, M., Moriarty, N.W., Eiteneer, B., Lissianski, J.V.V. and Qin, Z. (2000) [www http://www.me.berkeley.edu/gri_mech/]

[7] Lutz, A. E., R. J. Kee, J. F. Grcar, and F. M. Rupley. "OPPDIF: A Fortran Program for Computing Opposed-flow Diffusion Flames." Sandia National Laboratories Report SAND96-8243 (1997). Office of Scientific and Technical Information, OSTI, U.S. Department of Energy. Web. 12 Aug. 2011. <http://www.osti.gov/bridge/servlets/purl/568983-AkVFPW/webviewable/568983.pdf>.

[8] CHEMKIN-Pro, "Theory Manual." Reaction Design: San Diego, 2008.

[9] Klose, W., Damm, S. and Wiest, W. (2000) Pyrolysis and activation of different woods-Thermal analysis (TG/EGA) and formal kinetics. Oral presentation at 4th International Symposium of Catalytic and Thermochemical Conversions of Natural Organic Polymers, Krasnoyarsk. May 30 to June 3. <www http://ite-ws2.ite.maschinenbau.uni-kassel.de/silke/artikel/artikel.html>

[10] CHEMKIN-Pro, "Input Manual." Reaction Design: San Diego, 2008. pg 86.

[11] Som, Ramirez, Hagerdorn, Saveliev, and Aggarwal, 2008. "A numerical and experimental study of counterflow syngas at different pressures." *Fuel*, 87: 319-334.

[12] Bryden and Hagge, 2003. "Modeling the combined impact of moisture and char shrinkage on the pyrolysis of a biomass particle." Fuel, 82: 1633-1644.

[13] Lee, Yang, Yan, and Liang, 2007. "Prediction of gaseous products from biomass pyrolysis through combined kinetic and thermodynamic simulations." Fuel, 87: 410-417.

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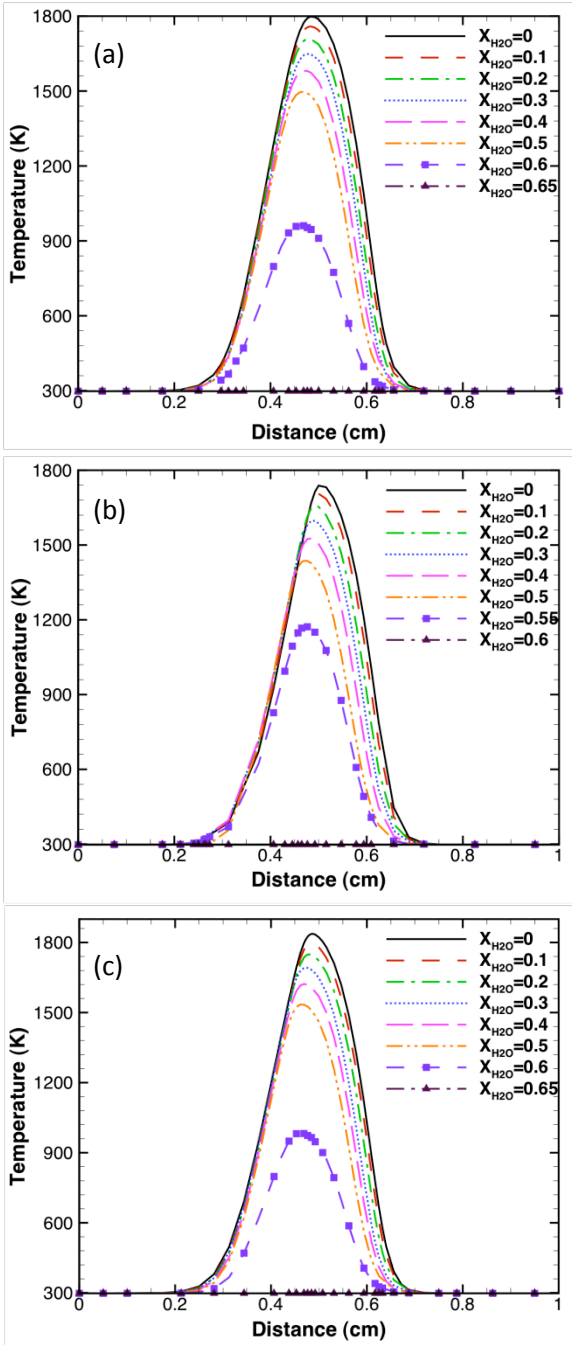

Figure 1. Spatial distribution of temperature in diffusion flame for different woods; (a) aspen; (b) beech; (c) larch.

