

INDUCING OPTIMALLY DIRECTED INNOVATIVE DESIGNS FROM CHEMICAL ENGINEERING FIRST PRINCIPLES

V. AELION,¹ J. CAGAN² and G. POWERS^{1†}

¹Department of Chemical Engineering and ²Department of Mechanical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, U.S.A.

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Abstract—A computational methodology is presented for the innovation of chemical engineering designs from first principle equations developed from the fundamental physics, chemistry, manufacturing and safety constraints of a system. The 1stPRINCE methodology, originally developed for mechanical design, generates optimally directed novel designs from previously known configurations. Design space expansion is performed by *dimensional variable expansion* which expands a design into multiple regions with independent properties. Symbolic optimization directs the search within the design space via monotonicity analysis. Trends over generations of designs are observed and the limiting designs are determined. In some design problems the 1stPRINCE methodology eliminates the need for a prepostulated superstructure for finding the optimal solution. The domain independence of 1stPRINCE is demonstrated in an application to the innovative design of a mixed flow reactor for maximum conversion.

1. INTRODUCTION

Designing a process or an artifact may be broken into three activities: (a) conceptualization; (b) generation of alternative solutions and selection among them; and (c) detailed analysis and evaluation. Currently conceptualization has the smallest computer-aided support, while in contrast, detailed analysis and evaluation is best supported in engineering disciplines (Westerberg, 1989).

The generation and selection of alternatives, step (b), is of great interest in all design activities, because even relatively small problems can have combinatorially many alternative solutions. Grossmann *et al.* (1987) have shown that the retrofit design of a separation sequence has an explosively large number of alternatives. The generation and selection of alternatives is often supported by a postulated superstructure of the design space and by qualitative knowledge about the design domain using artificial intelligence and expert systems technology. However powerful these techniques may be, they generally do not generate novel design concepts. In fact, superstructures are required *because* new designs are not automatically generated.

The task of a designer is to produce a *good* design. One way of accomplishing this is to search for the *best* design in a fixed (prepostulated) design space, a non-trivial task which rests on the imaginative application of optimization techniques. The incorporation of integer variables in large-scale optimization is an

important means of supporting the evaluation of alternative structures (Duran and Grossmann, 1986). Finite element representations and subsequent design by parameter optimization supports the *best shape* design of solid objects intended to perform specific functions (Hrymak *et al.*, 1985). The use of process simulation with optimization has provided insight on the critical factors of both the design of new processes and the operation of existing ones (Biegler and Hughes, 1982). In all of these approaches the design space is predefined and no innovative designs can be discovered.

Another way to produce better designs is by searching for design alternatives which lie beyond the boundaries of the design space currently explored. 1stPRINCE, the design methodology presented in this paper, provides one way of formalizing such a search. It has been introduced by Cagan (1990) and Cagan and Agogino (1987, 1990, 1991) for mechanical design. Unlike other heuristic methods to design innovation (Lenat, 1983; Murthy and Addanki, 1987; Ulrich and Seering, 1987; Joskowicz and Addanki, 1988), 1stPRINCE has its roots in formal optimization theory. This paper aims to introduce this methodology to the chemical engineering literature and demonstrate its cross-disciplinary nature.

1stPRINCE generates *superior* designs by expanding the *dimensional variables* (variables associated with the geometry) of an initial design, which is described by its first principle equations (*first principles* means the algebraic equalities and inequalities developed from the fundamental physics, chemistry, manufacturing and safety constraints of a system).

†To whom all correspondence should be addressed.

This manipulation increases, with certain restrictions, the *degrees-of-freedom* of the design space, thereby making possible innovation in the new designs. Optimization information drives the expansion, and at every iteration of this design process the resulting design is optimized. If the product of this optimization is not deemed satisfactory, then the methodology attempts to introduce design modifications which are guaranteed to perform at least as well as the design of the previous iteration. If trends of improvement appear when iteratively expanding a dimensional variable, this methodology recognizes them and uses induction to generalize these trends, thus achieving the limit of improvement with respect to that particular dimensional variable. New designs are generated from the fundamental equations that describe a previously known design, so the need for prepostulated superstructures for describing the design space is reduced.

