

Numerical modeling and analytical modeling of cryogenic carbon capture in a de-sublimating heat exchanger

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Abstract. Both a numerical and analytical model of the heat and mass transfer processes in a CO₂, N₂ mixture gas de-sublimating cross-flow finned duct heat exchanger system is developed to predict the heat transferred from a mixture gas to liquid nitrogen and the de-sublimating rate of CO₂ in the mixture gas. The mixture gas outlet temperature, liquid nitrogen outlet temperature, CO₂ mole fraction, temperature distribution and de-sublimating rate of CO₂ through the whole heat exchanger was computed using both the numerical and analytic model. The numerical model is built using EES [1] (engineering equation solver). According to the simulation, a cross-flow finned duct heat exchanger can be designed and fabricated to validate the models. The performance of the heat exchanger is evaluated as functions of dimensionless variables, such as the ratio of the mass flow rate of liquid nitrogen to the mass flow rate of inlet flue gas.

Keywords: Cryogenic CO₂ Capture, heat exchanger, numerical integration

1. Introduction

In history and modern society, especially developing countries where the energy sector is highly dependent on coal, will still use fossil energy as the primary power source for industrial development [2]. For example, coal represents 68.8% of the primary Chinese domestic energy sources in 2011[2]. The developed countries have the same issue. Take US as an example, the generation of electricity through combustion of coal is the largest component of greenhouse gas emissions in the United States, and globally coal combustion constitutes 40% of carbon dioxide (CO₂) emitted to the atmosphere due to energy consumption [3]. The large amount of CO₂ will cause global warming. We all know the importance of reducing CO₂ emissions. In order to reduce carbon emissions and achieve clean coal fired power generation, a demonstration unit to capture 0.12 million tons/year of CO₂ from flue gas has been put into operation [4].

There are three ways to capture CO₂: post-combustion, pre-combustion and oxy-fuel combustion. Post-combustion technologies are most likely to be commercialized and used in existing coal-fired power plants. Cryogenic CO₂ capture (CCC) is one of the post-combustion technologies with great potentials. It uses cryogenic refrigeration techniques to separate CO₂ from the other components of the flue gas. Although CCC techniques are still in the research phase, a variety of promising systems have been proposed. [5] It seems ridiculous to cool the hot gas to a very cold temperature to de-sublimate the CO₂ because in the first glance, it will consume huge energy. But research shows that by cooling to 156K, 90% of the CO₂ will be captured, by cooling to 138K, 99% will be captured, and the energy costs to this method are reasonable and competitive. [6]

In heat exchanger, there is lots of research on condensing heat exchanger especially for water condensing. In CCC, we need a heat exchanger to de-sublimate the CO₂. The difference between the condensing heat exchanger and the heat exchanger to de-sublimate the CO₂ is that we will separate the target gas by cooling it to solid, which needs much lower temperature than water condensing.

In this paper, we develop an analytical model and manipulate it in a numerical way to design a heat exchanger to capture the CO₂. This paper describes an analytical model of the heat and mass transfer process in a counter-flow rectangular duct heat exchanger with cooling nitrogen inside and a mixture of CO₂ and nitrogen outside the ducts. Then numerical integration of the governing equation technique is applied in EES (Engineering Equation Solver).



2. Heat exchanger structure

The plate heat exchanger operating in a counter-flow configuration is shown schematically in Figure 1. In the hot-side of the heat exchanger, a gas mixture (N₂-CO₂) at $P_H = 1\text{atm}$ and $T_{H,in} = 176.8\text{K}$ enters one set of channels (i.e., every other channel). The total mass flow rate of the gas mixture passing through all of the hot-side channels is $\dot{m}_H = 1.5\text{ kg/s}$. Nitrogen gas at $P_C = 1\text{atm}$ and $T_{C,in} = 160\text{K}$ enters the other set of channels (the cold-side of the heat exchanger) with a total mass flow rate $\dot{m}_C = 1.5\text{ kg/s}$. Each plate is $th_m = 0.5\text{ mm}$ thick and is composed of aluminum. The plates are $L = 100\text{ cm}$ long in the flow direction and $W = 35\text{ cm}$ wide (into the page). The plate separation distance (i.e., the channel height) is $th_H = th_C = 2.2\text{ mm}$. There are $N_{ch} = 100$ pairs of channels.