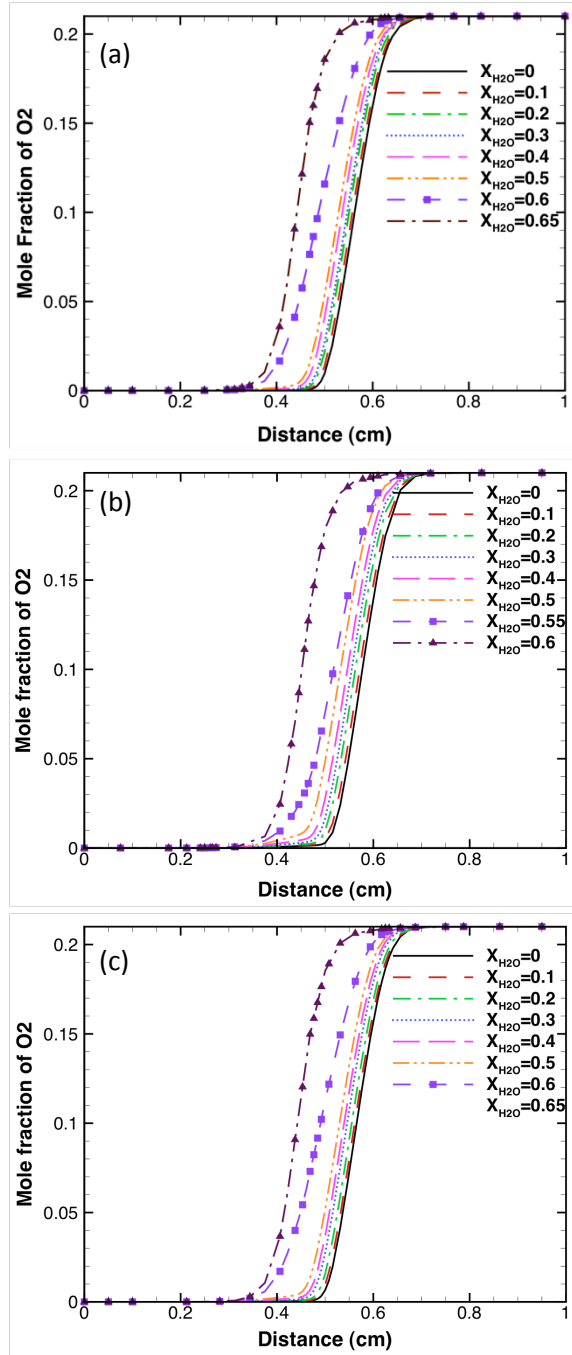

Figure 2. Mole fraction of O_2 in the diffusion flame for different woods; (a) aspen; (b) beech; (c) larch.

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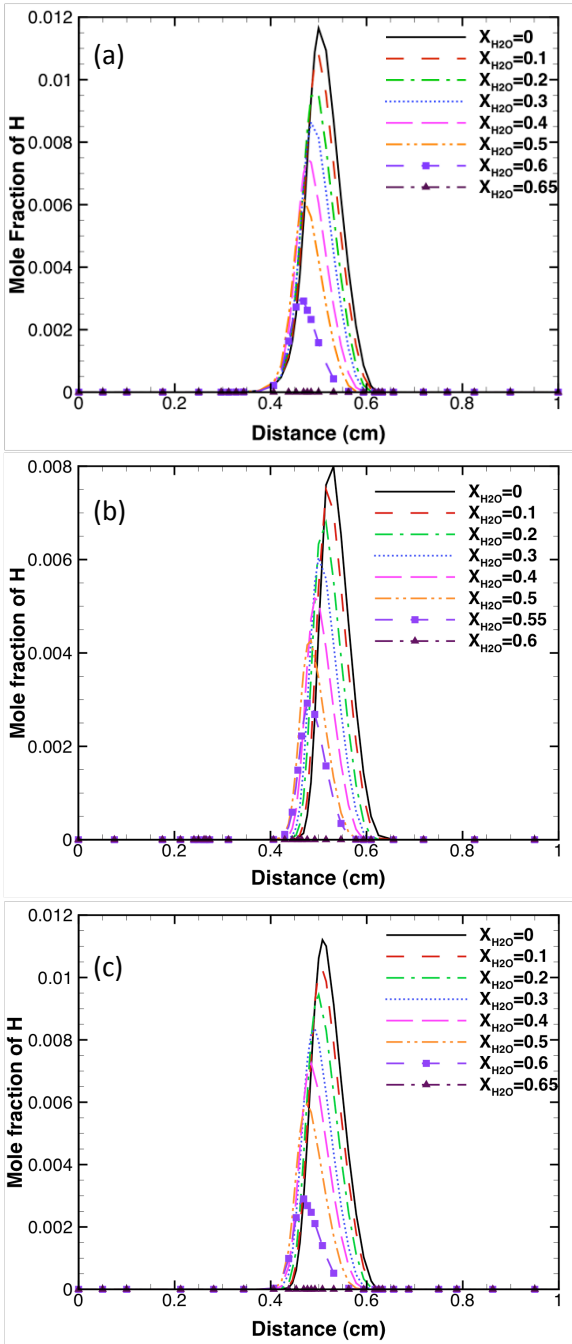

Figure 3. Mole fraction of H in the diffusion flame for different woods; (a) aspen; (b) beech; (c) larch.

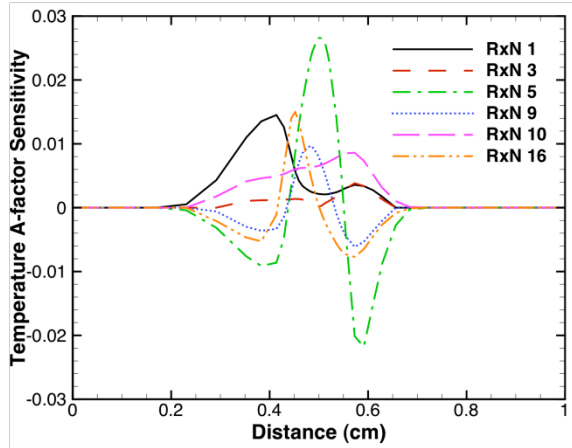

Figure 4. Sensitivity of temperature A-factor to various reactions for an H_2O mole fraction of 0.5 for aspen.

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