

## THE SIMULATION OF A THERMAL-FLUID SYSTEM USING AN INTEGRATED SYSTEMS CFD APPROACH

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### ABSTRACT

Complex thermal-fluid systems may consist of many interacting components such as pipes, heat exchangers, turbines and boilers. The first of two major design challenges is to predict the performance of all the thermal-fluid components on the system level and the second is to predict the performance of the integrated plant consisting of all its sub-systems. The solution to both is an integrated Systems CFD (Computational Fluid Dynamics) approach that deals with various levels of complexity between individual models. To account for the interaction between components on system level a progressive approach can be followed by first using lumped models for all components and then refining individual models where necessary.

To illustrate the application of a progressive analysis, this paper presents the practical example of a coal-fired boiler at a power station. A one-dimensional pipe network was used to determine the quality of the steam mixture and the heat transfer in the boiler riser tubes and these were linked to the detailed three-dimensional CFD model of the furnace. Results from the CFD model showed gas flow patterns and heat distributions inside the furnace. From the network model the temperatures and steam quality inside the riser tubes were obtained and it illustrated the process of steam generation inside the riser tubes.

### NOMENCLATURE

$A$	area
$\bar{B}$	body resistance force
$E$	total specific energy
$e$	specific internal energy
$\bar{g}$	gravitational acceleration vector
$\bar{n}$	unit vector normal to surface
$\bar{q}$	heat flux vector
$q'''$	heat generated per unit volume
$\bar{V}$	velocity vector
$\forall$	volume of control volume
$\varepsilon$	porosity
$\rho$	density
$\Gamma$	stress tensor
$f$	fluid
$s$	solid

### INTRODUCTION

Engineers are faced with two major challenges when carrying out the thermal-fluid design of complex thermal-fluid systems consisting of many interacting components such as pipes, valves, heat exchangers, compressors, turbines, pumps and reactors. Examples of such systems are nuclear power plants, coal-fired power plants and oil refineries. The first challenge is to predict the performance of all the individual thermal-fluid components (Becker & Laurien, 2003). The second challenge is to predict the performance of the integrated plant consisting of all its sub-systems (Greyvenstein & Rousseau, 2003). System performance predictions must be done for both steady-state and transient conditions. Steady-state analyses are required to study normal operating conditions and to generate initial values for transient analyses. Transient simulations are required for control studies and for studying operating procedures such as start-up, load rejection and load following, as well as for the analysis of accident events. The complexity associated with the thermal-fluid design of complex systems requires the use of a variety of analysis techniques and simulation tools. These range from simple one-dimensional models (Rousseau & Greyvenstein, 2003) that do not capture all the significant physical phenomena to large-scale three-dimensional CFD codes (Becker & Laurien, 2003) that, for practical reasons, can not simulate the entire plant as a single integrated model.

Various approaches have been developed to model complete thermal-fluid systems. One approach is to build a custom computer model for a specific system layout or to use commercially available modelling tools such as SPECTRA (Stempniewicz, 2002) or Aspen Custom Modeller (Kikstra, 2001). Another approach that is widely used is the (pipe-)network approach (Ji, 2004). With this approach models of standard lumped and one-dimensional models are developed that can be interconnected in any arbitrary way. Three-dimensional CFD codes and network codes have also been linked (Klein & Rüdiger, 2003). In such cases the 3D code would be used to simulate the detailed flow in a component, whilst the network would simulate the remainder of the system and thus provide the boundary conditions for the 3D code. In simulations such as these the main emphasis is on the detailed flow in the component and they are in essence controlled by the 3D code.

However, the simulations could also be managed by the network code. In this case the network code serves as the framework to link the models of the various components

together and to control the solution. The models of the components can be of varying degrees of complexity. These can range from simple lumped models to complex full three-dimensional CFD models. A heat exchanger for example can be represented by a single lumped model, a network of one-dimensional models or a full three-dimensional CFD model. The choice of model will amongst others depend on the nature of the simulation, the importance of the component(s) and the influence that it has on the system and vice versa. This philosophy has been coined the systems CFD approach. This has, over the last decade, gradually evolved from a mainly network approach (Greyvenstein & Laurie, 1994) to a more advanced strategy (Greyvenstein, 2002) and finally a comprehensive methodology (Du Toit et al., 2006). The thermal-fluid research and development work associated with the pebble bed modular reactor (PBMR) power plant currently being developed in South Africa provided a particular impetus in the evolution of the systems CFD approach.

