Numerical Method for Optimizing Stirrer Configurations

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Abstract

A numerical approach for the numerical optimization of stirrer configurations is presented. The methodology is based on a parametrized grid generator, a flow solver, and a mathematical optimization tool, which are integrated into an automated procedure. The flow solver is based on the discretization of the Navier-Stokes equations by means of the finite-volume method for block-structured, boundary-fitted grids with multi-grid acceleration and parallelization by grid partitioning. The optimization tool is an implementation of a trust region based derivative-free method. It is designed to minimize smooth functions whose evaluations are considered expensive and whose derivatives are not available or not desirable to approximate. An exemplary application illustrates the functionality and the properties of the proposed method.

Key words: Stirrer, numerical optimization, derivative-free optimization, computational fluid dynamics, parallel computing.

1 Introduction

The mixing of different substances with stirrers is a process that is frequently used in many industries such as chemical, pharmaceutical, biotechnological,

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and food processing. In chemical industry, for example, very often one is faced with the problem of mixing reacting substances as fast as possible in order to achieve an efficient reaction. In this case a stirrer is needed which produces a highly turbulent flow to achieve a sufficient segregation in order to minimize the mass and energy transport limitation for the chemical reaction. On the other hand, in biochemistry it is often necessary to suspend microorganisms in bioreactors. This has to be done very carefully without exposing the microorganism to high shear rates that can lead to the destruction of the cells.

Besides the mixing properties, important economic issues for the stirring process is the minimization of the amount of energy needed for the creation of certain mixing conditions, the material costs for the stirrer, as well as the lifetime and the breakdown security of the system. The above aspects strongly depend on the various geometrical parameters of the stirrer and the vessel as well as on the rotation rate and the fluid properties.

The variety of mixing tasks has led to a tremendous number of different types of stirrers (and vessels) which are in use nowadays. Due to the variety of influence factors it is very difficult to select or design a "good" stirrer for a specific process with respect to the criteria indicated above. For this, experimental investigations usually are very costly and time consuming. Here, the numerical investigation of the flow in a stirrer system together with mathematical optimization methods can be a very useful tool, which can offer new possibilities for a higher product quality, a reduction of costs, and a lowering of energy consumption.

Numerical simulation techniques provide a great flexibility concerning geometrical parameter variations. To employ such techniques for optimization purposes an integrated approach combining geometry variation, flow simulation, and mathematical optimization is desirable. In the present work a corresponding methodology is presented, which is based on developments in [1].

While for structural mechanics applications such approaches have been investigated and applied quite frequently (usually within the framework of the finite-element method), their application for general fluid mechanics problems up to now remained comparatively limited. Of course, this is mainly due to the fact that already the reliable simulation of a single flow configuration often can be a rather difficult task requiring a significant amount of computational resources. This, in particular, applies to stirring processes. Complex geometries (see Fig. 1 for an example) and complex interacting phenomena including turbulence, chemical reactions, heat transfer, or mass transfer make the simulations highly pretentious to the underlying computational methods. Often for a single simulation run many systems of equations each with millions of unknowns have to be solved.

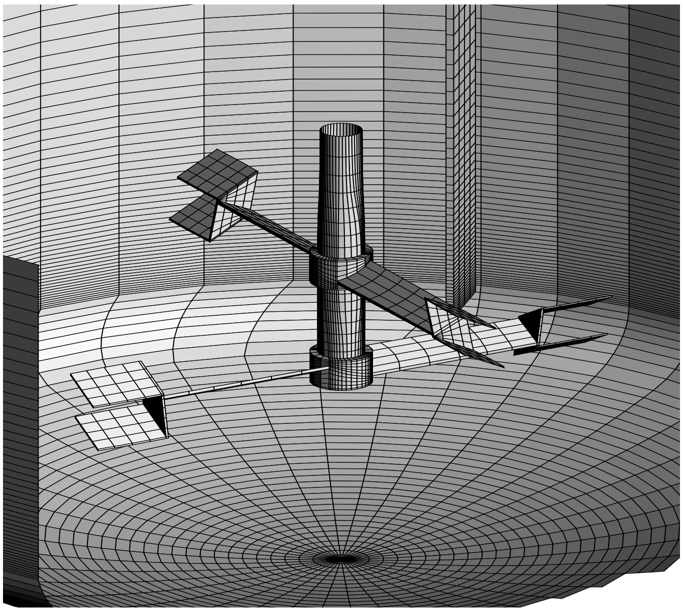

Fig. 1. Example of complex stirrer geometry (intermig).

