VALIDATION OF A TEMPERATURUE DEPENDENT 3D NUMERICAL DROPLET IMPIGNEMENT SIMULTATION PROCEDURE TO PREDICT SPLASH/NON-SPLASH BEHAVIOR

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ABSTRACT

A Computational Fluid Dynamics-based simulation procedure to study splash/non-splash behavior of single-component n-paraffin droplets impacting on a dry, horizontal surface is proposed. The capability of the simulation procedure to predict momentum-induced (cold surface) and boilinginduced (superheated surface) splash over a wide range of impingement conditions is evaluated. The Volume-of-Fluid model is combined with a vaporliquid interface reconstruction scheme. For droplet impingement on a cold surface good agreement with experimental data obtained from literature is observed. For droplet impingement on a superheated surface heat and mass transfer rates close to the surface have to be accounted for. The simulated splash/non-splash transition agrees reasonably well with the experimental data. The numerical procedure is capable of predicting the onset of splash for impinging hydrocarbon droplets.

1. INTRODUCTION

Insight into the behavior of droplets impinging on a solid surface is important in many applications including spray drying, film coating, spray painting, ink-jet printing, internal combustion engines, petrochemical process equipment fouling and many more.[1] In these applications droplet impact on a solid surface is a frequent event and results in a wide range of phenomena such as stick, splash, breakup and rebound. All of the above mentioned applications benefit from a specific impingement behavior. In spray dryers droplet deposition needs to be minimal. In spray painters and ink-jet printers a controlled deposition preventing droplet collision, is desired.[2] When applying a film coating, a uniform deposited liquid layer with a controlled thickness is crucial for the efficiency of the process.[3] On the contrary, in internal combustion engines splashing of the droplets upon impact on the combustion chamber results in the formation of smaller droplets, facilitating fuel evaporation.[4] In the petrochemical industry, liquid deposition on a heated wall is one of the important steps in surface fouling. The formed liquid film is exposed to high wall temperatures, promoting thermal cracking, which results in the formation of a so-called "coke" layer. In order to control the operation and, more preferably, predict the frequency of required shutdowns, the local coke layer thickness has to be determined.[5-7] In all the mentioned applications, simulations can help to accurately describe the – desirable or undesirable – deposited liquid film.

1.1. Droplet properties

For an incoming spherical droplet the dimensionless Weber number is a measure of the relative importance of the inertial forces compared to the fluid surface tension:

We =
$$\frac{\rho u^2 d}{\sigma}$$
 (1)

where ρ is the fluid density, *u* the droplet velocity, *d* the droplet diameter and σ the liquid surface tension. The ratio of the viscous forces to the inertial and surface tension forces is described by the Ohnesorge number:

$$Oh = \frac{\sqrt{We}}{Re} = \frac{\mu}{\sqrt{\rho\sigma d}}$$
(2)

with μ the fluid dynamic viscosity. The Reynolds number relates the inertial forces to the viscous forces.

1.2. Droplet impingement phenomena

Impingement on a cold surface

A droplet impacting on a solid dry surface passes through different phases due to the balance of several physical forces: inertial effect, viscous dissipation and capillary forces.[8] During the *spreading phase* of the impacting droplet, the droplet radially expands, forming a liquid film. Simple analytical models describe how during spreading the droplet kinetic energy changes to surface energy and to work done to overcome liquid viscosity.[9-11] When the droplet is at its maximum spreading, further expansion is restricted by the viscosity and surface tension. Next, capillary forces become dominant and the droplet starts receding, gaining in kinetic energy. This is known as the *relaxation phase*. If impact velocities are sufficiently high the inertial forces unbalance the capillary effects and the droplet disintegrates: the spreading phase results in splash.[12] When the droplet does not rebound, the surface is partially wetted. This is known as the *equilibrium phase*.

