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DESIGN OPTIMIZATION METHODOLOGY APPLIED TO A MIXER

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SUMMARY

The inverse design problem is the optimization of the design geometry to obtain functional performance which depends on this geometry. This work presents an integrated, highly systematic and generally applicable approach to the inverse design problem. In numerical terms the problem is formulated as the multi-dimensional maximization of a target function. This target function is defined as the numerical result of a decision making matrix consisting of a set of criteria, their weighting factors and a mark obtained for each criteria. In this paper the developed methodology is applied to the design of a straight blade turbine mixer centrally placed inside a cylindrical mixing vessel.

INTRODUCTION

Traditionally, design is governed exclusively by intuition, ingenuity and creativity of the engineer and therefore a good measure of arbitrariness and luck. This approach has yielded most of the ingenious and beneficial technical accomplishments to mankind and probably will continue to do so in the future. In no way shall this be belittled by the following praise and outline of a more methodological design approach nor shall it be denied that every design no matter how methodically conducted can only thrive on intuition, ingenuity and creativity.

However, it is desirable to work methodical wherever possible for the sake of

- transparency
- repeatability
- accountability

Seldom is a design problem posed in a straight forward manner, i.e. a geometry can be directly derived from the required functional behavior of the object. More likely it is posed as an inverted design problem where the functional behavior is dependent on the design geometry or more generally the choice of independent design variables, but the geometry can not be derived from the requirements. Further, no design of practical interest has to fulfill only a single requirement of its functional behavior and seldom are all requirements of equal importance. This type of problem is traditionally solved by trial and error, evolution and experience.

Designs that have to fulfill functional requirements and are related to fluid flow are particularly difficult because of the nonlinear behavior of the fluid mechanics equations.

Figure 1 shows the flow chart of an algorithm that was developed through strong inspiration by methods developed by Marshall et al., 1994. It tackles iteratively the task of optimizing the design.

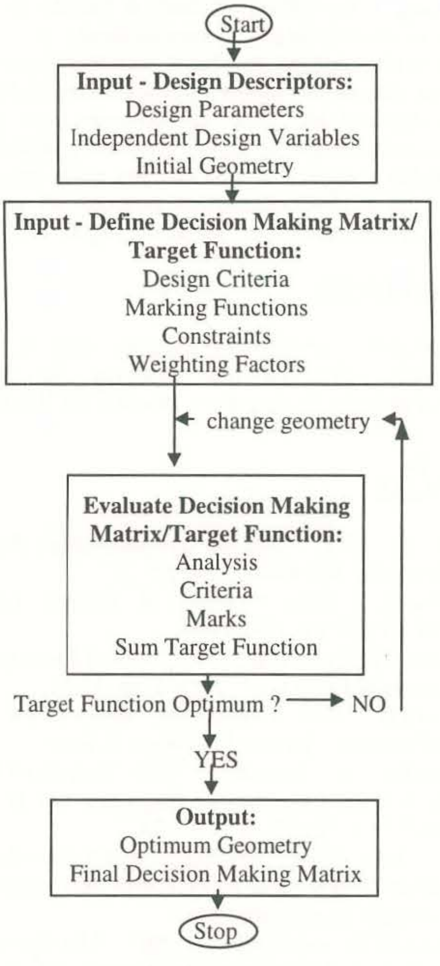

Figure 1 - Flow Chart for Design Optimization

DESCRIPTION OF OPTIMIZATION METHOD

If the goodness of a design can be expressed in a single number then the problem of finding the best design can be reduced to the optimization of a target function, F, which depends on a number of independent design variables, n_v.

$$F = F(x_1, x_2, \dots, x_{nv}) \quad (1)$$

The main task of the design optimization is to describe the formulation of a target function that takes account of the varied design requirements in a rigorous manner.

Definition of Design Descriptors. The first step in formulating the design problem is to establish a complete set of design variables and fixed parameters, the design descriptors, which describe the pertinent features of all possible solutions to the problem,. These may contain geometry, material, color, etc. Given the multitude of possible descriptors one must exercise restraint in only selecting those which significantly determine the function, e.g. where color may be a significant variable in determining the functional behavior of a solar collector it is probably less the case for a tool machine.