Thus, the simulations carried out so far in industrial practice are performed mainly in order to understand the flow behavior in a specific stirrer in order to conclude possibilities for an improvement of the configuration, but not for a systematic optimization requiring many runs with different parameter sets. Here, high-performance computing techniques with advanced numerical methods and parallel computers provide new possibilities making multiple runs within an optimization method feasible.

The major components of the proposed numerical optimization tool are:

- a specially designed parameterized grid generator for stirrer geometries,
- an efficient parallel multigrid flow solver,
- a derivative-free optimization method.

The grid generator allows the parametrized generation of block-structured grids for stirrer geometries, which, for instance, can vary in number, size and form of impeller blades or in form of vessels. Due to the parametrization, modifications of grids, which are necessary when applying an optimization tool searching for an optimized geometry, are easily possible. The flow solver is based on a fully conservative finite-volume method for non-orthogonal boundary-fitted block-structured grid, allowing a flexible discretization of even very complex stirrer geometries. The discrete systems are solved in each (implicit) time step by a nonlinear multigrid method with a pressure-correction smoother. For the parallelization a block-structured grid partitioning method with automatic load balancing and strongly implicit block coupling is used. The grid movement of the stirrer grid as against the vessel is handled by a clicking mesh approach. The solver already was applied in the past for a variety of different problems in stirrer technology and has proven that it can compute complex problems on parallel computers with high numerical and parallel efficiency (e.g. [2,3]).

Concerning numerical optimization of fluid flows, by far the most work can be found in the field of aerodynamics. An overview to the subject is given by Mohammadi and Pironneau [4]. For general fluid flow applications the resulting nonlinear optimization problems typically are solved by employing descent algorithms based on gradient information (e.g. [5–7]). However, the computation of the gradient of the objective function with respect to the design variables is usually very laborious and error-prone, e.g. when using a sensitivity analysis. Here, gradient-free methods may offer advantages. To this respect, there are also works applying genetic and evolutionary algorithms either directly (e.g. [8–10]) or in combination with gradient-based methods (e.g. [11]), but we will not follow this direction here. The optimization tool we employ here is the DFO package developed by Conn and co-workers (see [12–14]. The method is based on a derivative-free trust region method approximating the objective function by a second-order polynomial, which is then minimized by a sequential quadratic programming (SQP) method.

After introducing the individual components of the procedure and describing their integration we consider a representative test case to illustrate the capabilities of the approach.

2 Basic Numerical Concepts

In the following sections, after briefly introducing the flow model considered, we give a short description of the employed numerical tools (detailed information can be found in the corresponding references). Then the coupling of the components within a control program, which acts as master process, is discussed.

2.1 Governing Equations of Fluid Dynamics

We consider the flow of an incompressible Newtonian fluid in an arbitrary domain, which is described by the well-known Navier-Stokes equations:

$$\begin{aligned} \frac{\partial u_i}{\partial x_i} &= 0 \,, \\ \frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_j u_i)}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial p}{\partial x_i} &= \rho f_i \,, \end{aligned} \tag{1}$$

where u_i are the velocity vector components with respect to the Cartesian coordinates x_i, t is the time, p is the pressure, ρ is the fluid density, and f_i are the components of the vector of external forces. The viscous part of the stress tensor τ_{ij} for incompressible Newtonian fluids is given by

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{2}$$

with the dynamic viscosity μ. If further transport processes are involved into the problem, e.g. heat or mass transfer, additional balance equations of the form

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho v_i \phi)}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial \phi}{\partial x_i} \right) = \rho g \, . \tag{3}$$

have to be solved. Here, ϕ is the transported quantity, e.g. the temperature or species concentrations, α is a diffusive coefficient, and g are external sources.

