

NUMERICAL MODEL OF DISPOSAL SYSTEM FOR CHEMICAL WARFARE AGENTS

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Abstract

World War II has brought a lot of destruction to the world. Unfortunately, we can observe its effects until today. One of the effects is the tons of chemical warfare agents (CWAs) left at the Baltic Sea bottom. The paper undertakes the problem of numerical research on the innovative disposal system for chemical warfare agents. The system is being built within the Polish development project devoted to localization, transferring from the bottom to the water surface, and disposal of submerged CWA.

At the beginning of the paper, the introduction with the project description is included. Then, the analysis of functional and constructional assumptions for the CWA disposal system is presented. Next, the mathematical model with the results of numerical research is inserted. In the end, conclusions from the study with the future research schedule are formulated.

Keywords: disposal system, chemical warfare agents, linear production model

1. INTRODUCTION

After World War II, many kinds and tons of conventional and chemical ammunition were dumped in the sea, including the Baltic Sea. Explosives have medium toxicity to aquatic organisms, earthworms, and indigenous soil microorganisms [4]. Therefore, environmental monitoring and consequent disposal are required. This paper undertakes problems of numerical modeling of a disposal system for Chemical Warfare Agents (CWAs). It includes the research results carried out in the first stage of the project aiming at CWA disposal system development [2].

The main goal of this project is to carry out R&D processes aimed at developing comprehensive technology, embracing the process of precise location, identification, retrieval, and disposal of Chemical Warfare Agents (CWA) deposited on the bottom of sea basins, which pose a very high threat to the ecosystem (with particular regard to the Baltic Sea character).

As a result of the project, innovation will be achieved in the form of service unique on the world scale, available to customers and commercial clients, mainly: maritime wind farm investors, investors of infrastructural objects at sea (including investments at the Baltic Sea, North Sea, Danish Straits), port authorities, municipalities, maritime administrations, appropriate (competent) ministries and entities carrying out investments requiring interference with the seabed, where potentially dangerous substances, such as CWA, may be located.

Due to its' innovative character and features, the new service can be implemented supplementary to the offer in the field of seabed remediation from conventional weapons. It will be a response to the market needs in this range. The service will integrate the following systems: a unique method of location, identification, retrieval, and CWA disposal directly at sea (mobile installations mounted (installed) aboard the vessel are the critical elements of the innovative service). The project results are of particular importance from protecting the marine environment point of view and the prevention of its' further degradation by the release of CWA to the marine ecosystem.

The team of Applicant's and Subcontractor's employees will be involved in the implementation of R&D works, including the Polish Naval Academy team, a specialized diving team, and the entity responsible for developing a unique CWA extraction system and a laboratory responsible for analyzing bottom sediment samples.

The next section is devoted to materials and methods. It includes the subsections focused on a structure of the Chemical Warfare Agent Disposal System (CWADS), a selection of CWAs, and a description of the CWADS mathematical model. In the third section, numerical research results on CWADS with discussion on received results are presented. In the end, the conclusions and bibliography are inserted.

2. MATERIALS AND METHODS

2.1. Structure of CWADS

According to the application for financing the project on CWAs disposal, the following assumptions were made for the CWADS implementation [5]:

1. Net mass of neutralized CWA min. 7 kg/day,
2. Possibility of neutralization of CWA at sea state min. 3.

The second assumption will be fulfilled using the stabilization platform for the CWADS mounted on board the ship. The first one is planned to be initially verified using numerical research included in this paper.

Based on the project's initial conception phase, the linear structure of CWADS was accepted [1][3]. The subsequent subsystems of the CWADS with their main parameters are illustrated in Table 1. In practice, some subsystems will be duplicated for separate processing of compounds, including arsenic or arsenic-free.

No.	Subsystem	Parameters
1.	CWA preparation subsystem for pumping	1. CWA dilution subsystem: 1.1. Chemical-resistant pump with fittings; 1.2. Diluter tank. 1.3. Operating parameters: • Power supply: 300 W; • Capacity: 20 dm³/min. 2. Microwave system for heating the CWA solution: 2.1. Generator; 2.2. Radiator; 2.3. Power Supply. 2.4. Operating parameters: • Microwave power: 6 kW; • Power supply: 10 kW.
2.	CWA pumping subsystem	1. Chemical-resistant pump with fittings: • Capacity 20 dm³/min; • Power supply: 300 W. 2. Intermediate tank for diluter: • 50 dm³ capacity; • Material: stainless steel.