This paper gives a broad overview of the philosophy of the systems CFD approach. It is illustrated at the hand of an example of boiler simulation. It is not the purpose of the paper to discuss any validated results in detail. As such it serves only to illustrate the use of the Systems CFD technique in a possible application environment.

## METHODOLOGY

### Theory

The point of departure for such a methodology is the equations for the conservation of mass, momentum and energy for the fluid(s) and the conservation of energy for the solid(s). We therefore start with the equations for a control volume in integral form. The conservation equations for the fluid is then given as (Peyret & Taylor, 1983)

$$\frac{d}{dt} \int_{\mathcal{V}} \rho d\mathcal{V} + \int_A \{ \rho \vec{V} \cdot \vec{n} \} dA = 0 \quad (0.1)$$

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{V}} \rho \vec{V} d\mathcal{V} + \int_A \{ (\vec{n} \cdot \vec{V}) \rho \vec{V} - \vec{n} \Gamma \} dA \\ = \int_{\mathcal{V}} \rho \vec{g} d\mathcal{V} - \int_{\mathcal{V}} \vec{B} d\mathcal{V} \end{aligned} \quad (0.2)$$

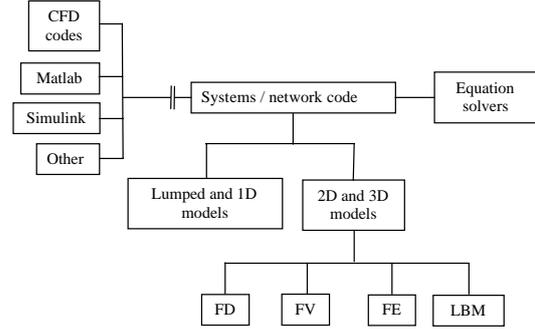
$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{V}} \rho E d\mathcal{V} + \int_A \vec{n} \cdot \{ \rho E \vec{V} - \Gamma \vec{V} + \vec{q} \} dA \\ = \int_{\mathcal{V}} (\rho \vec{g} \cdot \vec{V} + q''') d\mathcal{V} \end{aligned} \quad (0.3)$$

whilst the conservation equation for the solid is given as (Peyret & Taylor, 1983)

$$\frac{d}{dt} \int_{\mathcal{V}} \rho_s e d\mathcal{V} + \int_A \vec{n} \cdot \vec{q} dA = \int_{\mathcal{V}} q''_s d\mathcal{V} \quad (0.4)$$

The energy equations (3) and (4) are linked to each other at the fluid-solid interfaces through the appropriate convection boundary conditions. In the case where flow through a porous medium such as a packed bed reactor (Du Toit et al., 2006) is considered the porosity has to be incorporated in equations (1) to (4). Depending on the processes and phenomena that must be modelled the appropriate closure equations have to be added.

The underlying philosophy of the systems CFD methodology is that for the analysis of large thermal-fluid systems it must be possible to link models of various levels of abstraction and varying degrees of complexity together to simulate such systems. The level of abstraction and the degree of complexity of the models are determined by the nature of the simulation, i.e. a first order analysis or a detailed analysis, and the detail and character of the information required. It is therefore essential to have a framework which makes this possible and ensures that the fundamental conservation principles are satisfied at all times.



**Figure 1** : Schematic representation of the systems CFD framework

A schematic representation of the systems CFD framework is shown in Figure 1. The heart of the framework is a systems or network code. The network code in essence controls and drives the simulation process and links all the components together. It distributes the necessary data to the various components and then gathers all the required information to set up the global systems of equations that must be solved. It also manages the exchange of information with external codes. Two modes of coupling or linking between the network code and the other components of the systems CFD framework can occur, namely internal or external coupling. In the case of the internal coupling (represented by the blocks in the lower part of Figure 1) the components are intimately linked to the network code and merely provide the required information for the coefficients of the global systems of equations. In the case of the external coupling (represented by the blocks in the upper left handside of Figure 1) the network code and the relevant external codes exchange the required information through an appropriate interface at set intervals.

