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A heat transfer corrected isothermal model for CFD modeling of biomass devolatilization in fluidized beds

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Abstract

Isothermal models, which neglect particle internal heat transfer, are commonly used in computational fluid dynamic (CFD) modeling of biomass devolatilization in fluidized beds. However, for large biomass particle, the particle internal heat transfer influences significantly the devolatilization, and therefore needs to be considering in CFD modeling. In this work, a heat transfer corrected isothermal model presented in our pervious paper [1] was implemented in Eulerian-Eulerian methods to simulate a batch bubbling fluidized bed for biomass devolatilization. Compared to the conventional isothermal model, the heat transfer corrected isothermal model shown similar computational efficiency of CFD simulations, but for large biomass particles resulted in a lower heating rate and devolatilization rate, which are in better agreement with the observations in particle-scale experiments and simulations. The results demonstrate that the developed heat transfer corrected isothermal model is applicable in CFD modeling of devolatilization of large biomass particles in fluidized beds.

Keywords: biomass, devolatilization, internal heat transfer, CFD, fluidized bed

1. Introduction

Eulerian-Eulerian methods and Eulerian-Lagrangian methods have been widely used in CFD modelling of biomass devolatilization in fluidized beds [2–5]. In these two approaches, biomass particles are usually described by an isothermal model that neglects particle internal heat transfer. Such an isothermal model is simple and cost-effective to couple with CFD. However, it is only reasonable for the particles with small Biot Number (Bi) (e.g. $Bi < 1.0$) [5]. With the increase of Bi , the internal temperature gradient becomes large, resulting in thermally-thick biomass particles can not be described by isothermal model [6–9]. Therefore, non-isothermal model is favourably applied in this case [7,9–13].

Only a few of the exiting non-isothermal models have been implemented in CFD simulations. A detailed non-isothermal model, including heat diffusion equation for an isotropic particle has been implemented into ANSYS Fluent[®] by Papadikis et al. [14–16]. The model can reveal more detailed information of biomass devolatilization in fluidized bed (e.g. internal temperature gradient), compared to an isothermal model. However, the simulation is time-consuming, due to the extremely high amount of memory allocation for particle information and the increase of computational complexity [15]. Therefore, the model is not suited for large-scale CFD simulation of biomass devolatilization in fluidized beds. In other way, Thunman et al. [17] proposed a four layers model (moist wood, dry wood, char, and core layers) to represent a whole wood particle. Only ordinary differential equations (ODEs) are required to solve. Thus, it improves the computational efficiency as compared to detailed isothermal model. But the model is has only been investigated in fixed beds [12,18,19], with rare applications in fluidize beds.

Compared to non-isothermal model, isothermal model is still the most applicable method to simulate biomass devolatilization in large-scale CFD modelling [20–22]. However, modification is needed to model thermally-thick particles (e.g. $Bi > 1.0$). Johansen et al. [4] attempted to modify the kinetic parameters by fitting CFD modelled non-reacting biomass particle temperature history versus experimental conversion, instead of using directly experimental-determined kinetic parameters. Simone et al. [23] adopted a similar method to simulate biomass devolatilization in a drop tube reactor. In this way, CFD modelling performance is improved [4,23]. However, several CFD simulations are required to obtain the modified kinetic parameters, and the kinetic parameters should be updated with operating conditions (e.g. temperature and gas velocity).

In this paper, a heat transfer corrected model presented in our previous work [1] was implemented in CFD to simulate devolatilization of large biomass particles in a batch bubbling fluidized bed. First, the heat transfer corrected isothermal model was validated at particle-scale. Then it was coupled with

Eulerian-Eulerian method to investigate the biomass devolatilization with different particle sizes in the batch fluidized bed.