3.	CWA dosing subsystem	1. Chemical resistant dosing pump with fittings: • Capacity: 1 dm³/min; • Power supply: 300 W. 2. Ultrasonic nebulizer: • Efficiency: 50 cm³/min; • Power supply: 1 kW. 3. Carrier gas: • Gas type: argon Ar or nitrogen N₂; • Flow: 20 dm³/min.
4.	Plasma reactor	1. Plasmatron: 1.1. Type - external arc plasmatron; 1.2. Cooling - water; 1.3. Working gas - argon Ar or nitrogen N₂; 1.4. Operating parameters: • Power supply: 35 kW; • Water: 60 dm³/min. 2.1. Capacity - approx. 500 dm³; 2.2. Material - high-temperature ceramics, external water cooling.
5.	Scrubbers for the neutralization of BST decomposition products	1. Scrubber for the neutralization of CWA breakdown products: 1.1. Capacity - 200 dm³ each; 1.2. Execution - chemically resistant materials. 2. Equipment: • Subsystem for introducing CWA breakdown products; • Neutralizing agents dosing systems; • pH meter; • Pump for circulation and emptying of scrubbers.
6.	Wastewater treatment subsystem	

Table 1. Parameters of CWADS subsystems

Source: Documentation of project no. POIR.01.01.01-00-0540/19, 2020.

It was assumed that both the plasma reactor and the scrubber must operate for 0.5 hours to process the product contained in their tanks.

The CWADS handling systems are built inside the container, although it is allowed that some components may be installed outside. The last of the stabilization systems will allow for stabilization against the container vessel rolling with on-board systems installed on one typical frame or only the container itself with CWADS.

2.2. CWAs

The following CWA variants were used to test the performance and/or optimize the parameters of CWADS:

1. KC-50 bomb filled with sulfur yperite (19 kg),
2. KC-50 bomb filled with adamsite (14 kg),
3. KC-250 bomb filled with sulfur yperite (99.9 kg),
4. KC-250 bomb filled with lewisite (106.7 kg),
5. KC-250 bomb filled with tabun (93.44 kg).

To calculate the CWA volume included in the bombs, the substance densities listed in Table 2 were used.

No.	CWA type	Density [g/cm ³] (in temperature)	Includes arsenic
1.	Tabun	1,073 (25 ⁰ C)	
2.	Sulphuric yperite	1,274 (20 ⁰ C), 1,338 (13 ⁰ C), 1,37 (0 ⁰ C)	
3.	Nitrogen yperite	1,09 (25 ⁰ C) HN-1, 1,15 (20 ⁰ C) HN-2, 1,24 (25 ⁰ C) HN-3	
4.	Lewisite	1,89 (20 ⁰ C)	X
5.	Chloroacetophenone	1,318 (20 ⁰ C)	
6.	Clark I	1,422 (20 ⁰ C)	X
7.	Clark II	1,45 (20 ⁰ C)	X
9.	Trifenyloarsine	1,22 (20 ⁰ C)	X
10.	Fenylodichloroarsine	1,65 (20 ⁰ C)	X
11.	Arsenic oil	1,66 (20 ⁰ C)	X
12.	Adamsite	1,65 (20 ⁰ C)	X

Table 2. Parameters of different CWAs

Source: Documentation of project no. POIR.01.01.01-00-0540/19, 2020.

2.3. Mathematical model of CWADS

To model CWADS, a linear model of the production line was adopted in the form of components connected in series, i.e., subsystems specified in Table 1. The product flow, i.e., CWA with the diluter and water used to cut the bomb body, runs from warehouse no. 1, i.e., the CWA preparation subsystem for pumping to warehouse no. 2, i.e., the CWA pumping subsystem through individual stations illustrated in Table 1. Product flow is described in terms of real numbers (a purely deterministic model). The model is discretized with a time step of 1 s.

The system of two interconnected stations works with the actual efficiency equal to:

$$S'_i = \min(S_i, S_{i+1}) \quad (1)$$

where:

S'_i – the actual system efficiency of two adjacent stations,

S_i, S_{i+1} – the passport efficiency of neighboring stations.

