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ORTHOGONAL ARRAYS: AN INTRODUCTION AND THEIR APPLICATION IN OPTIMIZING UNDERRELAXATION FACTORS IN 'SIMPLE'-BASED ALGORITHM

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SUMMARY

The primary aim of this paper is to demonstrate how the 'design-of-experiments' techniques which are successful in physical experiments could also be adapted to a numerical simulation code.

As an example this technique is applied to a general finite difference code used for predicting three-dimensional turbulent recirculating flows. Here the equations for velocities and continuity are solved using the algorithm called SIMPLE, which stands for semi-implicit method for pressure-linked equations. Physical modelling of turbulence is taken care of by means of kinetic energy and turbulence dissipation rate equations.

The objective is to optimize the underrelaxation factors of primary and secondary flow variables so that the number of iterations required for convergence is minimum. This is done by the orthogonal array technique (a particular type of design-of-experiment technique).

The geometry considered for this purpose is that of a simple gas turbine can combustor and the study is restricted to the isothermal non-reacting condition.

Tests are carried out on three different grid configurations. In each case the underrelaxation factor for velocities contributed most to speed up the rate of convergence. Also, for each grid configuration the underrelaxation factor settings for minimum iterations for convergence was found to be same. Hence it is proposed that when doing grid independence tests for any similar flow situation, all the underrelaxation factors could be optimized on coarse grids.

KEY WORDS Orthogonal arrays Underrelaxation factors SIMPLE Grid independence Design of experiments

INTRODUCTION

The classical one-factor-at-a-time strategy used for performing experiments fails to detect interactions between the variable factors. The design-of-experiment technique overcomes this deficiency and is now gaining popularity in industries throughout the world. This concept can also be extended to computer simulation of any system with some modifications. This paper deals with such an attempt.

The first few sections are devoted to introducing the design-of-experiment technique to the CFD world. For the sake of brevity only the bare essentials are provided. For more details the reader is referred to References 1–3.

The remaining sections demonstrate the application of this technique in optimizing the underrelaxation factors in a SIMPLE-based finite difference code for three-dimensional turbulent recirculating flows.

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TERMINOLOGY

Some fundamental terms associated with design of experiments are defined as follows.

(i) *Factor.* This is a controlled or an uncontrolled variable which influences the result of an experiment. It may be quantitative, e.g. temperature, time, pressure, etc., or qualitative, e.g. different machines, different operators, switch on or off.

(ii) *Level.* The values of the factors being examined in the experiment are called levels. For quantitative factors each chosen value becomes a level; for example, if an experiment is conducted at four different temperatures then the factor temperature has four levels. In the case of qualitative factors, e.g. if a machine is run by two operators independently, the factor operator has two levels. Levels are denoted as 1, 2, 3 and so on.

(iii) *Treatment.* A treatment is a single level assigned to a single factor during an experimental run, e.g. pressure at 1 atm. A treatment combination is the set of levels for all factors in a given experimental run; for example, an experiment with a chemical process at a pressure of 1 atm, a temperature of 500 K and using a catalyst 'A' constitutes one treatment combination.

(iv) *Main effects.* The change in response produced by the change in level of a factor is called the main effect of that factor, e.g. the increase in power output of a two-stroke engine by a change of port timing alone.

(v) *Interaction.* Interaction is the simultaneous influence of two or more factors on the response. If the effect of one factor is different at different levels of one or more factors, the two factors are said to interact. For example, consider the following case.

The yield of a product depends on two factors A and B. Each factor has two levels (1 and 2). When A is at level 1, increasing B from level 1 to level 2 results in an increase in yield by x kg. If the same increase (within the range of experimental errors) is not obtained by increasing B from level 1 to level 2 when A is at level 2 then the factors are said to interact. Symbolically the interaction is denoted as $A \times B$ and is known as first-order interaction. If the interaction between two factors A and B is different at different levels of a third factor C then there is said to be an interaction between the three factors. This is called second-order interaction and is denoted by $A \times B \times C$. Similarly, higher-order interactions can be defined.

(vi) *Randomization.* If the sequence of experiments is determined in a random manner, it is called randomization. This minimizes the effect of uncontrolled variables (noise factors) and personal bias of the experimenter.

(vii) *Replication.* Replication is the repetition of an observation or measurement in order to increase the precision. Replication provides an opportunity for the effects of uncontrolled factors or factors unknown to the experimenter to balance out and thus with randomization acts as a bias-decreasing tool. Replication also helps to detect gross errors in the measurements.

(viii) *Contribution ratio (CR).* The contribution ratio of a factor is a measure to estimate the extent to which the factor contributes towards the variation of response.

STEPS IN DESIGN OF EXPERIMENTS

The following are the steps to be taken for a good experimental design.

(i) *Recognition and statement of the problem.* A clear statement of the problem often contributes substantially to a better understanding of the phenomena and the final solution of the problem.

(ii) *Choice of factors and levels.* All the independent variables or factors of the product or process that could possibly influence the quality or performance of the end products or process should be specified. The levels of factors should also be decided and their values should be within a reasonable range of interest.

(iii) *Selection of a response variable.* In choosing a response or dependent variable, the experimenter must be certain that the response to be measured really provides information about the problem under study.

(iv) *Choice of experimental design.* The formal plan for conducting the experiment is called the experimental design. A detailed description of several types of experimental design can be found in Reference 2. We will concentrate only on factorial and fractional factorial designs, which are described in subsequent sections.