At the highest level of abstraction we have the lumped and 1D models typically associated with a network code. These, however, follow from a rigorous analysis starting out from the basic conservation equations. At the lowest level of abstraction we may have a full 3D lattice Boltzmann (LBM) formulation. The notion is that in setting up the global systems of equations the values of the coefficients may be evaluated in any appropriate way using any valid formulation. The only requirement is that the formulations, and therefore the contributions to the coefficients, must be compatible. We may therefore elect to evaluate the coefficients of the global systems of equations for one part of the problem using a finite element formulation (FE), whilst for another part we may prefer to use a finite difference (FD) or finite volume (FV)

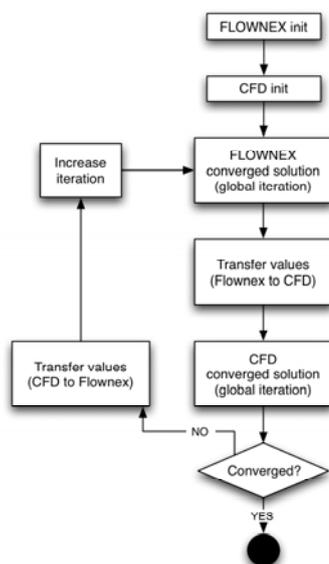
approach. The particular choice will amongst others be determined by the character of the problem and the suitability of the formulation.

The systems CFD methodology therefore provides the engineer with the basis for the progressive analysis of a problem. The investigation will start out with a first order analysis consisting of 1D and lumped models. This will provide the initial indications of the characteristics of the system and the areas that might need more attention. This also enables the engineer to start developing a feel and an understanding for the dynamics, peculiarities and intricacies of the system. The complexity of the simulation can then gradually and selectively be increased and eventually also the level of abstraction until the required degrees of complexity and levels of abstraction are reached. As mentioned before, this will all be determined by the nature of the simulation and the detail and character of the information required.

**Solution Algorithm**

A general algorithm for solving a steady-state integrated systems CFD problem is depicted in Figure 2. The process starts by initialising the models and obtaining separate, converged, steady-state solutions with each of the two codes. The initial boundary values used as input conditions for the models should be as close as possible to the values of the linked boundary elements during a coupled solution. This helps to reduce large variations in the solutions during the iteration process when the network and CFD codes are linked together.

When the steady-state solutions have been reached for both codes, the communications link between the codes is established and information transfer is initiated. The algorithm then follows an iterative procedure where the network code completes an iteration and transfers the necessary boundary values to the CFD code. The CFD code then completes its corresponding iteration and transfers the values back to the network code. Only after this handshaking process is completed, does the “integrated” global iteration advance.



**Figure 2 :** Solution algorithm for steady-state systems CFD models

The process is ended when the applicable convergence criteria are satisfied for both codes, or when a set number of integrated iterations have been completed.

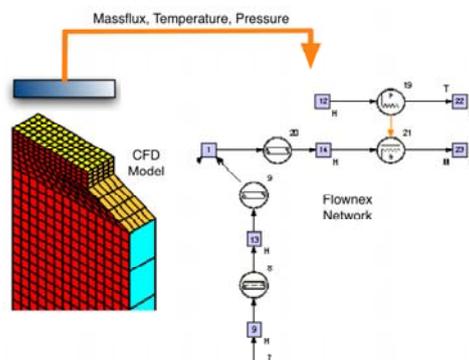
Transient integrated problems are solved using the same algorithm for information exchange, except that an extra time-step iteration loop is added outside of the integrated system’s iteration process. For each time-step, converged solutions must then be sought for both codes in order to determine the transient behaviour of the linked system.

The different elements of an integrated simulation are discussed in the next sections by describing the information transfer between the codes and the practical example of the Lethabo Power Station boiler and riser tube network.