Efficiencies are expressed in the volume of the product per unit of time [dm^3/min].

Most of the workstations have their handy storage, called a reservoir. The amount of product accumulating in the reservoir in a situation that two stations are connected in series and the first one works with greater efficiency than the second one is calculated from the dependence:

$$Z_i = f^+(S'_{i-1} - S_i), \text{ for } i = 2 \dots k \quad (2)$$

where:

Z_i – the degree of filling a reservoir,

i – the station ordinal number,

k – the total number of stations,

$f^+(x) = \max(0, x)$ prevents the reservoir from holding a negative amount of product.

The tank filling is controlled according to the two-position control principle with a hysteresis loop:

$$u_{ij} = \begin{cases} 1 & \text{dla } Z_{ij} \leq Z_{imax} - Z_{iH} \\ 0 & \text{dla } Z_{ij} \geq Z_{imax} \end{cases} \quad (3)$$

where:

u_{ij} – the control signal of the filling reservoir at the i -th position in the j -th time moment,

Z_{imax} – the maximum degree of filling the reservoir on the i -th station,

Z_{iH} – the hysteresis loop width of the tank control at the i -th station.

The last station's actual efficiency at the linear installation is the global capacity S_g of the entire CWADS. The quantity of the product in the j -th time moment in warehouse 2, i.e., at the last k -th position of B_{kj} , can be calculated from the following formula:

$$B_{kj} = S_g \sum_{i=1}^k t_{ij} \quad (4)$$

where:

t_{ij} – the time of the product flow between the i -th and the $i+1$ -th station at the j -th time moment.

The total operating time of the installation is equal to:

$$t_t = \sum_{i=1}^k t_{il} + \sum_{i=1}^k \tau_{il} \quad (5)$$

where:

t_{il} – the time of product flow between the i -th and the $i+1$ -th station to the last l -th time moment,

τ_{il} – operating time of the i -th station until the last i -th time related to the processing of the product by this station, e.g., the plasma reactor's operating time needed to neutralize the CWA contained in the tank.

Most CWADS subsystems consume electric energy during their operation. Electric energy consumption W_t is measured in [kWh]. It can be calculated using the following formula:

$$W_t = \sum_{i=1}^k P_{1i} t_{il} + \sum_{i=1}^k P_{2i} \tau_{il} \quad (6)$$

where:

P_{1i} – the electric power needed for the product flow between the i -th and $i+1$ -th station,

P_{2i} – the electric power required for the i -th station's work for the product processing at this station.

3. RESULTS AND DISCUSSION

During the research, the product flow of 5 different variants of CWAs with diluter was investigated. Fig. 1 shows the changes in CWA volume with a solvent in subsequent points of the disposal installation and the corresponding electricity consumption for the KC-250 bomb filled with lewisite.

For different CWA variants, including solvent, different processing times and electric energy consumption were obtained (Table 3).

Variant of CWAs	The volume of CWA with diluter on input [dm ³]	Processing time of CWA [h]	Consumption of electric energy [kWh]
KC-50 with sulphur yperite	175,13	3,82	53,37
KC-50 with adamsite	110,84	2,72	40,19
KC-250 with sulphur yperite	894,14	18,37	219,35
KC-250 with lewisite	674,55	13,92	173,94
KC-250 with tabun	980,5	19,67	234,91

Table 3. Results of processing 5 variants of CWAs

Source: Documentation of project no. POIR.01.01.01-00-0540/19, 2020.

Based on the results of processing all the CWA variants, the “bottleneck” is the dosing system, which causes cyclical stoppage of the pumping process (Fig. 1.a - orange line).

The additional "bottlenecks" in the case of KC-250 bombs are also reactor and scrubber. Due to a large amount of diluter, the entire process will have to be stopped due to the overfilling of the plasma reactor reservoir, which will extend the disposal time by the reactor's operating time. At the same time, it can be seen that the scrubber reservoir is smaller than the reactor vessel, which will result in additional delays, i.e., the reactor reservoir cannot be emptied until the product processing in the scrubber reservoir is completed.

