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Numerical Study of the Solidification and Macrosegregation Formation of the Binary System Al-4.1%wt Cu in a Rectangular Mold

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Abstract: Numerical study of both the solidification of the binary alloy Al-4.1%wtCu and macrosegregation formation have been carried out. The Bennon and Incropera continuum model was used in the development of the mathematical model representing the solidification phenomena. This model included the conservative equations; these equations were disctretized by using the finite volume method. The numerical solution of the disctretized conservative equations was performed by means of the SIMPLER algorithm.

Key words: Solidification, segregation, Al-4.1%wt Cu, continuum model, simpler algorithm, casting

INTRODUCTION

Solidification occurs in many metals growth processes, like foundry, welding, ingot casting, crystal growth, laser processing etc. The main feature in the solidification of a metallic alloy is the liquid-solid interface phase change associated with the release of latent heat and the solute redistribution. The solutes are often redistributed non-uniformly in the fully solidified product, which leading to segregation.

Segregation may be defined as any departure from uniform distribution of the chemical elements in the alloy. Because of the way in which the solutes in alloys partition between the solid and the liquid during freezing, it follows that all castings are segregated to some extent.

Some variation in composition occurs on a microscopic scale between dendrite arms, known as microsegregation. It can usually be significantly reduced by a homogenizing heat treatment because the distance, usually in the range 10-100 μm, over which diffusion has to take place to redistribute the alloying elements, is sufficiently small.

Macrosegregation cannot be removed. It occurs over distances ranging from 1 cm to 1 m and so cannot be removed by diffusion. We define positive segregation which refers to the solute concentration above the nominal concentration C_{ini}. While negative segregation refers to the solute concentration below the nominal concentration. The non-uniform distribution of chemical composition can significantly affect the mechanical properties of castings and therefore its prediction is very important.

Localised microsegregation causes macrosegregation as a result of physical movement of liquid and solid phases, most important being flow of interdendritic liquid.

Microsegregation results from freezing of solute-enriched liquid in the interdendritic spaces. But it does not constitute a major quality problem, since the effects of microsegregation can be removed during subsequent soaking and hot working. The basic principles of formation of microsegregation in castings and ingots were understood more than 50 years ago, (Flemings, 1974; Beckermann, 2002). These were extended thirty years ago to include the quantitative description of diffusion in the solid during solidification.

Macrosegregation, on the other hand, is non-uniformity of composition in the cast section on a larger scale. For example, a high degree of positive segregation in the central region of a continuously cast section is known as centreline segregation and poses quality problems. Macrosegregation affects the mechanical properties of casting products, (Schneider and Beckermann, 1995).

Solidification has been reviewed in books dealing with solidification Campbell (2003) and works due to Flemings (1974) Schneider and Beckermann (1995) and Ghosh (2001).

Likewise, experimental and theoretical studies on solidification phenomena have been carried out by several researchers (Singh and Basu, 2001a,b). In these studies; the mechanisms of different types of macrosegregation are well identified. It results from the relative motion in the liquid and solid phases. Motion in liquid phase can be induced by the solidification shrinkage and essentially by

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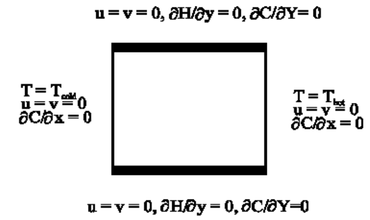

Fig. 1: Schematic of mold and boundary conditions

Table 1: Thermo-physical properties for Al-4.1% Cu From (Samanta and Zabaras, 2005)

Symbol	Quantity	Value in SI [a]
Ks	Thermal conductivity of solid	0.19249 kW m^{-1} °C
Kl	Thermal conductivity of liquid	0.08261 kW m^{-1} °C
cs	Specific heat of solid	1.0928 kJ kg^{-1} °C
cl	Specific heat liquid	1.0588 kJ kg^{-1} °C
Hf	Latent heat	397.5 kJ kg^{-1}
κp	Partition coefficient	0.17
β_T	Thermal expansion coefficient	4..95×10^{-5}°C^{-1}
β_S	Solutal expansion coefficient	-2.0 wt %$^{-1}$
ρ_s=ρ_l	Density, assumed here to be constant	2400 kg m^{-3}
μ	Viscosity	0.003 kg m^{-1} s
T_{ini}	Initial melt temperature	662°C
T_{cold}	Cold wall temperature	546°C
T_{hot}	Hot wall temperature	662°C$_r$
T_e	Eutectic temperature	548°C
T_f	Pure Al fusion temperature	660°C
C_{ini}	Initial concentration	4.1wt%
C_e	Eutectic concentration	33wt%
D_l	Melt diffusivity	3.0×10^{-9} m^2 s^{-1}
m	Liquidus slope assumed from Binary diagram	-353 K/wt%
N	Buoyancy ratio	-114.47
λ_1	Primary dendrite spacing assumed	161×0^{-6} m

the buoyancy forces and possibly by external forces, such as electromagnetically Lorentz force (Mechighel and Kadja, 2006).