Further, since only the design variables determine the dimension of the optimization problem, and therefore its complexity, it is advisable to make as many descriptors into parameters as possible based on previous experience or simple analysis of the physics involved in the design.

Criteria and Constraints. The next step is to identify the criteria and constraints for the design, e.g. cost, safety, velocity, stress, efficiency, etc.

The criteria are the standards of judgment for the goodness of the design and must be phrased in a numerical fashion. They will determine which features of the design will be rewarded and which will be penalized. Not enough care can be taken with their selection, marking and weighting.

Constraints limit the possible design solution to a subset of the n_v-dimensional solution space.

Target Function. The target function is the combination of all the criteria established. Its evaluation can be seen as a weighted averaging process.

To evaluate the target function the marking functions as well as the weight factors of each criterion with respect to the others must be known. The value of the target function is a single number that expresses the goodness of one particular selection of design variables in the light of the identified criteria and constraints.

The evaluation of each criterion may require a conventional analysis or analysis by computerized methods, such as Finite Element Analysis (FEA) for stresses and natural frequencies, Computational Fluid Mechanics (CFD) for flow patterns, pressure drop or efficiency or computer based expert systems. This analysis is integral part of the optimization to avoid any need for intermediate user interfacing.

Optimization. For optimization of a multidimensional constraint problem a number of algorithms are available from mathematical software libraries. The algorithms suitable for this application have to make due without the explicit evaluation of the function gradient because it is generally not known.

Initially, a Direction Set Method was selected for this work. This method consists of sequential one-dimensional (1D) optimization in all n_v directions of the solution space of the target function. These directions of 1D optimization are selected such as to gain the largest progress to the maximum for the specific shape of function to be optimized (PRESS et al., 1992, ch 10.5)

To get started the algorithm needs an initial guess of the geometry and a set of basis vectors for the solution space. These are selected as the n_v unit vectors if no better information about the principal directions of the target function exists. In some cases this algorithm was not able to proceed to the (known) maximum of a target function without an initial guess very close to the actual maximum.

Therefore, the optimization method was changed to a Downhill Simplex Method (Press et al., 1992, ch 10.4). This method needs not only a single starting guess (a n_v-dimensional vector), but n_v+1 vertices, the corners of a n_v-dimensional simplex. This simplex is then reflected, stretched and contracted along the target function's topology to arrive at a maximum. This algorithm always proceeded robustly to the maximum of the target function regardless of the initial guess.

GOVERNING EQUATIONS FOR MIXER

The design optimization was carried out for a single turbine mixer of the flat blade turbine type revolving inside a cylindrical mixing tank. The geometry and nomenclature of this standard configuration is given in Figure 2.

This definition sketch serves to illustrate the geometrical design descriptors

DT	=	tank diameter [m]
DI	=	impeller diameter [m]
NB	=	number of turbine blades [m]
Q	=	height of turbine blades [m]
HI	=	height of impeller in tank [m]
HL	=	height of liquid in tank [m]

Further parameters describe the fluid type, in the simple case discussed in this work the density, ρ, and the kinematic viscosity, ν, of a Newtonian fluid.

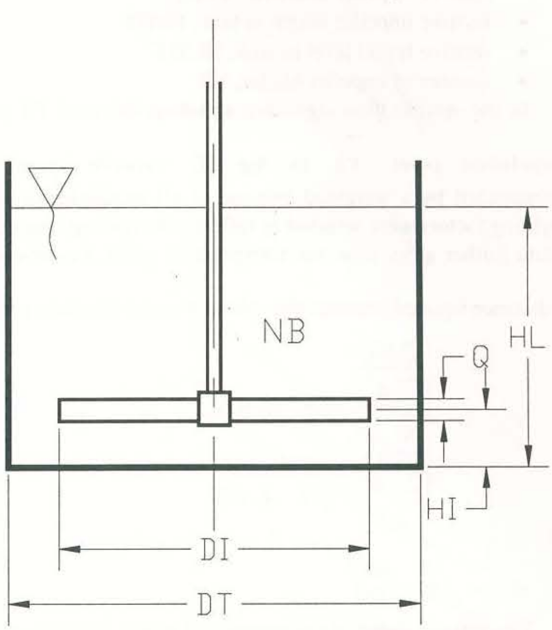

Figure 2 - Definition Sketch of Mixing Tank with Impeller

The first principal quantity of interest is the amount of power consumed by the mixing process. Dimensional analysis according to the Buckingham π-theorem (STERBACEK, 1965 or HOLLAND, 1966) yields a relationship between the non-dimensional numbers

