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The Impact of Design Correlations on Rate-based Modeling of a Large Scale CO2 Capture with MEA

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Abstract

Hydrodynamics and mass transfer correlations for the design of structured packed columns have been studied in order to compare the effect of different design correlations on the rate-based modeling of a large scale CO_2 capture process with a chemical solvent. The commonly used correlations like the Bravo et al.,[1] and Billet and Schultes [2] were applied in this study for the prediction of mass transfer in an absorber column. Two cases are considered: absorption of CO_2 from a gas-fired power plant (430 MWe) and absorption of CO_2 from a coal-fired power plant (800 MWe). In this work a scale-up analysis with respect to the effect of correlations used on the performance of the system for CO_2 capture with MEA was done within the Aspen RateSep simulator. The study showed that there is significant uncertainty associated with applying the proposed correlations for large scale packed columns for capturing CO_2 from gas-fired and coal-fired power plants. The height of packed column varies in both gas-fired and coal-fired power plants with the selected correlations. It was found that there is more uncertainty in using the selected correlations for absorption of CO_2 from gas fired power plant compared to a coal-fired power plant because of the lower CO_2 concentration. The differences are caused by both the mass transfer and the effective interfacial area models.

Keywords: Rate-based; Scale-up; Coal-fired power plant; Gas-fired power plant; Hydrodynamics and mass transfer correlations.

1. Introduction

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Although post-combustion CO_2 capture by chemical absorption has been tested in pilot plant and industrial applications, there is still much uncertainty associated with the scale-up of the technology. The volume of flue gas from power plants is high and with low partial pressure of CO_2. Therefore the energy requirement to separate out CO_2 is high and the installation is costly.

Nomenclature

a	Specific surface area of packing, m^2m^{-3}
C	Constant
C_E	Correction factor for surface renewal
d	Diameter, m
D	Diffusion coefficient, m^2s^{-1}
Fr	Froude number defined by u_L^2a/g
F_{SE}	Packing surface enhancement factor
Ft	Correction factor for total holdup
H	Hatta number
k	Mass transfer coefficient, m/s
Re	Reynolds number
S	Corrugation side length, m
u	Superficial velocity, m/s
We	Weber number

Greek letters

α	Corrugation inclination angle, deg
γ	Contact angel between solid and liquid film, deg
ε	Void fraction of packing
ν	Kinematic viscosity, m^2/s
μ	Viscosity, kg/m.s
ρ	Density, kg/m^3
σ	Surface tension, N/m

Subscripts

e	Effective
G	Gas
h	Hydraulic
L	Liquid

Thus, optimal design of both absorber and stripper for the duty in question must be aimed at, creating low pressure drop and heat requirement while still maintaining the appropriate separation target. In the design of large-scale columns, important design parameters like column diameter, packing type and size, height of packed section, pressure drop, physical properties of chemical system, and hydrodynamic parameters should be considered to achieve the best design[3]. A comprehensive comparison of different correlations for hydrodynamics and mass transfer in an absorber column without chemical reaction was done by Razi et al.,[3]. The comparison showed that the different correlations were not in correspondence with one another. The reason could be model assumptions, methods of measurement, packing type, physical properties of systems, etc. In the present study, the effect of two selected mass and interfacial area correlations on the performance of the absorption column were compared for a 430 MWe gas-fired power plant and 800 MWe coal-fired power plant.

2. The case study

The flue gas composition for the 800 MWe supercritical power plant and 430 MWe NGCC, which were used in this study are presented in Table 1 and Table 2 respectively [4].

Table 1: Coal-fired power plant flue composition

Flue gas flow rate (kg/s)	782
Solvent flow rate (kg/s)	3637
Temperature ℃	50
Pressure (kPa)	101.6

Compositions	Wet gas (Vol.%)
O_2	3.65
CO_2	13.73
Ar	0.005
N_2	72.855
H_2O	9.73
SO_2 (mg/Nm^3)	85
NOx (mg/Nm^3)	120
Particulate (mg/Nm^3)	8

Table 2: Gas-fired power plant flue composition

Flue gas flow rate (kg/s)	690
Solvent flow rate (kg/s)	915
Temperature ℃	90
Pressure (kPa)	101.6