The solidification processing of castings involves complicated phenomena such as: heat transfer with phase change, redistribution of solutes in liquid and solid phases; thermo-solutal convection in liquid and mushy zones, fluid flow driven by solidification shrinkage; transport of solute; transport of energy and thermal stresses and deformations in solidifying castings. The complicated transport phenomena result in defects such as shrinkage, macrosegregation, distortions and cracks, (Liu, 2005).

Solidification shrinkage is a result of the interface liquid-solid phase change. The solidification shrinkage induces the liquid motion and the solid deformation. Also, thermal contraction is another important feature in the solidification of castings.

In this study we interesting only to the study of solidification and macrosegregation formation in the system Al-4.1wt% Cu.

MATHEMATICAL MODEL FOR SOLIDIFICATION

Considering the molten Al-4.1%wt Cu alloy, filled in a rectangular mold, as shown in Fig. 1 where, the boundary conditions are illustrated. Moreover, the thermo-physical properties for this system are presented in Table 1 (Samanta and Zabaras, 2005). Suddenly, the left wall is cooled to a temperature below to the eutectic temperature and maintained at this temperature. The right wall temperature is maintained equal to the initial temperature of the melt. The other top and bottom walls are insulated and adiabatic. Under these conditions the directional solidification commences.

Assumptions: We assume that the solid phase is fixed and rigid (both in the mushy zone and in the solid zone). The movement of liquid is driven by the double diffusive convection. The behavior of the liquid metal is Newtonian. Fluid flow in the mushy zone obeys the Darcy's law. Also, we assume the following assumptions, (Ma *et al*., 2004).

- The flow is laminar and no turbulence is occurred.
- The permeability in the mushy is isotropic.
- The local thermal and phase equilibrium is satisfied in the mushy zone.
- The diffusion of solute within the solid is negligible,
- There is no motion or stress in solid phase.
- Densities in the solid and liquid are constants except for the variations in the volume force term (Boussinesq approximation).
- Diffusionlike and advectionlike terms in both energy and species conservation equations are considered.

Governing equations for solidification: The following Eq. 1-4 are derived based on the mass, momentum, energy and solute transfer conservations for binary alloy solidification, respectively. These equations are based on continuum model due to Bennon and Incropera (1987):

$$\frac{\partial \rho}{\partial t} + \nabla \bullet \left(\rho \vec{V}\right) = 0 \tag{1}$$

$$\frac{\partial(\rho u)}{\partial t} + \nabla \bullet \left(\rho \vec{V} u\right) = -\frac{\partial p}{\partial x} + \nabla \bullet \left(\mu_l \frac{\rho}{\rho_l} \nabla u\right) - \frac{\mu_l}{K}\frac{\rho}{\rho_l} u \tag{2}$$

$$\frac{\partial(\rho v)}{\partial t} + \nabla \bullet \left(\rho \vec{V} v\right) = -\frac{\partial p}{\partial y} + \nabla \bullet \left(\mu_l \frac{\rho}{\rho_l} \nabla v\right) - \frac{\mu_l}{K}\frac{\rho}{\rho_l} v + \rho_l g\left[\beta_T\left(T - T_{ref}\right) + \beta_S\left(f_l^{\alpha} - f_{l\,ref}^{\alpha}\right)\right] \tag{3}$$

$$\frac{\partial(\rho h)}{\partial t}+\nabla\bullet(\rho\vec{V}h)=\nabla\bullet\left(\frac{k}{Cps}\nabla h\right)+\nabla\bullet\left(\frac{k}{Cps}\nabla(h_s-h)\right)-\nabla\bullet\left(f_s\rho\vec{V}(h_l-h_s)\right) \quad (4)$$

$$\frac{\partial(\rho f^{\alpha})}{\partial t}+\nabla\bullet(\rho\vec{V}f^{\alpha})=\nabla\bullet(\rho D\nabla f^{\alpha})+\nabla\bullet\left(\rho D\nabla(f_l^{\alpha}-f^{\alpha})\right)-\nabla\bullet\left(f_s\rho\vec{V}(f_l^{\alpha}-f_s^{\alpha})\right) \quad (5)$$

In this dimensionless form, Mechighel and Kadja (2006): We defining characteristic scales for: Length, velocity, time, temperature, enthalpy, species concentration. The Eq. 1-4 in dimensionless form become, respectively.