- power number, $N_P = \dfrac{P}{\rho \cdot N^3 \cdot DI^5}$ (2)
- Reynolds number, $\mathrm{Re} = \dfrac{N \cdot DI^2}{\nu}$ (3)
- Froude number, $Fr = \dfrac{N^2 \cdot DI}{g}$ (4)

with

P	=	hydraulic power consumption [W]
N	=	speed of impeller rotation [rpm]
g	=	gravity acceleration [m/s²]

Generally, the power number depends on both the Froude and Reynolds numbers

$$N_P = N_P(\mathrm{Re}, Fr)$$

(5)

where the dependency on Froude number is merely due to the effect of vortexing of the fluid in the container which makes the mixing less efficient. The Froude number dependency of power consumption can be eliminated by placing suitable baffle plates on or near the wall of the container. The design of suitable baffle plates is considered a secondary design problem which can be solved independently of the principal design of the tank and impeller. Therefore, it shall not be subject to the further treatment of the design optimization and we obtain the relationship:

$$N_P = N_P(\mathrm{Re}) \tag{6}$$

This function, N_P can be approximated by the product of a geometry dependent factor, C1, and a normalized function, φ.

$$N_P = C1 \cdot \varphi(\mathrm{Re}) \tag{7}$$

The geometry factor, C1, the value of the power function at Re = 1, is tabulated by Sterbacek and Tausk, 1965 and Holland and Chapman, 1966 for a multitude of experimental results dependent on the following geometric variables:

- relative impeller height, Q/DI
- relative impeller diameter, DI/DT
- relative impeller height in tank, HI/DT
- relative liquid level in tank, HL/DT
- number of impeller blades, NB

In the optimization algorithm an interpolation of C1 at the interpolation point $\vec{x}_0$ in the 5D variable space was accomplished by a weighted average of all available data. The weighting factors were selected to reflect a decreasing importance of data further away from the interpolation point, i.e. inverse to the distance squared between the point $\vec{x}_0$ and this data point.

$$C_{10} = \begin{cases} \dfrac{\sum_{i=1}^{n} \frac{C_{1i}}{d_i^2}}{\sum_{i=1}^{n} \frac{1}{d_i^2}} & for \quad d_i \neq 0 \\ C_{1i} & for \quad d_i = 0 \end{cases} \tag{8}$$

with

$$d_i = |\vec{x}_i - \vec{x}_0|$$

The general shape of the normalized power function, φ, can be described by

$$\varphi(\mathrm{Re}) = \begin{cases} 1 \cdot \mathrm{Re}^{-1} & for \quad \mathrm{Re} < 10 \\ 0.214 \cdot \mathrm{Re}^{-0.331} & for \quad 10 \le \mathrm{Re} < 100 \\ 0.040 \cdot \mathrm{Re}^{0.036} & for \quad 100 \le \mathrm{Re} < 1000 \\ 0.013 \cdot \mathrm{Re}^{0.198} & for \quad 1000 \le \mathrm{Re} < 10000 \\ 0.080 & for \quad 10000 \le \mathrm{Re} \end{cases} \tag{9}$$

The second quantity that is important to know in the mixing process is the time required to obtain a mixed solution. Khang and Levenspiel, 1976 presents results for Re > 10000 and determines the mixing time by observing the decay of the amplitude of concentration of a solution that is admixed into a tank.

Figure 3 shows the general shape of φ as well as the mixing rate number, Mx.

- mixing rate number,

$$Mx = \frac{N}{K} \cdot \left(\frac{DI}{DT}\right)^{2.3} \tag{10}$$

with

K = decay exponent [1/s]

The decay exponent, K, describes the exponential decay over time of the concentration amplitude that a sensor measures if placed at a fixed location in the tank during progressive mixing.