Compositions	Wet gas (Vol.%)
O_2	12.57
CO_2	3.88
Ar + N_2	75.34
H_2O	8.2
SO_2 (mg/Nm^3)	-
NOx (mg/Nm^3)	-
Particulate (mg/Nm^3)	-

The following base cases were defined:

- 90% CO_2 capture efficiency
- 30 wt. % solvent concentration (MEA)
- CO_2 lean loading 0.27 (mol CO_2/mol MEA) for coal-fired power plant
- CO_2 lean loading 0.25 (mol CO_2/mol MEA) for NGCC power plant
- CO_2 rich loading 0.47 (mol CO_2/mol MEA) for coal-fired power plant
- CO_2 rich loading 0.45 (mol CO_2/mol MEA) for NGCC power plant
- Packing type Mellapak 250 Y

In this study flue gas flow rates, solvent circulation rates, and lean loading for the two cases (a combined cycle power plant and coal-fired power plant) are assumed constant. For a specific diameter of column, the height of packing is varied to remove 90% of CO_2 in both power plants. The effect of selected mass transfer and effective interfacial area correlations on the design performance of the absorber are compared in this study.

3. Mass transfer and interfacial area correlations

A large number of empirical and semi-empirical published correlations for estimation of liquid and gas mass transfer coefficients exist similarly for effective interfacial area applied to packed columns. These correlations are developed and verified based on different assumptions and test systems. Two different correlations for calculation of mass transfer coefficients and interfacial area in an absorber column equipped with Mellapak 250Y structured packing are shown in Table 3. The Bravo et al., [1] correlation and Billet and Schultes[2] correlations are commonly used to predict the mass transfer in packed columns. The methods, experimental specifications, and system used for developing the correlations are given in Table 4 these correlations are applied in this study.

Table 3: Correlations for Mass Transfer and Effective Interfacial Area

Bravo et al., (1992) correlation [1]

$$k_G=0.054\frac{D_G}{S}\left(\frac{(u_{Ge}+u_{Le})\rho_G S}{\mu_G}\right)^{0.8}\left(\frac{\mu_G}{D_G\rho_G}\right)^{0.8}$$

$$\frac{a_e}{a}=F_{SE}F_t$$

$$k_L=2\left(\frac{D_L u_{Le}}{\pi s C_E}\right)^{0.5}$$

$$F_t=29.12\left(We\,Fr\right)_L^{0.15}\frac{S^{0.359}}{Re_L^{0.2}\varepsilon^{0.6}\left(1-0.93\cos\gamma\right)\left(\sin\alpha\right)^{0.3}}$$

$$\cos\gamma=0.9 \quad \text{for} \quad \sigma<0.055\frac{N}{m}$$

$$\cos\gamma=5.211\times10^{-16.835\sigma} \quad \text{for} \quad \sigma>0.055\frac{N}{m}$$

Billet and Schultes (1993) [2]

$$k_G=D_G C_G(a/d_h)^{(1/2)}(\upsilon_G/D_G)^{(1/3)}(u_G/a\upsilon_G)^{(3/4)}(1/(\varepsilon-h_L)^{0.5})$$

$$a_e/a=1.5(ad_h)^{(-0.5)}((u_L d_h)/\nu_L)^{(-0.2)}((u_L^2\rho_L d_h)/\sigma_L)^{0.75}(u_L^2/gd_h)^{(-0.45)}$$

$$k_L = C_L \left(\frac{\rho_L g}{\mu_L}\right)^{0.167} \left(\frac{u_L}{a}\right)^{0.333} \left(\frac{D_L}{d_h}\right)^{0.5}$$

Table 4: Assumptions and testing systems to develop correlations

Correlation	Packing	Testing system	Chemical system (measuring interfacial area)	Unit operation	Assumptions
Bravo et al., (1992) correlation [1]	Gempak 2A Gempak 2AT Mellapak 250Y Mellapak 350Y Mellapak 500Y Flexipac-2 Intalox 2T Maxpak Sulzer BX	Cyclohexane/n-hexane o/p-xylenes ethylbenzene/ethanol chlorobenzene/ethylbenzen i-butane/n-butane	Based on Shi and Mersmann [5] Physical model: measuring the liquid width during liquid flows over the surface	Distillation column (total reflux)	Sheet-metal packings F_{SE} factor was accounted for Surface enhancement. The surface of packing assumed partly wetted.
Billet and Schultes (1993) [2]	over 70 types of packings (random, structured)	More than 50 testing systems (surface tension positive-negative)	Theoretical model	Distillation column (total reflux)	The area of packing was assumed not uniformly wetted.