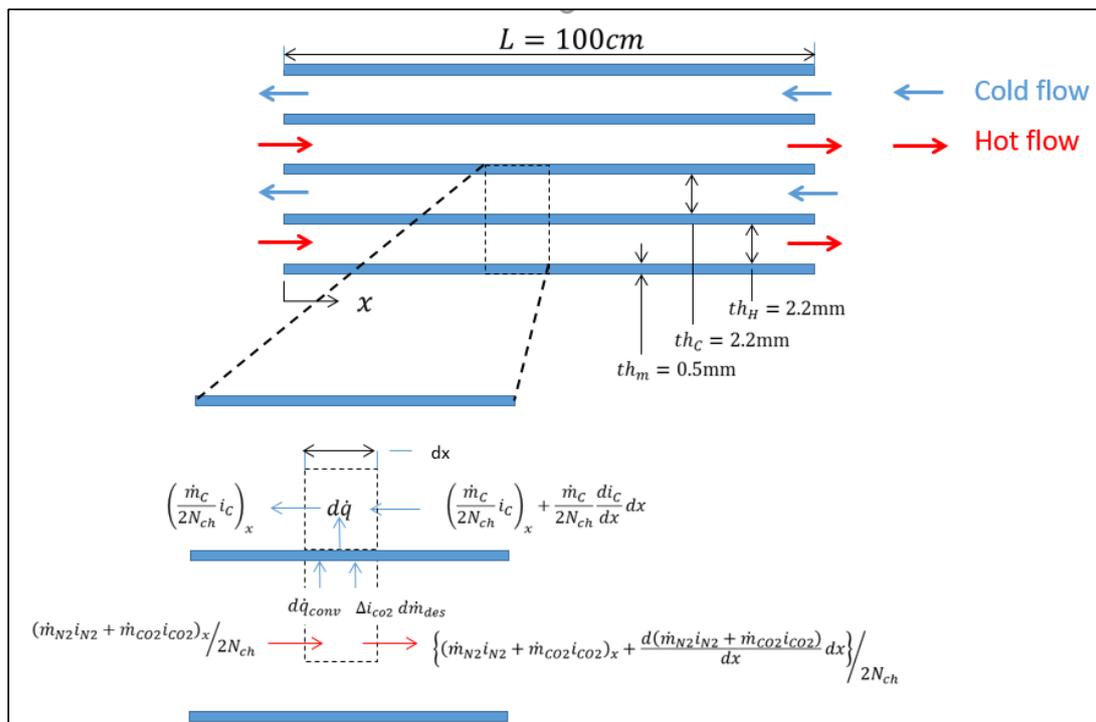


Figure 1. Plate heat exchanger in a counter-flow configuration

The fins are also added to the hot channels as is shown in figure 2. The length of the fin, L_{fin} is half of the hot channel height so that it is adiabatic in the end when we analyse it. The thickness of the fin th_{fin} is 0.001 m. The number of fins in each channel is 50. We can calculate the fin area of one channel by the following formula:

$$A_{s,fin} = L \times th_H \times (N_{fin} - 1) \quad (1)$$

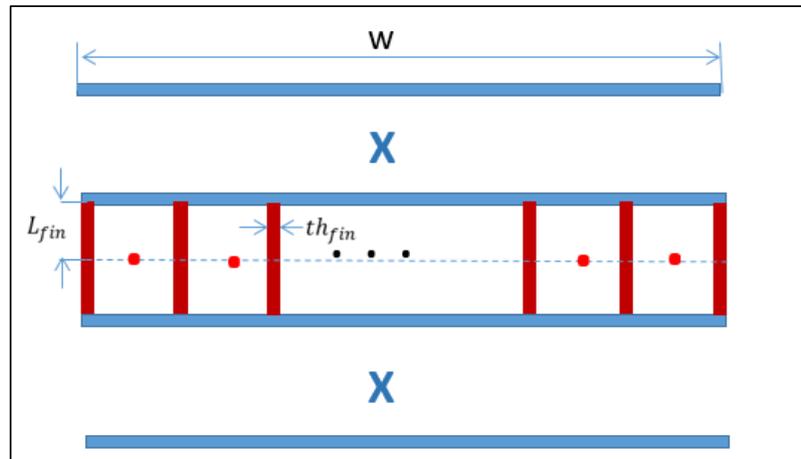


Figure 2. The cross-sectional area of the heat exchanger

3. Assumption and Analytical model

Assumption:

1. Any CO₂ that hits the wall will stick to the wall.
2. The thermal resistance of the CO₂ layer can be ignored
3. The pressure drop can be ignored. Based on the output, the total pressure drop is just 700 Pa.
4. The total inlet pressure is ambient pressure.

