EuroCC@Turkey

https://eurocc.truba.gov.tr/

This document is prepared by EuroCC@Turkey for EuroCC under GA NO 951732

CASE STUDY REPORT

Simulation-Optimization of a Patented Design with Parallel Computing on TRUBA cluster

NCC Partner	*Name*
Company*	*Design and Simulation Technologies Inc. – http://www.dstechno.net/*
Expert	*Ender Demirel, Ph – edemirel@dstechno.net*
Start & End Date	*07.06.2021-08.09.2021*
Approved by	*NCC Project Management Team – Date*

***Company** accepts that the Case Study Report is shared with the EuroCC Project and the community through the EuroCC@Turkey awareness creation activities and platforms.

Date	Author	Comments	Version

1. Problem Identification

Design and Simulation Technologies (DSTECH) Inc. is an SME company supplying and services with customers in the solution of complex engineering problems encountered in different disciplines such as Environment, Energy and Aerospace sciences. In the scope of this case study, DSTECH intends to first optimize a design patented by EPO (European Patent Office) for the efficiency enhancement of a mixing system used in potable water treatment plants (Aral and Demirel, 2019). Definition of the problem, solution strategy and proposed optimization procedure are identified in this document.

Treatment of surface waters in large cities has emerged as a critical point of interest for governments in recent years with increasing clean water demand and development of energy intensive water treatment technologies such as ozone and ultraviolet. Raw water is mixed with the disinfectant in a multi-chambered contact tank (Fig. 1a) at the last stage of the treatment procedure to remove viruses and pathogens from the water. Although an efficient contact system is required for the effective disinfection of water with less disinfectant dosages and energy usage, conventional mixing systems suffer from low mixing and high energy consumptions due to the recirculation and short-circuiting effects (Fig. 1b) inside the chambers (Demirel and Aral, 2018a).

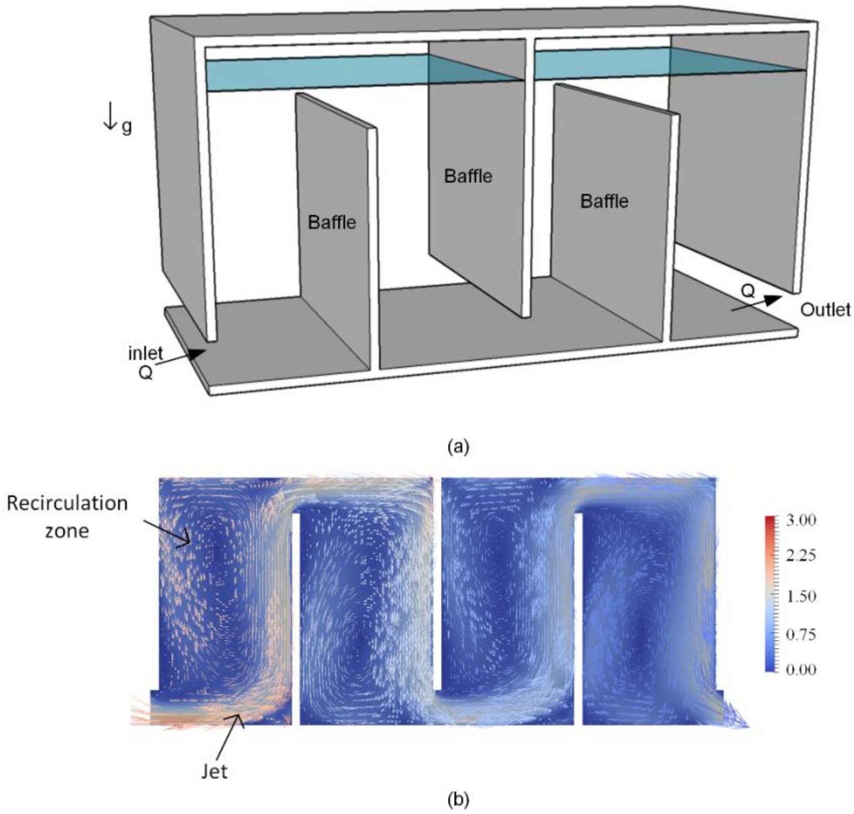


Figure 1. Schematic view of the flow inside a multi-chambered contact system: a) Three-dimensional view of the tank geometry and b) flow structure inside the tank.

