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Using air dispersion modeling to evaluate stack characteristics

The modern science of air pollution modelling began in the 1920's when military scientists in England tried to estimate the dispersion of toxic chemical agents released in the battlefield under various conditions. Rapid developments in the 1950's and 1960's, including major field studies and advances in the understanding of the structure of the atmosphere, led to the development of the first regulatory air pollution models in the U.S.

1. Introduction

Dispersion modeling is a mathematical simulation of emissions as they are transported throughout the atmosphere. Nowadays the term "air pollution model" usually refers to a computer program, but in the past it has also included hand calculations or use of charts and tables from simple handbooks. Dispersion models replicate atmospheric conditions, (which includes wind speed and direction, air temperature and mixing height), and provide an estimate of the concentration of pollutants as they travel away from an emission source. These models can also generate estimates of the formation of secondary pollutants by incorporating atmospheric chemistry into the model. Dispersion models can be used to determine whether a new source will adversely impact an area or to predict if the control of an individual source will have a beneficial effect. Dispersion models are used when prediction of ambient concentrations is necessary, such as in the design of a new source, existing sources performance review or even in evaluating emissions reduction plans. The available dispersion models vary in their complexity. At a minimum, most of the models require meteorological data, defined receptors of interest and details about the emission sources in question (stack height, emission rates, gas exit velocity, etc). Some of the more complex models require topography information, chemical species characteristics and land use data. The output from this type of models is a spatial and temporal distribution of the pollutant concentration throughout the modeled domain, ie. region (which depends on the model chosen).

Dispersion models have acceptable reliability in estimating the value of the highest concentrations occurring somewhere within the observed area. Typical accuracy of the results obtained by modeling are in the range of 10 to 40 per cent in the assessment of the maximum concentration.

In this paper air dispersion modelling is used in order to investigate impacts on ambient air quality in case of possible stack height reduction. Within the project of installation of flue gas desulphurization system (FGD) in old units of thermal power plant "X" (TPP X), it is planned to build new "wet stacks"¹ instead of the existing one. TPP X consists of three units (X1, X2 and X3). According the Basic Project design, the old units (X1 and X2) should be connected on a double inner 200 m height "wet stack", while the X3 unit is a new one with FGD system and its own 150 m high "wet stack". The Modelling in this paper aims to evaluate the feasibility for reduction of initial (Basic Project design) 200 m high "wet stack". With that aim, three different scenarios, which incorporate various stacks construction characteristics for X1 and X2 units, are investigated:

- Scenario 1: 170 m high double inner tube concrete stack;
- Scenario 2: 180 m high double inner tube concrete stack;
- Scenario 3: 180 m high single concrete stack.

The main criteria for possible stack reduction decision is that reduced stack height ensures that ground level concentrations of the released pollutants remain within acceptable limits, prescribed by the applicable National Legislation.

2. Description of used model

In order to analyze the influence of TPP X, the standard model of the US EPA (US Environmental Protection Agency) AERMOD is used, which is based on the Gaussian model. AERMOD includes a wide range of possibilities for modeling the effects of released pollutants on ambient air quality. This model includes modeling of multiple sources of pollution including point, line, area and volume sources. Model contains algorithms for analyzing aerodynamic flow in the vicinity of and around buildings (building downwash). Values of pollutants from the source can be treated as constants during the period of analysis, and may vary within a month, a period of time, or an optional hour time change.

2.1 The Diffusion Equation and the Gaussian Plume Model

By performing a mass balance on a small control volume, a simplified diffusion equation, which describes a continuous cloud of material dispersing in a turbulent flow, can be written as:

$$\frac{dC}{dt} + U\frac{dC}{dx} = \frac{d}{dy}\left(K_y\frac{dC}{dy}\right) + \frac{d}{dz}\left(K_z\frac{dC}{dz}\right) + S \tag{1}$$

^{1 &}quot;Wet stack" implies special construction of the stack used in wet FGD systems, which allows that saturated gases exiting the system's absorber could be directly sent to the stack without reheating and drying.