4. Case study results and discussion

Table 5 shows a summary of the simulation results from the four cases in Aspen plus RateSep. The column diameter was determined at 80% flooding condition for both power plants. The flow rate of flue gas coming from the coal-fired power plant is approximately 1.13 larger than the flue gas flow rate of the gas-fired power plant. Accordingly, a slightly larger diameter is needed to handle the extensive flow from the coal-fired power plant. High concentration of CO_2 in the flue gas coming from the coal-fired power plant requires a large solvent rate to remove 90% of CO_2 from flue gas, and the amine circulating rate has an impact on the size of absorber column through the flooding condition. As can be seen from Table 5, the height of packing calculated for 90% CO_2 removal based on Billet and Schultes correlations (1993) [2] is smaller than that based on the Bravo et al., (1992) correlation [1] for both the gas and coal-fired power plants. Therefore, a lower total volume of packings will be required. Since the same equilibrium and kinetics models were used the differences seen in Table 5 must be caused by the mass and heat transfer models including the effective interfacial area model which may be the main factor. According to Table 4, for the used correlations, different methods were applied to measure effective interfacial area. The correlations are tested on a wide range of particular packings and test systems. However, none of these are for absorption systems, let alone reactive absorption. Applying mass transfer and interfacial area correlations based on distillation data must be deemed unreliable when used for simulation of CO_2 capture with MEA. Table 5 gives an indication of the uncertainty associated with using these correlations in design of a large scale CO_2 capture system.

Table 5: Simulation results from Aspen plus RateSep for two power plants

	Gas-fired power plant		Coal-fired power plant	
Correlations	Bravo et al., (1992)[1]	Billet and Schultes (1993)[2]	Bravo et al., (1992)[1]	Billet and Schultes (1993)[2]
Column diameter (m)	17.5	17.5	23	23
Maximum u_L (m/s)	0.003774	0.0037788	0.0091461	0.009177
u_G (m/s)	2.46	2.46	1.61	1.61
Lean loading	0.25	0.25	0.27	0.27
Rich loading	0.45	0.45	0.47	0.47
LOG	1.592	1.592	5.65	5.65
L/G	7	7	7	7
Height of packed column (m)	25	17	27	23
Pressure drop (mbar/m)	2.38	2.38	1.77	1.88
Total volume of packing (m^3)	5864	3993	11284	9382
Interfacial area (m^2/m^3)	52	83	72	111

Necessary interfacial areas predicted by the Billet and Schultes (1993)[2]correlations tend to be higher than those calculated from Bravo et al., (1992)[1] method and thus results in lower volume and height of packing.

The simulated gas and liquid phase temperatures, CO_2 concentration profiles, and pressure drops per height of packings are shown Figures 1-12 for gas (430 MWe) and coal-fired (800 MWe) power plants. The values on the x axis of the graphs are the distances from the top of the absorber packing.

The inlet flue gas absorbs part of the heat of the rich amine at the bottom of the absorber, and the flue gas temperature increases from bottom to near the top of the absorber. In the top part, heat from flue gas is transferred to the lean amine to increase the temperature of the lean amine (Fig.1.and Fig.2.).The liquid phase and the gas temperature profiles seem to be very alike, although shorter for one set of correlations than for the other. This implies that the heat transfer coefficients must be quite large. The gas and liquid temperature profiles cross each other near the bulge temperature, and the location and shape of the temperature bulge depends on where CO_2 is absorbed into MEA in the absorber, the flow rate of flue gas and liquid, and the heat of reaction. The absorber temperature bulge is approximately at the same position for both the gas and coal-fired case but for the coal fired case it extends further down into the packing. For both cases the lean solution rapidly absorbs CO_2 but the driving force is limited and there is a need for more interfacial area to absorb the larger amount of CO_2 on the coal-fired case. Also the temperature bulge is larger for the coal fired case as there is more CO_2 captured per unit of liquid and gas flowing.