(v) *Performing the experiment.* Particular attention should be paid to randomization, measurement, accuracy and maintaining as uniform an experimental environment as possible.

(vi) *Data analysis.* Statistical methods such as analysis of variance (ANOVA) should be used in analysing the results. The contribution ratios of all the factors and interactions considered are then found.

(vii) *Conclusions and recommendations.* Recommendations may include a further round of experiments, since experimentation is usually an iterative process with one experiment answering some questions and simultaneously posing others.

FACTORIAL EXPERIMENTS

A popular method of experimentation used so far by researchers is the one-factor-at-a-time approach. Each factor in turn is varied while all the rest of the factors are held at some fixed, constant levels. This strategy is inefficient because it fails to detect interaction between the variable factors and there is a possibility of false optimum setting being achieved. Hence this method is now rapidly being replaced by the technique of factorial experiments. Factorial experiments can estimate interactions between the factors and are also the most efficient way of estimating the main effects even if no such interactions are present. These advantages of a factorial experiment over one-factor-at-a-time experiment are illustrated as follows.

Let us consider a chemical reaction which results in a certain product. Suppose the amount of product produced depends on two factors, namely pressure and temperature. The aim is to optimize the settings of pressure and temperature so that the yield of the product is maximum. For the sake of simplicity we conduct experiments at only two levels of pressure (P_0 and P_1) and two levels of temperature (T_0 and T_1).

The one-at-a-time strategy proceeds as follows (see Table I). The experimenter tries out the setting T_0P_0 which yields 4 kg. Then, keeping the pressure at the same level P_0, he tries out the combination T_1P_0 which yields 2 kg. The experimenter infers that T_1 results in less yield, so he reverts to the temperature setting T_0 and tries out the combination T_0P_1 which produces 6 kg. He repeats these trials and gets the same results within experimental errors. He now concludes that T_0P_1 is the best combination for maximizing the yield. He has not tried the setting T_1P_1 at all because he feels that since the yield was reduced by 50% (from 4 to 2 kg) when the temperature was changed from T_0 to T_1 with the pressure at P_0, the same would be the case if the temperature were changed from T_0 to T_1 with the pressure at P_1.

He expects the yield for T_1P_1 to be only around 3 kg (i.e. 50% of 6 kg). His prediction will be correct only if the pressure and temperature factors do not interact with each other; but if they do, the yield for the combination T_1P_1 may be much higher or much lower than 3 kg. It is also possible that the combination may result in the maximum yield, say 10 kg, in which case the one-at-a-time experiment strategy has missed the optimum setting T_1P_1.

Table I. A simple hypothetical factorial experiment

Pressure	Temperature	
	T_0	T_1
P_0	4	2
P_1	6	?

In factorial experiments all possible combinations of levels of factors are tried out and hence the possibilities of such mishaps are averted.

Even if there is no interaction between pressure and temperature, it is advantageous to perform factorial experiments.

In the one-at-a-time strategy detailed above the combinations T_0P_0, T_1P_0 and T_0P_1 have been tried out. It is evident from Table I that the effect of changing the temperature from T_0 to T_1 is to reduce the yield by 50% and the effect of changing the pressure from P_0 to P_1 is to increase the yield by 50%. It is necessary to repeat the experiment at least once. This is done and similar results are obtained within the limits of experimental error. Thus we have two pieces of evidence to confirm the effect of pressure and temperature on the yield of the product. In all, six trials have been performed.

Now, if factorial design is adopted then each possible combination of factors is tried out once, i.e. four trials in all. Since there is no interaction, combination T_1P_1 will yield 3 kg. Here also we have two pieces of evidence to prove that the change of temperature from T_0 to T_1 results in a 50% decrease in yield (from 4 to 2 kg for combinations T_0P_0 and T_1P_0 and from 6 to 3 kg for combinations T_0P_1 and T_1P_1) and also two pieces of evidence to prove that the change of pressure from P_0 to P_1 results in a 50% increase in yield (from 4 to 6 kg for combination T_0P_0 and T_0P_1 and from 2 to 3 kg for combinations T_1P_0 and T_1P_1).

Thus the findings with factorial design are as precise as those obtained by performing one-at-a-time experiments twice; but while the latter strategy took six trials, the same preciseness was achieved by factorial experiments in only four trials.

In general, if there are m levels for each of N factors, the factorial design involves m^N trials.

FRACTIONAL FACTORIAL DESIGN

When the number of factors is too large, the full factorial design calls for a large number of experiments. For example, if there are five factors with two levels each, we require $2^5 = 32$ experiments to estimate all the main effects and interactions. This may not be economical and therefore one should go for fractional factorial experiments.

When there are several factors, the effects of higher-order interactions are generally not significant and in some cases are also difficult to interpret. Hence information on these higher-order interactions is deliberately lost to reduce the number of experiments.

In the above example of five factors each at two levels, all the main effects and first-order interactions can be estimated with a half-factorial design of $\frac{1}{2} \times 2^5 = 16$ trials. All the main effects can be estimated with a quarter-factorial design of eight trials. Such designs are known as fractional factorial designs.

ORTHOGONAL ARRAYS AND LINEAR GRAPHS

Orthogonal arrays (Tables II–IV) are the means to design factorial and fractional factorial experiments.