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where:

x = along-wind coordinate measured in wind direction from the source,

y = cross-wind coordinate direction,

z = vertical coordinate measured from the ground,

C (x, y, z) = mean concentration of diffusing substance at a point $(x, y, z) [kg/m^3]$,

 K_{y} , K_z = eddy diffusivities in the direction of the y- and z- axes [m²/s],

U = mean wind velocity along the x-axis [m/s],

S = source/sink term [kg/m³-s].

The eddy diffusivities $(K_y \text{ and } K_z)$ are a way of relating the turbulent fluxes of material to the mean gradients of concentration:

$$\overline{v'c'} = -K_y \frac{\partial C}{\partial y}, \ \overline{w'c'} = -K_z \frac{\partial C}{\partial z}$$
(2)

Here primed coordinates refer to the turbulent fluctuations of terms about their mean values; for example, etc. Typically in the atmosphere c(t) = C + c', u(t) = U + u', etc. Typically in the atmosphere $K_y > K_z$, that explains why the cross-section of a plume often takes on an elliptic shape (Figure 1).

A term-by-term interpretation of Equation (1) is as follows:

$$\frac{dC}{dt} + U\frac{dC}{dx}$$
Time rate of change and advection of the cloud by the mean wind.

$$\frac{d}{dy}\left(K_y\frac{dC}{dy}\right)$$
, etc.
Turbulent diffusion of material relative to the center of the pollutant cloud.
(The cloud will expand over time due to these terms.)
S
Source term which represents the net production (or destruction) of pollutant due to sources (or removal mechanisms).

Equation (1) is grossly simplified, since several assumptions are made in its derivation:

- 1. The pollutant concentrations do not affect the flow field (passive dispersion).
- 2. Molecular diffusion and longitudinal (along-wind) diffusion are negligible.
- 3. The flow is incompressible.
- 4. The wind velocities and concentrations can be decomposed into a mean and fluctuating component with the average value of the fluctuating (stochastic) component equal to zero. Mean values are based on time averages of 10-60 minutes.
- 5. The turbulent fluxes are linearly related to the gradients of the mean concentrations as in Equation (2).
- The mean lateral and vertical wind velocities V and W are zero, so we have also restricted our analysis to steady wind flow over an idealized flat terrain.

The Gaussian plume model, which is at the core of almost all regulatory dispersion models, is obtained from the analytical solution to Equation (1). For a continuous point source released at the origin in a uniform (homogeneous) turbulent flow the solution to Equation (1) is:

$$C(x, y, z) = \frac{Q}{4\pi x \sqrt{K_y K_z}} \exp\left(\frac{-y^2}{4K_y \frac{x}{U}}\right) \exp\left(\frac{-z^2}{4K_z \frac{x}{U}}\right)$$
(3)

Unfortunately, the turbulent diffusivities K_y and K_z are unknown in most flows, and in the atmospheric boundary layer K_z is not constant, but increases with height above the ground. In addition, K_y and K_z increase with distance from the source, because different scales of turbulence in the atmosphere affect the diffusion as the plume grows. Despite these limitations, the general Gaussian shape of Equation (4) is often. If we define the following Gaussian parameters:

$$\sigma_{y} = \sqrt{2K_{y}\frac{X}{U}} \text{ and } \sigma_{z} = \sqrt{2K_{z}\frac{X}{U}}$$
 (4)

Then the final form of the Gaussian plume equation, for an elevated plume released at $z = H_p$ is:

$$C(x, y, z) = \frac{Q}{2\pi U_p \sigma_y \sigma_z} \exp\left(\frac{-y^2}{\sigma_y}\right).$$

$$\cdot \left[\exp\left(-\frac{(z - H_p)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + H_p)^2}{2\sigma_z^2}\right)\right]$$
(5)

Schematic representation of the principle of dispersion of pollutants based on Gaussian model, or a coordinate system that is used in them is given in Figure 1. In these models as the origin implies that the emitter, while calculating the concentration and expansion of the plumes observed in the model domain.



Figure 1: Plume dispersion: definition sketch

2.2 Modeling approach

The results presented in this paper were obtained using a model which included the emissions of SO_2 , NO_2 and PM_{10} from the X1-X3 units. Model included only stacks of X1-X3 units, while neither other sources of emissions, nor background concentrations wereincluded.. The focus of this modeling exercise and the case study is not to evaluate the overall air quality in the project area, but rather to present a representative assessment of the impact of *TPP X* on air quality in the model domain.