We restrict ourselves here to stirrers working in the laminar regime, since the specific problems related to turbulence are not in the focus of the present work. However, the generalization of our considerations to turbulent flows is straightforward by replacing the above Navier-Stokes equations by their Reynolds-averaged counterpart together with some appropriate statistical turbulence model (e.g. [15]). In principle, large eddy simulation techniques, which recently also found application to stirrer flows (see e.g. [16]), can be employed as well, however, at the cost of a significant higher computational effort.

2.2 Grid Generation Tool

The grid generation tool involves an algebraic method based on transfinite interpolation for the generation of multi-block boundary-fitted grids, which facilitates the accurate representation of the complex geometries associated with stirrer configurations. It includes a built-in library of impellers commonly used in the chemical and process industries (e.g. blade, propeller, anchor, horseshoe, helix, and intermig stirrers) and, in principle, allows for any combination of impeller, baffle, and vessel geometries.

In order to allow an easy design variation, the grid generation is parametrized with respect to the characteristic geometric quantities for the different stirrer types. Thus, the input parameters are radii of hub, shaft, disk, vessel or numbers and dimensions of blades, baffles and so on. Additionally specifying the number of control volumes for different stirrer sections the grid then is created automatically by respecting basic criteria with respect to grid quality, i.e. skewness, aspect ratio, and expansion factor (see e.g. [17]), as far as possible. Following this concept the geometrical input parameters directly can be used in an easy way as design parameters for the optimization purpose.

2.3 Numerical treatment of the flow problem

Within the optimization procedure a relatively large number of individual flow simulations may be necessary and the geometry variations may lead to "nasty" grids. Thus, important prerequisites for the flow solver are its numerical efficiency and robustness, in particular, also in situations when the grid is distorted.

We employ here a finite-volume solver which specially takes into account the above aspects. It is based on a fully conservative finite-volume scheme for general non-orthogonal block-structured grids, which is described in detail, for instance, in [17]. A special interpolation is employed for approximating cell face values by nodal values within the finite-volume discretization proposed in [18]. This is based on a multi-dimensional Taylor series expansion and ensures second-order spatial accuracy regardless on the grid distortion. The pressure-velocity coupling is established by using a pressure-correction technique of SIMPLE type (see [19]). Also here, a special variant is employed (see [20], which, in particular, is characterized by good robustness properties also for highly skewed grids). To solve the various sparse linear systems within the pressure-correction scheme an iterative ILU decomposition following Stone [21] is used. For convergence acceleration a nonlinear multi-grid scheme is implemented [22], which has proven its high numerical efficiency for many applications (e.g. [23–28]). The overall solution procedure is also applicable on a multi-processor architecture by means of a block-structured grid partitioning technique [29].

The rotation of the stirrer is handled with the clicking mesh technique, which is described in detail in [30]. Here, the basic idea is to compute parts of the grid related to the impeller and the vessel in a rotating and stationary frame of reference, respectively, accompanied by an data transfer via a corresponding coordinate transformation at the interface of the two grid parts.

2.4 Numerical principles of the optimization tool

In general, a nonlinear optimization problem with possible nonlinear constraints formally can be written as:

$$\begin{aligned} & \min f(\alpha) \\ \text{subjected to} \quad & \alpha_i^l \leq \alpha_i \leq \alpha_i^r \ , \quad i = 1, ..., N \ , \\ & g_j(\alpha) \geq 0 \ , \quad j = 1, ..., J \ , \\ & h_k(\alpha) = 0 \ , \quad k = 1, ..., K \ , \end{aligned} \tag{4}$$

where f is the objective function to be minimized, $\alpha = (\alpha_1, \cdots \alpha_n)$ denotes the vector of the N design variables (restricted to the intervals $[\alpha_i^l, \alpha_i^r]$), g_j are J equality constraints, and h_k are K non-equality constraints. In our context of stirrer applications, the objective function may correspond to the Newton number, mixing time, stresses, etc., which are derived from the flow field. The design variables can be quantities determining the stirrer geometry or operating parameters like the rotational speed. Constraints can be restrictions of the stirrer geometry, of operational parameters, or of other quantities depending on the flow field (e.g. minimum value of mixing time). The most frequently encountered constraints are are simple bounds on the variables $\alpha_i^l \leq \alpha_i \leq \alpha_i^r$ which are called as 'easy' or 'box' constraints, which re also used in the stirrer configuration.