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{V})=0 \quad (6)$$

$$\frac{\partial(\rho U)}{\partial t}+\nabla\cdot(\rho\vec{V}U)=-\frac{\partial P}{\partial x}+\frac{1}{Gr^{0.5}}\nabla\cdot(\rho\nabla U)-\frac{1}{Da\,Gr^{0.5}}\frac{(1-\varepsilon_l)^2}{\varepsilon_l^3}\rho U \quad (7)$$

$$\frac{\partial(\rho V)}{\partial t}+\nabla\cdot(\rho\vec{V}V)=-\frac{\partial p}{\partial y}+\frac{1}{Gr^{0.5}}\nabla\cdot(\rho\nabla V)-\frac{1}{Da\,Gr^{0.5}}\frac{(1-\varepsilon_l)^2}{\varepsilon_l^3}\rho V+(\Theta+NX_l) \quad (8)$$

$$\frac{\partial(\rho H)}{\partial t}+\nabla\cdot(\rho\vec{V}H)=\frac{1}{PrGr^{\frac{1}{2}}}\nabla\cdot\left(\frac{1+\varepsilon_s(Rk-1)}{CP}\nabla H\right)+\frac{1}{PrGr^{\frac{1}{2}}}\nabla\cdot\left(\frac{1+\varepsilon_s(Rk-1)}{CP}\nabla(H_l-H)\right)-\nabla\cdot\left[f_s\rho\vec{V}(H_l-H_s)\right] \quad (9)$$

$$\frac{\partial(\rho X)}{\partial t}+\nabla\cdot(\rho\vec{V}X)=\frac{1}{Sc\,Gr^{\frac{1}{2}}}\nabla\cdot\left((1-f_s)\rho\nabla X\right)+\frac{1}{ScGr^{\frac{1}{2}}}\nabla\cdot\left((1-f_s)\rho\nabla(X_l-X)\right)-\nabla\cdot\left[f_s\rho\vec{V}(X_l-X_s)\right] \quad (10)$$

With Blake-Kozeny model for isotropic permeability (Guo and Beckermann, 2003):

$$K=K_0\varepsilon_l^3/(1-\varepsilon_l)^2 \text{ and } K_0=6.10^{-4}\lambda_1^2 \quad (11)$$

Also, with the full coupling, in the mushy zone, of the temperature and solute concentration through equation.

$$T=T_f+mC$$

NUMERICAL SOLUTION PROCEDURE

The system of the governing equations, with the coupling of the temperature and concentrations, has been discretized by means of volume based finite difference method Patankar (1980). For the resolution of discretized equations obtained the SIMPLER Algorithm is used. And for the resolution of the algebraically system equations obtained the Thomas Algorithm (TDMA) is used. A mesh of 50*50 nodes in the domain is used.

RESULTS AND DISCUSSION

The solidification of Al-4.1wt% Cu in two-dimensional rectangular mold was numerically simulated for the following dimensionless times of 10 and 350.

Temperature field: Figure 2 illustrate the isotherms at the previous times of solidification, in the casting (solid