Any $N \times k$ matrix **A** with entries from a set of s ($\geqslant 2$) elements is called an orthogonal array of size N, k constraints, s levels, strength d and index λ if in any $N \times d$ submatrix of **A** the combination of levels for a particular row appears with the same frequency λ.

For an example, refer to Table III. This is an array of size eight, seven constraints and two levels. If we consider columns 1 and 2 (i.e. 8×2 submatrix), we find that the combination levels (1 1), (1 2), (2 1) and (2 2) appear with same frequency i.e. two times each.

Again, if we consider columns 1, 2 and 3 (i.e. 8×3 submatrix), we find that the combination levels (1 1 1), (1 2 2), (2 1 2) and (2 2 1) appear with same frequency (two times each). The same is true for any submatrix. Hence the array is said to be orthogonal.

Each orthogonal array has associated with it a set of linear graphs (Figures 1–3 for Tables II–IV respectively).

The concept of such linear graphs was propounded by Taguchi,[3] a well-known figure in the field of statistical quality control (SQC). The use of linear graphs makes it possible to design and analyse complicated experiments without requiring the basic knowledge of the constructions of design using finite geometrics and Galois fields.

A linear graph associated with an orthogonal array represents the information about the interactions between some specified columns of that array. It consists of a set of nodes and a set of lines, each of which joins a certain pair of nodes. A node represents the column of the array which is to be assigned to the main factor. A line joining any two nodes denotes the column of the array

Table II. L4 array

Experiment	Column number		
	1	2	3
1	1	1	1
2	1	2	2
3	2	1	2
4	2	2	1

Table III. L8 array

Experiment	Column number						
	1	2	3	4	5	6	7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

Table IV. L16 array

Experiment	Column number														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2
3	1	1	1	2	2	2	2	1	1	1	1	2	2	2	2
4	1	1	1	2	2	2	2	2	2	2	2	1	1	1	1
5	1	2	2	1	1	2	2	1	1	2	2	1	1	2	2
6	1	2	2	1	1	2	2	2	2	1	1	2	2	1	1
7	1	2	2	2	2	1	1	1	1	2	2	2	2	1	1
8	1	2	2	2	2	1	1	2	2	1	1	1	1	2	2
9	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2
10	2	1	2	1	2	1	2	2	1	2	1	2	1	2	1
11	2	1	2	2	1	2	1	1	2	1	2	2	1	2	1
12	2	1	2	2	1	2	1	2	1	2	1	1	2	1	2
13	2	2	1	1	2	2	1	1	2	2	1	1	2	2	1
14	2	2	1	1	2	2	1	2	1	1	2	2	1	1	2
15	2	2	1	2	1	1	2	1	2	2	1	2	1	1	2
16	2	2	1	2	1	1	2	2	1	1	2	1	2	2	1

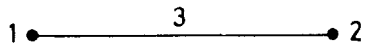

Figure 1. Linear graph of L4 table

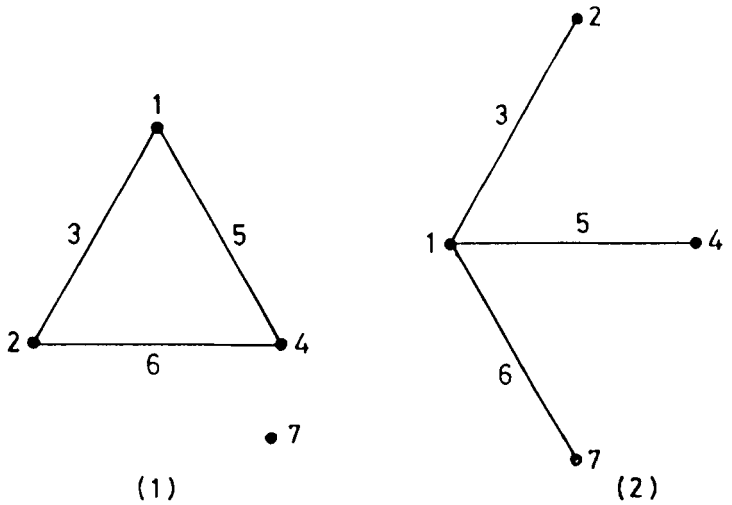

Figure 2. Linear graphs of L8 table

which is to be assigned to the interaction effect of the main factors associated with nodes being joined.

For a two-level experiment the orthogonal arrays are classified as L4, L8, L16 and so on. Here L4 for example means that this orthogonal table can be used if the minimum number of