To solve problem (4) we employ the optimization package DFO which is based on developments described in [12–14]. The basic idea of this approach is to construct a multivariable derivative free optimization algorithm that uses a surrogate model for the objective function f within a trust region method. In DFO the points are sampled to obtain a well-poised interpolation set and to build a well-defined interpolation model. This interpolation model is achieved by using the Newton fundamental polynomials and is at least a linear one to guarantee the local convergence, although the aim is to build a quadratic model for the objective function. For a detailed description of the DFO algorithm, and in general derivative free optimization, readers are encouraged to see [12–14] and the references therein.

The main benefit of this approach is that the local gradient of f with respect to the design variables, which is not directly available for the complex discrete Navier-Stokes system, does not have to be provided by the flow solver. However, the character of this approach is still similar to the frequently applied gradient based optimization algorithms, since the solution space is evaluated on a path rather then the entire space using an incomplete set of interpolation points. Moreover, because the termination criteria used in derivative free algorithms are not based on the gradient and the stationary points of the objective function these methods are often more likely to obtain a global rather than locally optimal solutions. Since no rigorous convergence properties for globally optimal solutions have yet been discovered, the optimal solutions presented in this work should be considered locally. However, it is always possible to search for a better local optimum, for instance in cases where simple geometries are concerned, can be carried out by giving a set of initial solutions to the derivative free optimization algorithm.

DFO was successfully applied as a black-box optimization routine in optimizing energy systems [31] and for the helicopter rotor blade design [32], where some practical aspects of DFO were described. Numerical tests in both papers show that DFO works faster and more accurate than the derivative based methods like the Quasi-Newton to find an optimum solution in those kind of problems with noisy function evaluations.

The essential elements of DFO are:

- Building either at least a linear model using $n+1$ interpolation points or at most a quadratic model with $(n+1)(n+2)/2$ interpolation points based on Newton's fundamental polynomials.
- The model is then minimized not over the whole feasible region but over the trust region (an n-dimensional ellipsoid around the current iterate) subject to the constraints (or models of the constraints) intersected with the feasible set. If, however, the trust region is infeasible then an exact penalty function incorporating the model is used. The minimization of the possibly quadratic model is done by applying a standard optimization procedure, i.e. a sequential quadratic programming (SQP) method (e.g. [33]) and in our case, an interface to IPOPT [34], which is also provided by the DFO package, is used. After computing the optimal point, the achieved reduction in the objective function is compared to the reduction obtained by the model.
- The next step is the updating of interpolation points which is the most critical part. If the reduction of the objective function compared to the reduction of the model is good enough, this point will be included in the interpolation set, otherwise a new point is added to the interpolation set which will improve the approximation model. Interpolation points far from the current iterate are removed from the interpolation set. Usually one wants to use as many as possible interpolation points at which functions values are known referred as sample points. Not all new points are taken in the interpolation set, they have to satisfy some geometric requirements, the so called 'well-poisedness' [12,32,31] because of non-uniqueness of quadratic interpolation polynomial.
- After evaluation of the true objective function value and depending on the quality of the optimization of the model either the new point is accepted and the trust region radius is increased or rejected and the trust region radius is decreased.

The DFO uses for the minimization of the quadratic model the smallest Frobenius norm. Minimal trust region radius of size $\Delta_{\min}$ is used as stopping criteria. $\Delta_{\min}$ varies between $10^{-3} - 10^{-5}$ depending on the number of parameters and accuracy requirements.

DFO is available as an open source code and designed so that all the parameters can be tuned according to user requirements.

2.5 Control Program

The components described in the preceding sections are combined within an integrated optimization tool by means of a control script (following [1]), which is illustrated schematically in Fig. 2. After the initializations the procedure involves the following major steps:

(1) *Optimizer:* The optimizer is started and computes a new set of design variables. Afterwards it turns into a waiting state.
(2) *Grid variation:* Getting the signal that the new design variables are available, the grid generation tool becomes active and creates the new geometry and the corresponding numerical grid.
(3) *Flow simulation:* Getting the signal that the new grid is available, the flow solver computes the flow field and the corresponding objective function for the new geometry. As starting value the solution from the previous simulation is used.
(4) *Test of flow solver convergence:* If the flow solver is converged, the optimizer gets a signal to continue. It may happen that the flow solver does not converge. Then another run with more "conservative" numerical parameters, i.e. reduced relaxation factors, is started. If this also fails, corresponding set of design variables is excluded.
(5) *Test of optimizer convergence:* The optimizer decides by a given criterion, if the current value of the objective function is accepted as optimum. If yes, the procedure is finished, if not, the procedure is continued with step (1).