2. Heat transfer corrected isothermal model

To take into account of the internal heat transfer, two heat transfer corrected coefficients: H_T and $H_{R,i}$ was introduced to consider the difference between isothermal model and non-isothermal model. The two factors can be expressed as Eq. (1) and (2). H_T and $H_{R,i}$ is a binary function of particle temperature and heat convection coefficient with constant gas and wall temperatures. The scheme to obtain H_T and $H_{R,i}$ is described in our pervious paper [1], along with the models for thermo-physical properties, drying, and devolatilization. In following discussion, for brevity, we refer to the heat transfer corrected isothermal model as this work.

$$H_T = \frac{q_{non-iso}}{q_{iso}} = \frac{h_c(T_g - T_{surf}) + \varepsilon\sigma(T_w^4 - T_{surf}^4)}{h_c(T_g - T_p) + \varepsilon\sigma(T_w^4 - T_p^4)} \quad (1)$$

$$H_{R,i} = \frac{R_{non-iso,i}}{R_{iso,i}} \quad (2)$$

Where $q_{non-iso}$ is the heat flux to a particle predicted by the non-isothermal model, q_{iso} is the heat flux predicted by the isothermal model, $R_{non-iso,i}$ is the devolatilization rate of reaction i predicted by the non-isothermal model, $R_{iso,i}$ is the devolatilization rate of reaction i predicted by the isothermal model. T_g , T_p , T_{surf} and T_w is the gas, particle, particle external surface and wall temperature, respectively. ε is the emissivity of the particle, assumed to be 0.85. σ is the Stefan–Boltzmann constant. i represents different reactions.

The experimental data of Lu et al.[7] was used to validate the heat transfer corrected isothermal model at particle-scale. For the case of Lu et al., 9.5 mm spherical wood particle with a moisture content 6.38 wt% (dry based) was combusted in a single particle combustor (SPC). The content of volatiles and fixed carbon and ash in the wood is 90 wt%, 9.5 wt%, and 0.5 wt%, respectively. The gas and wall temperature in the combustor was 1050 K and 1276 K, respectively. Both particle surface and center temperature was measured by thermocouples, and the weight loss was measured from the wood particles extracted from the combustor at different residence time [7].

Figure 1. shows that H_T (correction of heat transfer), $H_{R,v}$ (correction of devolatilization rate), and $H_{R,w}$ (correction of evaporate rate) of the case of Lu et al.[7]. At the two ends, $\theta=0$ and $\theta=1$ (θ is dimensionless temperature: $\theta=(T_p-T_{p0})/(\max(T_w, T_g)-T_{p0})$, T_p is particle temperature, T_{p0} is initial particle temperature, 298 K), both H_T , $H_{R,v}$ and $H_{R,w}$ is 1, due to no internal temperature gradient. H_T decreases with the increase of θ , while $H_{R,v}$ and $H_{R,w}$ first increase with the increase of θ and then decrease and finally become 1. For $H_{R,v}$ and $H_{R,w}$, the point changed to 1 is different due to the different reaction temperature zone of devolatilization and evaporation. In this case, H_T is in a range of 0~1, $H_{R,v}$ is 10^{-2} ~ 10^9 and $H_{R,w}$ is 10^{-4} ~ 10^4 , implying a significant difference between isothermal model and non-isothermal model.

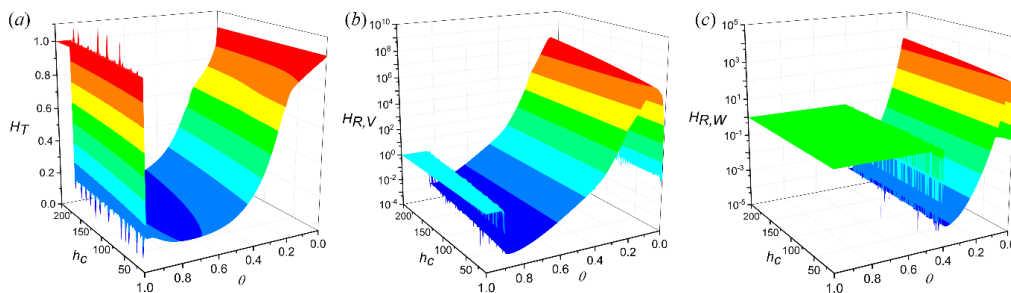


Figure 1. H_T (correction of heat transfer), $H_{R,v}$ (correction of devolatilization rate), and $H_{R,w}$ (correction of evaporate rate) of the case of Lu et al. [7].

