Use of Navier Stokes in Extractive Metallurgical Systems

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Abstract

This paper provides an overview of the use of Navier-Stokes equations in extractive metallurgical processes. It explores the relationship between these equations and extractive metallurgical processes and techniques. The paper further delves into the applications of Navier-Stokes equations within these processes, as well as the reactions involving their use. The paper highlights the recent advancements in computational fluid dynamics and its effects on extractive metallurgical processes. Finally, the paper addresses the challenges and limitations of applying Navier-Stokes equations in extractive metallurgy. The paper aims to provide a deep understanding that Navier-Stokes equations remain a powerful tool for improving efficiency and sustainability in extractive metallurgy, with ongoing research aimed at overcoming current limitations.

1 Introduction to Navier-Stokes Equations - Yash

1.1 Overview

The Navier-Stokes equations govern the motion of fluids. The Navier-Stokes equations are partial differential equations that describe motion in terms of the instantaneous velocity, pressure, and spatial position relationship of viscous fluids. The equations can be seen as Newton's second law of motion for fluids. They mathematically express momentum balance for Newtonian fluids and make use of conservation of mass. They often include an equation of state relating to pressure, temperature and density. Although they have a wide range of applications, it has not yet been proven whether smooth solutions always exist in three dimensions, that is, whether they are infinitely differentiable or even just bounded at all points in the domain.

1.2 Models to solve Navier-Stokes equations

Computational Fluid Dynamics (CFD) methods which can be used to solve the Navier-Stokes equations holding a large number of industrial applications and use cases are:

- 1. **Direct numerical simulation** (DNS) does not need a turbulence model and directly solves the NS equations. Although this simulation method is a high-accuracy solution, it is computationally expensive.
- Reynolds-averaged Navier-Stokes (RANS) models rely on RANS equations and are the most frequently used models for computational fluid dynamics simulation in the extractive metallurgical field due to their industrial applications. These turbulence models approximate the NS equation to save computational costs.
- 3. Large-eddy simulations (LESs) focus on a large-scale turbulence structure with simplified small-eddy effects and approximations in the NS equations. LES has been drawing increasing popularity because of the increased computational power and the requirement to capture relatively detailed flow information.

CFD models which are also used are Detached Eddy Simulation(DES), which combines aspects of LES and RANS, Finite Element Method(FEM) and Pseudo-spectral Method. Despite the type of CFD models, the CFD workflow to solve the Navier-Stokes equations majorly consists of three steps,

Figure 1: Navier-Stokes Equations

that is, pre-processing (building models, generating grids, and setting boundary conditions), solving (selecting appropriate solvers and calculation), and post-processing (data analysis and visualization). e

2 Introduction to Extractive Metallurgy - Vatsal

- 1. Extractive metallurgy is a branch of metallurgical engineering that focuses on how metals are extracted from their natural ores. It involves studying different types of ores, processes like washing, concentration, and separation, as well as chemical methods to extract pure metals. These metals are then alloyed or processed further, either for direct use or to create materials with specific properties for various applications.
- 2. It involves various processes like Mining, Crushing, Grinding, Concentration, Smelting, Refining, Casting and some important techniques such as Hydrometallurgy, Pyrometallurgy and Electrometallurgy. The processes to be used in extraction and refining are selected to fit into an overall pattern, with the product from the first process becoming the feed material of the second process, and so on. It is quite common for hydrometallurgical, pyrometallurgical, and electrolytic processes to be used one after another in the treatment of a single metal.
- 3. Extractive metallurgy is truly advanced engineering. Experts in this field design complex reactors like blast furnaces for iron, Hall-Héroult cells for aluminum, and the Siemens process for silicon. These designs rely on principles of physics, thermodynamics, reaction kinetics, and transport phenomena. Creating these reactors also involves expertise in high-temperature experiments and computer simulations, often using methods like finite element or finite volume techniques. Additionally, many extractive metallurgy processes are applied to treat and manage air, water, and solid waste.
- 4. Extractive metallurgy is essential for producing materials critical to modern industries. It enables the extraction of steel for construction, aluminum for transportation, copper for electrical wiring, and rare earth metals for renewable energy technologies like wind turbines and EV batteries.