The first step in obtaining the numerical solution is to derive the state equations that must be integrated numerically through the heat exchanger. These are obtained from the differential energy balances on the cold stream and hot stream, shown in Figure 1.

3.1 energy balance on cold and hot stream

The energy balance on the cold stream is:

$$dq = -\frac{\dot{m}_c}{2 \cdot N_{ch}} \cdot c_c \cdot \frac{dT_c}{dx} \cdot dx \quad (2)$$

The energy balance on the hot stream:

$$dq = -\frac{d(m_{N_2} i_{N_2} + m_{CO_2} i_{CO_2})}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (3)$$

Pull out the mass flow rate of nitrogen:

$$dq = -m_{N_2} \frac{d(i_{N_2} + mr \cdot i_{CO_2})}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (4)$$

And expand into an equation of $\frac{dT}{dx}$:

$$dq = -m_{N_2} \left[\frac{\partial(i_{N_2} + mr \cdot i_{CO_2})}{\partial T} \right]_{sat} \cdot \frac{dT}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (5)$$

Expand by chain rule:

$$dq = -m_{N_2} \left[\frac{\partial(i_{N_2})}{\partial T} + mr \frac{\partial(i_{CO_2})}{\partial T} + i_{CO_2} \left(\frac{\partial(mr)}{\partial T} \right)_{sat} \right] \cdot \frac{dT}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (6)$$

It can be expressed in terms of c_{N_2} and c_{CO_2} :

$$dq = -m_{N_2} [c_{N_2} + mr c_{CO_2} + i_{CO_2} \left(\frac{\partial(mr)}{\partial T} \right)_{sat}] \cdot \frac{dT}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (7)$$

Then it can be expressed in terms of c''_{N_2} (the specific heat capacity of the N_2 - CO_2 mixture expressed on a per mass of N_2 basis)

$$dq = -m_{N_2} [c''_{N_2} + i_{CO_2} \left(\frac{\partial(mr)}{\partial T} \right)_{sat}] \cdot \frac{dT}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (8)$$

The term within the square brackets in Eq. (8) is referred to as the saturation specific heat capacity $c''_{a,sat}$ (along the saturation line). Then we get

$$dq = -m_{N_2} c''_{N_2,sat} \cdot \frac{dT}{dx} \cdot dx / (2 \cdot N_{ch}) \quad (9)$$

Where,

$$c''_{N_2,sat} = \left(\frac{\partial i_{N_2}}{\partial T} \right)_{sat} \quad (10)$$

The saturation specific heat capacity can be evaluated numerically according to [7]:

$$\begin{aligned} c''_{N_2,sat} &= \left(\frac{\partial i_{N_2}}{\partial T} \right)_{sat} \\ &\approx [i_{N_2}^*(T + \Delta T) - i_{N_2}^*(T - \Delta T)] / (2 \cdot \Delta T) \end{aligned} \quad (11)$$

3.2 the heat transfer rate from mixture gas to the wall:

On the mixture-side, the differential rate of energy transfer from the mixture gas to the wall, $d\dot{q}$, is associated with both convection heat transfer from the mixture to the wall ($d\dot{q}_{conv}$) as well as energy carried by the desublimating CO_2 . The rate of energy carried by the desublimating CO_2 is the product of the mass flow rate of desublimation (d) and the latent heat of desublimation of CO_2 (Δi_{des}):

$$d\dot{q} = d\dot{q}_{conv} + \Delta i_{des} d\dot{m}_{des} \quad (12)$$

Convection heat transfer from the mixture to the wall ($conv d\dot{q}$) is given by:

$$d\dot{q}_{conv} = \eta_0 A_{tot} h_0 (T_h - T_w) \frac{dx}{L} \quad (13)$$

η_0 is the overall surface efficiency and h_0 is the local mixture side heat transfer coefficient.