Pressure drop per height of packing increases from bottom to near the top of the column then it decreases (Fig.3. and Fig.4.). The pressure drop is related to the volumetric superficial gas velocity and this will change mainly with temperature. Thus the pressure drop profiles follow the temperature profiles closely. The Bravo et al.(1992)[1] and Billet and Schultes (1993)[2] correlations are quite similar with regard to pressure drop.

The required absorber height is directly affected by specific effective interfacial area and liquid and gas mass transfer coefficients. The higher interfacial area and the smaller required height of absorber were predicted by the Billet and Schultes (1993)[2] correlation (Fig. 11. andFig.12.). For a specific height of packed column, the liquid mass transfer coefficient is larger than the gas mass transfer coefficient.

The profiles for the gas and liquid mass transfer coefficients are shown in Fig. 5-8. Both the mass transfer coefficients are relatively constant through the packing for both the coal and gas cases; the only exception being the large changes for the coal case close to the top of the packing. The temperature has a direct effect on the gas side mass transfer coefficient, but the temperature variation is not believed to be large enough to cause this rapid variation, and why should the mass transfer coefficient decrease rapidly a little further down in the packing where still the temperature is high. No good explanation for this behavior has been found. The two sets of correlation predict quite different gas side mass transfer coefficient, the Billet and Schultes (1993)[2] predictions being about 30% higher than the Bravo et al.(1992)[3] results. The liquid side mass transfer coefficients see Figures 7 and 8; rise markedly when going down in the packing. One would not expect the physical liquid side mass transfer coefficient to change this much, so this change probably stems from variations in the enhancement factor E which must be low at the top and very high at the bottom of the packing where the loading is high and the driving forces small. Small driving forces can give very high enhancement factors, see Astarita et al(1983)[6], but the effects seem very strong. Higher liquid side mass transfer coefficients are seen for the coal-fired case mainly due to higher gas temperatures.

The overall mass transfer coefficients, K_G, as given by Eq. 1 and in Figures 9 and 10, are seen to be dominated by the liquid side resistance and follow the shape of the liquid side mass transfer coefficient closely.

$$1/K_G = 1/k_g + H/k_l \qquad (1)$$

In figures 11 and 12 are given specific effective interfacial area predictions. The interfacial area are alsmost constant throught the column both for the coal and gas case. This is reasonable and expected as the liquid velocity and liquid properties do not change significantly through the packing. The gas velocity changes but in the correlations tested, gas velocity does not enter into the effective interfacial area calculations. It is seen that the Bravo et al., (1992)[1] correlation consitently predicts substantially lower interfacial areas than the Billet and Schultes(1993)[2]correlation. So both overall mass transfer coefficient and effective interfacial area are predicted higher in the Billet and Schultes(1993)[2]correlations, resulting of course in a lower packing height.

The present exercise gives an idea about the accuracy one may expect when trying to make "from scratch" design of an absorber column, and it is seen that large uncertainties must be expected

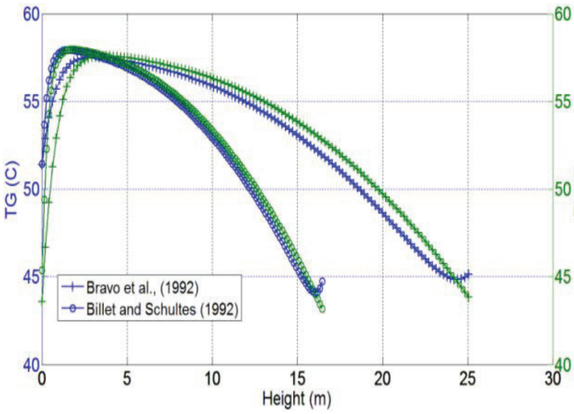

Fig.1. Gas phase and liquid phase temperature (gas-fired power plant 430 MWe)