The modeling procedure included the following steps: 1. Preparation of the facilities plan, including sources and facilities; 2. Defining the modeling domain and the receptors' locations; 3. Developing source inventories and categorization of all considered sources; 4. Processing of required meteorological data; 5. Terrain data processing; 6. Modeling runs and analysis of the results. Based on the input parameters for all sources, emissions and meteorological data, modeling resulted in the spatial distribution of ground level concentrations of selected pollutants over the selected averaging periods of 1 hour, 24 hours and one year averages

2.2.1 Terrain data

A modeling domain of 50 km x 50 km (2500 km²), with TPP X in its center is selected for this study. Cartesian coordinate system with the distance of 400 m between adjacent points (receptors) is used, which implies that the models processed 15876 points (receptors). To obtain necessary terrain data, SRTM3 - Shuttle Radar Topography Mission data (resolution: ~ 90m, 3 arc-sec) is used (Figure 2).



Figure 2: Processed terrain elevation and Cartesian receptor grid at model domain

2.2.2 Meteorology data

AERMET, a meteorological preprocessor, prepares hourly surface data and upper air data for use in AERMOD. The surface data are hourly observations of surface level parameters such as wind speed and direction, ambient temperature, and cloud cover that are used by AERMET to generate a surface file for use in AERMOD. The upper air data file provides information on the vertical profiles of atmospheric parameters. This includes the altitude, pressure, dry bulb temperature, and relative humidity. Meteorological data that are used for the preparation of model included hourly values of:

- wind speed,
- wind direction,

- ambient temperature,
- relative humidity,
- atmospheric pressure,
- cloud cover-opaque.

Since upper air data was not available, AERMET Upper Air Estimator used hourly meteorological data for the period 2010-2014 to simulate the upper air data.. Meteorological data from the closest meteorological station (operated by Hydrometeorological Institute of Serbia) was used. Figures 3-8 demonstrate wind roses (blowing from), based on meteorological data for period 2010-2014 and for each single year.









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Figure 5: Wind rose and frequency analysis 2011



Figure 6: Wind rose and frequency analysis 2012



Figure 7: Wind rose and frequency analysis 2013



Figure 8: Wind rose and frequency analysis 2014

Based on presented wind statistics (wind roses) it could be concluded that none of the observed year has shown significant differences and that the prevailing wind direction is from east-southeast followed by the southeast direction. This implies that most of the time, released pollutants will be dispersed towards west-northwest and northwest from the source.

2.2.3 Sources charecteristics

For the modeling process the following parameters have to be obtained either by measurements or by calculations so to accurately characterize each of the emission sources:

- the type of pollutants,
- physical stack height, •
- geographic coordinates of stack,
- diameter of the stack,
- the flow rate of flue gases through the stack,
- the temperature of flue gases exiting the stack,
- pollutant concentrations. .

All sources characteristics presented in this paper are calculated.

2.3.3.1 Scenario 1 and 2

Scenario 1 considers future state of TPP X with three units X1-X3 and built-in FGD system at X1 and X3 units. In this scenario units X1 and X2 are connected to the double inner tube concrete stack 170 m high. The difference between Scenario 1 and Scenario 2 is only in the height of the inner tube concrete stack, which is 180 m in case of Scenario 2. For both scenarios characteristic of the future B3 unit remain the same. All necessary data of TPP X units in case of conditions of Scenario 1 and Scenario 2 are presented in tables below (Table 1 and Table 2).

Table 1. Scenario 1 – Units parameters

Unit	Stack height (m)	Stack inner diameter (m)	Exit temp (°C)	Flue gas flow (m ³ /h)	SO ₂ emis- sion rate (g/s)	NO ₂ emis- sion rate (g/s)	PM ₁₀ emis- sion rate (g/s)
X1	170	6.7	66.22	2509640	71.19	71.19	10.4
X2	170	6.7	66.22	2509640	71.19	71.19	10.4
X3	150	6.7	64.00	1971569	49.00	65.50	3.30