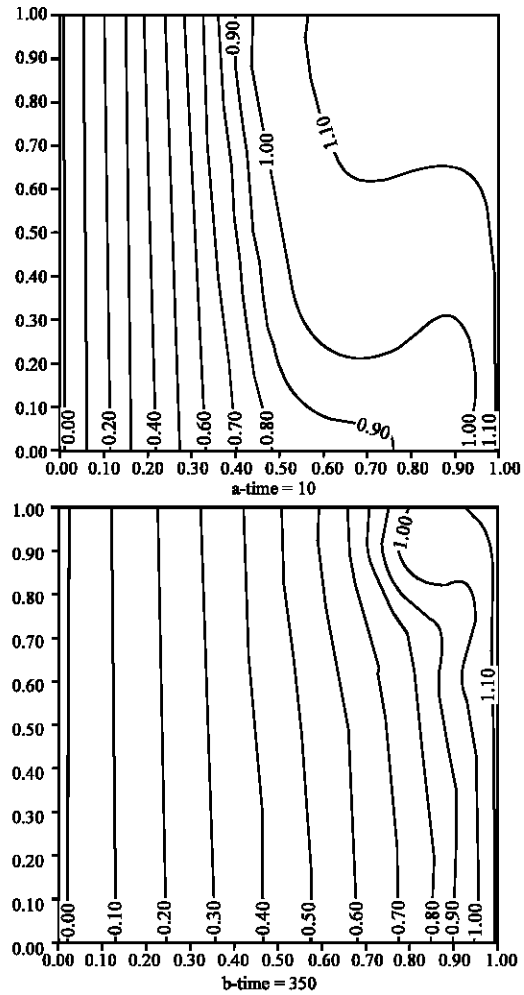

Fig. 2: Isotherms

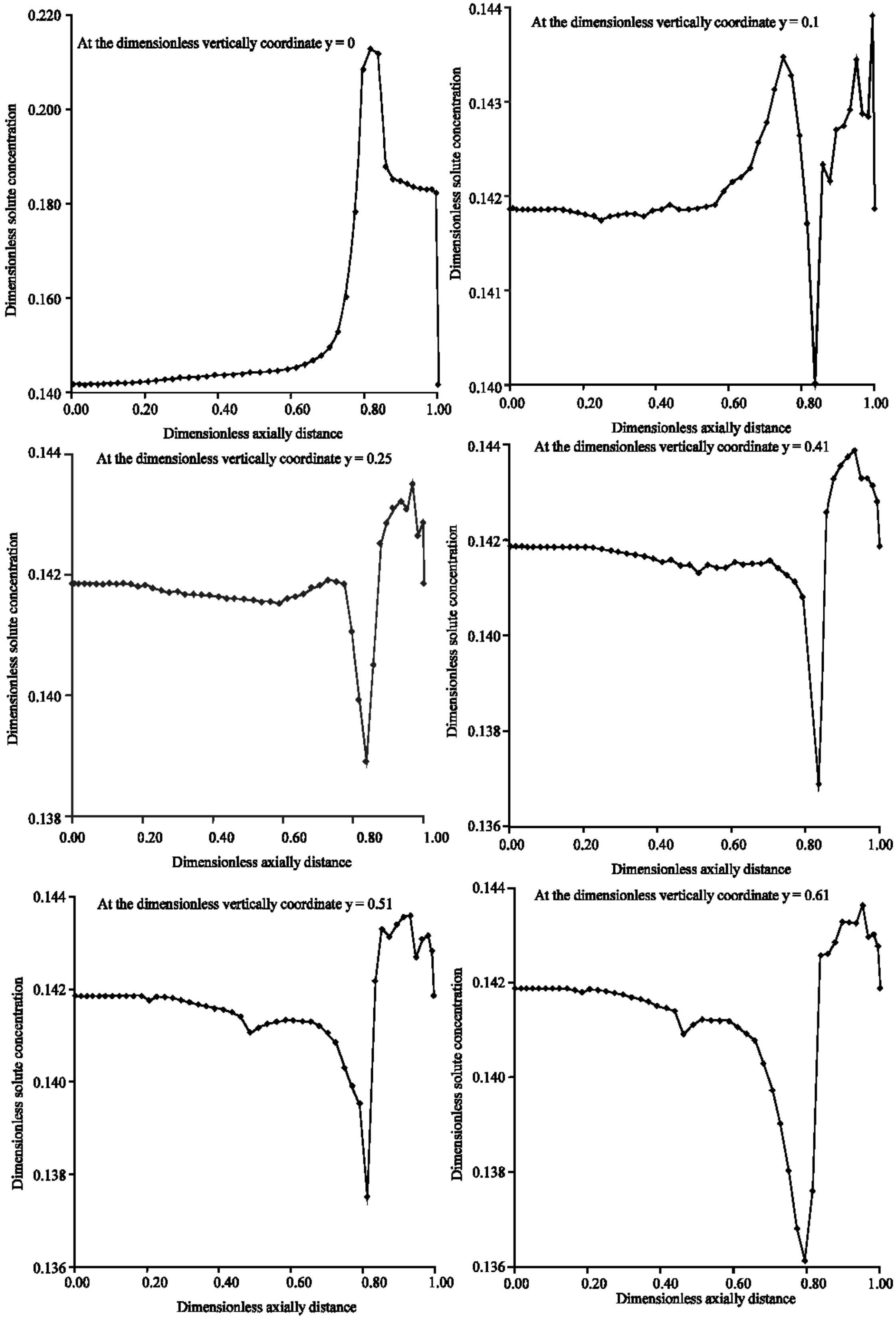

Fig. 6: Macrosegregation at the time = 350

formed) the isotherms is regular and along of the profile of casting. The temperature gradients centralize along the sides of the casting and the temperature in the interior of casting is planar, which signified that only conduction is presented in casting.

In the melt, the isotherms are not planar, which signified the presence of the convection. The temperature decreases since the solidification front advances.