Figure 2. (a) shows the total conversion $((m-m_\infty)/(m_0-m_\infty))$, m is particle mass, m_0 is initial particle mass, m_∞ is finally mass after devolatilization and drying) predicted by different models and its comparison

with experimental data. The total conversion history predicted by the heat transfer corrected isothermal model and non-isothermal model are in good agreement with experimental data, while the conventional isothermal model underestimates the conversion at the beginning and overestimates the conversion at a later time. In Figure 2. (b), after the isothermal model modified with heat transfer corrected coefficients, it can predict similar particle average temperature profiles with non-isothermal model, while the isothermal model overestimates heating rate. Therefore, the heat transfer corrected isothermal model can predict much more reasonable devolatilization behavior of biomass particle than the conventional isothermal model.

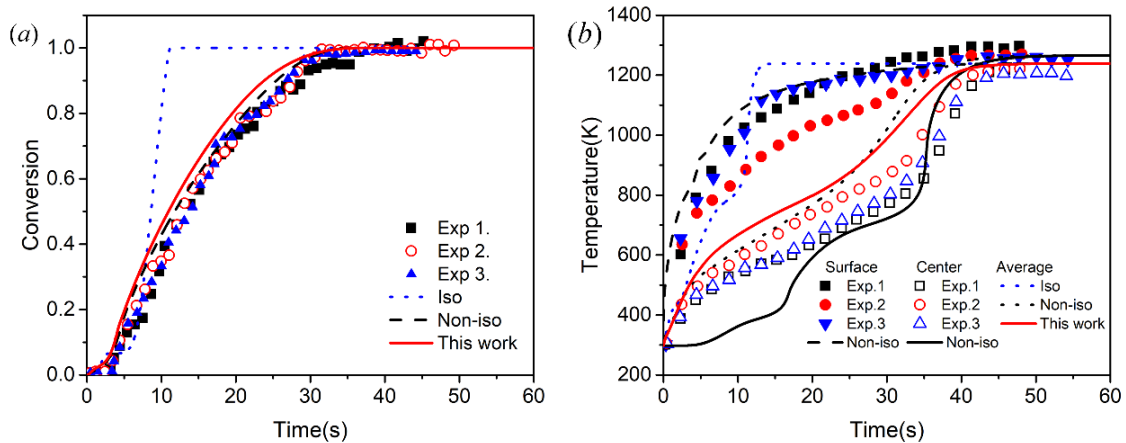


Figure 2. Total conversion (a) and temperature (b) comparison of a spherical wood particle during devolatilization in nitrogen ($d_p = 9.5$ mm, $T_w = 1276$ K, $T_g = 1050$ K)

3. CFD modeling a batch fluidized bed

3.1 CFD model and Simulation settings

The Eulerian multi-fluid model in ANSYS Fluent® 18.0 is used to simulate biomass devolatilization behavior in the batch fluidized bed. In the model, the gas phase, biomass, and sand particle are treated as inter-penetrating continua. The kinetic theory of granular flow (KTGF) is applied to close the solids stress [24]. More details can be found in the user guide of ANSYS Fluent® 18.0. The algebraic form of the granular temperature model is chosen for both sand and biomass particle instead of the full granular energy balance model, because it can save computational time and has better numerical convergence [25–27]. The no-slip and the partial-slip boundary condition were prescribed for the gas phase and solid phase, respectively. The specular coefficient is specified as 0.001, as suggested by Vashisth et al. [28]. The momentum exchange between gas and solid phase was derived by Gidaspow [24], which has been applied to model biomass devolatilization in a bubbling fluidized bed reactor [14,15,29]. The interaction forces between the different solid phases are expressed in terms of the drag force and the enduring contact force in the plastic regime as described in Syamlal et al. [30]. The heat exchange between the fluid and solid phase is determined by the model derived by Gunn [31]. The correlation of physical properties is the same to our previous work [1].

To compare the results of conventional isothermal model and the heat corrected isothermal model, both models are implemented in ANSYS Fluent® by using User Defined Functions (UDFs). The difference between this work and isothermal model is that all reaction source term and heat transfer between biomass and gas phase of the new model are modified with H_T and H_R obtained from the heat transfer corrected isothermal model. H_T and H_R are stored in ANSYS Fluent®, and the two-dimensional linear interpolation method [32] is used to calculate H_T and H_R in each cell by using UDFs. The grid size adopted here is 2.5 mm × 2.5 mm and total number of meshes is 1600. The grid size is approximately 5 times of sand size and fine enough to obtain grid convergence results for Group B particle as discussed in Li et al. [33]. The total conversion of biomass volatiles and particle temperature are monitored. After biomass totally converted and biomass particle temperature reach steady state, the CFD simulation is stopped. All simulations were carried out by using 16 cores in HPC system of Technical University of Denmark (<http://www.hpc.dtu.dk/>). More simulation settings are summarized in

Table 1.