η_0 can be calculated using the adiabatic tip condition:

$$\eta_0 = \tanh(mL) / (mL) \quad (14)$$

$$mL = \sqrt{\frac{2 \cdot h_0}{k \cdot t_{fin}}} \cdot L_{fin} \quad (15)$$

Here, k is the conductivity of the fin material

The differential mass flow rate at which CO_2 is de-sublimated ($d\dot{m}_{des}$) can be expressed in terms of a local mass transfer coefficient (h_D).

$$d\dot{m}_{des} = \eta_0 A_{tot} h_D \rho_{N_2} (mr_{sat,center} - mr_{sat,wall}) \frac{dx}{L} \quad (16)$$

ρ_{N_2} is the density of the nitrogen. $mr_{sat,center}$ is the mass ratio of the saturation state on the centreline of the stream and $mr_{sat,wall}$ is the mass ratio of the saturation state on the wall.

Combining equations (12), (13) and (16), we get the heat transfer rate, $d\dot{q}$:

$$d\dot{q} = \eta_0 A_{tot} h_0 (T_h - T_w) \frac{dx}{L} + \Delta i_{des} \eta_0 A_{tot} h_D \rho_{N_2} (mr_{sat,center} - mr_{sat,wall}) \frac{dx}{L} \quad (17)$$

3.3 calculate the h_0 and h_D

h_0 is the local mixture side heat transfer coefficient, and the Nusselt number is calculated using the built-in function in EES:

Call ductflow_n_local(Re,Pr,LoverD_h, Aspect,RelRough: Nusselt_T_x, Nusselt_H_x, f_x), where Re is Reynolds number, Pr is the Prandtl number, LoverD_h is the ratio of the length and hydraulic diameter. Aspect is the ratio of the channel height and the gap between fins. RelRough is set to zero. The heat transfer coefficient is then obtained in the standard way:

$$h_0 = Nu \frac{k_m}{D_h} \quad (18)$$

A similar approach also can be applied to h_D , the local mass transfer coefficient:

Call ductflow_n_local(Re,Sc,LoverD_h, Aspect,RelRough: Sh_t, Sh_h, f_x_s) where Sc is the Schmidt number and Sh is the Sherwood number. Finally, we have

$$h_D = Sh \frac{D_{CO_2,m}}{D_h} \quad (19)$$

$D_{CO_2,m}$ is the mass diffusion coefficient.

3.4 The heat transfer rate from the wall to the cold flow

The heat transfer rate from the wall to the cold flow, which also can be expressed as $d\dot{q}$, can be calculated by the formula shown as below:

$$d\dot{q} = (T_w - T_c) / (th_m / (k_w \cdot w \cdot deltax) + 1 / (h_c \cdot w \cdot deltax)) \quad (20)$$

It is the temperature difference divided by the thermal resistance.

4. Numerical model

The numerical model is composed by combining equations (2), (9), (17) and (20) and applying them for each control volume. The boundary conditions are specified for the inlet temperature of the hot and cold flows. By applying the numerical integration technique, we can calculate $\frac{dT}{dx}$ and obtain the temperature distribution and other properties.

The Euler method is applied in this problem. The temperature at the end of each time step is computed based on the temperature at the beginning of the time step and the governing differential equation. Euler's method approximates the rate of temperature change within the time step as being constant and equal to its value at the beginning of the time step. Therefore, for any time step j :

$$T_{j+1} = T_j + \frac{dT}{dt} \Big|_{T=T_j, t=t_j} \Delta t \quad (21)$$

Because the temperature at the end of the time step (T_{j+1}) can be calculated explicitly using information that is available at the beginning of the time step (T_j), Euler's method is referred to as an explicit numerical technique. [7] We can also apply a higher order numerical integration technique, such as the Runge-Kutta fourth order method, or fully implicit method such as Crank-Nicolson Method.

5. Results and discussion

By varying the inlet temperature of the cold nitrogen flow, we plot the CO2 mass rate to the wall versus time (figure 3) and the CO2 mass flow rate in the stream versus time (figure 4) for each pair of channels.