Impingement on a heated surface

When the surface is heated, the behavior of the impinging droplets changes. A droplet in contact with a superheated surface (surface temperature exceeding the boiling point of the impinging fluid) boiling different experiences mechanisms. depending on the surface temperature. In case the surface is slightly overheated, the droplet experiences nucleate boiling. Bubbles are formed at the surface, resulting in a very efficient surface-toliquid heat transfer.[13] During nucleate boiling the heat flux from the surface to the droplet increases until it reaches the critical heat flux and a vapor film is formed on the surface. In contrast to bubble formation, film formation lowers the mass transfer rate in the transition boiling regime. At the Leidenfrost temperature, the vapor film is fully developed and *film boiling* starts.[14] Heat transfer rate and, consequently, vapor-liquid mass transfer rate are at their minimum. If the surface temperature exceeds the Leidenfrost temperature, the developed vapor film drastically changes the droplet impingement behavior. A droplet impinging at film boiling conditions, floats on the developed vapor film. This results in a different impingement behavior such as rebound without breakup at very small Weber numbers (We < 60) and splash at moderately high Weber numbers.[12]

To conclude, there are two main mechanisms that result in the disintegration of impinging droplets: momentum-induced splash and boilinginduced splash. For that reason, the results of droplet impingement studies are mostly mapped by incoming momentum, characterized by the Weber number, and by the surface temperature.

1.3. Numerical simulations

A vast number of experimental studies has been performed to investigate the complex droplet impingement behavior over a wide range of impingement conditions, and for different applications.[1, 9, 15-20] However, in the last decade, detailed numerical studies of droplet impingement on a surface are gaining in popularity due to the increased accessibility of computing infrastructures, the flexibility of operating conditions and the vast amount of data typically obtained by numerical studies. Various numerical two-phase simulations have been performed to study droplet impingement dynamics.[21-27] These numerical studies aim at precisely tracking the droplet vapor-liquid interface during the droplet impingement and, consequently, at accurately modeling the interface phenomena. The Volume-of-Fluid (VOF) method is the predominant modelling technique since it is conservative and can deal with topology changes at the interface. Lunkad et al.[25] introduced a static and dynamic contact angle in the VOF model to determine the spreading diameter of glycerin droplets. Briones et al.[28] adopted the VOF model with the dynamic contact angle approach to simulate the spreading of a micrometersized water droplet on a dry surface, showing good agreement with experimental data. Malgarinos et al.[27] implemented a new wetting force model to simulate wetting of the surface without a priori knowledge of the dynamic contact angle. This study of droplet impingement on hydrophilic and hydrophobic surfaces using the new wetting force model yielded reasonable agreement with experimental data.

The majority of the numerical studies on droplet impact investigated the spreading and recoiling behavior of the droplet for impact at low incoming Weber number. At lower Weber numbers, the droplets exhibit non-splash behavior, i.e. stick and rebound. Mahulkar et al.[26] constructed a heavy hydrocarbon droplet impingement regime map based on data obtained in an extensive numerical study. The VOF model, combined with an interface reconstruction algorithm, was applied to study the dynamic droplet impact behavior. The behavior of single and multicomponent hydrocarbon droplets impinging on a surface at temperatures starting from 400 up to 900 K and with incoming Weber numbers ranging from 1 to 1000 was simulated. As such, an extensive regime map covering a wide range of droplet impingement conditions was constructed.

In the present study, an updated numerical procedure is presented and validated using experimental data from literature reported by Vander Wal et al.[18, 29] and Kompinsky et al.[16]. In particular, both momentum-induced and boilinginduced splash are studied to cover a wide range of splash/non-splash droplet impingement dynamics. Hence, prediction of the transition from the nonsplash to the splash regime caused by, on the one hand, relatively high Weber numbers and, on the other hand, high surface temperature, is investigated and validated using the experimental data from Vander Wal et al.[18, 29] and Kompinsky et al.[16].

2. NUMERICAL MODEL AND SIMULATION APPROACH

The balance between physical forces controls the dynamic behavior observed when a droplet impinges on a surface, as depicted in Figure 1. These physical forces are mainly governed by droplet properties, such as droplet diameter and incoming velocity, by liquid properties, such as density, surface tension and viscosity, and by properties of the solid surface, e.g. temperature. All of these parameters have to be accounted for in a numerical simulations to accurately describe droplet-surface interaction.



Figure 1: Physical forces and phenomena dominating droplet impingement behavior.

2.1. Geometry

In this work, the simulation domain as designed by Mahulkar et al.[26] is adopted. A domain of two coaxial cylinders, as illustrated in Figure 2, is constructed to limit the size of the simulation domain and, consequently, to reduce the number of grid cells to a minimum. Close to the surface a cylinder with high radius-to-height ratio allows full spreading of the droplet. The diameter of the second cylinder, confining the path of the incoming droplet, is reduced to limit the mesh size. A mesh selectivity study results in a mesh with 1.2 million cells.