To this end, DSTECH invented a slot-baffle design (Fig. 2), in which slots are created at specific locations of the baffle in order to improve mixing efficiency of the system by increasing interaction between two neighboring chambers (Aral and Demirel, 2017).

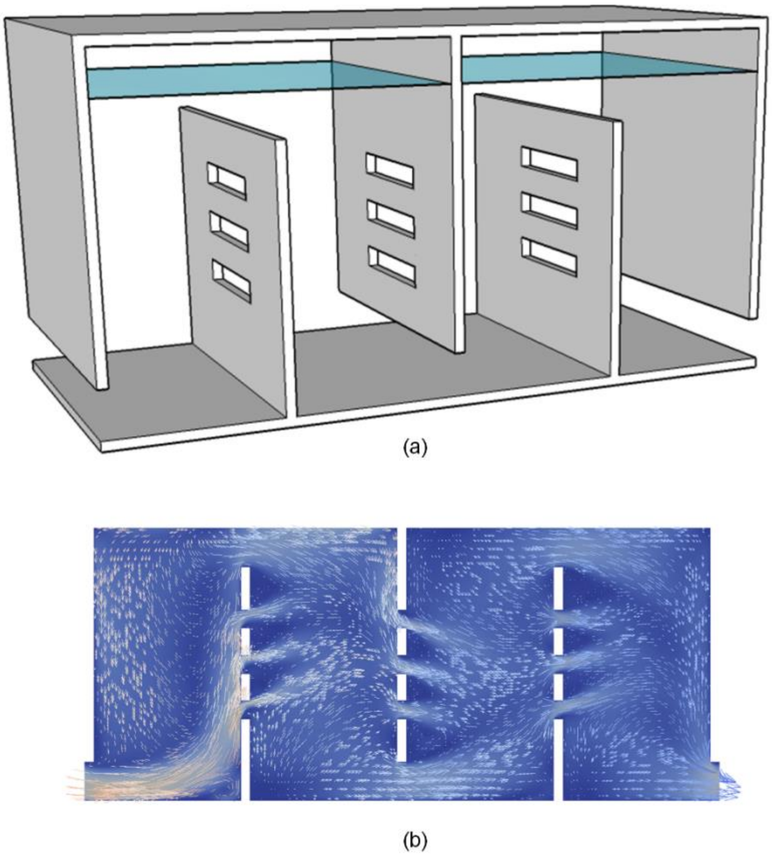


Figure 2. Schematic view of the slot-baffle design: a) Three-dimensional view of the slot-baffles inside the tank and b) velocity vectors emerging from the slots.

Although slot-baffle design has been proved to significantly increase the efficiency of a multi-chambered contact system in several published technical papers so far (Aral and Demirel 2017, Demirel and Aral 2018a, Demirel and Aral 20218b), geometrical properties of the design have not been optimized yet since an intense computational resource and time are required for the optimization of the design. In this case study, we aim at optimizing the patented design with an augmented simulation and optimization framework developed by the DSTECH team.

2. First Suggestion

Each contact tank facilitated at potable water treatment plants has its own flow conditions depending on water resources and water consumption ratios in modern cities. Geometrical specifications of the design such as width and location of the slots need to be investigated and optimized to achieve the highest efficiency of a disinfection contact system. Such dynamic systems should be optimized using a simulation and optimization framework to find out design parameters without using a blind-search approach. DSTECH has developed an open source simulation and optimization framework augmented with OpenFoam (OpenFoam, 2015), Dakota (Adams et al., 2019) and Python, which can be freely used on HPC clusters without any restrictions such as license, commercialization and parallelization (https://github.com/DSTECHNO/simOptDST/tree/main/EUROCC).

Hydraulic and mixing efficiencies of a contact system should be assessed using metrics such as baffling factor (θ_{10}), Morrill (Mo) and Aral-Demirel (AD) indexes (Demirel and Aral, 2018b). Environmental Protection Agency (US EPA 2013) suggested the baffling factor as 1 for the hydraulic efficiency and Morrill index (Mo) as 2 for the mixing efficiency of a perfect disinfection system. Thus, the design is optimized according to the following objective function for the overall efficiency of the mixing system:

$$|Mo - 2| \rightarrow 0 \tag{1}$$

Consider that the above procedure is not interrupted by a human hand since the augmented open source platform follows the above procedure with a strong interaction of open source codes with each other. Thus, this augmented platform will be run with parallel computing using multi processors on the TRUBA (Turkish National Science e-Infrastructure) cloud-computing center. Optimization studies are carried out as three stages given in the following parts.