Note also the modularity of the approach, which makes it straightforward to modify or replace individual components of the procedure.

3 Exemplary Results

In the following we consider a Rushton turbine as a representative test case for a practical stirrer configuration to illustrate the functionality of the proposed approach. Prior to the optimization task, at first, computations for validation are carried out.

3.1 Stirrer Configuration

A schematic sketch of the considered stirrer configuration is shown in Fig. 3. The system consists of a flat bottomed cylindrical vessel with diameter T and

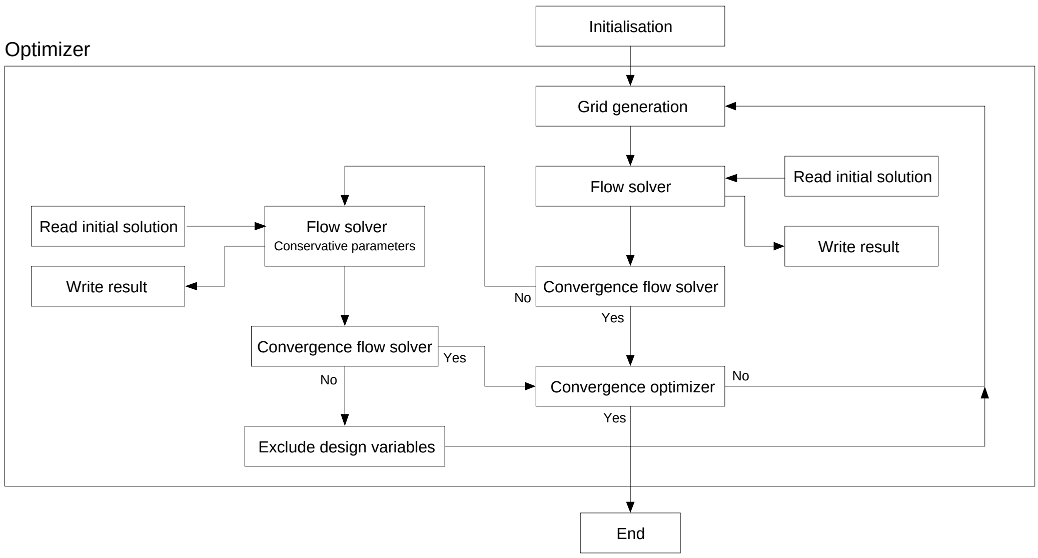

Fig. 2. Flow chart of control script for automated optimization.

height H which equals the height of the liquid. Four baffles having width W are spaced equally around the vessel. The shaft of the impeller is concentric with the axis of the vessel. The impeller is a six bladed Rushton turbine with a diameter D, a blade height w, a blade length ℓ, and a bottom clearance C. The actual geometrical parameters, which we consider as the standard configuration, are summarized in Table 1. The working Newtonian fluid is a glucose solution with density $\rho = 1330\,\mathrm{kg/m^3}$ and viscosity $\mu = 0.105\,\mathrm{Pas}$.