Figure 2: 3D geometry visualizing the simulated domain used in present work.

2.2. Conservation equation

Simulations are performed using the commercial software package ANSYS FLUENT[®] 15.0. For the governing conservation equations the reader is referred to Mahulkar et al. [26]. The VOF model is used to model the vapor-liquid flow. In the VOF model a single set of equations is solved for both phases. The mass fraction of both phases in the computational domain is obtained by solving an additional balance equation for the mass fraction of one of the phases, including mass transfer between the phases for simulations where boiling occurs[30]:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l) + \nabla(\alpha_l \rho_l \vec{u}) = m_{\nu \to l} - m_{l \to \nu}$$
(3)

where $m_{\nu \to l}$ and $m_{l \to \nu}$ represent the mass transfer from vapor to liquid phase and from liquid to vapor phase, respectively. When solving the complete set of equations, the time step is varied to keep a Courant number of 2 in order to limit simulation time but retain stability.[31]

2.3. Interface phenomena

The behavior of a droplet impacting on a surface is mainly determined by interface effects such as surface tension, wall adhesion and evaporation. Accurately quantifying interface forces and evaporation requires tracking of the vapor-liquid interface changes during droplet impingement. To reach that goal, the VOF model is combined with the Piecewise Linear Interface interpolation (PLIC) scheme, Geo-reconstruct.[32]

Surface tension

The surface tension model implemented in ANSYS FLUENT[®] 15.0 is the continuum surface force model developed by Brackbill.[33] In this model the surface tension is approximated by a volume force acting in each cell where a vapor-liquid interface is located.

Wall adhesion

Adhesion of a liquid to a surface is set by imposing a contact angle for the vapor-liquid-solid system as shown on Figure 1. Two main approaches to model the contact angle are used in numerical droplet impingement studies, i.e. the static and dynamic contact angle approach. The latter accounts for a different contact angle during the spreading and recoiling. This approach is proven to drastically improve results when simulating the spreading phase of droplet impact. However, predicting the onset of splash does not require the use of a dynamic contact angle approach. The static contact angle approach, i.e. a constant value of contact angle during spreading, is seen to accurately predict the onset of splash.[12] Given the goal of the present study, determining transition from non-splash to splash behavior, the static contact angle approach is adopted.

The contact angle, θ , can be calculated from the equilibrium relation known as Young's equation:

$$\sigma_{s-\nu} = \sigma_{s-l} + \sigma_{\nu-l} \cos \theta \tag{4}$$

which defines mechanical equilibrium for a droplet under the action of three interfacial tensions: solidvapor interaction ($\sigma_{s-\nu}$), solid-liquid interaction (σ_{s-l}) and vapor-liquid interaction ($\sigma_{\nu-l}$). As the three interfacial tensions depend on liquid, vapor and solid properties, Young's equation defines a single, unique contact angle for each liquid-vapor-solid combination. In the present work contact angles taken from literature will be imposed in the numerical simulations. The work of Lam et al.[34] provides values for the advancing contact angle for a wide range of hydrocarbons.

3. EXPERIMENTAL VALIDATION DATA

The numerical model described above is validated by stepwise comparing simulation results with two sets of experimental data for hydrocarbon droplet impingement, covering both splash/non-splash behavior. First, droplet impingement on a surface at room temperature, excluding evaporation, is simulated. The absence of evaporation reduces the impingement behavior to momentum-induced splash. For this initial validation the experimental dataset of Vander Wal et al.[18, 29] is used. Next, the surface temperature is changed to study boilinginduced impingement. For this second study, the experimental dataset of Kompinsky et al.[16] is used.