3. Numerical Model and Optimization Toolbox

Incompressible and turbulent flow inside the contact tank is simulated using the following Reynolds Averaged Navier–Stokes (RANS) equations:

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{2}$$

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = \frac{-1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\nu \frac{\partial U_i}{\partial x_j} - \overline{u'_i u'_j}\right) + S_i \tag{3}$$

$$\frac{\partial \varphi}{\partial t} + U_i \frac{\partial \varphi}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D \frac{\partial \varphi}{\partial x_i}\right) + S \tag{4}$$

Flow quantities are calculated as the summation of mean and fluctuation components of flow variables:

$$U_i = \overline{U_i} + u'_i \tag{5}$$

$$p = \overline{p} + p' \tag{6}$$

$$\varphi = \overline{\varphi} + \varphi' \tag{7}$$

The standard *k-ε* model turbulence model proposed by Launder and Spalding (1974) is employed to close the equations. Turbulent viscosity ν_t is determined using Boussinesq approach:

$$\nu_t = C_\mu \frac{k}{\varepsilon^2} \tag{8}$$

Here, the turbulence model constant C_μ is set to 0.09 for the present problem. Initial values of *k* and *ε* in the RANS solution are calculated from the following equations:

$$k = \frac{3}{2}(UI)^2 \tag{9}$$

$$\varepsilon = C_\mu^{\frac{3}{4}} \frac{k^{\frac{3}{2}}}{l} \tag{10}$$

Numerical solutions of the governing equations are carried out in the framework of finite volume method using open source Computational Fluid Dynamics (CFD) code OpenFoam. Steady-state solution of the governing equations is achieved using the SIMPLE algorithm (OpenFoam, 2015). Concentration of the tracer is monitored at the outlet of the tank and cumulative Residence Time Distribution (RTD) curve is obtained using the following equation (Danckwerts, 1953).

$$F(t) = \frac{C_{out}(t)}{\sum_{i=1}^{n} C_{out-i}} \tag{11}$$

Two characteristic dimensionless time quantities are determined from the cumulative RTD plot to calculate Morril index:

$$Mo = \frac{\theta_{90}}{\theta_{10}} \tag{12}$$

Regulations used in the treatment of potable waters suggest that Mo approaches 2 for a perfectly mixing system. Thus, the objective function for the optimization of the mixing system is constructed as $|2 - MI| = 0$ (Teixeria and Siqueira, 2008).

Open source software Dakota is employed as an optimization-toolbox in the present study. Dakota includes various optimization algorithms such as uncertainty quantization by sampling, reliability, stochastic expansion and interval estimation methods, parameter estimation and experimental design with nonlinear least squares methods, and parameter study capabilities and sensitivity/variance analysis (Trucano et al., 2006). Preliminary numerical studies conducted in the scope of this case study suggest that the *conmin_frcg* algorithm is the most efficient algorithm among the algorithms available in Dakota.

3.1 Fletcher-Reeves Conjugate Gradient Method

This method is derived from the Conjugate Gradient Method (Hestenes and Steiffel, 1952) based on simultaneous linear equations including a symmetric positive definite coefficients matrix (Fletcher and Reeves, 1964).

$$Ax = b \tag{13}$$

$$b = Ah \tag{14}$$

Here, A is the orthogonality condition in the solution of the equations. Solution of these equations in the directions $(p_0, p_1, \ldots)$ are generated such that p_{i+1} is a linear combination of $-g_{i+1}$. The simplest equation is obtained when coefficients are arranged:

$$p_{i+1} = -g_{i+1} + \beta_i p_i \tag{15}$$

$$\beta_i = \frac{{g_{i+1}}^2}{{g_i}^2} \tag{16}$$

Eqs. 13 and 14 reveal the general minimization algorithm, where x_0= arbitrary value, $g_0 = g(x_0), p_0 = -g_0$, x_{i+1} = position of the minimum of $f(x)$ on the line through x_i in the direction p_i, $g_{i+1} = g(x_{i+1})$. This system finds the local minima of functions having *n* variables with the iteration number *n*. Here, selected arbitrary values should not exceed the specified boundary conditions. Linear search method is adopted to the Davidon cubic interpolation method. In addition, the variables in the equation set were arranged according to the Flecther and Powell Method. Thus, Eq. 16 is given for linear search (Adams et al., 2019).