Precious metals like gold and silver, vital for electronics and financial systems, are also refined through metallurgical processes, driving industrial and technological progress.

3 Relation Between Navier-Stokes and Extractive Metallurgy -Vedant

1. Introduction

"Free surface flows" describe a diverse range of flows in pyrometallurgical unit operations. Examples of important free surface flows in pyrometallurgy include pouring and skimming operations, bubbling from gas injection, slopping from molten metal baths, and splashing induced by gas injection.

In recent years, the intensification and development of new bath smelting processes, such as the Ausmelt and HiSmelt processes have led to use of well developed fluid dynamics models. These tools, have been very handy in gaining the insights of smelting and furnace operations in metal melting.

2. Computational Models

Primarily, two working models have been used in the computation of surface flows:

Single Fluid Model The single fluid model, in which the gas—liquid mixture that makes up the volume of the flow domain, is considered as a single fluid of variable density determined from the volume fraction distribution of bubbles in liquid.

Two Fluid Model Two-fluid models have been more widely used than single-fluid models in the studies of flows in metallurgical vessels because they require less knowledge about the gas distribution compared with single-fluid models. However, significant empiricism is also required in the two-fluid model to estimate the phase interactions between the two phases.

An alternative approach to the CFD modeling of free surface flows in metallurgical vessels is to attempt to capture the transient nature of these flows and model the fundamental physics driving these flows. Numerical methods based on *interface tracking* within transient numerical simulations can be subdivided into **Lagrangian** and **Eulerian** methods for tracking complex free surface motions.

3. Numerical Modeling

The Navier-Stokes equations play a crucial role in improving extractive metallurgy processes by enabling accurate modeling and simulation of fluid dynamics.

The dimensional velocity formulation of the equations governing incompressible isothermal multifluid flow is:

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

The elaborated form of the Navier-Stokes equation is:

$$\frac{\partial U}{\partial t} + \nabla \cdot UU = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \nabla \cdot \tau + g + \frac{1}{\rho} S, \tag{2}$$

where U is the velocity, P is the pressure, τ is the viscous stress tensor, g is the acceleration due to gravity, S is the surface tension force, ρ is the density, and t is time.

4 History Of Navier Stokes Equation- Varun Malviya

1. Navier has a background in higher analysis at the École Polytechnique and in practical engineering at the École des Ponts et Chaussées put him in a good position to contribute to the science of fluid flow by realizing that fluid friction was the main cause for the deviation of experiments from theory. In his developments, Navier begins by using Laplace's molecular program that considers bodies as made up of particles which are close to each other and which act on each other by means of two opposing forces - one of attraction and one of repulsion - which, when in a state of

equilibrium, cancel each other out. When the fluid moves, and all the molecules, being carried away by a common motion, preserve their respective situations, the state of these molecules does not change, and no new action is established in the interior of the fluid. However, when there is difference in velocities between two molecules, the repulsive force between these two molecules will change. According to Navier, a quantity given by the difference in velocities between the two molecules, multiplied by a function of the distance of these two molecules 2 (which decreases very fast as the distance increases), and by a constant relative to the viscosity, gives the repulsive force between them. Because of contradictory experimental results, Navier's main concern was to know what would be the correct boundary conditions to be satisfied at solid boundaries, for cases where the molecules of the walls exert a particular action upon those of the fluid. Lastly by applying Lagrange's method of moments, obtains again the Navier-Stokes equation, but with new boundary conditions.

2. In 1845, Sir George Stokes found the equation of motion of a viscous flow by adding Newtonian viscous terms, thus the Navier-Stokes Equations was brought to its final form, which is used to generate numerical solutions for fluid flow .

5 Reactions in extractive metallurgy involving the use of N-S equation:- Varun Malviya

In extractive metallurgy , Navier-stokes equation is used in designing fluid flow, heat transfer and mass transport across various process. The few metallurgical reactions and the use of Navier stokes equation in these processes is described below:-

1. Smelting and matte converting: Reactions are as follows: -

• Iron ore reduction in blast furnace:

$$\mathrm{Fe_2O_3} + \mathrm{3CO} \rightarrow \mathrm{2Fe} + \mathrm{3CO_2}$$

• Sulfide oxidation in matte smelting:

$$2Cu_2S+3O_2\rightarrow 2Cu_2O+2SO_2$$

Here N-S equation helps to find the circulation pattern that is the movement of slag and different substances and also predict their movement under the influence of buoyancy, surface tension and many more.