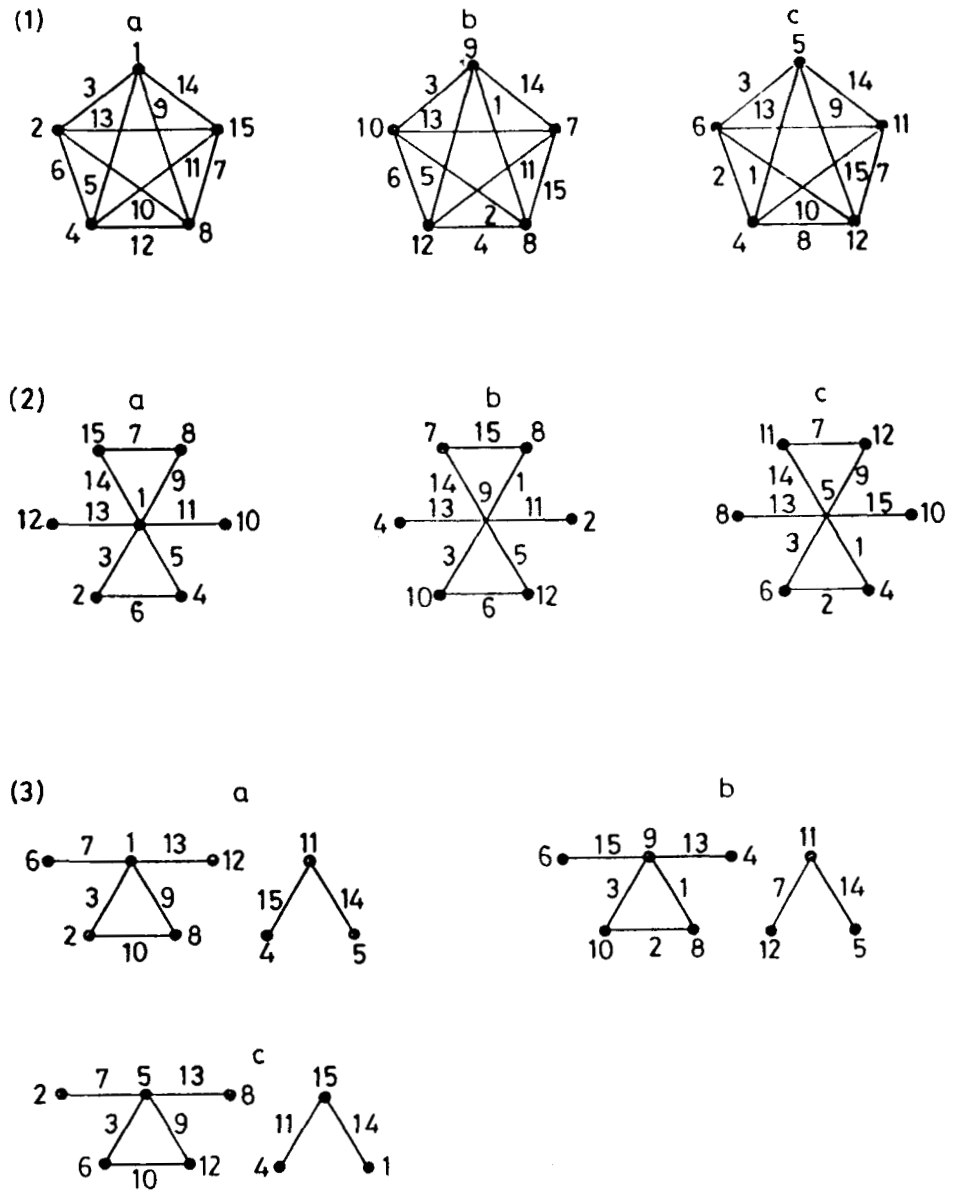

Figure 3. Linear graphs of L16 table

experiments required to be conducted is four. The L4, L8 and L16 arrays along with their associated linear graphs are shown in Tables II–IV and Figures 1–3.

EXPERIMENTAL DESIGN FOR COMPUTER SIMULATION CODES

The design-of-experiment techniques used for physical experiments can also be applied to computer simulation codes since these codes are analogous to the real life situation, the only difference being that the physical phenomenon is replaced by mathematical models.

An additional advantage when this technique is applied to such codes is that there are no uncontrolled variables (unlike in a physical system) and the ideal situation exists. Hence replication and randomization need not be done. There is also some modification to be done when analysing the data obtained from numerical studies. This is explained in detail a little later.

In an application-oriented simulation package involving several differential equations the situation is as complex as any real life situation. It may not be easy to infer by examination alone the effect of variation of a particular term in a particular equation. Design-of-experiment techniques will be of help in such cases. These techniques will also be of great use in parametric studies with simulation packages.

In the CFD area this technique can be used for several purposes, e.g.

(i) optimization of relaxation factors in finite difference codes
(ii) numerical estimation of the effects of swirlers, injection holes, flame holders, etc. on the recirculation zone in gas turbine combustion chambers
(iii) estimation of the effects of various algorithms and their interaction with grid size and relaxation factors on the convergence rate
(iv) determination of various adjustable constants to be substituted in the differential equations to match the real life variation of any factor.

The rest of the paper demonstrates the use of orthogonal array design for optimizing underrelaxation factors in a finite difference code.

PROBLEM DESCRIPTION

A finite difference code for three-dimensional turbulent recirculating flow is used for the present study.

The governing partial differential equations for mass, momentum and energy can be generalized as

$$\frac{\partial}{\partial t}(\rho\phi)+\operatorname{div}(\rho\mathbf{V}\phi-\Gamma\operatorname{grad}\phi)=S_\phi,$$

where ϕ is any dependent variable, ρ is the density, Γ is the diffusion coefficient, $\mathbf{V}$ is the velocity vector and S_ϕ is the source term for ϕ.

This code solves for continuity, the velocity in three directions, turbulent kinetic energy and turbulence dissipation rate using the algorithm SIMPLE (semi-implicit method for pressure-linked equations).[4]

The essential feature of SIMPLE is the replacement of the continuity equation with a Poisson type of pressure correction equation. This pressure correction equation is prone to divergence in the iterative solutions. Hence underrelaxation factors are introduced when solving for the dependent variables to ensure convergence.