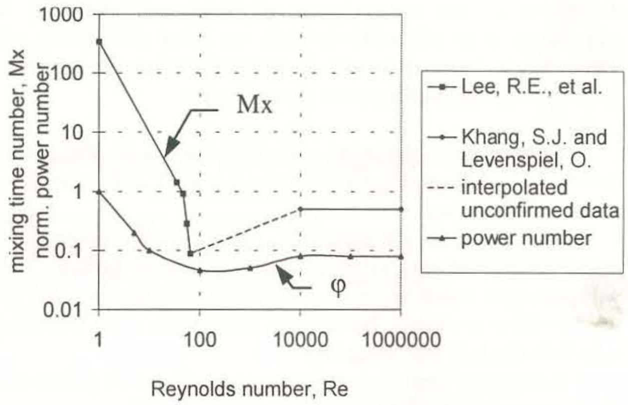

Figure 3 - Normalized Power Function and Mixing Rate Number for Flat Blade Turbine Mixer

It relates the time and remaining concentration fluctuation after addition of a substance of concentration 1 by

$$A = 2 \cdot e^{-K \cdot t_m} \tag{11}$$

with

A = final value of fluctuation amplitude [-]

t_m = mixing time [s]

Lee et al., 1957 used in their experimental investigations of mixing time a visual observation of dye dispersion. The Reynolds number range covered is Re < 65. To make the experimental results comparable to the ones by Khang and Levenspiel, 1976 the final amplitude, A, that is comparable to a completely mixed dye solution (by visual inspection) is considered to be 1%. This makes the equivalent decay exponent

$$K = \frac{-\ln(0.5\%)}{t_m} \tag{12}$$

and data from both publications can be plotted on the same scale as seen in Figure 3.

By interpolation between the known data the relationship of mixing time with the Reynolds number is given by

$$Mx(\mathrm{Re}) = \begin{cases} 340 \cdot \mathrm{Re}^{-1.54} & for \quad \mathrm{Re} < 46.5 \\ 4.34 \cdot 10^{11} \cdot \mathrm{Re}^{-7.0} & for \quad 46.5 \le \mathrm{Re} < 65 \\ 0.021 \cdot \mathrm{Re}^{0.343} & for \quad 65 \le \mathrm{Re} < 10000 \\ 0.5 & for \quad 10000 \le \mathrm{Re} \end{cases} \tag{13}$$

APPLICATION OF DESIGN OPTIMIZATION METHODOLOGY TO MIXER

Two-Dimensional Design Problem. The first application of the design methodology shall be the optimization of only impeller diameter, DI, and speed, N, for an otherwise fixed mixer configuration. This 2D design problem allows a graphical representation of the target function and therefore a check on the optimization algorithm.

The fixed parameters of a given container and fluid were selected to be

- tank diameter, DT = 0.1 m
- number of mixer blades, NB = 6
- impeller position, HI/DT = 0.33
- impeller blade height, Q/DI = 0.25
- liquid level, HL/DT = 1.0
- fluid: water, $\rho = 1000\ \mathrm{kg/m^3}$, $\nu = 1.e\text{-}6\ \mathrm{m^2/s}$