1stPRINCE has been used to invent optimally directed tapered beams, hollow tubes, composite rods and, of course, the wheel (Cagan and Agogino, 1987, 1990, 1991). In the following sections, the concept of *optimally directed design* is defined and illustrated by applying 1stPRINCE to the design of a beam under flexural load. 1stPRINCE is then applied to the design of a chemical reactor for optimal conversion to demonstrate domain independence.

2. FIRST PRINCIPLE COMPUTATIONAL EVALUATOR (1stPRINCE)

Cagan and Agogino (1987, 1990, 1991) and Cagan (1990) present the 1stPRINCE methodology for innovative design. Their theory was developed for the domain of mechanical structures. In chemical engineering this methodology can be used in the retrofit design of processes or processing components, based on an initial feasible design.

In this section we review the 1stPRINCE methodology with a discussion of design innovation, an explanation of the design space expansion technique known as *dimensional variable expansion* (DVE) and a discussion of the inductive techniques utilized by 1stPRINCE to observe trends in the design space. An example application of 1stPRINCE for the design of a flexural beam is demonstrated. A discussion of the symbolic optimization analysis technique of monotonicity analysis is also included; monotonicity analysis is used in directing the search and analysis of the design space.

2.1. Classes of design

Cagan (1990) defines a *primitive-prototype* as the model of a design problem, specified by an objective function and a set of inequality and equality constraints within the design space. A *prototype* is defined as a solution from the analysis on a primitive-

prototype which can be instantiated to at least one feasible artifact. The *artifact* in mechanical design is the final product. In chemical engineering the product can be a process as well as an object.

Designs are classified by Cagan (1990) based on the prototype as *routine* or *non-routine*. A *routine design* is defined as a prototype with the same set of variables or features as a previously known prototype, i.e. the structure of the prototype does not change. A *non-routine design* demonstrates a prototype with an expanded set of variables or features as compared to a previously known prototype. In this case new variables or features are introduced in the structure of the prototype.

Non-routine designs are further classified as *innovative designs*, which incorporate new design variables or features in a prototype based on existing variables or features from a previously known prototype, and *creative designs*, which introduce new design variables or features in a prototype demonstrating no obvious similarity to variables or features in a previously known prototype. Innovative designs are often generated by modification of a prototype while creative designs are often generated utilizing outside knowledge.

2.2. Dimensional variable expansion

The 1stPRINCE methodology produces innovative designs by creating new variables within the design space. These variables can introduce new design features and thus support innovation. The new variables are created by manipulating the mathematical formulation of the primitive-prototype. 1stPRINCE incorporates DVE as the technique to expand the design space. First it is determined which variables are potentially critical, defined as those variables which have an influence on the objective function and which, when expanded, will create new variables which may also influence the objective. This variable expansion cannot contract the design space, because the expanded design space incorporates all original variables into the new set of variables and thus, if superior, the initial design can be regained.

Once critical variables are selected, mathematical manipulations of those variables expand the design space. DVE introduces new variables in the primitive-prototype by expanding a single region into multiple regions, where a *region* is a section of an artifact which may be independently modeled and may have independent properties and features. Thus the model of an artifact is subdivided into a group of regions which together define a new primitive-prototype and artifact during DVE. If there is a coordinate system which is not of physical dimensions, DVE remains valid although not necessarily physically intuitive.

Cagan (1990) presents the formal theory for DVE. The intuition behind DVE can be viewed by observing a continuous integral of a function of variables x

and w divided into a series of continuous integrals over smaller ranges as:

$$\int_{z_0}^{z_n} f(\chi, w) dw = \int_{z_0}^{z_1} f(\chi_1, w) dw + \int_{z_1}^{z_2} f(\chi_2, w) dw + \dots + \int_{z_{n-1}}^{z_n} f(\chi_n, w) dw, \quad (1)$$

where n is the number of divisions, often of number two, and subscripts designate distinct variables. If the body remains homogeneous after division, the equality in equation (1) remains consistent; analysis of either side of the equality would produce the same design. 1stPRINCE uses the right-hand side of equation (1) as a starting point for its procedure. DVE is first utilized to discretize the integral over a critical variable and then the properties within each subregion are made independent. Thus the equality in equation (1) no longer applies. Rather, a completely different prototype than the one implied in the left-hand side of the equation may result. Cagan shows that, with restriction, the *degrees-of-freedom* of the expanded design space often increases, indicating an increased likelihood of a novel design being generated.