$$t_e = b - \left(\frac{y'(b)+w-z}{y'(b)-y'(a)+2w}\right) \quad (17)$$

$$z = 3\,\frac{y(a)-y(b)}{b-a} + y'(a) + y'(b) \quad (18)$$

$$w = \sqrt{\left(z^2 - y'(a)y'(b)\right)} \quad (19)$$

In Eq. 19, a: initial time, b: last time, t_e: estimate time, $a < t_e \leq b$. Iterations are terminated when the ${g_i}^2$ term approaches to zero in the equation system and hence x_i becomes minimum. This condition also clearly proves the existence of the convergence criterion (Adams et al., 2019). The optimization framework will search the optimized design to minimize the objective function (Eq. 1) using the following steps:

1. Geometry and mesh of the computational domain are generated for the geometrical specifications of slots using blockMesh utility in OpenFoam.
2. Turbulent flow is simulated using open source CFD code OpenFoam.
3. Tracer simulation is performed using OpenFoam for the flow and turbulence field predicted in the previous step.
4. Efficiency indexes and objective function (Eq. 1) are calculated using the developed Python code.
5. Optimization software Dakota reads the calculated objective function and predicts the next geometrical specifications of the slots using Fletcher-Reeves conjugate gradient method.
6. The procedure is repeated from step 1 to step 5 using the new parameters of the slots until the optimization is achieved.

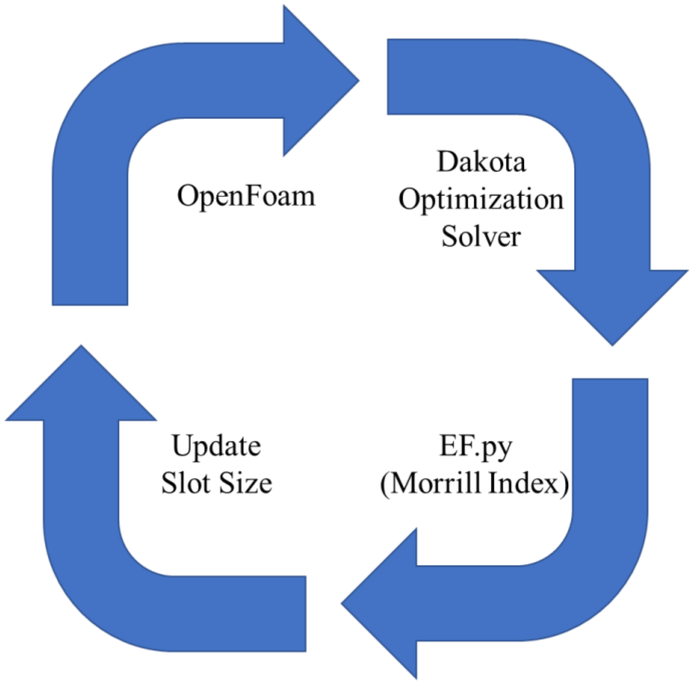


Figure 3. Schematic view of the loop for the simulation-optimization of the slot-baffle design.

4. Solution Stages

The slot-baffle design shown in Fig. 2a has its own design specific parameters such as width, height and position of the slots created on the solid baffle. Optimization of the slot-baffle design is achieved in three separate stages in the present study instead of optimization of all parameters in a single stage since increasing the number of variables results in uncertainty and deviation during optimization procedure.

4.1 Stage 1: Optimization of the slot dimensions simultaneously

As seen in Figure 4, height and width of the baffle are 0.18 m and 0.23 m, respectively. Here, the aim of this solution phase is to optimize the dimensions of the slot for specific locations. Note that dimensions of the rectangular slots are changed diagonally such that width and height of a slot increase and decrease simultaneously during an optimization cycle. Central coordinates of the slots in vertical direction are given in Table 1. Here, slots are placed at the center of the baffle in a spanwise direction.