• N-S Equation:

$$ho\left(rac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot
abla \mathbf{v}
ight) = -
abla P + \mu
abla^2 \mathbf{v} + \mathbf{F}$$

• Continuity equation: assuming to be incompressible

$$\nabla \cdot \mathbf{v} = 0$$

where:

- ho = density of the molten metal or slag
- v = velocity field (flow of molten metal or slag)
- P = pressure
- μ = dynamic viscosity
- F = external forces (gravity, buoyancy, surface tension,

Assumption for smelting furnace flow are as follows, it also comprises of the equation that is used along with N-S:

• Using the boussiness approximation we assume:

$$\rho = \rho_0(1 - \beta(T - T_0))$$

Where the terms are as:

- ρ_0 = reference density
- β = coefficient of thermal expansion
- \bullet T = local temperature
- \bullet T_0 = reference temperature

The buoyancy term in the equation is:

$$\mathbf{F} =
ho g \mathbf{\hat{k}} =
ho_0 g eta (T - T_0) \mathbf{\hat{k}}$$

• The term -rho*g*k represents a constant hydrostatic pressure gradient due to the weight of the fluid moreover we are mainly concerned with how buoyancy drives fluid motion thus we ignore this hydrostatic term.

Putting this in the momentum equation we get the N-s equation as follows:

$$ho_0 \left(rac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot
abla \mathbf{v}
ight) = -
abla P + \mu
abla^2 \mathbf{v} +
ho_0 geta(T-T_0)\mathbf{\hat{k}}$$

• Surface tension effects: This effect occurs at the interface between molten metal and slag, its dependency on the temperature is as follows:

$$\sigma = \sigma_0 - \gamma (T - T_0)$$

$$\gamma = rac{d\sigma}{dT}$$

 $\gamma = rac{d\sigma}{dT}$ is the surface tension gradient

The force per unit area due to this surface tension is:

$$\mathbf{F}_{\sigma} = \nabla_{s} \sigma$$

Where ∇_s represent surface tension gradient

• The final reduced N-S equation is as follows:

After assuming:

Steady state conditions and neglecting inertia for slow flows which is Represented below:

$$(\mathbf{v} \cdot \nabla \mathbf{v} \approx \mathbf{0}) \qquad (\frac{\partial \mathbf{v}}{\partial t} = \mathbf{0})$$

Modified N-S equation:

$$0 = -
abla P + \mu
abla^2 \mathbf{v} +
ho_0 g eta(T - T_0) \mathbf{\hat{k}} +
abla_s \sigma$$

2. Electrolytic refining:

- Reaction involved are as follows:
- At the anode:

$$Cu o Cu^{2+} + 2e^-$$

• At the cathode:

$$Cu^{2+} + 2e^- \rightarrow Cu$$

- Here N-S is used to model ion transport and fluid flow due to convection and helps analyze bubble formation at electrodes.
- The general form of the equation:

$$rac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot
abla) \mathbf{v} = -rac{1}{
ho}
abla p +
u
abla^2 \mathbf{v} + \mathbf{f}$$

where $\mathbf{f} = \frac{\mathbf{F}}{\rho}$ represents body forces per unit mass.

• Electromagnetic force: when an electric field is applied then there will be the flow charges in copper refining and if a magnetic field is present then an external force will act which is the Lorentz force per unit mass given by:

$$\mathbf{f}_L = \frac{1}{\rho} (\mathbf{J} \times \mathbf{B}) \tag{3}$$

Where:

- $\mathbf{J} = \text{current density}$
- $-\mathbf{B} = \text{magnetic field}$
- Natural convection due to the heat generated due to electrolysis is handled by using boussineq approximation :

$$\rho = \rho_0 (1 - \beta (T - T_0))$$

The buoyancy force is:

$$\mathbf{F}_B = \rho_0 g \beta (T - T_0) \mathbf{\hat{k}}$$

- The mass transport equation is used along with the N-s equation and it describes the movement of ions due to diffusion, convection and other effects.
- The equation is as follows:

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = D\nabla^2 C + \frac{zF}{RT}C\nabla \Phi$$

where:

- $C = \text{concentration of metal ions (e.g., Cu}^{2+})$ R = universal gas constant
- D = diffusion coefficient
 - T = temperature
- ullet z = charge of the ion (e.g., z=2 for Cu^{2+})
- Φ = electrostatic potential

- F = Faraday's constant
- Final reduced equation, ignoring inertial effects and for slow flows we get:

$$0 = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{v} + g\beta (T - T_0) \hat{\mathbf{k}} + \frac{1}{\rho} (\mathbf{J} \times \mathbf{B})$$
(4)

Where:

- $-\frac{1}{a}\nabla P$ represents the pressure gradient force.
- $\nu \nabla^2 \mathbf{v}$ accounts for viscous effects.
- $g\beta(T-T_0)\hat{\mathbf{k}}$ represents natural convection due to thermal gradients.
- $\frac{1}{a}(\mathbf{J} \times \mathbf{B})$ represents the Lorentz force due to electromagnetic effects.

6 Uses of Navier-Stokes in Extractive Metallurgy - Vedant

- 1. Application of computational fluid mechanics in two areas of metallurgy is considered: solidification of liquid alloys and MHD turbulence.
 - The Navier-Stokes equations have been employed to model the flow of liquid steel during ingot casting. A numerical model for solving the hydrodynamic problem has been presented. The finite element method has been used to solve the problem. Numerical calculations have been performed using a developed computer program. The solutions have been accomplished for steady-state conditions.
- 2. Slag formation in the furnace during smelting of iron has a fundamental application of Navier-Stokes equations. Slag forms and rises through the liquid metal to float on the surface. Navier-Stokes equations can be used to model slag movement through liquid metal.
 - Understanding the behavior of nonmetallic inclusions (particles) or gas bubbles in molten steel is an important topic in primary and secondary metallurgy. Gas bubble flow in steelmaking vessels, melt stirring in ladles to maintain thermal homogeneity and reduce nonmetallic inclusions, melt flow and removal of nonmetallic inclusions in tundishes, blowing argon gas into submerged entry nozzles (SEN) during continuous casting to minimize the risk of clogging, etc.
- 3. The most common way of modeling the motion of bubbles/particles in molten steel and turbulent flow of the molten steel is by solving the Navier-Stokes equation together with corresponding turbulence equations. Gas stirring is an important process used in secondary metallurgy. It allows to homogenize the temperature and the chemical composition of the liquid steel and to remove inclusions which can be detrimental for the end-product quality. In this process, argon gas is injected from two nozzles at the bottom of the vessel and rises by buoyancy through the liquid steel, thereby causing stirring, i.e., a mixing of the bath. The gas flow rates and the positions of the nozzles are two important control parameters in practice. A continuous optimization approach is pursued to find optimal values for these control variables. The effect of the gas appears as a volume force in the single-phase incompressible Navier-Stokes equations.

7 Research on the Use of Navier-Stokes in Extractive Metallurgical Systems- Yash

7.1 Motivation

The current drive for research in extractive metallurgy is to incorporate and integrate advanced computational methods to improve efficiency, optimise existing approaches, minimise environmental impact, and ultimately foster a more sustainable future.

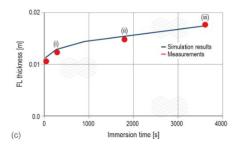


Figure 2: Comparison of the experimental results and simulation results of the Freeze Lining thickness development over immersion time.

7.2 Computational Methods in Metallurgical Systems

Computational methods like Computational Fluid Dynamics (CFD) or methods like Geo-metallurgical modelling are the primary techniques. Computational Fluid Dynamics (CFD) simulates fluid flow, heat transfer, and mass transport within metallurgical systems. By solving the governing equations of fluid mechanics and thermodynamics such as the Navier-Stokes equation. Almost all CFD problems are based on the solving of Navier-Stokes (NS) equations.

CFD is a powerful tool that allows for the detailed analysis of multiphase interactions, such as those occurring in furnaces during extractive metallurgical processes. This technique is at the forefront of optimization of the design and operation of metallurgical equipment and processes at the level of individual furnaces.