DVE has been incorporated into the 1stPRINCE design methodology to perform innovative design of mechanical structures. 1stPRINCE utilizes DVE and symbolic, qualitative optimization to reason about design problems from fundamental principles. The manipulations performed by 1stPRINCE are domain-independent. Their application, however, may require domain specific knowledge. This knowledge specifies which design variables can be expanded as dimensional variables. In Section 3 we used DVE in the design of a reactor system, based on the design equation of a well-mixed reactor.

2.3. Induction

1stPRINCE generates sets of active constraints, i.e. constraints which affect the location of the optimum. As DVE is repeatedly applied to generations of prototypes, trends in the design space can occur. To observe these trends, Cagan and Agogino (1990) have extended the 1stPRINCE methodology by incorporating inductive techniques on constraint activity. They take a heuristic approach to induction whereby if some set of facts are true for step 1 through step m , then they are assumed true for step $m + 1$. From this concept they define inductively active and inductively inactive constraints as follows:

Inductively active—If a constraint is active for m consecutive generations, then it is induced to be continuously active. As with unconditionally active constraints, variable backsubstitution of functional information can be performed.

Inductively inactive—If a constraint is inactive for

m consecutive generations, then it is induced to be continuously inactive. As with unconditionally inactive constraints, the constraint can be removed from the constraint set.

When a constraint is found to be inductively active, it is assumed active across the entire continuum. The number of iterations for the induction limit, m can be chosen by the user but is defaulted to be three. If a set of constraints is inductively active then the division of the corresponding critical variable is taken to its limit and the discrete regions are reintegrated into a continuously changing single region. As with all heuristic induction techniques, if an insufficient number of iterations is chosen as the induction limit, then the assumption that the constraint set is unconditionally active or inactive may be a poor assumption.

2.4. Monotonicity analysis

The prototypes innovated by 1stPRINCE are *optimally directed*. *Optimally directed design* is an approach which attempts to determine optimal regions of the design space by directing the search toward the objective and eliminating suboptimal regions. The result is to reduce the size of the search space and gain insight as to the desirable directions for improving the design variables. *Optimally directed design* is distinguishable from *optimal design* in that the goal is not to find a single optimum for a specific set of numerical parameters, but to determine ways, in symbolic form where possible, for improving the design relative to the objective (Cagan and Agogino, 1990).

DVE is relevant only if it can affect the location of the optimum. If a variable appears in a set of active constraints, it is potentially critical. This raises the question of determining constraint activity. Depending on the nature of the optimization problem, different methods exist for determining constraint activity. All these methods are based on the Karush–Kuhn–Tucker (KKT) optimality conditions. In linear and non-linear programming problems constraint activity can be determined from the values of the Lagrange multipliers.

Monotonicity analysis, presented by Papalambros and Wilde (1988), is one method based on the KKT conditions. It utilizes qualitative first derivative information (i.e. the algebraic sign of the direction of change of a variable) to determine candidate active constraint sets, which are guaranteed to bound the optimization problem. Monotonicity analysis is advantageous over other approaches because it does not require numerical parameter information for application. However, because the analysis is based on conditions which are only *necessary* and not sufficient to satisfy the KKT conditions, it can only determine *candidate* active constraint sets. Further, the KKT conditions are themselves only the *necessary* conditions for optimality. It is, however, suitable for exploring the properties of the design space in the

1stPRINCE environment, because we are interested in all the candidate active constraint sets, to produce alternative innovative designs. Three rules of monotonicity analysis define well-constrained monotonic optimization problems [a full discussion of monotonicity analysis is presented in Papalambros and Wilde (1988)]:

Rule One—If the objective function is monotonic with respect to a variable, then there exists at least one active constraint which bounds the variable in the direction opposite to the objective.