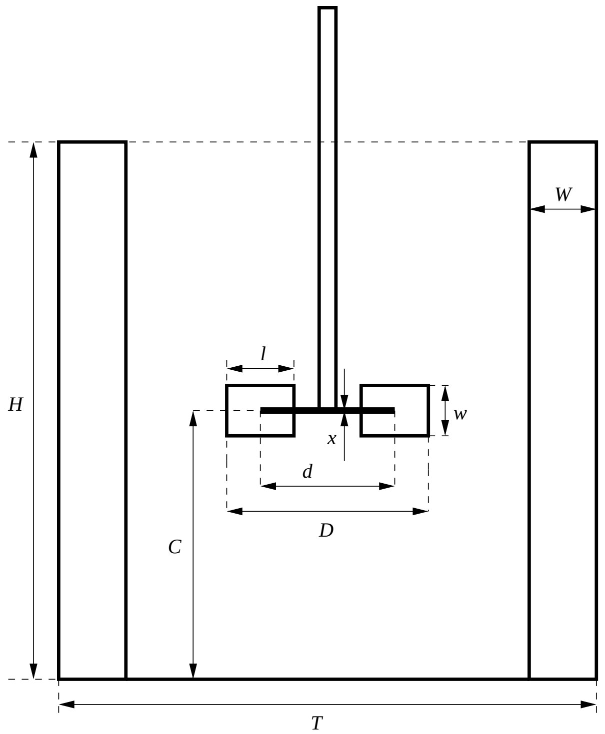

Fig. 3. Schematic sketch of stirrer configuration.

Table 1
Geometrical parameters of standard stirrer configuration

Parameter	Value
Tank diameter	$T = 0.15\,\mathrm{m}$
Impeller diameter	$D = T/3 = 0.05\,\mathrm{m}$
Bottom clearance	$C = H/2 = 0.075\,\mathrm{m}$
Height of the liquid	$H = T = 0.15\,\mathrm{m}$
Length of the baffles	$W = 3D/10 = 0.015\,\mathrm{m}$
Length of the blade	$\ell = D/4 = 0.0125\,\mathrm{m}$
Height of the blade	$w = D/5 = 0.01\,\mathrm{m}$
Disc thickness	$x = D/5 = 0.00175\,\mathrm{m}$
Diameter of the disk	$d = 3D/4 = 0.0375\,\mathrm{m}$

The numerical grid employed involves 22 blocks. 17 blocks are defined as rotating while the remaining 5 blocks are defined as stationary. The total number of of control volumes is 238 996. In Fig. 4 a sketch of the corresponding surface grid is shown.

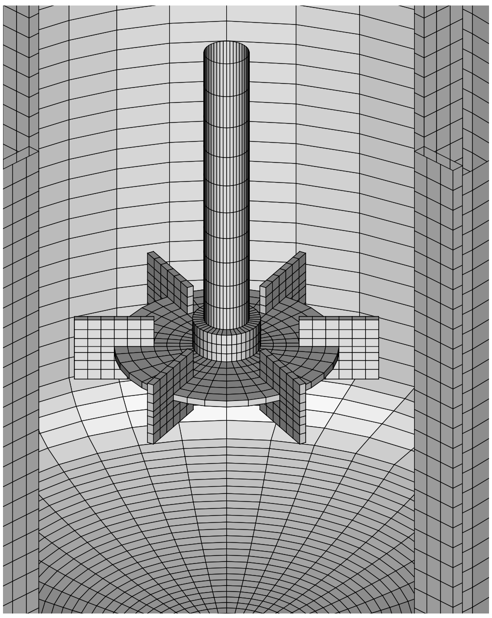

Fig. 4. Sketch of surface grid for standard stirrer configuration.

First, for validation the stirrer configuration is simulated for different Reynolds numbers $Re = \rho N D^2/\mu$. As a characteristic reference quantity the (dimensionless) Newton number is considered, which relates the resistance force to the inertia force. It is expressed as

$$Ne = \frac{P}{\rho N^3 D^5}\,, \tag{5}$$

where N is the rotational speed of the impeller and the power P is computed from the flow quantities by

$$P = -\int_S (p u_j + \tau_{ij} u_i)\, n_j \,\mathrm{d}S\,, \tag{6}$$

where S denotes the surface of the impeller and n_j are the components of the unit normal vector. A plot of Ne versus Re, i.e. the power curve, is shown in Fig. 5 also including experimental data reported in Bates et al. [35]. The predicted Newton numbers are in excellent agreement with the experimental results.