Specially designed algorithms that combine mathematical programming and metaheuristics can explore vast parameter spaces, tackle complex optimization problems inherent in metallurgical processes and identify optimal operating conditions that balance efficiency, environmental impact, and cost.

7.2.1 Steel-making processes

In steelmaking, CFD models help to optimize the gas flow and slag behaviour inside a metallurgical furnace, reducing gas emissions while improving metal yield. By simulating complex steel-making environments, we can predict how molten, gaseous, and solid charges will behave under varying conditions in the process of extractive metallurgy, allowing for more efficient process design, optimization of energy consumption, and minimization of emissions. These improvements align with the motivation that exists for the research.

The complexity of the steel-making process and other metallurgical processes, which involve multiple variables such as temperature, pressure, reaction kinetics, and resource inputs, are at the level of individual unit operations. Hence, there is a need for techniques that globally optimize the coordination and integration the unit operations.

7.2.2 Slag Freeze Lining

One of the most interesting and path-breaking uses of computational fluid dynamics in the field of extractive metallurgy is for slag freeze lining. Freeze lining (FL) is a protective layer of solidified slag formed on the inside of a furnace lining. It has a significant economic value in industrial processes specifically in steel-making. This technique is widely used in extractive metallurgical systems to protect furnaces and refractory linings from corrosive molten slag and acts as a thermal barrier to minimise energy consumption.

A novel computational fluid dynamics (CFD) model and framework capable of simulating FL formation across various applications has been developed recently. Extensive validation to confirm the model's robustness and versatility has provided positive results. This model has created a way for more efficient and cost-effective processes

Future research could include incorporating new fundamental knowledge of FL formation kinetics, its response to thermal and compositional fluctuations, and modelling the mobile phase. comparison of the experimental results and simulation results of the FL thickness development over immersion time. We can thus see that the simulation results are validated by experimental data

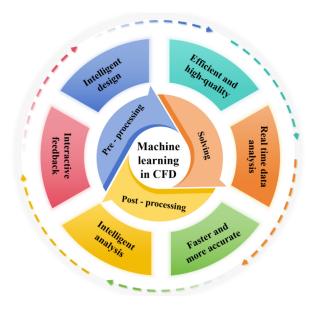


Figure 3: Use of Machine Learning in computational fluid dynamics

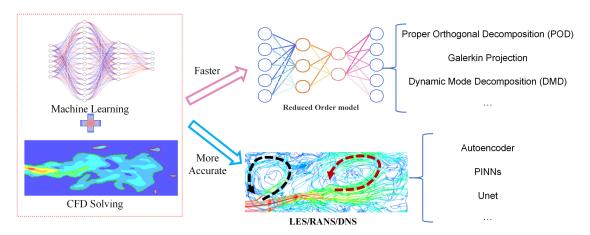


Figure 4: The main ways of applying machine learning to the computational fluid dynamics (CFD) solving process

7.3 Future Research Potential

Future research will focus on developing innovative extraction methods to address challenges such as decreasing ore grades and complex mineralogies, energy shortage or water scarcity. Research could also include developing advanced numerical methods alongside machine learning techniques to solve the Navier-Stokes equation more efficiently. To solve the complex Navier-Stokes equations in 3D simulations supercomputers could be leveraged.

The development of machine learning could improve the CFD performance. The machine learning or parametric modelling methods may reduce the pre-processing time of CFD by three orders in the estimate. The solving step is expected to be accelerated by 5 to 1000 times using machine learning. ML could be tailored for each step of the CFD simulation process, providing a convenient and efficient modelling framework to break through many bottlenecks of current CFD.

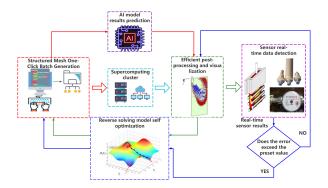


Figure 5: Proposed framework to combine parametric modelling or meshing with ML for real-time CFD prediction and close-loop online control

8 Challenges and Limitations in the using navier Stokes in Extractive metallurgy- Vatsal

The Navier-Stokes equations are essential tools for understanding fluid dynamics and are commonly used to simulate fluid flow in diverse areas, including extractive metallurgy. However, using these equations in extractive metallurgy comes with difficulties and restrictions because of the intricate nature of the processes involved. The following points highlight some of the main hurdles and limitations:

8.1 Complexity of Multiphase Flows

r Extractive metallurgy frequently deals with multiphase systems, like the interactions between gases, liquids, and solids (for example, in smelting, slag formation, or flotation).