Fluid flow: Figure 3 and 4, respectively, illustrate fluid flow and solid fraction at the early stage (time = 10) and the later stage (time = 350), respectively. As the solidification process has proceeded for the time of 10, the temperature gradient has been established and the solidification occurs. At the beginning the fluid is superheated and the fluid flow is affected almost only by temperature gradient because the permeability keeps maximum everywhere in the casting. The downward flow, provoked by thermal gradient, occurs along the side wall of the solid formed, i.e., in the mushy zone, where the horizontal temperature gradients exist.

With the solidification proceeding, the fluid flow is affected by not only the temperature but also the solid fraction and the solute concentration. The solid fraction affects the fluid flow by changing the permeability in the mushy zone.

For Al-4.1 wt% Cu alloy, the primary solid phase is Aluminum-rich, whereas the interdendritic liquid becomes enriched in Copper, the denser of the two constituents. Therefore, solutal and thermal buoyancy forces augment each other (Beckermann, 2002). So the flow is weak in the depth of the mushy zone though in which the gradient of temperature is very high. The effect of the solute concentration is strong in the mushy zone because (buoyancy ratio is N = -114). The mushy zone, where the gradient of solute concentration is large, is very large for such system. So the fluid is mainly driven by the temperature and concentration fields and affected by solid fraction.

Macrosegregation formation: Figure 5 illustrate the solute concentration corresponding to time of 350. The negative segregation (where solute concentration is lower than nominal solute concentration 0.1418) forms along the side walls especially in the upper corners of the mold because the solidification begins at the side walls. The interdendritic solute-rich liquid moves downward and takes the solute away. The solute-rich liquid moves into the liquid pool in the centre of the casting so the solute in the center of the casting increases. With the solidification advancing, the solute accumulates in the centre continuously, so the highest positive segregation forms at the bottom corner of the mold where the highest temperature and highest solid fraction exist.

Numerical predictions of macrosegregation at the time of time = 350 is shown in Fig. 6. Figure 6 shows the composition in a horizontal sections at nta Y = 0, 0.1, 0.25, 0.40, 0.50 and 0.60, respectively.

It may be noted that in Fig. 1 the concentration profile is not smooth but is marked by random oscillations. These fluctuations occur on macro-and semi-macro scales.

These fluctuations are the consequence of the manner in which segregated spots get distributed. Such distribution is again closely linked with morphological features of the casting section.

CONCLUSION

The continuum model, due to Bennon and Incropera, to simulate macrosegregation induced by fluid flow in the mushy zone under the effect of thermal-solutal convection is presented and the transport behavior in a Al-4.1wt% Cu alloy is predicted with this model. The conservative transport equations are discretized by mean of finite volumes method and for their resolution SIMPLER algorithm is used.

The fluid flow in the melt was found affected by the temperature and solute concentration fields and by solid mass fraction.

NOMENCLATURE

Cin	=	Reference concentration
T_{ini}	=	Initial temperature of the molten alloy
T_e	=	Eutectic temperature
T_{cold}	=	Temperature of the colder wall
T_{liq}	=	Liquidus temperature
T_{ref}	=	Reference temperature
T	=	Time
L	=	Length or height of the mold
V	=	Vector velocity of flow field
T_f	=	Melting point
L_H	=	Latent heat
cp	=	Specific heat
k	=	Thermal conductivity
D	=	Solute liquid diffusivity
m	=	Slope of the liquidus line
m^{ad}	=	Dimensionless slope of the liquidus line
kp	=	Partition coefficient
Da	=	Darcy number
Gr	=	Grashof number
Pr	=	Prandtl number
Sc	=	Schmidt number
CP	=	Dimensionless specific heat ratio

Rk	=	Dimensionless heat conductivity ratio
N	=	Boyancy ratio
K_0	=	Parameter
U,	=	Vdimensionless mixture velocity components
X	=	Dimensionless mixture composition
H	=	Dimensionless mixture enthalpy
P	=	Dimensionless mixture pressure
ΔT	=	Temperature scale
ΔC	=	Concentration scale
C	=	Concentration
u,v	=	Components of velocity
h	=	Enthalpy
x, y	=	Cartesian coordinates
		Greek symbols:
ρ	=	Density
β_T	=	Thermal expansion coefficient
β_S	=	Solutal expansion coefficient
μ	=	Viscosity of the melt
λ_1	=	Primary dendrite arm spacing
v	=	Kinematic viscosity of the melt
α	=	Thermal diffusivity
ε	=	Volume fraction
Θ	=	Dimensionless temperature
		Subscripts
s	=	Used to identify properties of the solid phase
l	=	Used to identify properties of the liquid phase
ref	=	Used for the reference case

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