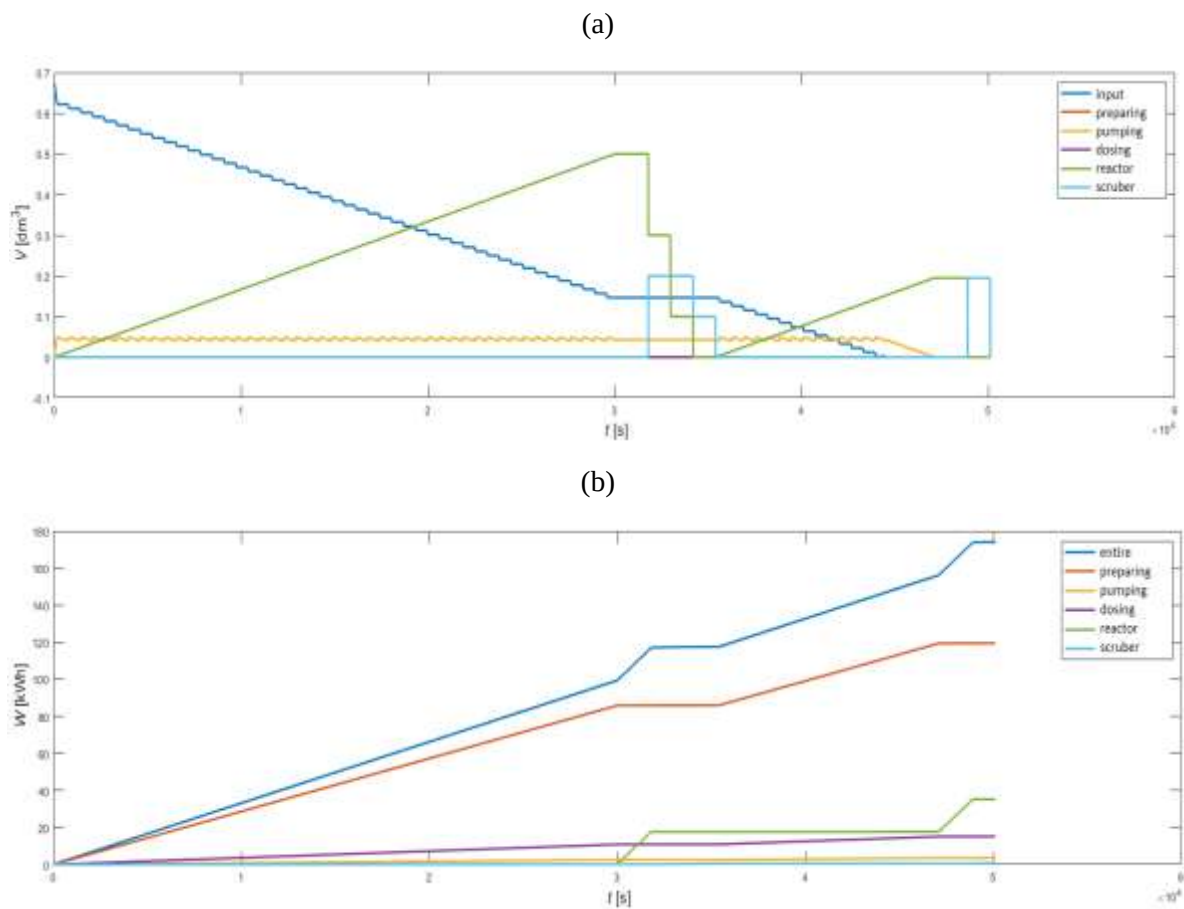


Fig. 1. Product flow of KC-250 with lewisite: (a) volume changes, (b) electric energy consumption changes

Source: Documentation of project no. POIR.01.01.01-00-0540/19, 2020.

Then, the research was conducted to estimate the better efficiency of the dosing subsystem and volumes of the reservoirs for reactor and scrubber. As shown in Fig. 2, an increase in dosing efficiency can cause even a 50% decrease in processing time and consumed electric energy (KC-250³).