**Information Transfer**

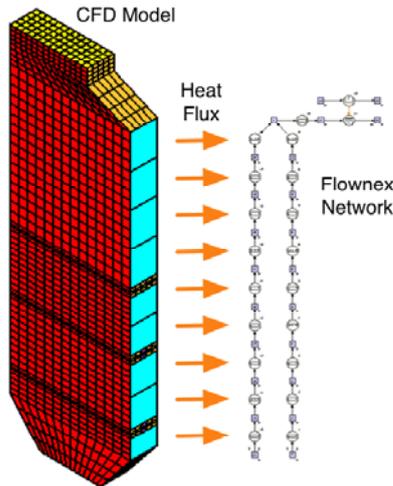
Information coupling between the network and CFD codes can be accomplished in two different manners. One method is an “internal”-coupling where the equations generated by individual component models are assembled into a single global matrix system and solved as an implicit, inter-dependant system. The other method – used in this study and illustrated in Figure 2 – is to use an “external”-coupling where information is explicitly exchanged across boundaries between two parts of the systems CFD model. Explicit coupling can be accomplished by using boundary- and node-averaged values or by directly linking cells and elements.

The link by using values averaged on the boundary is illustrated in Figure 3. To use this type of coupling, the property values on a certain boundary patch in the CFD model is averaged and applied to a single network node. The average value is determined by using area, volume or density weighted properties, depending on the type of property and the mesh geometry. In reversal, the property value at a node is uniformly applied to the corresponding patch in the CFD model. This assumes that the uniform boundary condition is a suitable approximation in the context of the rest of the model. In practice, this is enforced by defining the location of the linked boundary in regions where close-to-uniform distributions in properties are expected. Node-averaged values are useful in situations where properties such as inlet and outlet velocities are transferred to-and-fro between the network and CFD codes.



**Figure 3 :** Boundary averaged information exchange

Improved per-element accuracy can be achieved by linking elements and cells directly, as shown in Figure 4. The network elements are linked exclusively to corresponding cells in the CFD model and property values are directly transferred without undergoing any averaging or conversion processes. The only modification needed is to ensure that compatible units are used between codes. The researcher has a great degree of freedom in choosing numerical resolutions for the CFD mesh and network models and as such the integrated model's accuracy can readily be modified to achieve a solution suited to the requirements of the simulated problem.



**Figure 4 :** Element and cell based information exchange

## EXAMPLE

### Lethabo boiler test case

To illustrate the unique modelling possibilities available when using the integrated systems CFD approach, a simulation test case was selected with features requiring detail CFD and network methods. The boiler and riser-tube system in a modern coal-fired power station is a practical example where both methods can be shown in action. The Lethabo Power Station is one of the more recent coal-fired power stations commissioned in the last two decades by the South African national electricity utility company ESKOM and the boilers have been the subject of a previous study as published by ESKOM (1995). It was decided to use the Lethabo boiler (specifically the combustion chamber) and typical operating conditions as basis for the test case presented to emphasize the feasibility of the Systems CFD approach in modelling actual plant situations. The test case is however not intended to be a rigorous analysis of all the physical phenomena inside a boiler and does not present results that were validated against operational data. As such it serves only to illustrate the use of the Systems CFD technique in a possible application environment.

### Boiler simulations

The modern coal-fired boiler is a complex piece of thermal equipment where the chemical heat energy stored in coal is unlocked through combustion and transferred to water in the wall tubes to ultimately result in superheated steam to drive the turbine generators. In the case of the

Lethabo boiler, which is a radiant water-tube type, heat transfer between flue gas and riser tubes is mainly through convection and radiation.

Current CFD simulation codes have advanced capabilities with which to model the combustion of p.f. (pulverized fuel), the passage of flue gas through the boiler, radiation inside the combustion chamber and radiation/convection heat transfer to the walls of the chamber. To obtain optimum use of computing resources, the CFD model is typically subdivided into a separate model for the combustion chamber and another for the heat exchangers in the outlet passage of the boiler. This division of labour is necessitated by the different requirements of the two sections: the chamber has complex numerical models regulating the combustion process and a simple geometry, whilst the outlet passage uses ordinary gas models but with a complex heat exchanger geometry. By assuming at least 90% combustion, the fluid properties at the outlet of the combustion chamber can be linked through boundary values to the inlet of the heat exchanger passage.

### The combustion chamber

The primary objective of the CFD model of the combustion chamber is to determine the effectiveness of the combustion process. This is done by modelling the actual flames that result from the chemical combustion reactions and the resultant flow of flue gas through the chamber. The main phenomena investigated are: the transient shape of the flames, the active chemical reactions, radiation from the flames and heat-transfer between the gas, walls and water-tubes. The actual shape of the flames is determined by the interaction between all the physical processes, which makes for very costly simulations in terms of computational resources.