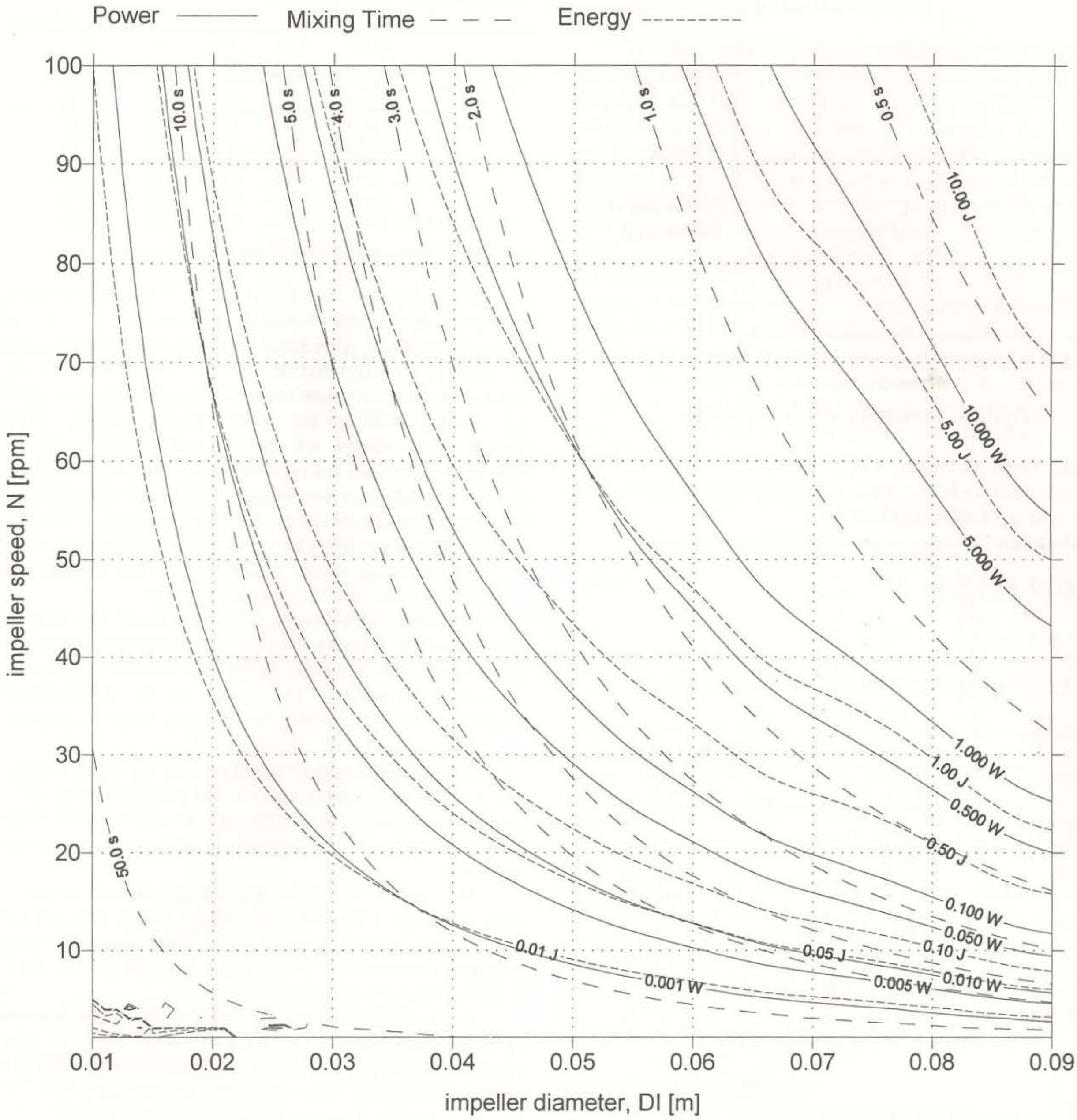

Figure 4 - Lines of Equal Power, Mixing Time and Energy Consumption in 2D Design Problem

Figure 4 shows the lines of equal power mixing time and energy consumption, in the 2D solution space that is bounded by the constraints on the mixer impeller to be between 10% and 90% of the tank diameter.

To define the target function the criteria were selected as

- mixing time to obtain a completely mixed solution
- energy, E, consumed during this time with

$$E \;=\; t_m \cdot P \tag{14}$$

For the marking scheme a scale of one to 10 was selected. The following marking functions, M_1 and M_2, are designed to translate the values of the criteria into marks that reflect the desired behavior of the mixer. Clearly it is desirable to have both , short mixing time and low energy consumption. Therefore, both marking functions display a negative slope.