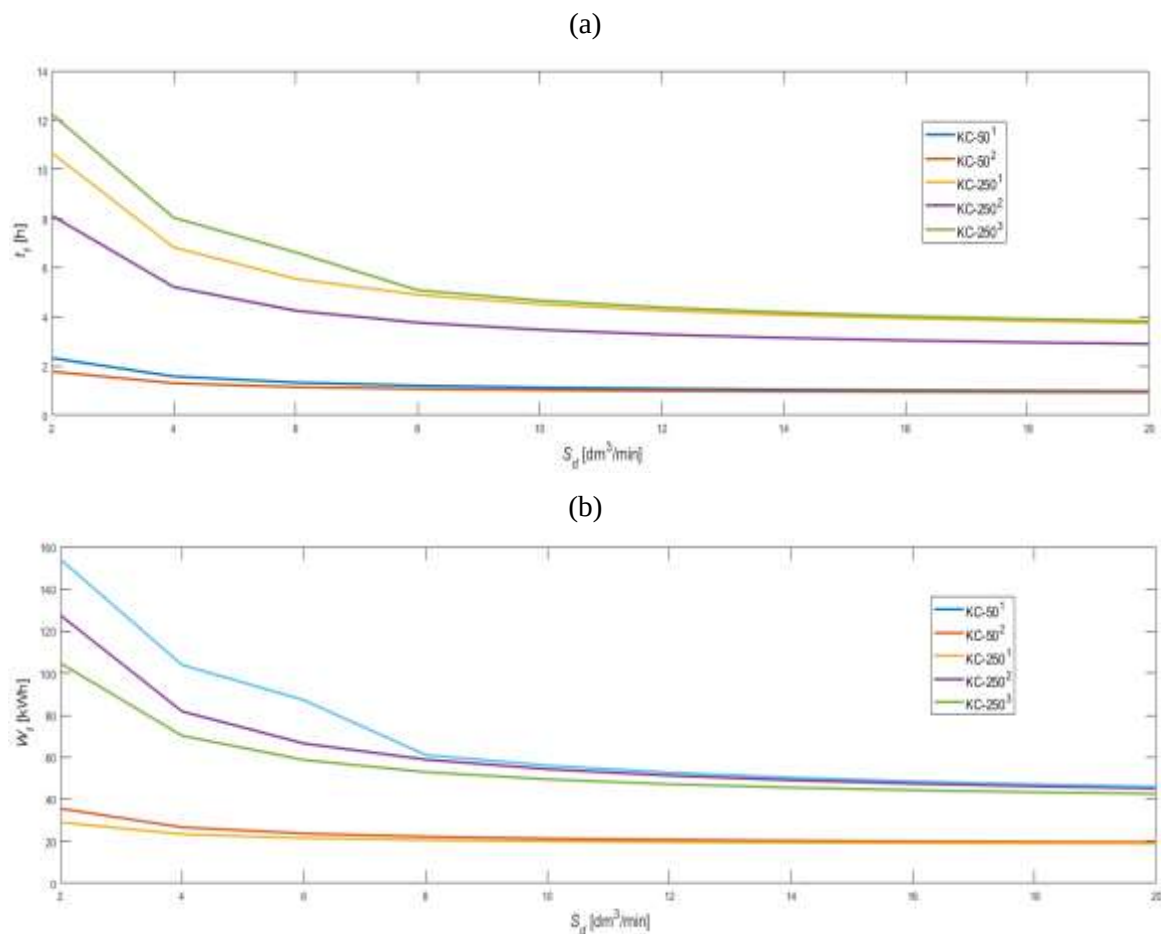


Fig. 2. Influence of dosing subsystem efficiency on (a) processing time, (b) electric energy consumption for five different CWA variants

Source: Documentation of project no. POIR.01.01.01-00-0540/19, 2020.

In Fig. 3, the influence of reservoir capacity of reactor and scrubber on processing time is visualized. The reservoirs have a smaller impact on processing time and consumed electric energy than dosing efficiency. However, the increase in reservoir capacity may lead to a decrease in processing time, reaching even 4-5 hours.