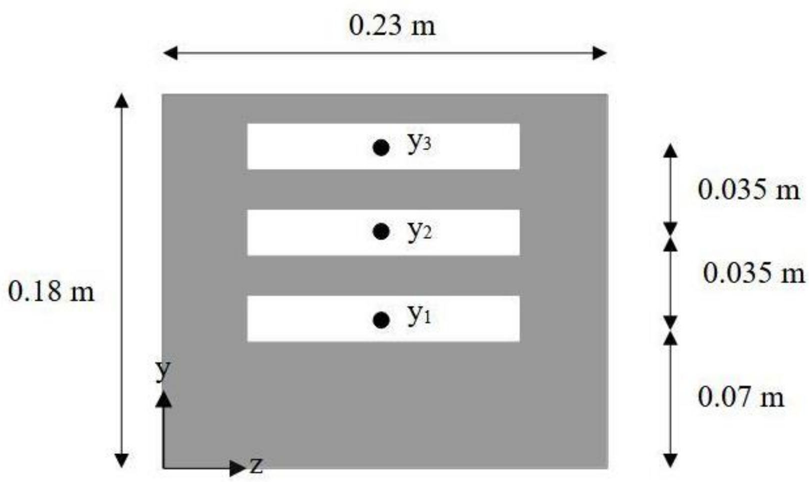
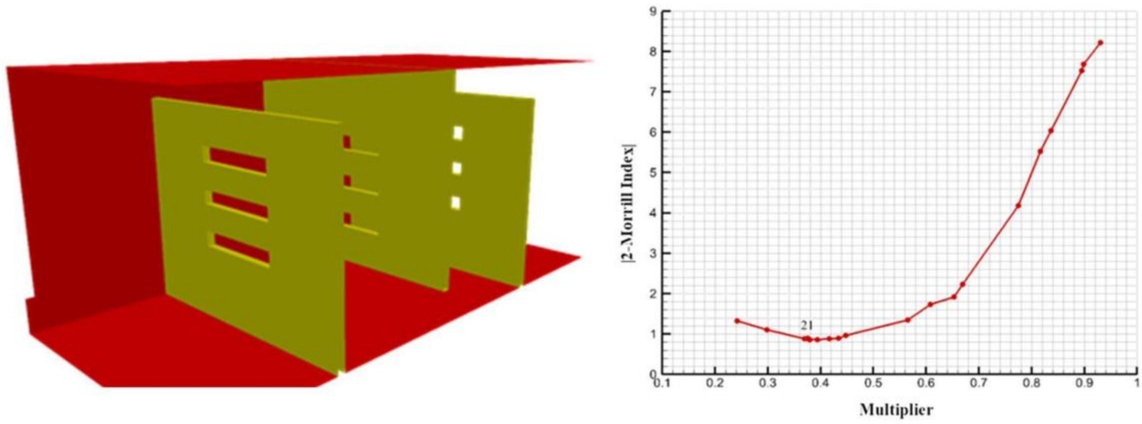


Figure 4. Geometrical parameters of the slots.

Table 1. Vertical coordinates of the baffles.

Coordinate	**Value (m)**
y_1	0.070
y_2	0.105
y_3	0.140

Dimensions of the slots are changed with Δ in the diagonal direction of the rectangular shaped slot as one variable in the optimization cycle. Then width and height are calculated from the corresponding increment. Note that dimensions of the slots should be limited to the dimensions of the baffle to overcome an unphysical situation during the search algorithm. As the dimensions of the slots change, mesh is regenerated for the new baffle configuration and flow and tracer simulations are carried out successively to determine Mo index, which is used for the calculation of the corresponding object function. The convergence tolerance of the *conmin_frcg* method is selected as 10^{-4} during iterations. As seen in the following figure, dimensions of the slots are optimized in 21 iterations and the minimum value of the objective function was determined as 0.8564 for the height of 0.175 m and width of 0.501 m of a slot.



(a) (b)

Figure 5. Optimization of the slot dimensions for constant locations. (a) Three-dimensional view of the optimized baffle and (b) variation of the object function with the iteration.

4.2 Stage 2: Optimization of width and height separately

Width and height of the slots were optimized for the same diagonal increment in Stage 1. However, width and height of a slot should be optimized independently to achieve higher efficiencies. Here, height and width of the slot were optimized separately using the increment values obtained from the first stage. Unlike Stage 1, slot dimensions are optimized with two-variables. Different optimization algorithms are employed for the two-variable optimization and results are summarized in Table 2 in terms of wall clock time, CPU time and iteration number. Gradient and Hessian based *optpp_newton* method could not optimize the present design. Here, *conmin_frcg* yielded the optimized solution using less CPU time than *ncsu_direct* and *mesh_adaptive_search* methods.

Table 2. Performance assessment of optimization algorithms.