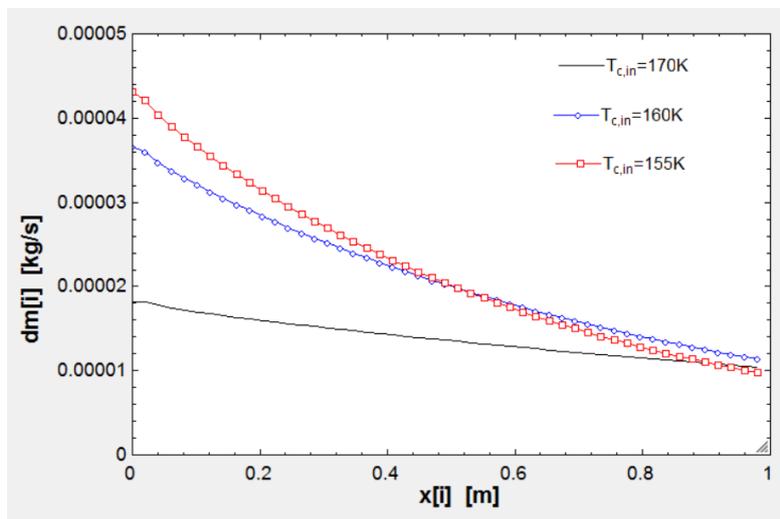


Figure 3. the mass rate to the wall versus position

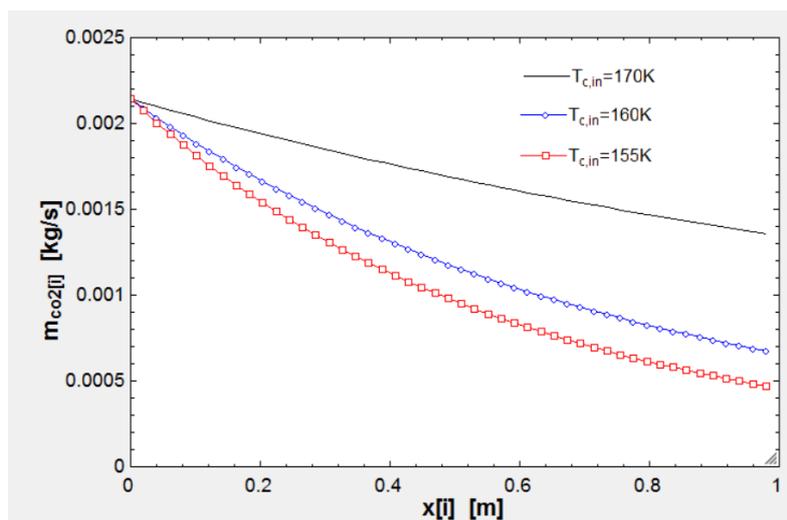


Figure 4. the CO2 mass flow rate in the stream versus position for different inlet temperature of cold flow

As the inlet temperature of the cold flow at the beginning of the duct decreases, the desublimating rate increases. However, near the cold inlet end of the duct, the desublimating rate with $T_{c,in}$ 155K is smaller than that with $T_{c,in}$ 160K. The reason is that the mass flow rate of CO2 in the centerline is smaller in the $T_{c,in}$ 155K case.

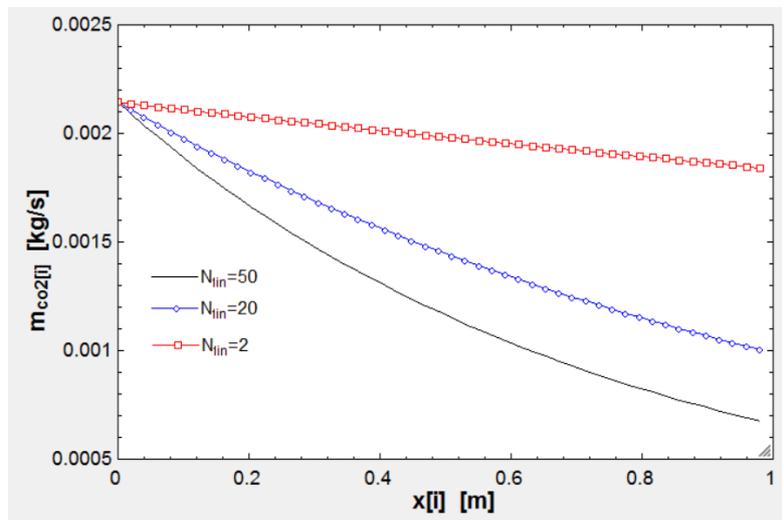


Figure 5. The CO2 vapour mass flow rate in the stream versus position for different fin numbers