3.1. Momentum-induced impingement

Vander Wal et al.[18, 29] experimentally studied the splash/non-splash behavior of nparaffins, n-alcohols and water droplets impinging on a dry surface at room temperature. In the experiments of Vander Wal et al., a droplet with a diameter of 2.0 mm was released above the surface at a selected height ensuring that the droplet reaches the targeted wall impact velocity due to gravitational acceleration. The droplet impinged on a diamondlathed aluminum surface. Vander Wal et al. concluded that the impingement behavior could be predicted based on incoming Weber number and Ohnesorge number only. Increasing the Weber number favors splashing, since high Weber numbers indicate that the incoming momentum exceeds the surface tension forces. The Ohnesorge number is a measure for the viscous momentum dissipation of a liquid. Momentum dissipation upon impact decreases the droplet kinetic energy and, consequently, lowers the splash tendency. Vander Wal et al. introduced a relationship delineating splash/non-splash behavior based on the Ohnesorge and Weber number of an impinging droplet:

$$Oh^{0.39}We^{0.3} = 0.85 \tag{5}$$

From the liquids experimentally studied by Vander Wal et al., the liquids most relevant for fuel applications are selected for validation purposes in this study. The Ohnesorge number does not depend on the incoming velocity as shown in Eq. 2. However, the Ohnesorge number depends on the characteristic length, namely the droplet diameter. Due to this dependency the reported Ohnesorge numbers cannot be regarded as a fundamental property of the fluid and should be regarded as a physical property of the droplet. Table 1 reports the droplet properties for different hydrocarbon droplets having a diameter of 2.0 mm.

Table 1: Liquid hydrocarbon droplet properties or	f
the droplet impingement study of Vander Wal e	t
al.[18, 29]	

	Viscosity	Surface tension	Density	Oh
	[10 ⁻³ Pa.s]	[10 ⁻³ N/m]	[kg/m ³]	[10-3]
Hexadecane	3.34	27.1	773	16.3
Tetradecane	2.04	26.7	763	10.1
Dodecane	1.35	25.4	750	6.9
Decane	0.925	24	730	4.9
Nonane	0.711	22.9	722	3.9
Heptane	0.409	20.1	684	2.5

In the present study, the impingement at room temperature of hydrocarbon droplets with a 2.0 mm diameter is simulated with incoming droplet velocities ranging from 1.09 to 4.22 m/s, corresponding to Weber number in the 100 - 1200 range.

3.2. Boiling-induced impingement

Kompinsky et al.[16] performed experiments studying the dynamic behavior of a fuel droplet impinging on a superheated surface. In addition to other observations, the condition for the transition from non-splash to splash behavior was reported. In the study, n-hexane and n-decane droplets with a diameter of 2.3 mm were injected towards a heated surface. The incoming Weber number ranged from 155 to 255. The relatively low incoming Weber numbers limit the inertia of the impinging droplet. As such, the splash/non-splash transition is due to heat transfer from the heated surface. The initial temperature of the droplet and the surroundings was 313 K. For each incoming Weber number the surface temperature was gradually increased until the transition from non-splash to splash behavior was observed. The study resulted in the definition of a critical temperature, i.e. the surface temperature at which the non-splash behavior turns into splash behavior. The critical temperature was found to be independent of the low incoming Weber numbers and to correspond to the Leidenfrost temperature, defining the onset of film boiling. For alkanes, the Leidenfrost temperature was experimentally determined to be the normal boiling point augmented with 52 K.[35] For n-decane, this results in a Leidenfrost temperature of 499 K.

In the present study, the proposed numerical droplet impingement model is validated by simulating the n-decane impingement behavior at the minimum and maximum incoming Weber numbers used in the experimental study, i.e. 155 and 255. The surface temperature is set 15 K below and 15 K above the experimentally determined critical surface temperature.

4. RESULTS AND DISCUSSION

4.1. Momentum-induced droplet impingement

In total 27 momentum-induced numerical droplet impingement simulations are performed according to the described procedure. The impingement behavior as simulated and as experimentally determined by Vander Wal et al. [18, 29] is shown in Figure 3.



Figure 3: Droplet impingement behavior for various n-paraffins (from top to bottom: hexadecane •, tetradecane •, dodecane •, decane •, nonane • and heptane •) as observed experimentally and numerically. Empty markers correspond to experimentally observed non-splash and filled markers to experimentally observed splash. The rectangle visualizes the region where splash is predicted by numerical simulations.