Algorithm	Total Wall Clock	Total CPU	Iteration Number for Optimization	Minimum |2-Morrill| Value	Description
conmin_frcg	112705	0.44	33	0.7625	Gradient Based
optpp_newton	106800	0.47	25	7.0320	Gradient and Hessian Based
ncsu_direct	201813	0.86	115	0.7365	Derivative Free
mesh_adaptive_search	116615	0.48	42	0.7640	Pattern Serach Derivative Free

Three-dimensional view of the optimized design is shown in Figure 6. Width and height of the slot are optimized as 0.023 m and 0.031 m, respectively, for a given flow rate. Moreover, the achieved minimum of the object function is less than that in Stage 1.

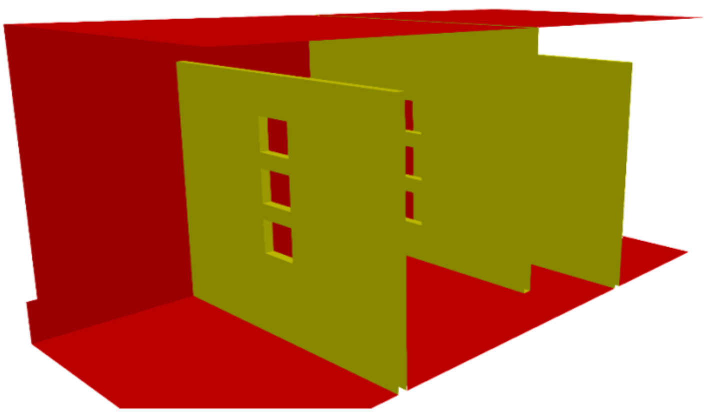


Figure 6. Slot baffle design with minimum |2-Morrill Index| value in phase two.

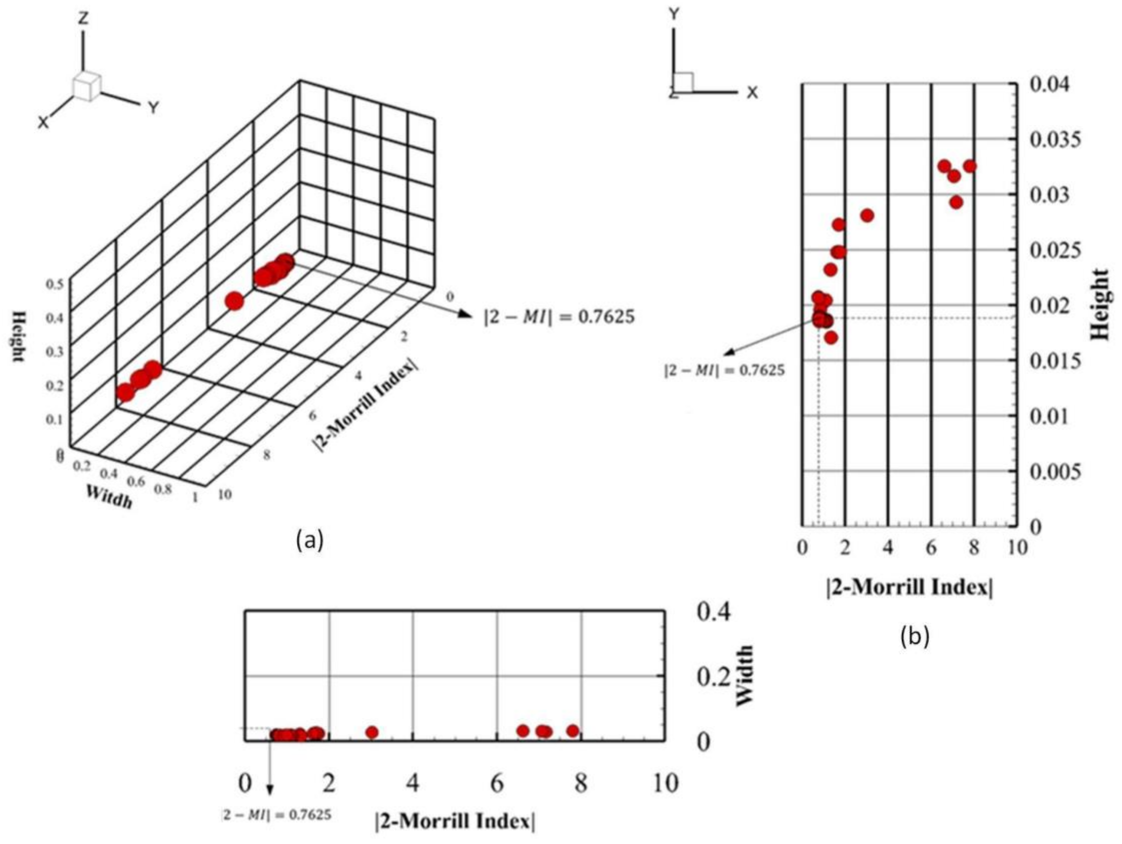


Figure 7. Variations of the parameters during optimization. (a) Variations of width and height, variation of (b) height and (c) width.