Table 2. Scenario 2 – Units parameters

Unit	Stack height (m)	Stack inner diameter (m)	Exit temp (°C)	Flue gas flow (m³/h)	SO ₂ emis- sion rate (g/s)	NO ₂ emis- sion rate (g/s)	PM ₁₀ emis- sion rate (g/s)
X1	180	6.7	66.22	2509640	71.19	71.19	10.4
X2	180	6.7	66.22	2509640	71.19	71.19	10.4
X3	150	6.7	64.00	1971569	49.00	65.50	3.30



Figure 9: 3D model of TPP X (view from south-east)



Figure 10: 3D model of TPP X (view from north)

As buildings could radically influence the dispersion of pollutants there is a need for building downwash analysis. Figures 9 and 10, present 3D models, developed by AERMOD, with units' future point sources (red stacks) of TPP X. Beside point sources, 3D model includes significant buildings (buildings higher than 10 m) layout in TPP from the downwash effect perspective.

2.3.3.2 Scenario 3

Scenario 3, as well, considers future state of TPP X with three units X1-X3 and built-in FGD system at X1 and X3 units. In this scenario units X1 and X2 are connected to a single concrete 180 m high stack. For this scenario, characteristics of the future X3 unit remain the same as in the previous two scenarios. All necessary data of TPP X units for Scenario 3 are presented in Table 3.



Figure 11: 3D model of TPP X (view from east)



Figure 12: 3D model of TPP X (view from west)

Following the same procedure, as for scenarios 1 and 2, a 3D model of TPP is prepared and presented at figures 11 and 12.

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Unit	t Stack height (m) Stack inn diamete (m)		Exit Flue gas temp flow (°C) (m ³ /h)		SO ₂ emis- sion rate (g/s)	NO ₂ emis- sion rate (g/s)	PM ₁₀ emis- sion rate (g/s)			
X1- X2	180	10.1	66.22	5019280	71.19	71.19	10.4			
X3	150	6.7	64.00	1971569	49.00	65.50	3.30			

Table 3.	Scenario	3 –	Units	parameters
Table J.	Scenario	5 -	Onus	parameters

3. Results and discussion

Since these models did not take into consideration the background pollution levels, results obtained by this modeling do not represent the overall ambient air quality with respect to SO_2 , NO_2 and PM_{10} concentrations in the modeling domain, but rather present only the contribution of the power plant emission sources. On the other side it is very important to note that these models represent the worst case scenarios, meaning that they consider that all pollutant sources emit at maximum emission rates 24 hours a day, 365 days a year, which certainly is not the case.

Within described scenarios, for each year, in period 2010-2014, model runs provided outputs as maximum concentrations of pollutants as presented in Table 4 for Scenario 1 and Table 5 for Scenario 2. Pollutants concentrations are presented, as per regulation requirements, as percentile and hourly, daily and annual concentrations depending on the pollutant.

Table 4. Maximum concentrations of pollutants obtained by modeling: Scenario 1 (Double inner tube concrete stack of 170 m)

	SO ₂ [μg/m³]			NO ₂ [μg/m³]			PM ₁₀ [μg/m ³]	
Year	1hr 99.73 perc.	24hr 99.18 perc.	Annual	1hr 99.79 perc.	24hr	Annual	24hr	Annual
2010	128.07	63.19	5.11	119.99	53.17	3.38	11.93	0.74
2011	128.71	38.01	3.05	130.37	94.68	3.38	13.83	0.37
2012	125.96	39.39	3.24	128.02	74.02	3.59	10.81	0.39
2013	128.66	76.24	4.86	129.24	87.04	4.91	12.71	0.70
2014	128.62	43.39	3.59	129.55	72.54	4.00	10.60	0.43

Table 5. Maximum concentrations of pollutants obtained by modeling: Scenario 2 (Double inner tube concrete stack of 180 m)

	SO ₂ [μg/m³]			NO ₂ [μg/m³]			PM ₁₀ [μg/m³]	
Year	1hr 99.73 perc.	24hr 99.18 perc.	Annual	1hr 99.79 perc.	24hr	Annual	24hr	Annual
2010	64.55	13.23	2.83	58.47	16.53	3.26	1.95	0.34
2011	69.39	13.26	2.90	80.02	19.19	3.24	2.55	0.34
2012	65.27	15.34	3.11	79.62	18.40	3.45	1.94	0.37
2013	79.47	13.75	2.78	89.84	23.09	3.10	2.31	0.33
2014	64.00	15.12	3.42	76.02	17.16	3.83	2.34	0.41