Table 1 Simulation settings of CFD modeling the batch fluidized bed

Unsteady formulation	Unsteady, 2nd-order Implicit
Granular viscosity	Gidaspow
Granular bulk viscosity	Lun et al.
Frictional viscosity	Schaeffer
Granular temperature	Algebraic
Frictional pressure	Based KTGF
Solid pressure	Lun et al.
Radial distribution	Lun et al.
Angle of internal friction	30
Drag model	Gidaspow
Time step	0.0001/0.0005 s

3.2 Geometry and operating conditions

Figure 3. shows the two-dimensional (2D) domain of the batch fluidized bed. The gas N_2 enters the bed from the bottom inlet with a uniform velocity 0.65 m/s, and exits from the top outlets. Operating pressure is atmospheric pressure. The temperature of both inlet N_2 gas and sand is 1173 K, and wall-temperature is fixed at 1173 K. The sand particles are piled up in the bottom of bed to a height of 0.1 m at the beginning of simulation, and the temperature of sand is 1173 K. The solid flux at different heights were monitored to determine when the simulation reach quasi-steady state during cold-state simulation. For the fluidization of sand, it reaches quasi-steady after 10 seconds in our simulations. Then the biomass particles are patch in a region (0.05 m \times 0.1 m with a center height of 0.25 m) as shown in Figure 3. with a volume fraction 0.01 and an initial temperature 298 K.

To simply CFD modeling, the wood particles in the batch fluidized bed are dry particle. The initial particle density is 580 kg/m³ with volatiles content 90 wt%. With the assumption of constant particle size, the char density is 58 kg/m³. More details of physical properties and operating conditions and biomass proximate analysis are shown in Table 2 and Table 3, respectively.

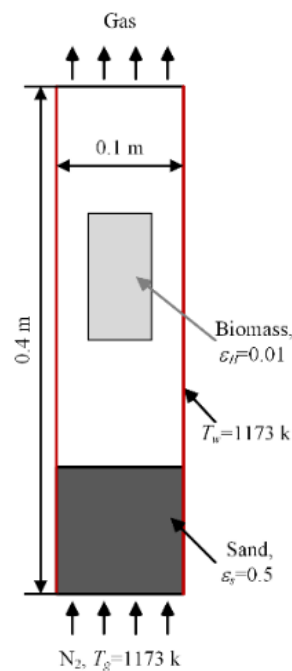


Figure 3. 2D domain of the batch fluidized bed system

Table 2. Physical properties and operating conditions

N ₂ inlet, m/s	0.65
Initial sand patch height, m	0.1
Sand patch volume fraction	0.55
Sand diameter, mm	0.5
Sand density, kg/m ³	2600
Biomass diameter, mm	1/3/6/10
Biomass mass, kg	0.029
Operating pressure, Pa	101325
Bed temperature, K	1173
Wall temperature, K	1173

Table 3. Biomass proximate analysis used in CFD simulation

Density, kg/m ³	580
Volatiles, wt%	90
Fixed carbon, wt%	9.5
Ash, wt%	0.5
Moisture, wt%	0.0
Char density, kg/m ³	58

3.3 Results and Discussions

Figure 4. shows a comparison of CFD modeling of biomass devolatilization rate by using the heat transfer corrected isothermal model and conventional isothermal model in the batch fluidized bed. For this work, the devolatilization of wood starts at ~ 500 K, reached a maximum rate at ~ 650 K, while the corresponding temperature for the isothermal model is ~ 600 K and ~ 750 K, respectively. Compared to the isothermal model, the wood devolatilization predicted by this work starts at lower temperature and ends at higher particle temperature. At particle average temperature $T_p \sim 500$ K, the temperature of particle outer layer is high enough for biomass devolatilization, but the particle average temperature is lower than devolatilization temperature. It is in the region of $H_R > 1$. Therefore, this work predicts higher devolatilization rate of biomass particle than isothermal model. At particle average temperature $T_p \sim 800$ K, the particle outer layer has high conversion or even totally converted due to high particle temperature at outer layer, only remains core layer occurs biomass devolatilization. It is in the region of $H_R < 1$. Therefore, this work predicts lower devolatilization rate. Such differences reflect the contribution of internal heat transfer.