Only two of the performed simulations predict an impingement behavior that does not agree with experimental observation. Vander Wal et al. introduced Eq. 5 to differentiate between non-splash and splash behavior (shown with the dashed curve on Figure 3). Since the contact angles used in the numerical simulations are taken from the work of Lam et al.[34], which is for a different substrate, it can be expected that the onset of splash does not perfectly match the experimental observations. Lam et al. reported contact angles for hydrocarbon droplets impinging on a FC-732-coated silicon wafer, whereas Vander Wal performed experiments on diamond-lathed aluminum disk. Overall, there is a scarcity of experimentally determined contact angles because of their dependency on all three interfacial surface tensions as illustrated by Eq. 4. The interfacial surface tensions reported are in turn dependent on temperature and require the solid

surface to be perfectly smooth. Because of the fact that the onset of splash is dependent on the contact angle, there is a slight difference between the simulated results and the experiments. Based on the impingement regime map shown in Figure 3, it is possible to conclude that at low Ohnesorge numbers, impinging droplets exhibit non-splash behavior over a wide range of Weber numbers. At higher Ohnesorge number, splash is observed from a given Weber number on, the value of which decreases when the hydrocarbon becomes heavier.



Figure 4: Snapshots over time for an n-decane droplet impinging on a non-heated surface for a Weber number of 272 (left) and a Weber number of 878 (right).

Figure 4 shows different snapshots over time for an n-decane droplet impinging at Weber numbers below and above the experimentally determined splash/non-splash transition line. Splashing with ring detachment is observed for the higher Weber number (right) after 0.8 ms.[26] At a Weber number of 272 the maximum spreading diameter is lower ensuring that the droplet can recover enough kinetic energy to contract and finally detach. For a Weber number of 878 the maximum spreading caused by the higher inertial forces is too high for the capillary forces to contract the droplet. This finally results in a partly wetted surface with the remainder of the droplet sticking to the surface.

Since the simulations agree reasonably well with the experimental observations, the proposed simulation procedure will be tested against the boiling-induced experimental dataset by Kompinsky et al.[16] Simulations will be performed for ndecane droplets impinging at Weber numbers of 155 and 255 and an Ohnesorge number of 4.6×10^{-3} . The Ohnesorge of the simulated n-decane droplet is slightly lower compared to the non-heated dataset as the impinging droplets have a slightly higher diameter, i.e. 2.3 mm instead of 2.0 mm, resulting in a lower Ohnesorge number according to Eq. 2. Taking into account the regime map shown in Figure 3, non-splash behavior is expected in this region for impingement on a cold surface. So in case splash behavior is observed when the surface temperature is modified, it is acceptable to state that the observed splash is boiling-induced.

4.2. Boiling-induced droplet impingement

Numerical modelling of boiling-induced impingement becomes more challenging, since droplet-surface heat transfer and vapor-liquid mass transfer become dominant phenomena and have to be accounted for accordingly. Prior to comparing the simulations to the data provided by Kompinsky et al.[16], the phenomena close to the surface during the droplet impingement are first studied more closely. Additional mesh refinement will be necessary to accurately model these interface phenomena.

Mesh independency study

The temperature gradient at the surface has to be fully resolved to obtain accurate interphase heat and mass transfer close to the surface. Accurately capturing the steep boundary temperature profile and the amount of evaporated liquid are highly related phenomena that require small cell sizes close to the heated surface. For the mesh independency study a droplet with a Weber number of 155 impinging on a heated wall with a temperature 15 K below the Leidenfrost temperature is simulated for three different meshes consisting of 1.4, 1.5 and 1.6 million cells (corresponding to an initial cell thickness of 4.6, 2.3 and 1.73 μ m close to the wall, respectively). The final mesh is selected based on the onset of evaporation. According to the mass transfer rate for different mesh sizes, a boundary layer thickness of 2.3 μ m is selected. By reducing the thickness to 1.73 μ m, the onset of evaporation shifts by 40 μ s only, suggesting that a mesh of 1.5 million cells is sufficiently small.

Model validation

The droplet impingement simulations are visualized in Figure 5.



Figure 5: Snapshots over time for an n-decane droplet impinging on a superheated surface 15 K below (left) and 15 K above (right) the Leidenfrost temperature for a Weber number of 155 (top) and a Weber number of 255 (bottom).