	SO ₂ [μg/m³]			NO ₂ [μg/m³]			PM ₁₀ [μg/m³]	
Year	1hr 99.73 perc.	24hr 99.18 perc.	Annual	1hr 99.79 perc.	24hr	Annual	24hr	Annual
2010	32.74	6.96	1.56	31.69	9.62	1.92	0.83	0.15
2011	36.03	7.56	1.61	52.10	9.56	1.95	0.80	0.16
2012	36.36	8.25	1.69	50.37	12.09	2.03	0.87	0.17
2013	38.95	7.32	1.54	52.74	15.98	1.86	0.96	0.15
2014	33.22	7.86	1.89	43.53	9.91	2.29	0.85	0.18

Table 6. Maximum concentrations of pollutants obtained by modeling: Scenario 3 (Single inner tube concrete stack of 180 m)

According to the presented results for Scenario 1 and 2, it is clear that a 10 m higher stack has positive influence on air quality. As for the hourly averages in case of SO_2 and NO_2 concentrations are almost two times lower, while in case of PM_{10} a three-fold reduction in ambient concentrations is obtained.. Daily averages show almost a six-fold difference in two scenarios for SO_2 and NO_2 , while for PM_{10} that reduction is about 3 times if a 180 m stack is chosen. Lower concentrations could be observed in case of annual averaging period, concentrations of SO_2 and PM_{10} are two-times lower, while concentrations of NO_2 remain the same or show minor reduction. Therefore, an increase of 10 m in stacks high, gives significantly wider dispersion and higher dilution of flue gases emitted from stacks that has a lower pollution at ground level as a consequence.

From the point of view of the air quality regulatory requirements (Table 7), according to the modelling results, presented in Table 6, it would not be recommended to reduce stacks height to 170 m, since the pollutant (NO_2) concentration would be probably higher than the limits outlined by the National Air Quality Objectives. In case of Scenario 2 all obtained results are below the prescribed limits.

Table 7. National Air Quality Objectives

Pollutant	Concentration (micrograms per cubic meter)	Measured as
Sulphur dioxide (SO ₂)	$350\mu\text{g/m}^3$ (not to be exceeded more than 24 times per year)	1 Hour Mean
	125 μg/m ³ (not to be exceeded more than 3 times per year)	24 Hour Mean
	50 μg/m³	Annual Mean
Nitrogen dioxide (NO ₂)	150 $\mu g/m^3$ (not to be exceeded more than 18 times a year)	1 Hour Mean
	85 μg/m³ 40 μg/m³	Annual Mean
PM ₁₀	50 μg/m ³ (not to be exceeded more than 35 times per year)	24 Hour Mean
	40 μg/m³	Annual Mean

Results from Scenario 2 and Scenario 3 show just about a double reduction of ground concentrations of given pollutants in favor of Scenario 3. Regardless the same stack height the reduction is a result of a single tube construction. Namely according to Equation (6), larger inner stack diameter of a single tube compared to the diameter of each individual stack tube in a double inner tube design case and joint flue gases in one tube give the higher buoyance flux parameter F, which directly influence plume rise, and with that, the effective emission height. Briggs' buoyancy flux parameter F:

$$F = gv_s r^2 \frac{(T_s - T_a)}{T_s} \tag{6}$$

Where:

 $g = 9,807 \text{ m/s}^2$, $v_s = \text{stack exit velocity [m/s]}$, r = stack exit radius [m], $T_s = \text{stack gas temperature [K]}$, $T_s = \text{ambient air temperature [K]}$.

According to the modeling results, Scenario 3 is the most favorable from the resulting ambient air quality point of view, within considered scenarios in this study. So beside the tabular presentation of modeling results for Scenario 3, a total of 8 isopleth maps (depicting contour lines obtained by connecting the receptors with the same ground level concentration values) are presented in Figures 13-20.