Figure 5 shows that the de-sublimating is more effective with increasing number of fins as one would expect. This simulation is under $T_{c,in}$ 160K. However, there may be a disadvantage to this approach since in such a case, it may be more challenging to design an appropriate dynamic scraper to collect the solid CO2. More fins will make the scraping process more difficult.

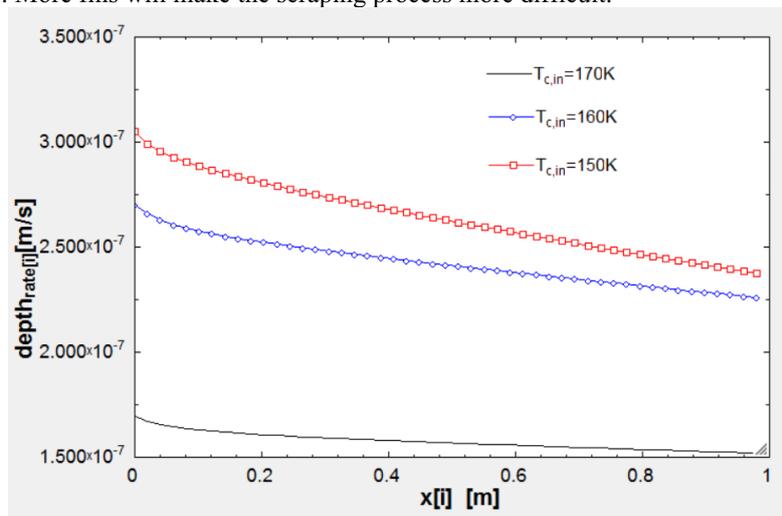


Figure 6. the depth rate of desublimation to the wall versus the position

Figure 6, displays the expected feature of a faster growth rate of the solid layer for, the lower inlet cold flow temperature. By calculation, in the condition of $T_{c,in}$ 160K, $N_{fin} = 50$, it takes 4070s to fill up the inlet duct.

In this heat exchanger, the total mass of de-sublimation of CO2 is 0.06023kg by using eq.22 to get the de-sublimating rate and multiplying the time (4070s).

$$\dot{m}_{des} = \frac{\dot{m}_H}{1 + mr_{in}} (mr_{in} - mr_{out}) \quad (22)$$

When $T_{c,in} = 160\text{K}$, and with 50 fins, we find that solid CO_2 also forms in the free stream because the centerline temperature drops very fast. For example, by taking the difference between the CO_2 mass flow rate at the exit as displayed in figure 5 and the summation of the mass rate going to the wall ($0.0003011\text{kg/s} - 0.0001359\text{kg/s}$), we find that the mass flow rate of solid CO_2 in free stream equals 0.0001652kg/s . In this case, the summation over the entire channel length of the mass rate going to the wall is 0.0001359kg/s . The ratio of the mass rate in the free stream over the mass rate going to the wall is then 1.215. In other words, a significant amount of the solid CO_2 that forms in the heat exchanger is not captured by the walls. Future analyses of heat exchanger geometries will be pursued in order to characterize the effectiveness of the ‘exchanger’ as a solid CO_2 capture device.

6. Conclusion:

An analytical model of heat and mass transfer processes in a mixture gas desublimating heat exchanger system was developed using fundamental heat and mass transfer relations. The modeling approach is based on conservation of energy and mass for the mixture gas and cooling nitrogen. All governing equations were solved using a numerical integration technique with appropriate assumptions. The analysis provides a means for calculating the rate of desublimation and thickness of solid formation on the walls as a function of time and location. Further analyses will explore the effectiveness of various heat exchanger designs for capturing the de-sublimated solid.

7. References

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