Variations of the width and height of the slot with the iteration number are shown in Figure 7. The local minimum of the function was found to be 0.7625, which is less than that in Stage 1. This result proves that the optimization of the design variables separately could yield higher efficiency than that in Stage 1.

4.3 Stage 3: Optimization of slot locations

Dimensions of the slots were optimized as 0.023 m height and 0.031 m width in Stage 2. Locations of the slots still need to be optimized to achieve higher efficiencies for the multi-chambered contact tank. In this stage, locations of the slots are optimized using a multi-variable optimization approach using the dimensions determined in Stage 2. To address this need, coordinates of the slots are optimized in two steps. Vertical coordinates y_i are optimized keeping the spanwise coordinate z constant in the first step and spanwise coordinates z_i are optimized in the second step using *conmin_frcg* method with the convergence tolerance 10^{-4} in Dakota. In order to prevent overlapping of the slots while shifting coordinates, locations of the slots are limited using the following expressions for each slot:

- First Slot: $y_{11}, y_{12}, z_{11}, z_{12}$.

$$y_{11} + H_S = y_{12}$$
$$z_{11} + W_S = z_{12}$$

- Second Slot: $y_{21}, y_{22}, z_{21}, z_{22}$.

$$y_{21} + H_S = y_{22}$$
$$z_{21} + W_S = z_{22}$$

- Third Slot: $y_{31}, y_{32}, z_{31}, z_{32}$.

$$y_{31} + H_S = y_{32}$$
$$z_{31} + W_S = z_{32}$$

Vertical coordinates of the slots are optimized in 34 iterations and results are given in Table 3.

Table 3. The values of the lower left corners of the slots on the y-axis

Variable	**Value**
y_{11}	0.057067
y_{21}	0.109823
y_{31}	0.147153

Spanwise coordinates of the slots are optimized in 39 iterations and results are given in Table 4. The objective function minimized to 0.5439 at the end of this stage which results in the highest efficiency for the corresponding contact tank. Optimized slot configuration is shown in Fig.8.

Table 4. The values of the lower left corners of the slots on the z-axis

Variable	Value
z_{11}	0.104361
z_{21}	0.124118
z_{31}	0.107937

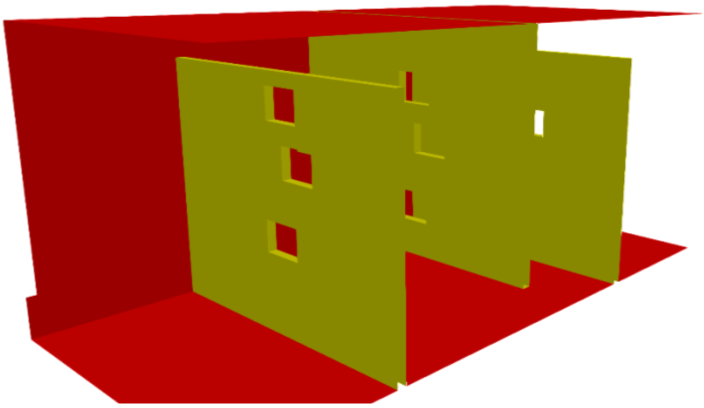


Figure 8. Optimized slot configuration in stage 3.

5. Results and Achievements

Contact tanks are the most critical infrastructures in potable water treatment plants for the disinfection of surface waters using different disinfection methods such as chlorine, ozone and ultraviolet. Conventional tank designs suffer from low mixing and disinfection efficiencies that may yield high disinfectant dosages and energy usages for the treatment of surface waters in modern cities. As an SME company, DSTECH invented a novel design, which substantially enhances the efficiency of a disinfection system to reduce disinfectant and energy usages in water treatment plants.