Figure 13: SO₂ 99.73rd percentile of hourly means $[\mu g m^{-3}]$ (2013)



Figure 14: SO, 99.18th percentile of daily means [µg m⁻³] (2012)



Figure 15: SO₂ annual mean concentration [μ g m⁻³] (2015)



Figure 16: NO₂ 99.79th percentile of hourly means[µg m⁻³] (2013)



Figure 17: NO₂ daily mean concentration [μ g m⁻³] (2013)



Figure 18: NO₂ annual mean concentration [μ g m⁻³] (2014)



Figure 19: PM10 daily mean concentration $[\mu g m^{-3}]$ (2013)



Figure 20: PM10 annual mean concentration [μ g m⁻³] (2014)

Since the source characteristics, such as: stacks heights, emission rates and inner stacks diameters, of a newly proposed double inner tube stack are different then ones proposed in the mentioned Basic design of the Project, it is not possible to make a simple comparison between results of a previously prepared environmental impact assessment study and results in this study. By analysis of results presented in this study it could be concluded that in terms of the ratio limit value/modeling result of a given pollutant the most problematic is NO₂. Based on those facts and in order to give quick insights in discrepancies between the two studies, additional modelling has been carried out with a newly proposed stacks data and the height of 200 m for a double inner tube stack as it was originally defined in the basic design. As well by analysis of modelling results for Scenario 3 as a most favorable of all presented scenarios, 2011 and 2013 have been chosen as years with highest concentrations of NO2. Results of modelling for 200 m double inner stack as well the corresponding results of Scenario 3 are given in Table 8 (maximum concentrations).

Table 8. Modelling NO₂ concentration (maximum values) $[\mu g/m^3]$

	Year	1hr 99.79 perc.	24hr	Annual
Conorio 2	2011	52.10	9.56	1.95
Scenario S	2013	52.74	15.98	1.86
200	2011	55.98	15.48	2.98
200 m	2013	61.63	18.44	2.88

Compering the results presented in Table 8 and spatial distribution it could be concluded that that Scenario 3 is not only the best solution between scenarios that have been presented in the study, but that stack design is, from the air quality point of view, is better than original solution that included two wet stacks with 200 m stack height. The explanation for this lies in stack construction and buoyance flux parameter F, detailed explained above.

4. Conclusion

In order to investigate the influence of stack construction on pollutants dispersion, this paper investigated three different scenarios that incorporated various stacks construction characteristics for X1 and X2 units, while X3 unit characteristics stayed unchanged:

- Scenario 1: 170 m high double inner tube concrete stack;
- Scenario 2: 180 m high double inner tube concrete stack;
- Scenario 3: 180 m high single concrete stack.

For each of those scenarios prepared for the five years (2010-2014) period of hourly sequential meteorological data from a representative measuring station, air dispersion modelling has been completed for thee major pollutants (SO₂, NO₂ and PM₁₀) and maximum concentrations have been presented in a tabular and in a graphical (isopleth maps) forms:

- SO₂ 99.73rd percentile of hourly means [μ g m⁻³],
- SO₂ 99.18th percentile of daily means [μ g m⁻³],
- SO₂ annual mean concentration [μ g m⁻³],
- NO₂ 99.79th percentile of hourly means [μ g m⁻³],

- NO₂ daily mean concentration [μ g m⁻³],
- NO₂ annual mean concentration [μ g m⁻³],
- PM_{10} daily mean concentration [$\mu g m^{-3}$],
- PM₁₀ annual mean concentration [µg m⁻³].

Considering that these model runs did not take into consideration background pollution levels, results obtained by this modeling do not represent overall ambient air quality (SO₂, NO₂ and PM₁₀ concentration) in the modeled area, but only considered the contribution of the power plant TPP X to overall air quality. Furthermore, these model outputs represent the worst case scenarios, i.e. that all pollutant sources emit at the maximum emission rate 24 hours a day, 365 days a year, which certainly is not the case.

According to the presented results, Scenario 3 (180 m high single concrete stack) is the most favorable from the resulting air quality perspective, within discussed scenarios in this study and compared to the originally proposed design (200 m stacks height). As well, based on the National Air Quality Objectives, ambient concentrations obtained as a result of Scenario 3 assumptions will be below the prescribed regulatory limits. Results of modeling runs presented in this paper show great influence of buoyance flux parameter F on plum rise and thereby on air quality. This gives possibilities for stack height reduction with influence on stack construction.

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