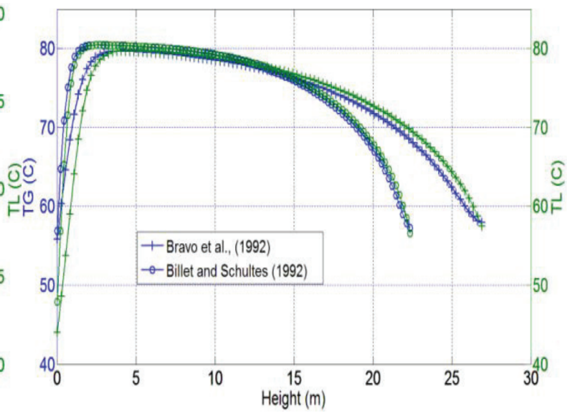

Fig.2. Gas phase and liquid phase temperature coal-fired power plant 800 MWe)

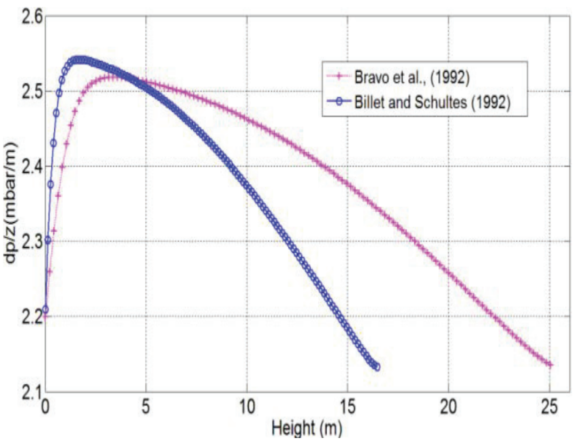

Fig.3. Profiles for pressure drop per height of packing (gas-fired power plant 430 MWe)

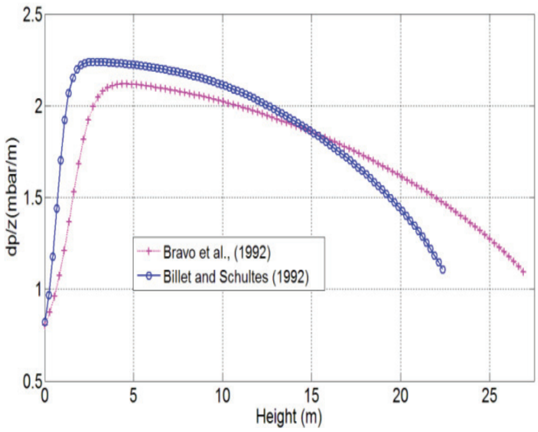

Fig.4. Profiles for pressure drop per height of packing (coal-fired power plant 800 MWe)

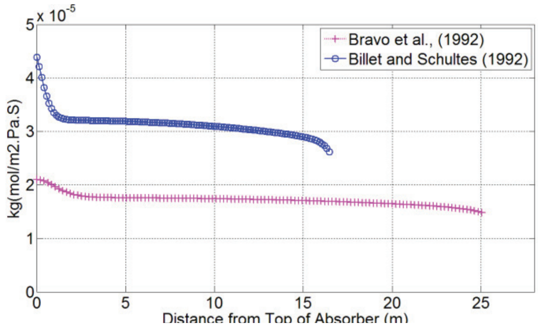

Fig.5. Profiles for gas mass transfer coefficients (gas-fired power plant 430 MWe)

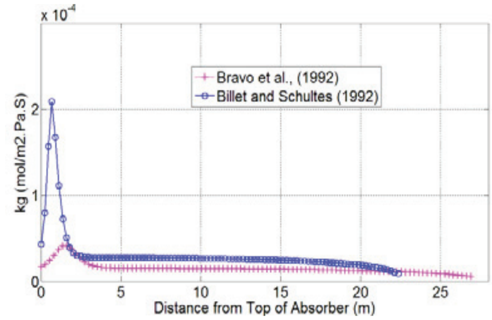

Fig.6. Profiles for gas mass transfer coefficients (coal-fired power plant 800 MWe)

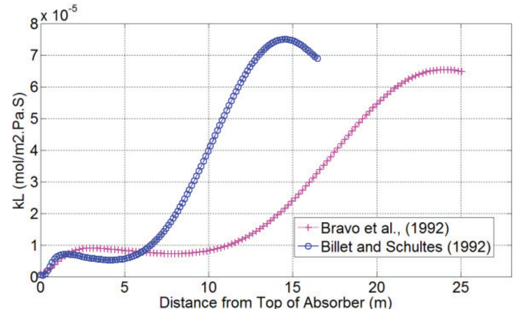

Fig.7. Profiles for liquid mass transfer coefficients (gas-fired power plant 430 MWe)