The simulations show that for surface temperatures above the Leidenfrost temperature the impinged droplet sticks to the heated wall. As the droplet spreads part of the droplet starts evaporating in the center, where the droplet thickness is significantly smaller than at the wave front. This phenomenon, in combination with film boiling, ensures that for high surface temperatures capillary forces cannot retrieve enough kinetic energy to contract the droplet. The droplet impinging at a Weber number of 255 on the surface below the Leidenfrost temperature (484 K) also appears to splash, as shown in Figure 5 (left This splash behavior is not in bottom). correspondence with the experimental dataset. However, Kompinsky et al.[16] explicitly mention that very small liquid fragments ejected during droplet impact could not always be detected by the high-speed camera.

Interphase mass transfer

The mass transfer rate, i.e. the evaporation rate, during the spreading phase of the droplet impingement shown in Figure 6. An increase in surface temperature by 30 K results in an earlier onset of evaporation because of the higher heat flux caused by the steeper temperature gradient. An earlier onset of evaporation is observed for the highest Weber number, this can be explained by the fact that all droplets are released at the same height above the surface. A higher Weber number directly relates to a higher droplet velocity and hence a sooner contact with the heated substrate. In case the surface temperature is above the Leidenfrost temperature a drop in mass transfer rate is observed about 0.5 ms after the onset of evaporation, corresponding to film boiling. For a more accurate understanding of the total mass transfer rate the spreading diameter, as reported in Figure 7, should also be taken into account.



Figure 6: Mass transfer rate for a n-decane droplet impinging on a heated surface.

The spreading diameter is a direct measure for the total contact area during the droplet impingement spreading phase. When the droplet starts receding, after 7.0 ms as shown in Figure 5, part of the liquid in the center will have evaporated, not only reducing the total contact area, but also causing the shape of the contact area to deviate from a circle. In general the droplet diameter increases the moment the droplet makes contact with the surface, a second

rapid increase is observed as spreading starts and the spreading diameter rapidly exceeds the original droplet diameter.



Figure 7: Spreading diameter for an n-decane droplet impinging on a heated surface.

In correspondence with Figure 6, the spreading diameter increases first for the higher Weber numbers, since the droplet velocity is higher. The higher Weber number droplets will reach the surface earlier. The maximum spreading diameter is higher for droplets with a higher incoming momentum, i.e. a higher Weber number. A higher contact area directly relates to a higher mass transfer rate. This explains why the total mass transfer rate is similar for the droplet with a low Weber number but a higher surface temperature and the droplet with a lower surface temperature but a higher total contact area. A discrepancy is observed in the spreading diameter profile for the higher Weber number simulations. This discontinuity is a direct result of the observed splash behavior. Small ligaments rapidly expand and detach from the droplet, resulting in a rapid increase in droplet diameter, directly followed by a decrease in droplet diameter as the ligaments detach from the droplet.

5. CONCLUSION

Momentum-induced and boiling-induced droplet impingement simulations are performed for a series of n-paraffins. The observed splash/nonsplash behavior agrees reasonably well with the behavior reported in scientific literature for the nparaffins (heptane, nonane, decane, dodecane, tetradecane and hexadecane). The described numerical procedure offers the opportunity to simulate the impingement of different hydrocarbons at Leidenfrost temperatures and offers a tool to predict whether fouling due to splash and stick will occur at specific process conditions using the information from the regime maps. This research focused on comparing the developed methodology with experimental observations reported in literature. With this validation in mind, the goal is to produce regime maps for multi-component mixtures. These impingement regime maps should help the process engineer to predict the fouling

dynamics of the process. Regarding future work, a more detail contact angle model will have to be developed to narrow the non-splash/splash boundary regime. This in turn will require more extensive modelling of the solid-liquid and solidvapor surface tension, contact angle described by Young's equation, as opposed to only the temperature-dependent modelling of the liquidvapor interface. For this reason experimental measurement of surface tension at different temperatures and experimental validation of the regime maps will remain crucial for this research.

NOMENCLATURE

- d diameter, m
- m mass transfer, kg/s
- Oh Ohnesorge number, dimensionless
- Re Reynolds number, dimensionless
- *u* velocity, m/s
- We Weber number, dimensionless
- α volume fraction, dimensionless
- μ dynamic viscosity, Pa s
- ρ density, kg/m³
- σ surface tension, N/me
- θ contact angle, rad

Subscript

- l liquid
- s solid
- v vapor

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