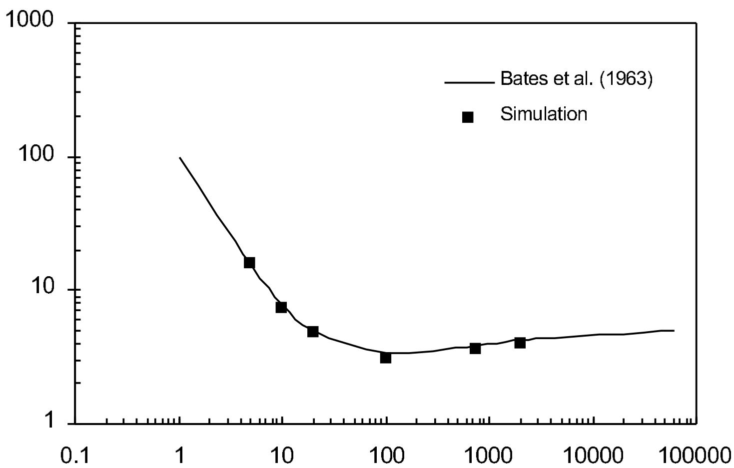

Fig. 5. Comparison of experimental and numerical power curves for standard stirrer configuration.

Concerning the computational requirements we remark that one time step approximately needs 20 seconds of computing time on an eight processor Redstone cluster machine. This results in about 8 hours computing time to reach a steady state flow in the sense of a frozen rotor computation, a criterion that we adopt for all cases.

4 Optimization of the Newton Number

As an exemplary application of the optimization tool we consider the minimization of the Newton number for the case $Re = 1000$, where the disk thickness x, the bottom clearance C, and the baffle length W are considered to be the design variables, for which the constraints $0.001 \leq x \leq 0.005$, $0.02 \leq C \leq 0.075$, and $0.005 \leq W \leq 0.03$ are prescribed. The other parameters are kept constant according to the standard configuration (see Table 1).

Figure 6 shows the Newton number versus the number of cycles of the optimization algorithm. It can be seen that the Newton number first sharply drops and then slowly approaches the minimum in a slightly oscillating manner. Finally, the optimized Newton number is about 37% lower than the one for the standard configuration. Differences in the flow patterns in the optimized and the standard geometry can be seen in Fig. 7 showing the velocity fields in a plane midway between two baffles for both cases. The overall computing time for the full optimization process took about 5 days on the eight processor Redstone cluster machine.

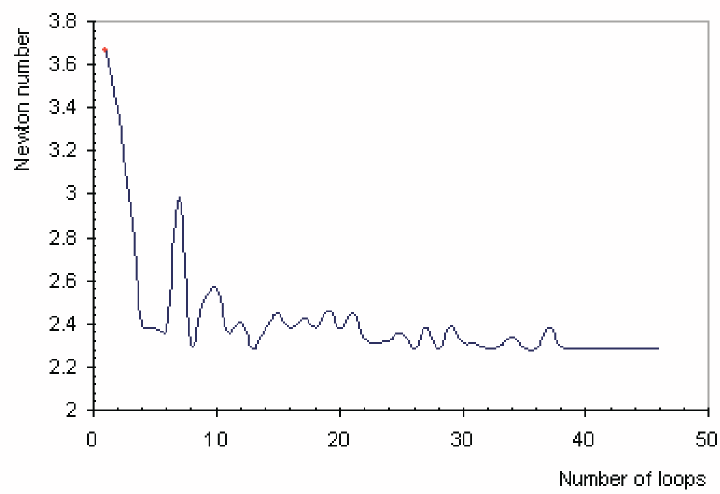

Fig. 6. Newton number versus number of optimization loops.

Figure 8 depicts the corresponding changes of the three design variables. The disk thickness approaches its upper bound, while the bottom clearance and the baffle length reach their optimum values in-between their given bounds.

5 Summary and Conclusions

In this study we have presented a method for optimizing practical stirrer configurations. The automated integrated procedure consists of a combination