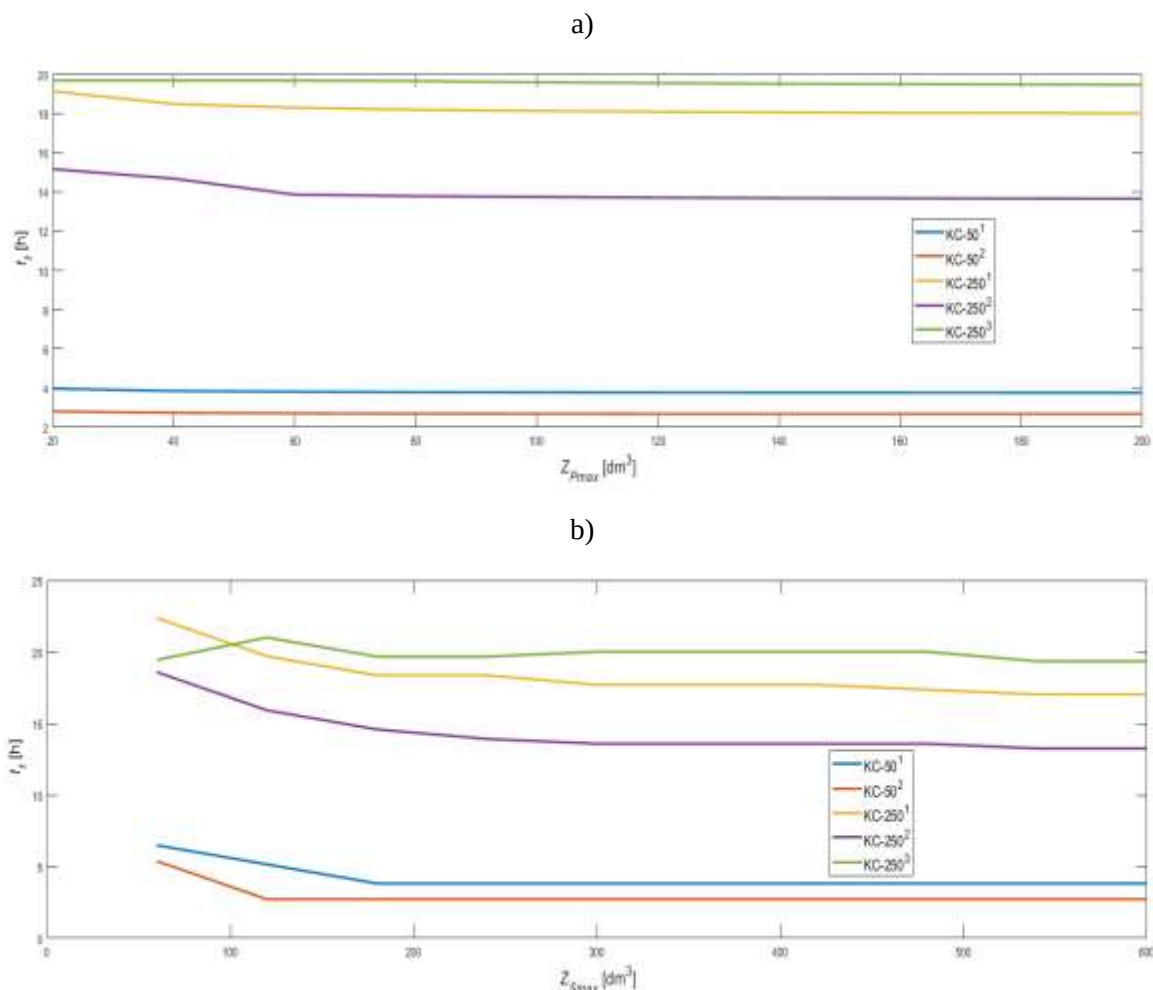


Fig. 3. Influence of (a) reactor reservoir and (b) scrubber reservoir on processing time for five different CWA variants

Source: Documentation of project no. POIR.01.01.01-00-0540/19, 2020.

4. CONCLUSIONS

The mathematical model of the CWADS was built and then implemented in Matlab. It enabled to carry out several numerical tests showing:

1. The flow at individual stations of the CWADS carried by the KC-50 and KC-250 bombs,
2. The influence of several selected parameters on the entire disposal process was examined, particularly the disposal time and consumed electric energy.

Disposal of KC-250 bomb causes many problems both at the system input (almost 1 m³ of CWA with solvent) and at the installation's output (the need to start the plasma reactor and the scrubber repeatedly at the adopted reservoirs of both disposal stations). For both KC-50 and KC-250 bombs, a "bottleneck" in the form of low dosing system efficiency can be noticed.

Due to the continuous process of improving the innovative CWADS, the mathematical model implemented in Matlab will also be modified later in the project. It is also planned to enrich the existing numerical model to analyze the flow/consumption of cooling water and carrier gases.

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