To mark the mixing time criterion it is assumed that the mixture consists of reactive components whose individual stability is such that only within the critical time t_0 a reaction can take place and thereafter no benefit results from further mixing. Therefore the marking function reaches the zero mark at t_0 with no marks gained for longer mixing time.

$$M_1(t_m) \;=\; \begin{cases} 10 - \dfrac{10}{t_0} \cdot t_m & for \quad t_m < t_0 \\ 0 \quad for \quad t_m \geq t_o \end{cases} \tag{15}$$

The energy consumption on the other hand yields ever lower marks with higher consumption asymptotically approaching zero while at very low energy levels, lower than E_0, the benefit of even lower energy consumption is insignificant and does not earn higher marks

$$M_2(E) \;=\; \begin{cases} 10 \quad for \quad E < E_0 \\ 10 \cdot E_0 / E \quad for \quad E \geq E_0 \end{cases} \tag{16}$$

Figure 5 shows the graph of the two marking function for

- critical time, $t_0 = 5$ s
- energy threshold, $E_0 = 5$ J

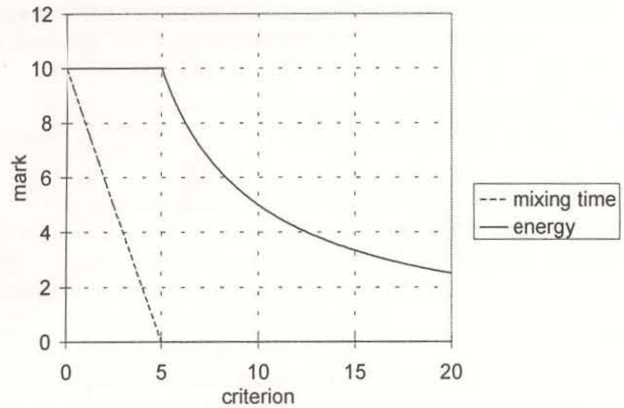

Figure 5 - Marking Functions, M_1 and M_2

The weighting factors, WF_1 and WF_2, were in this example selected as unity for both criteria, expressing equal importance of mixing time and energy consumption.

The target function, F, is now defined as

$$F(DI,N)=\sum_{i=1}^{n_c} M_i \cdot WF_i \tag{17}$$

with

n_c = number of criteria

Figure 6, displays the contour plot of the target function, F.

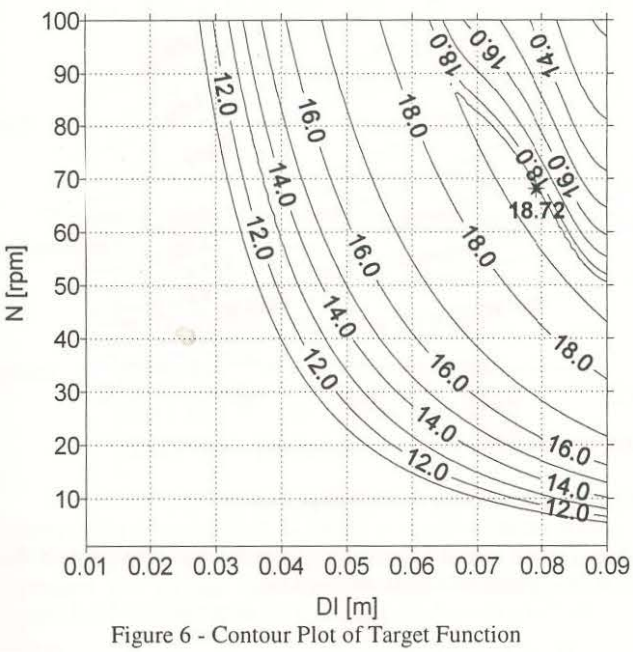

Figure 6 - Contour Plot of Target Function

It can be seen in Figure 6 that the unconstrained target function shows a maximum at

- DI = 7.93 cm
- N = 67.6 rpm

Depending on the required accuracy and the initial guess it takes different computational effort, i.e. number of evaluations of the target function, ITER. The existing maximum was reached regardless of the initial guess with only marginal influence on the computational effort. For an initial master vertex developed from the point 3.0 cm, 70.0 rpm the influence of the tolerance requirement for the incremental function value, FTOL, on the computational effort is summarized in Table 1.

Table 1 - 2D Design Optimization

	FTOL	ITER	DI [cm]	N [rpm]	F
unconstrained	1%	15	7.25	76.0	18.604
	0.1%	31	7.81	69.1	18.706
	0.01%	48	7.87	68.6	18.722
	0.001%	64	7.92	67.8	18.724
	10^{-6}	121	7.93	67.6	18.724
	10^{-8}	131	7.93	67.6	18.724
P < 5 W	0.01%	48	7.95	57.8	18.516
P < 5 W and N > 60 rpm	0.01%	67	7.80	60.3	18.515

It can be seen that the number of function evaluations increases significantly with an increase in the tolerance requirement. On the other hand, the return on the improvement in the value of the target function and the variables diminishes. A reasonable tolerance requirement was considered to be 0.01%.