### The riser tubes in the chamber walls

The phase change from feed water to steam takes place inside of the riser tubes situated in the walls of the combustion chamber. The tubes form a critical heat sink in the boiler and extract heat from the combustion process to drive the enthalpy increase of the water and steam mixture. Because of the strong interaction between phenomena inside the combustion chamber, the heat flux through the walls has a direct influence on the shape of the flames.

The status quo in CFD modelling is to use average approximations for the heat flux through the boiler walls. The heat flux values are then calibrated with local velocity profiles to obtain the known total heat flux through the walls. Because the actual phase change in the pipes cannot be modelled simultaneously with the combustion chamber with traditional CFD codes, this heat flux approximation is the "best guess" that can be made under the circumstances.

The above leads to the situation where the chamber is modelled using approximate heat fluxes and flame positions are determined from these guessed boundary conditions. This in turn means that predicted modifications for flame optimization cannot be done with a great deal of confidence because of the uncertain nature of the wall conditions.

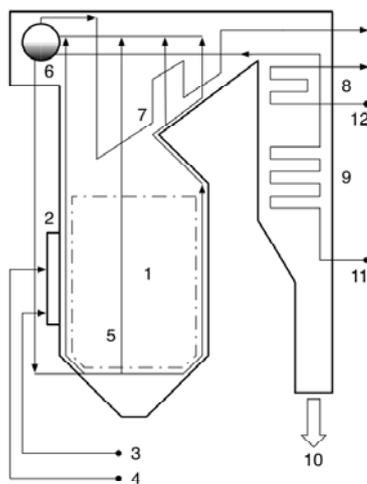
### Modelling riser tubes as separate pipe network

The problematic heat fluxes in the CFD model can be improved by modelling the riser tubes as a separate pipe network. With the network code, the flow conditions inside individual pipe elements can be calculated (e.g. the quality of the water/steam mixture, fluid temperature and convection coefficients) and are directly influenced by the heat flux per element. The temperatures and convection values can then be fed back to the CFD model in an iterative manner to obtain more realistic heat flux boundary values for the CFD model.

### Lethabo boiler thermal network

The illustration in Figure 5 shows the main components of the Lethabo boiler's thermal network. The heart of the boiler is the combustion chamber, where pulverized fuel is injected into the combustion chamber and ignited to burn at about 1300 °C. The p.f. is injected at a total rate of between 350 and 400 tons per hour through a maximum of 36 burners situated in the front and rear walls of the boiler. The coal is pulverized in rotating tube mills and transported by the primary air supply to the burners. The burners blend the primary and secondary air supplies to obtain the correct mixture between p.f. and air to sustain combustion at the correct rate to handle the load required of the boiler.

The demineralised feed water is fed to the steam drum at a pressure of 20.5 MPa and a temperature of 248 °C. In order to conserve energy, the feed water is pre-heated by flowing through the enclosure side walls and economiser. In the combustion chamber, the feed water in the riser tubes is heated by convection and radiation and through a process of natural convection flows to the steam drum situated at a height of 77 m. The saturated steam is separated from the water by cyclone separators and scrubbers - the water flows back to the boiler via the downcomers and the steam is passed through the boiler platen superheaters. The final condition of steam from the boiler is a superheated condition at 17.32 MPa, 540 °C at a rate of 509.7 kg/s.



- 1 Boiler combustion chamber
- 2 Boiler burners
- 3 Secondary air
- 4 Primary air
- 5 Riser tubes
- 6 Steam drum
- 7 Boiler platen superheater
- 8 Boiler reheater
- 9 Boiler economiser
- 10 Outlet to precipitators and chimney
- 11 Demineralised feed water
- 12 From HP turbine

Figure 5 : Coal-fired boiler thermal circuit

### DISCUSSION OF RESULTS

In this section, representative results are shown that gives an idea of the results that can be obtained through the use of an integrated model approach.