The discretized form of the governing partial differential equation is

$$a_{\mathrm{P}}\phi_{\mathrm{P}}=\sum a_{\mathrm{nb}}\phi_{\mathrm{nb}}+S_\phi,$$

where a denotes the coefficient of convective and diffusive fluxes. The subscripts 'P' and 'nb' denote the grid point under consideration and the neighbouring grid point respectively.

By introducing an underrelaxation factor α, we modify the above equation as

$$\frac{a_{\mathrm{P}}}{\alpha}=\sum a_{\mathrm{nb}}\phi_{\mathrm{nb}}+S_\phi+(1-\alpha)\frac{a_{\mathrm{P}}}{\alpha}\phi_{\mathrm{P}}^{*},$$

where ϕ_p^* is the value of ϕ from the previous iteration. The value of α should be between zero to unity. The optimum value of α may depend on the nature of the problem, the grid configurations and the type of algorithm employed. This study estimates the effects of variation in various underrelaxation factors employed when solving for velocities, pressure, kinetic energy k, turbulence dissipation ε and turbulent viscosity μ_t.

The possibility of convergence with the number of iterations depends on the magnitude of underrelaxation. If it is very low, convergence will be slow; if it is very high, oscillations will occur. Besides, every variable need not require the same magnitude of underrelaxation. Hence the problem is that of optimizing the underrelaxation factors.

Underrelaxation factors are said to be optimized if their settings minimize the number of iterations taken for convergence. The convergence criterion in this case is that the sum of absolute source terms should be less than 0·1% of the total inflow. Optimization is done using the orthogonal array technique as detailed in the next section.

The geometry of the physical system considered is that of a gas turbine can combustor as shown in Figure 4. However, for simplicity the flow considered is of non-reacting type. Air is set in swirling motion through the vane swirlers in the annular space and then admitted into the combustor. No fuel is injected. Additional air is injected radially through one row of holes (six in number) on the combustor walls. Also, air is directed tangentially through a circumferential slot around the combustor wall.

Analysis is done for an angular sector of 60° (because other sections are identical to the section considered) and for three grid configurations, namely $15 \times 12 \times 5$, $18 \times 14 \times 7$ and $20 \times 16 \times 9$.

CALCULATION OF CONTRIBUTION RATIO

Following the philosophy of design of experiments (DOE), the steps in calculating the contribution ratios are as follows.

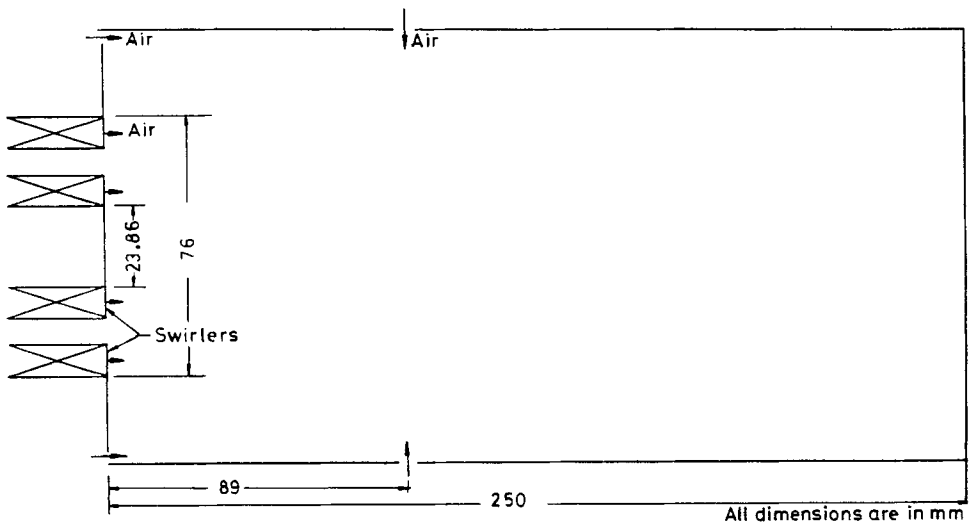

Figure 4. Combustion chamber geometry

(1) Decide upon the levels, factors, main effects and interactions.

We confine ourselves to two-level experiments. The main effects chosen to be estimated are underrelaxation factors (URFs) for velocities u, v and w; pressure (p); kinetic energy (k) and turbulence dissipation (ε); and turbulent viscosity (μ_t).

URFs for velocities in all three directions are grouped together as factor A. The individual effects of the three components of velocity are not being estimated for two reasons: one is that these components are obtained from the solution of the same type of differential equation having similar source terms; the other reason is that if the individual effects are estimated at this stage, the minimum number of experiments to be performed will be more, which may not be economical. By the same argument the URFs for k and ε are grouped together as C. The URFs for p and μ_t are denoted by B and D respectively.

Table V gives the values of the URF for various factors at two different levels. It has been found that URFs of 0·5 for velocity and 0·8 for pressure are satisfactory in a large number of flow situations.[5] Hence we have fixed the ranges of URFs for velocity and pressure around these values. The range for k, ε and μ_t is the same as that for velocity since the values of these terms depend to a great extent on the value of velocity.

We have chosen to estimate all five first-order interactions, namely A × B, A × C, A × D, B × C, B × D and C × D. We are not estimating the individual effects of higher-order interactions such as A × B × C, A × B × D, A × C × D, B × C × D and A × B × C × D since they are difficult to interpret and also their effects will not be significant, as will be evident later.