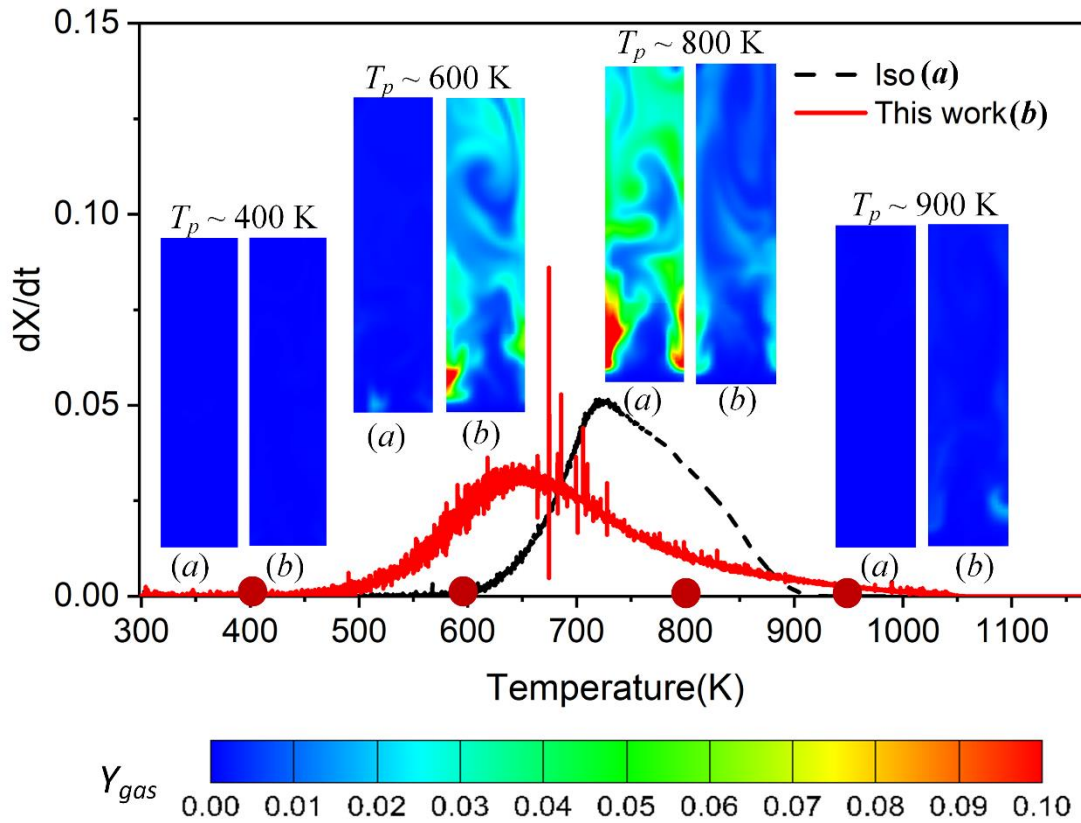


Figure 4. Comparisons of CFD modeling biomass conversion rates versus particle temperature and contour plot of volatiles mass fraction by using isothermal model and this work for the case of $d_p=10$ mm

Figure 5. shows biomass conversion history in the batch fluidized bed by using CFD simulation with isothermal model and this work. When $d_p=1$ mm, isothermal model predicts slightly shorter devolatilization time than this work, with a derivation of about 10%. With increasing of biomass particle size, the derivation between those two models becomes larger and larger. when $d_p= 6$ mm and $d_p=10$ mm, the derivation is over 50%. Moreover, for the case of $d_p= 6$ mm and $d_p=10$ mm, isothermal model predicts lower reaction rate at the beginning, while it predicts higher devolatilization rate after particle reach a certain temperature point. That is consistent what we found in our pervious paper [1].