To model these interactions, the Navier-Stokes equations must be linked with additional equations for each phase, which makes the calculations more complex.

It's difficult to accurately represent interfacial phenomena such as surface tension and phase boundaries.

8.2 High-Temperature and Reactive Environments

Extractive metallurgy processes typically take place at high temperatures (e.g., in furnaces or reactors), leading to substantial variations in fluid properties like viscosity and density.

Chemical reactions (e.g., reduction, oxidation) add further complexity to the system by introducing more variables and nonlinear behaviors. The Navier-Stokes equations alone cannot describe chemical reactions without being integrated with reaction kinetics models.

8.3 Turbulence Modeling

Turbulent flows are frequently observed in metallurgical processes, such as in stirred reactors or gas injection systems.

Direct numerical simulation (DNS) of turbulence using the Navier-Stokes equations demands significant computational resources.

Simplified turbulence models (e.g., k-E or Reynolds-averaged Navier-Stokes) are commonly employed, but they might not precisely capture all the important flow characteristics.

8.4 Non-Newtonian Behavior

Certain fluids in extractive metallurgy, like slags or slurries, display non-Newtonian behavior (e.g., shear-thinning or viscoelasticity).

The standard Navier-Stokes equations are based on the assumption of Newtonian fluids, which means they need to be modified or supplemented with additional constitutive equations to accurately model non-Newtonian behavior.

8.5 Boundary Conditions and Geometry

Extractive metallurgy systems often have complex geometries, such as those found in furnaces, ladles, or reactors, making it difficult to define appropriate boundary conditions.

Wall effects, like heat transfer and friction, can significantly influence the flow, but they are challenging to model accurately.

8.6 Computational Cost

Using the Navier-Stokes equations to simulate big metallurgical processes needs a lot of computer power. To get all the small details right, you often need very detailed models and long simulations, which makes it hard to do simulations quickly or for very large systems.

8.7 Material Property Variability

Material properties like viscosity, density, and thermal conductivity in extractive metallurgy can change a lot depending on what the material is made of, how hot it is, and the pressure it's under. Since we often don't have good data for these properties, simulations can be inaccurate.

8.8 Coupling with Other Phenomena

Extractive metallurgy frequently involves interconnected phenomena like heat transfer, mass transfer, and electromagnetism (as seen in electric arc furnaces).

Combining the Navier-Stokes equations with models for these phenomena increases the complexity of the simulations and requires more computational power.

8.9 Validation and Experimental Data

It's hard to prove that Navier-Stokes models are accurate for metallurgical processes because it's difficult to get good experimental data in very hot or dangerous environments.

This lack of data can make the model predictions uncertain.

8.10 Simplifications and Assumptions

To make the Navier-Stokes equations easier to work with, we often make simplifying assumptions (like assuming things are constant over time or that the fluid can't be compressed).

However, these assumptions might not be valid for all metallurgical processes, which can lead to inaccurate results.

8.11 Conclusion

While the Navier-Stokes equations provide a powerful framework for modeling fluid flow in extractive metallurgy, their application is limited by the complexity of the processes, computational costs, and the need for accurate data and coupled models. Advances in computational fluid dynamics (CFD), high-performance computing, and experimental techniques are helping to address some of these challenges, but significant work remains to improve the accuracy and applicability of these models in extractive metallurgy.

9 Conclusion

With the emerging need for optimal, calculated and easy to use solutions for engineering problems in metallurgical process, the Navier-Stokes equations becomes significantly important. Their implementation aided by improved computational facilities can predict the behavior of a metallurgical process under certain control parameters, which can be tuned to study their effects on overall efficiency and output enhancement. However with increasing complexities in engineering fields, the Navier-Stokes are also needed to reengineered involving more control parameters.

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