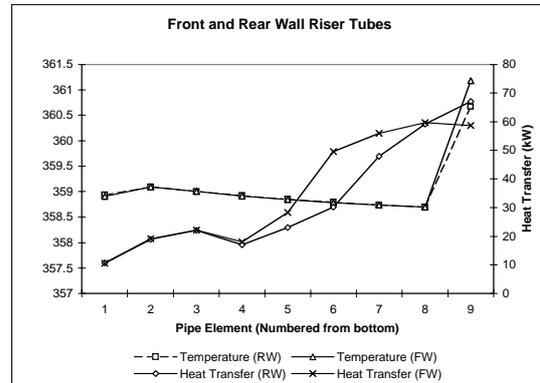


Figure 6 : Temperature and heat flux distributions in pipe elements

Figure 6 illustrates the calculated properties inside the front and rear wall riser tubes. The temperature distributions stay relatively constant in the lower 8 pipe elements due to the boiling of the water and the subsequent phase change. The variation in the temperature is due to the increase in height between pipe elements that lowers the pressure and results in lower saturation temperatures.

The effect of localized superheating can be seen in the top-most pipe (number 9) in the front and rear wall sections where the heat flux into the tubes is a maximum. At that point all the saturated mixture has been converted to steam and the temperature starts to increase again as the steam enters the superheated region. The non-uniform calculation of heat flux is markedly different from previous studies (Van Staden, 1994) that used a pre-determined, uniform heat flux boundary on the boiler's furnace walls. When Figure 7 is considered, the phase change is clear from the steam quality, which changes from liquid (at node zero) through saturated mixture (nodes 1 – 9) to superheated vapor (node 10).

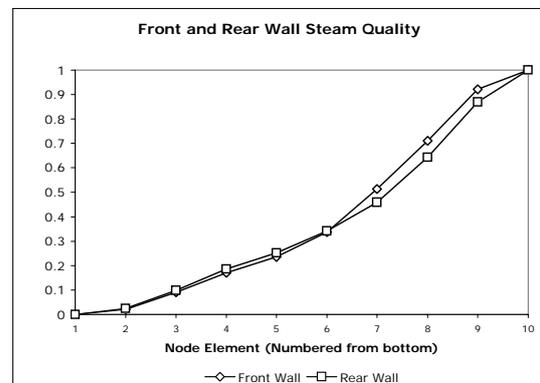


Figure 7 : Steam quality in node elements

Due to the rapid solution times of the network code, the iteration process to obtain the integrated model's solution is largely dependant on the convergence properties of the

CFD model. Because the combustion process is modelled with explicit heat sources in the enthalpy equation and the strong temperature influence on the fluid density, convergence for the CFD model was achieved after about 3000 iterations.

## CONCLUSION

Integrated Systems CFD is a methodology to link one-dimensional network codes with three-dimensional CFD models to model thermal systems as a whole, while retaining the added accuracy of the detail CFD component models. The coupling between codes for information exchange can be done on a per-cell/per-element basis, or by linking averaged boundary values to single nodes in the network.

The process was described at the hand of the practical test case of a coal-fired boiler where the furnace was modelled with CFD and the riser tubes in the furnace walls were represented by the pipes in a fluid network model. Gas flow inside the furnace was simulated using CFD and the network code calculated the temperatures and mass fluxes inside the riser network. Information was exchanged from the CFD to the network code via the heat flux across the furnace boundaries into the pipe elements. For the CFD model, the boundary conditions were obtained from the network code by specifying the fluid temperature and convection coefficients.

Results for the CFD model included the temperature, pressure and velocity distributions inside the boiler's furnace. In the pipe network, the variations in the heat flux along the furnace wall showed the quality of the water and steam mixture in the pipes to increase along the length of the pipes and at the top of the boiler superheated steam was obtained.

The results illustrate the advantages of using the Integrated Systems CFD approach to model coupled problems in situations where previous (uncoupled) assumptions in simulations proved to be rather inaccurate. For instance, the ability to model the liquid phase change in the pipes enabled the calculation of more realistic, non-uniform wall heat fluxes for the CFD model. By linking the two different methods, improved boundary values and system behaviour could thus be obtained from both the CFD model and fluid network model.

Future research on boiler simulation as presented in this study will incorporate more physical phenomena, e.g. combustion and radiation effects and realistic physical geometries. Operational effects such as the fouling of combustion chamber walls and incomplete combustion can also be investigated. By modelling different boiler loads the capabilities of the integrated system can be used to determine the varying steam conditions according to boiler load.

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