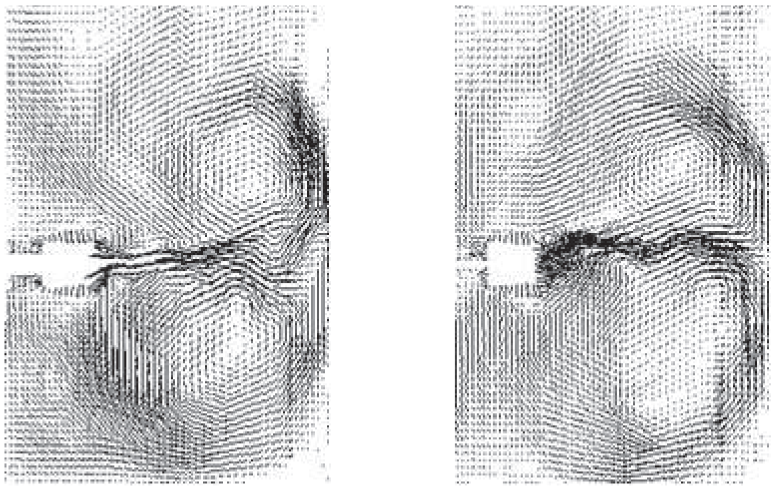

Fig. 7. Comparison of velocity fields in a vertical plane between two baffles for optimized (left) and standard (right) configuration.

of a parametrized grid generator, a parallel flow solver, and a derivative-free optimization procedure. The numerical experiments have shown the principle applicability of the considered approach. For the considered Rushton turbine it has been possible to achieve a significant reduction of the Newton number with relatively low computational effort.

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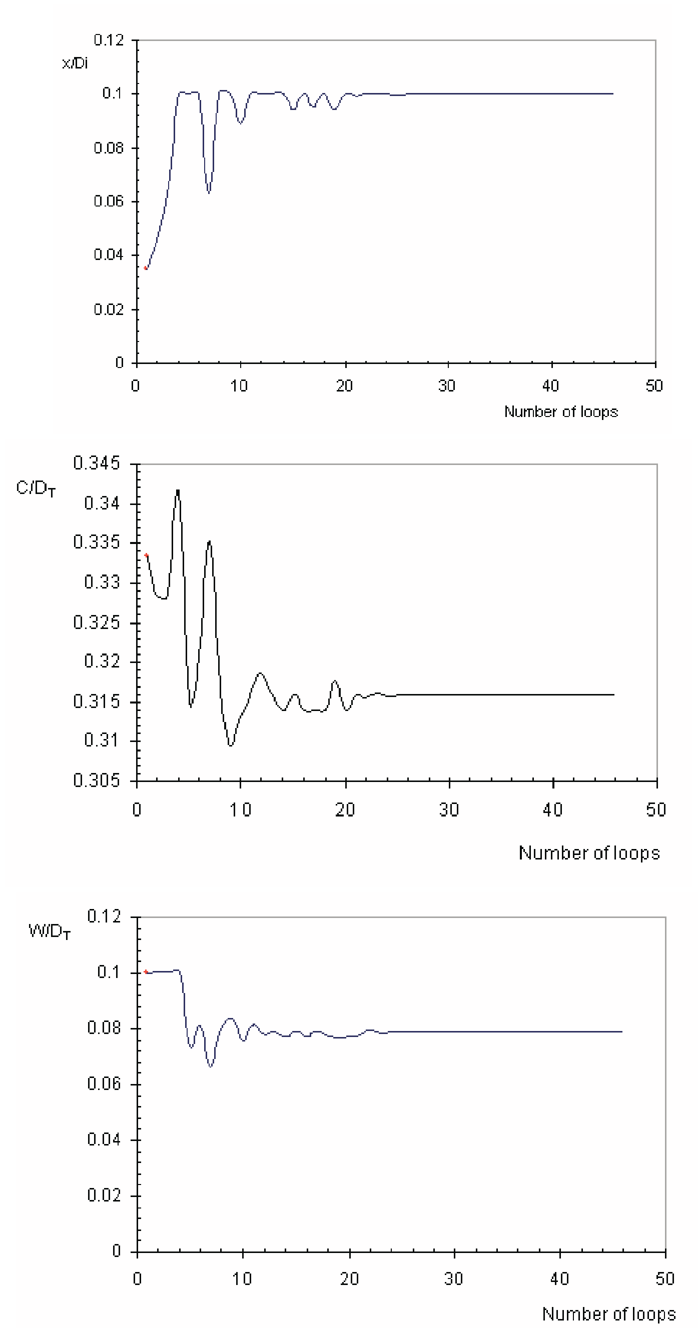

Fig. 8. Dimensionless impeller design parameters versus number of optimization loops: disk thickness (top), bottom clearance (middle), baffle length (bottom).

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