(2) Compute the minimum number of degrees of freedom required to estimate all the effects that are of interest.

As evident from Table VI, the minimum number of degrees of freedom in this case is 10.

(3) Calculate the minimum number of experiments (MNE) required:

$$\text{MNE} = \text{minimum number of degrees of freedom} + 1 = 11.$$

(4) Choose an orthogonal array (OA) just greater than the value of MNE.

The OA just greater than MNE is L16 (Table IV). We choose this array. The total number of degrees of freedom is now $16 - 1 = 15$.

(5) Express the information required in an experiment by linear graphs representing the main effects by nodes and interactions between two factors as a line joining the nodes. This is known as the required linear graph (RLG) and is shown in Figure 5(a).

(6) Compare the standard linear graph (SLG) of the chosen array with the RLG and modify the SLG to correspond to the RLG.

We choose SLG 1(a) associated with the L16 table (Figure 3) and modify it to correspond to the RLG by deleting the lines connecting nodes 2 and 15, 4 and 15, 2 and 4, and 1 and 2.

Table V. Values of URFs for various factors

Factors		Levels	
		1	2
URF for u, v, w	(A)	0·3	0·6
URF for p	(B)	0·5	0·8
URF for k and ε	(C)	0·3	0·6
URF for μ_t	(D)	0·3	0·6

Table VI. Degrees of freedom for various factors

Factor	Level	Degrees of freedom (number of levels − 1)
A	2	1
B	2	1
C	2	1
D	2	1
A × B	2	1
A × C	2	1
A × D	2	1
B × C	2	1
B × D	2	1
C × D	2	1
Minimum number of degrees of freedom		10

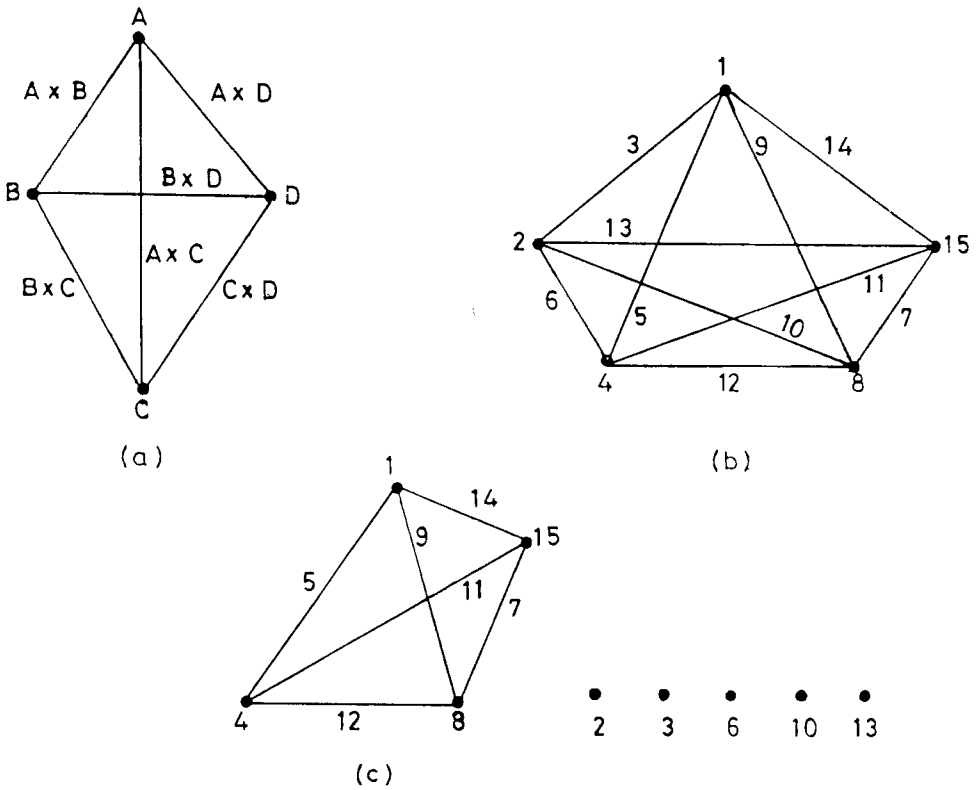

Figure 5. (a) Required linear graph (RLG). (b) Standard linear graph (SLG). (c) Modified SLG

When this is done, the deleted nodes and lines become independent nodes, namely 2, 3, 6, 10 and 13 as shown in Figures 5(b) and 5(c).

(7) Allocate the factors and interactions to the respective columns by comparing the modified SLG with the RLG.

In this case, comparing Figures 5(a) and 5(c), we make the following allocations:

A → 1	B →4	C → 8	D →15
A×B→ 5	A×C→9	A×D→14	B×C→12
B×D→11	C×D→7		

(8) The experimental layout is determined by copying these columns from the orthogonal table.

Here we have the experimental lay-out as per Table VII.

The numbers 1 and 2 indicate the level of the factors. For example, in experiment 4 the levels of factors A and D are at 1 and those of B and D are at 2. This means that the experiment is performed with URFs for A and D at 0·3, URF for B at 0·8 and URF for C at 0·6.

If physical experiments were being done, the sequence of experiments would have been randomized and also each observation would have been replicated; but since we are performing numerical experiments, these are not necessary since the situation is ideal.