DSTECH developed a simulation and optimization framework integrating open source CFD and optimization software, which is freely accessible in TUBITAK open archive Aperta (Kuzay et al. 2021). The present simulation and optimization framework is employed to optimize the slot-baffle design in three stages without any convergence issues. Numerical simulations are performed with parallel computing strategies using an intense computational resource allocated on the TRUBA infrastructure. Numerical simulation results in the present study show that the efficiency of the conventional design can be improved by 12.47% when the optimized design is implemented to the present tank.

Table 6. Improvements achieved at each stage.

Stage	Mo	Improvement (%)
Main Case	2.9125	-
Stage 1	2.8564	1.93 %
Stage 2	2.7625	5.15 %
Stage 3	2.5493	12.47 %

A patented design could be optimized by the partnership of an SME company and high performance computing center in the present case study. This study is a good example of using high performance computing center by an SME company for the optimization of an engineering design with an augmented open source simulation-optimization framework.

6. References

Adams, B. M., Bohnhoff, W. J., Dalbey, K. R., Ebeida, M. S., Eddy, J. P., Eldred, M. S., ... & Winokur, J. G. 2019. DAKOTA, a multilevel parallel object-oriented framework for design optimization, parameter estimation, uncertainty quantification, and sensitivity analysis: version 6.11 user's manual. *Sandia National Laboratories, Tech. Rep. SAND2010-2183*. https://dakota.sandia.gov/content/manuals.

Aral, M. M., and Demirel, E. 2017. "Novel Slot-Baffle Design to Improve Mixing Efficiency and Reduce Cost of Disinfection in Drinking Water Treatment. " *Journal of Environmental Engineering (United States)* 143 (9): 1–5. https://doi.org/10.1061/(ASCE)EE.1943-7870.0001266.

Aral, M. M. and Demirel, E. 2019. “Baffle Design to Improve Mixing and Reduce the Flow Through Energy Requirements in Chlorine and Ozone Contact Tanks,” USA Patent and Trademark Office, USA Patent # 62/498,260, USA and EUROPEAN Union.

Danckwerts, P. V. 1953. "Continuous flow systems: distribution of residence times." *Chemical engineering science* 2 (1): 1-13. https://doi.org/10.1016/0009-2509(53)80001-1.

Demirel, E. and Aral M. M. 2018a. “An Efficient Contact Tank Design for Potable Water Treatment.” *Teknik Dergi/Technical Journal of Turkish Chamber of Civil Engineers* 29 (2): 8279–94. https://doi.org/10.18400/tekderg.322491.

Demirel, Ender, and Mustafa M. Aral. 2018b. “Performance of Efficiency Indexes for Contact Tanks.” *Journal of Environmental Engineering* 144 (9), 04018076. https://doi.org/10.1061/(asce)ee.1943-7870.0001431.

Fletcher, Reeves, and Colin M. Reeves. 1964. "Function minimization by conjugate gradients." *The Computer Journal* 7 (2): 149-154. https://doi.org/10.1093/comjnl/7.2.149

Hestenes, M. R., and Stiefel, E. 1952. *Methods of conjugate gradients for solving linear systems*. Vol. 49. No. 1. Washington, DC: NBS.

Kuzay, M., Nasyrlayev, N. ve Demirel, E. (2021). Simulation-Optimization of a Patented Baffle Design with Parallel Computing on TRUBA. doi:10.48623/aperta.227987

Launder, B.E., Spalding, D.B., 1974, “The numerical computation of turbulent flows.” *Comput.Methods in Appl.Mech.Eng.* 3 (2): 269-289. https://doi.org/10.1016/0045-7825(74)90029-2.

OpenFOAM, 2015. *The OpenFOAM Foundation*; OpenCFD Ltd., Bracknell, UK.

Teixeira, E.D. and Siqueira, R.N. 2008. "Performance assessment of hydraulic efficiency indexes." *Journal of Environmental Engineering* 134 (10): 851-859. https://doi.org/10.1061/(ASCE)0733-9372(2008)134:10(851).

Trucano, T.G., Swiler, L.P., Igusa, T., Oberkampf, W.L. and Pilch, M. 2006. “Dakota: User Manual.” *Reliability Engineering & System Safety* 91 (10–11): 1331–57.

http://linkinghub.elsevier.com/retrieve/pii/S0951832005002437.

US EPA. 2003. "Disinfection Profiling and Benchmarking Technical Guidance Manual." *U.S. Epa*, 210.