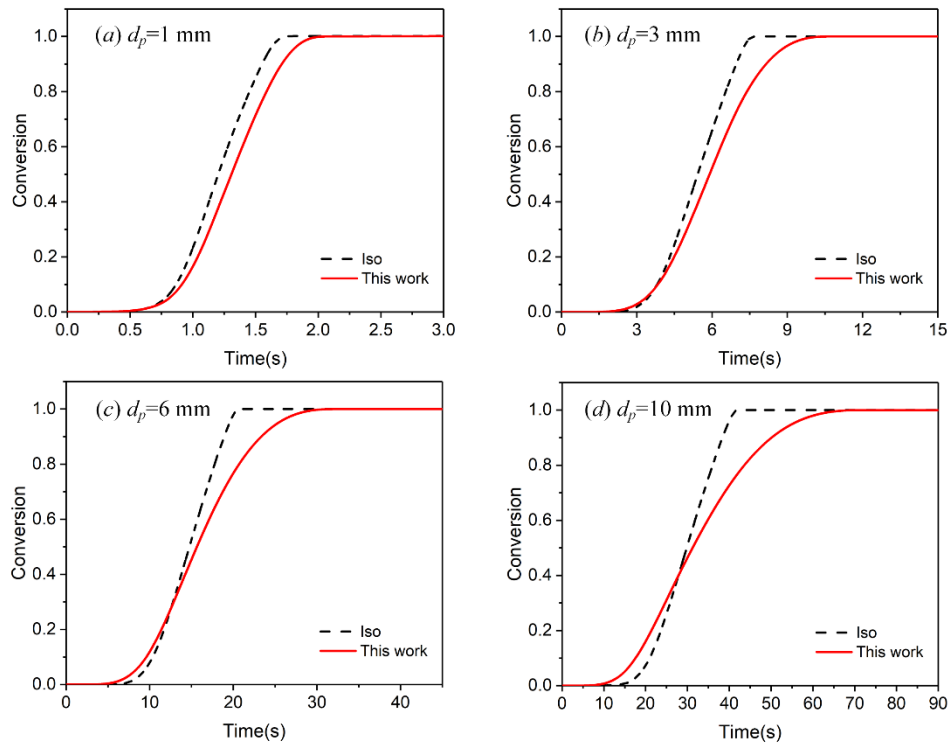


Figure 5. CFD modeling biomass conversion history with different particle size (1/3/6/10 mm) in the batch fluidized bed by using isothermal model and this work

Table 4 compares the computational speed (simulation time per time step) of the isothermal model and this work. The computational speed of the two models is in the same order of magnitude, about 1 s/time-step. Therefore, this work, which included the effects of internal heat transfer, have the same computational efficiency of isothermal model. For the case with 300000 meshes and a time-step of 0.001 s, 10 min of CFD simulation biomass devolatilization in fluidized bed can be finished within 2 weeks with 32 CPU cores. Such a number of meshes can be used to simulate pilot or large scale fluidized bed. As compared to the model of Papadikis et al. [14,15] and, Ström and Thunman [12], the biomass particle does not require to be discretized radially in a number of grid points or marked with different particle layout, which requires additional computational cost for internal grid points. we can except that the heat transfer corrected isothermal model has better performance on computational efficiency.

Table 4 A comparison of computational speed by using isothermal model and this work

Particle size	Computational speed (s/time step)	
	Isothermal model	This work
$d_p=1, \text{ mm}$	0.92	0.88
$d_p=3, \text{ mm}$	0.97	0.92
$d_p=6, \text{ mm}$	0.95	0.98
$d_p=10, \text{ mm}$	0.93	1.15

4. Conclusion and future work

In this paper, the heat transfer corrected isothermal model which presented in our pervious paper [1] was firstly verified by modeling biomass devolatilization in a single particle combustor. Then the model was implemented in Eulerian-Eulerian method for CFD modeling biomass devolatilization in a batch bubbling fluidized bed. This work predicts high devolatilization rate at low temperature but lower at high temperature. The heating rate predicted by this work is lower, as compared to the conventional isothermal model. Moreover, the derivation between the isothermal model and this work increases with the increase of particle size. Those results indicate that internal heat transfer has significantly effects on biomass devolatilization and it should be considered in CFD simulations to improve the performance.

The computational speed of this work and isothermal model is in the same order of magnitude, implying that this work is applicable to simulate biomass devolatilization or combustion in large-scale fluidized beds.

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