Having solved the unconstrained design problem (unconstrained except for the geometry requirement of an impeller smaller than the tank diameter) we can proceed to ask the question what the best design according to our criteria is if the largest available drive can deliver a maximum of 5 W to the mixer. Table 1 also shows the results for the constrained cases. In the power constrained case we fill find the best combination of diameter and speed at 7.95 cm and 57.8 rpm.

Additional constraints can be introduced. For example if the minimal drive speed due to transmission restrictions is 60 rpm we will find the best impeller diameter at 7.80 cm and 60.3 rpm

An observation in this context is that the presence of constraints also increases the computational effort significantly.

Multi-Dimensional Design Problem. Up to this point the real power of this methodology has not presented itself very well because we could have gained all the insight about optimum design without ever bothering to device an optimization algorithm.

This notion will falter immediately when we enter the multi-dimensional solution space. Where are the hills and valleys of the target function topology in n_v dimensions? The tools of graphical representation of the target function will not have the power to solve this question for us.

So the further discussion shall treat the optimization of an open flat blade turbine mixer for a volume of water of 7.85398 liters (incidentally the same volume as in the 2D example to have a point of reference). The six relevant variables are then

- impeller diameter, DI [m]
- impeller speed, N [rpm]
- number of blades, NB [-]
- relative impeller height in container, HI/DT [-]
- relative impeller blade height, Q/DI [-]
- relative liquid height in container, HL/DT [-]

The impeller and tank diameter and the impeller speed influence directly the power, energy and mixing time criteria. The other variables only enter the power and energy criterion via the geometry factor C1. This makes for a group of variables with strong and another group with weak influence on the target function. Therefore, we will tackle the problem cautiously with an intermediate step at the 3D design problem with DI, N and DT as variables. Table 2 summarizes the optimization results.

Following the same strategy as outlined on the 2D problem, i.e. starting from an initial guess of 3.0 cm and 70 rpm at a relative liquid height of 1.0 we go through a sequence of tougher and tougher tolerance requirements to assure a stable target function maximum. As a second check we start the search for the maximum from this just found maximum and confirm it is there, at impeller diameter 8.94 cm, 58.7 rpm and a liquid level of 1.07. Further, the target function has a higher value than what we obtained in the 2D case, i.e. we found a better solution.

All this indicates that we could be satisfied and implement our optimized design.

Table 2 - 3D Design Optimization

	FTOL	ITER	DI [cm]	N [rpm]	HL/ DT	F
initial			3.00	70.0	1.00	
final	1%	26	8.52	58.7	1.07	18.871
initial			3.00	70.0	1.00	
final	0.01%	75	8.92	58.9	1.03	18.904
initial			3.00	70.0	1.00	
final	10^{-6}	145	8.94	58.9	1.02	18.905
initial			3.00	70.0	1.00	
final	10^{-8}	181	8.94	58.9	1.02	18.905
initial			8.94	58.9	1.02	
final	10^{-6}	131	8.94	58.9	1.02	18.905

However, thinking smarter we can also use the insight we gained on the 2D design and start the search from an initial vertex at the 2D optimum. Table 3 shows the sequence of using the found solution as the new initial vertex and progress in this manner to another stable maximum. All we can do at this point is note that the target function at this maximum at impeller diameter 7.27 cm, 107 rpm and a liquid level of 1.90 has a higher target function value than the previous found which makes that maximum only a local one.

Further quest into solution space starting from 500 rpm yields a maximum at 473 rpm which proves not to be stable by the restart from itself, but converges onto the previously found absolute maximum.