The responses, i.e. the number of iterations required for convergence, for the three grid configurations tested are also indicated in Table VII.

(9) Calculate the contribution ratio for each factor and interaction considered.

When analysing the data of physical experiments, it is essential to confirm the contribution ratio calculated by subjecting the data to an analysis of variance (ANOVA) test. Without this test we cannot say for certain whether the change in response obtained by changing the settings is really different from that of the original settings or whether it falls within the range of response

Table VII. Experimental lay-out and results

	Main effects and interactions										Number of iterations per grids		
	A	B	C	D	A×B	A×C	A×D	B×C	B×D	C×D			
Column:	1	4	8	15	5	9	14	12	11	7	I	II	III
Experiment													
1	1	1	1	1	1	1	1	1	1	1	320	464	732
2	1	1	2	2	1	2	2	2	2	1	314	459	724
3	1	2	1	2	2	1	2	2	1	2	308	435	697
4	1	2	2	1	2	2	1	1	2	2	305	413	665
5	1	1	1	2	1	1	2	1	2	2	318	461	729
6	1	1	2	1	1	2	1	2	1	2	316	461	725
7	1	2	1	1	2	1	1	2	2	1	310	437	699
8	1	2	2	2	2	2	2	1	1	1	304	411	663
9	2	1	1	2	2	2	1	1	2	2	294	378	527
10	2	1	2	1	2	1	2	2	1	2	191	333	497
11	2	2	1	1	1	2	2	2	2	1	229	321	467
12	2	2	2	2	1	1	1	1	1	1	191	301	464
13	2	1	1	1	2	2	2	1	1	1	291	379	530
14	2	1	2	2	2	1	1	2	2	1	203	332	494
15	2	2	1	2	1	2	1	2	1	2	239	319	486
16	2	2	2	1	1	1	2	1	2	2	193	303	466

Grid I: 15 × 12 × 5.
Grid II: 18 × 14 × 7.
Grid III: 20 × 16 × 9.

that could be obtained with the original settings themselves. This is because the presence of uncontrolled variables causes the individual observations to scatter around a mean value in most real life situations. By the ANOVA test we can quantify this uncertainty. We say that a particular change in setting of a factor has a significant effect on the response only if this test shows an uncertainty below 5% (or in other words a confidence level of 95%).

However, in numerical experiments (except those involving random number generation) such tests are not necessary, because we can say with 100% confidence that whatever results we get due to changes in the settings are really a departure from that of the original settings. Hence it is enough to calculate only the contribution ratio.

The steps in the calculation of the contribution ratio for each factor are as follows.[3]

(i) *Average response* (*AR*)

$$\mathrm{AR} = G/N,$$

where G is the grand total of all responses and N is the number of responses.

(ii) *Total sum of squares* (*TSS*)

$$\mathrm{TSS} = \sum_{i=1}^{N} (x_i - \mathrm{AR})^2,$$

where x_i denotes the individual response.

(iii) *Sum of squares due to each factor* (*SS*)

$$\text{For a factor A:} \quad \mathrm{SS_A} = \mathrm{SS_{A,1}} + \mathrm{SS_{A,2}},$$

where

$$\mathrm{SS_{A,1}} = n_{\mathrm{A},1} \times (\text{mean of all responses with A at level 1} - \mathrm{AR})^2,$$

$$\mathrm{SS_{A,2}} = n_{\mathrm{A},2} \times (\text{mean of all responses with A at level 2} - \mathrm{AR})^2,$$

where $n_{\mathrm{A},1}$ and $n_{\mathrm{A},2}$ denote total numbers of responses with A at levels 1 and 2 respectively. Similarly calculate $\mathrm{SS_B}$, $\mathrm{SS_C}$, $\mathrm{SS_D}$, $\mathrm{SS_{A\times B}}$, $\mathrm{SS_{A\times C}}$, etc.

$$\mathrm{SS_{residuals}} = \mathrm{TSS} - (\text{sum of SS of all the main factors and interactions})$$

$\mathrm{SS_{residuals}}$ will include the effects of all the remaining possible interactions among A, B, C and D. In physical experiments it also accounts for the effects due to uncontrolled variables.

(iv) *Contribution ratio* (*CR*)

$$\mathrm{CR} = 100 \times \frac{\mathrm{SS}}{\mathrm{TSS}}.$$

RESULTS AND DISCUSSION

Table VIII shows the contribution ratios for all the main effects and interactions for the three different grid configurations. The following facts are evident from the table.

(i) Within the range of values of URFs chosen, the URF for velocities turns out to be the major contributing factor in all the grid configurations. Its effect increases with increasing number of grid points, the CR being as high as 94·6% for the $20 \times 16 \times 9$ configuration.

(ii) The CRs of the URFs for pressure and for kinetic energy and dissipation rate are less than 15% in all cases.

Table VIII. Contribution ratios of main effects and interactions

Factors	Contribution ratios (%)		
	Grid I	Grid II	Grid III
A (u, v, w)	67·48	83·04	94·6
B (p)	4·32	11·60	4·02
C (k, ε)	13·04	3·55	0·9316
D (μ_t)	0·03918	0·0244	0·0002936
A × B	1·13	0·0912	0·01438
A × C	10·18	0·6102	0·0002642
A × D	0·14	0·0078	0·01178
B × C	1·72	0·0183	0·0005513
B × D	0·0055	0·8982	0·01726
C × D	0·0006	0·0001	0·01178
Residual	1·94	0·1594	0·3931
Total	100·0	100·0	100·0

(iii) The CR for effective viscosity is negligible in all cases.
(iv) The interaction effects are negligible in all cases, except in the case of $15 \times 12 \times 5$ grid where the A × C interaction contributes 10·18%.