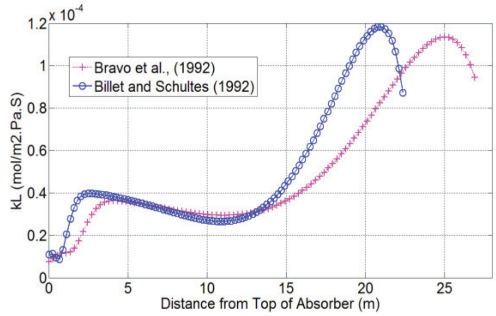

Fig.8. Profiles for liquid mass transfer coefficients (coal-fired power plant 800 MWe)

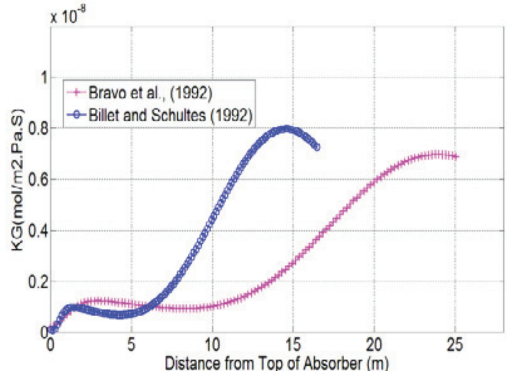

Fig.9. Profiles for overall gas mass transfer coefficients (gas-fired power plant 430 MWe)

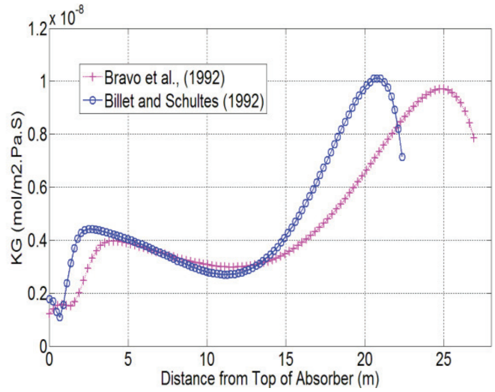

Fig.10. Profiles for overall gas mass transfer coefficients (coal-fired power plant 800 MWe)

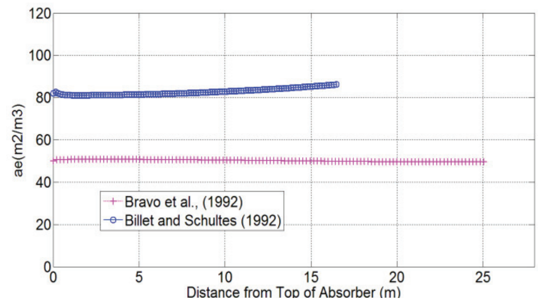

Fig.11. Profiles for effective interfacial (gas-fired power plant 430 MWe)

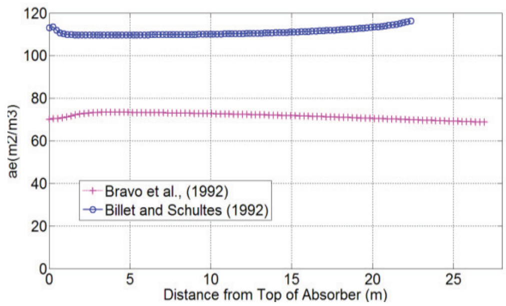

Fig.12. Profiles for effective interfacial (coal-fired power plant 800 MWe)

5. Conclusions

In this study the effect of two commonly used mass transfer and interfacial area correlations on the performance of CO_2 capture from power plants were compared using a rate-based model. The study shows how the effective interfacial area and overall mass transfer coefficient calculations may differ between two sets of correlations and how this can affect the determination of the size of the absorber. It was found that the variation was very large giving significant uncertainty in the design predictions. The correlations used in this study were developed and are tested for specific chemical systems and packing types but not for reactive absorbent systems. Therefore, applying these correlations into Rate-based simulations of large scale absorber systems requires awareness of the uncertainties involved. It is believed that more confidence could be obtained if the underlying correlations were based on testing with reactive absorbents.

6. References

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