Table 3 - 3D Design Optimization

	FTOL	ITER	DI [cm]	N [rpm]	HL/ DT	F
initial			7.93	67.6	1.00	
final	10^{-6}	197	7.27	82.3	1.90	19.217
initial			7.27	82.3	1.90	
final	10^{-6}	130	7.27	107	1.90	19.397
initial			7.27	107	1.90	
final	10^{-6}	160	7.27	107	1.90	19.397
initial			3.00	500	1.00	
final	10^{-6}	157	2.43	473	1.90	18.307
initial			2.43	473	1.90	
final	10^{-6}	407	7.27	107	1.90	19.397

Having probed the solution space from various locations we conclude that the global maximum is probably at

- impeller diameter, DI = 7.27 cm
- impeller speed, N = 107 rpm
- relative liquid level, HL/DT = 1.90

However, we can not be absolutely sure about this since we do not have comprehensive knowledge about the topology of the target function in the 3D solution space. This means that the art of optimization in multi-dimensional solution space finds itself a bit probing in the dark and has to rely on good engineering judgment and a bit of luck.

This is even more the case now, that we introduce the remaining three variables and optimize the 6D design problem. Table 4 shows a sample solution output for the optimized design after having followed a strategy as described for the 3D optimization of increased tolerance refinement and restart on earlier found solutions.

The found 6D solution again improves the target function value slightly and therefore provides a better solution than the 3D solution.

CONCLUSIONS AND FUTURE WORK

In this work a design optimization algorithm was developed. With the use of numerical analysis tools criteria were evaluated and then summed up according to their individual value to the design, expressed in a marking function and weighting factor. The resulting target function, representing the goodness of the design according to the specified criteria, was then maximized using a simplex downhill optimization algorithm. This methodology was successfully applied to the design of an open straight blade turbine mixer centrally mounted in a cylindrical vessel. In this application no advanced numerical simulation was employed, but existing experimental results were interpolated to find values for the criteria of power, energy and mixing time. It certainly is an area of expansion of the algorithm to include numerical simulation, in particular Computational Fluid Dynamics (CFD) of the mixing process. Other expansions may include a variety of mixer types and a wider range of design variables.

Table 4 - 6D Design Optimization

	DI (m)	N(rpm)	NB	HI/ DT	HL/DT	F
initial	.07260	107	3.00	.33	1.90	19.396
final	.07260	109.1	3.00	.2814	1.89	19.408
initial	.07260	107	3.00	.33	1.90	19.151
final	.06260	109.1	3.00	.2844	1.89	19.408
initial	.07260	109	3.00	.33	1.90	19.407
final	.07260	109.1	3.00	.2906	1.89	19.408
initial	.07260	107	3.00	.33	1.90	19.396
final	.07260	109.1	3.00	.2789	1.89	18.408
initial	.07260	107	4.00	.43	1.90	19.396
final	.07260	109.1	3.00	.2825	1.89	19.408
initial	.07260	107	3.00	.33	1.90	19.396
final	.07260	109.1	3.00	.2858	1.89	19.408
initial	.07260	107	3.00	.33	1.80	19.370
final	.07260	109.1	3.00	.2855	1.89	19.408

Formulation of the design problem led to a 6D optimization problem which was solved by a strategy of successive optimization of the 2D and 3D subspace. The effects of design constraints were presented for the 2D case only.

However, in this type of optimization where the topology of the target function is unknown it will always remain uncertain if the found optimum is truly a global one or only local.

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REFERENCES

Lee, R.E., Finch, C.R., and Woodledge, J.D. 1957 "Mixing of High Viscosity Newtonian and Non-Newtonian Fluids", Ind.and Eng. Chemistry, vol 49, 11, pp 1849-1854,

Sterbacek, Z., Tausk, P. 1965 "Mixing in the Chemical Industry", Pergamon Press, Oxford.

Holland, F.A., and Chapman, F.S. 1966 "Liquid Mixing and Processing in StirredTanks", Reinhold Publishing Co. NY.

Khang, S.J., and Levenspiel, O. 1976 "The Mixing-Rate Number for Agitator Stirred Tanks", Chemical Eng. pp 141-143.

Press, W.H., Teukolsky, S.A., Vetterling, W.T., and Flannery, B.P. 1992 "Numerical Recipes in FORTRAN", Sec Ed, Cambridge University Press.

Marshall, R., Hudspith, R.C. and MacHattie, D. 1994 "Engineering Design and Communication", unpublished lecture notes, McMaster University, Hamilton, Canada.