In addition, from Table VII we can infer that the treatment combination for the minimum number of iterations required for convergence is the same for all the grids. This is when all factors are at level 2.

An attempt is made to minimize the number of iterations further by varying only the URF for the most significant factor (in this case the URF for velocity). The other URFs are kept at level 2. The results are depicted in Figure 6. We find that when the value of the URF is greater than 0·65 in the case of the $15 \times 12 \times 5$ grid and greater than 0·625 in the cases of the $18 \times 14 \times 7$ and $20 \times 16 \times 9$ grids, divergence occurs. Hence the URF value of 0·625 is considered to be ideal.

CONCLUSIONS

In this flow situation the URF of velocity is found to have a very dominant effect on convergence for all the grids. This dominance increases with increasing number of grid points.

When performing grid independence tests, the number of iterations for convergence increases with increasing number of grid points. If the URFs are optimized for the minimum number of iterations for convergence, the computing costs can be reduced.

From the results of our case we can infer that for similar flow situations the URFs can be optimized on coarser grids and the same settings can then be used when executing the code on finer grid configurations.

Table IX shows the CPU time taken to achieve convergence with optimized setting for all the grid configurations. It is evident that the coarsest grid ($15 \times 12 \times 5$) takes only 10% of the time taken for convergence by the finest grid ($20 \times 16 \times 9$). Also, as mentioned earlier, the settings are the same for all the grid configurations.

This indicates that a tremendous amount of computer time can be saved when the URFs are optimized on coarser grids rather than on the finer grids where the final results are required.

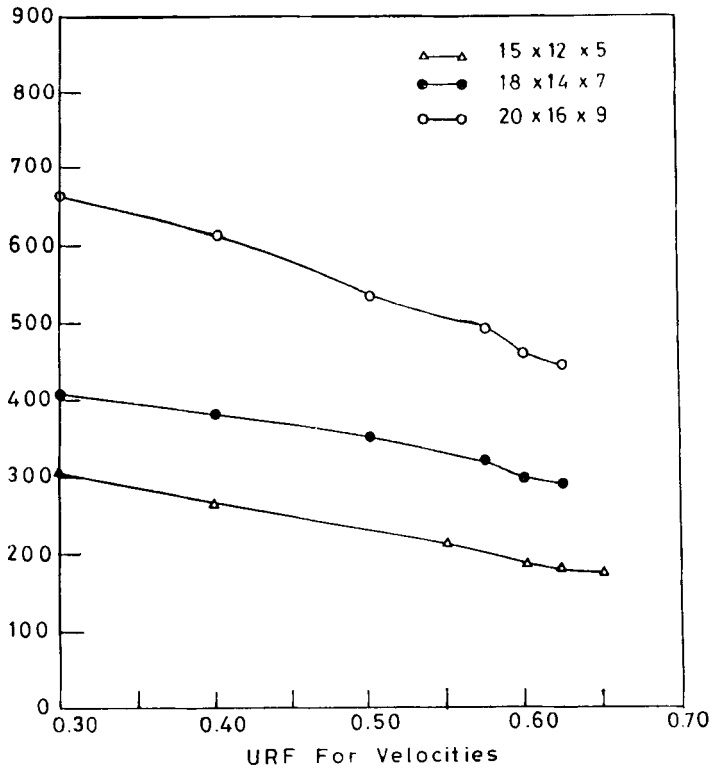

Figure 6. Effect of URF for velocities on convergence

Table IX. Comparison of CPU times for various grids

Grid size	CPU time (minutes) for convergence (for optimized setting)
15 × 12 × 5	2·9
18 × 14 × 7	10·3
20 × 16 × 9	28·7

CLOSURE

The primary aim of this paper is to introduce the design-of-experiments technique to researchers working in the field of mathematical modelling and computer simulation. Since we are involved in the mathematical modelling of gas turbine combustion-chambers, the example chosen was from this field, but the technique is of a general nature and can be applied to any code for parametric studies.

Also, it should be borne in mind that this paper is only a demonstration case of a particular technique. However, we get some guidance on how to optimize the URFs for similar flow situations. We also do not claim that this technique leads to the best possible optimization of URFs, but we do feel that the final settings obtained are a good trade-off between the constraints of CPU time and the best possible settings.

Design-of-experiments techniques are not limited to the OA technique alone. Other techniques are detailed in the references listed. The OA technique itself can be made more sophisticated: (i) by opting for three or more levels of factors in order to adequately resolve the response characteristics for some sensitive systems where there is a strong peak or valley in the response curve in a narrow window of the range of values admitted by a particular system variable; (ii) by using a dummy level technique for accommodating a two-level factor in a three-level OA series, a three-level factor in a four-level series, and so on; (iii) by using a multilevel technique which accommodates a higher-level factor in a lower-level array. Work in these areas is in progress.

To sum up, we feel that the purpose of this paper is served if it motivates researchers in the numerical simulation area to apply design-of-experiment techniques in their respective fields and comment on the efficacy of such methods.

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