Rule Two—If a variable is not contained in the objective function then it must be either bounded from both above and below by active constraints or not actively bounded at all (i.e. any constraints monotonic with respect to that variable must be inactive or irrelevant).

Rule Three (the maximum activity principle)—The number of non-redundant active constraints cannot exceed the total number of variables.

For non-monotonic functions these rules can be applied in piecewise monotonic intervals. A qualitative analysis of the design problem is completed utilizing monotonicity analysis. Certain valid, distinguishable design prototypes occur via active constraints. Functional information for design modification can be extracted from the relationships of the various parameters within those active constraints. A mathematical functional analysis can then be performed on each of the cases by backsubstituting the known, active information into the objective function. Monotonicity analysis within the 1stPRINCE methodology is demonstrated in the design of an innovative mixed reactor in Section 3.

2.5. Beam example

In this paper we demonstrate that the 1stPRINCE design methodology is interdisciplinary. 1stPRINCE has previously been applied to various structures and dynamics problems. By minimizing weight, hollow tubes and composite rods from a solid cylindrical rod under torsion load been innovated. Also by minimizing weight from a solid rectangular cross-section rod under flexural load, the 1stPRINCE design methodology has innovated a hollow tube and an I-beam. By minimizing resistance to spinning, a wheel has been invented from a solid rectangular block. In each of

these examples, a qualitative optimization analysis after DVE has produced optimally directed prototypes in closed form when possible.

In this section we briefly show how the 1stPRINCE methodology has been used by Cagan and Agogino (1990) on a solid beam of circular cross-section of radius r , under flexural load P , while minimizing weight of given material density, ρ . The beam can be seen in Fig. 1 where the only concern is the bending stress σ , not violating the yield stress σ_y . The primitive prototype is thus represented by:

$$\begin{aligned} &\text{minimize } W = \rho \pi r^2 (l_1 - l_0), \\ &\text{subject to } \sigma \leq \sigma_y, \\ &\quad \sigma_1 = 4 P l_1 / (\pi r^3), \\ &\quad l_0 = 0, \\ &\quad l_1 = L. \end{aligned}$$

Omitting the analysis [see Cagan and Agogino (1990) or Cagan (1990) for details], the optimally directed solution has bending stress at its yield active. The solution is given in Fig. 2a. The closed form solution has radius given by:

$$r_1 = \left(\frac{4 P L}{\pi \sigma_y} \right)^{1/3}. \quad (2a)$$

The beam weight is then found to be:

$$W = \rho \pi \left(\frac{4 P L^{5/2}}{\pi \sigma_y} \right)^{2/3}. \quad (2b)$$

After DVE is applied along the length of the beam with $n = 2$, the beam has two separate regions of distinct material properties. Analysis shows that the optimally directed solution has the bending stress at yield in each region and the solution appears as in Fig. 2b [a similar but more complicated closed-form solution as given in equations (2) is available but will be omitted here]. After DVE is applied once more the beam appears as in Fig. 2c and the bending stress is again active in each region. Note that this is the third iteration.

Since the induction limit is chosen to be three iterations, 1stPRINCE can now determine if any constraints are inductively or inactive. In this example, the bending stress is active in each region and considered to be inductively active across the continuum. 1stPRINCE then determines that the superior solution is a tapered beam as shown in Fig. 2d and the radius as a function of length (x) is determined in closed form to be:

$$r = \left(\frac{4 P x}{\pi \sigma_y} \right)^{1/3}. \quad (3)$$

In this example, a single material has been used to demonstrate the induction of constraint activity. 1stPRINCE does not require a single material; rather, via DVE 1stPRINCE permits *discontinuities* in material properties across regions demonstrating powerful composite solutions. If material had been a variable and different materials were selected for various regions, the beam of Fig. 2c could have taken

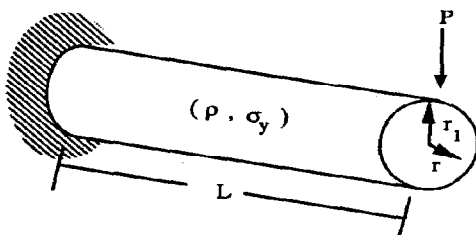


Fig. 1. Beam under flexural load.

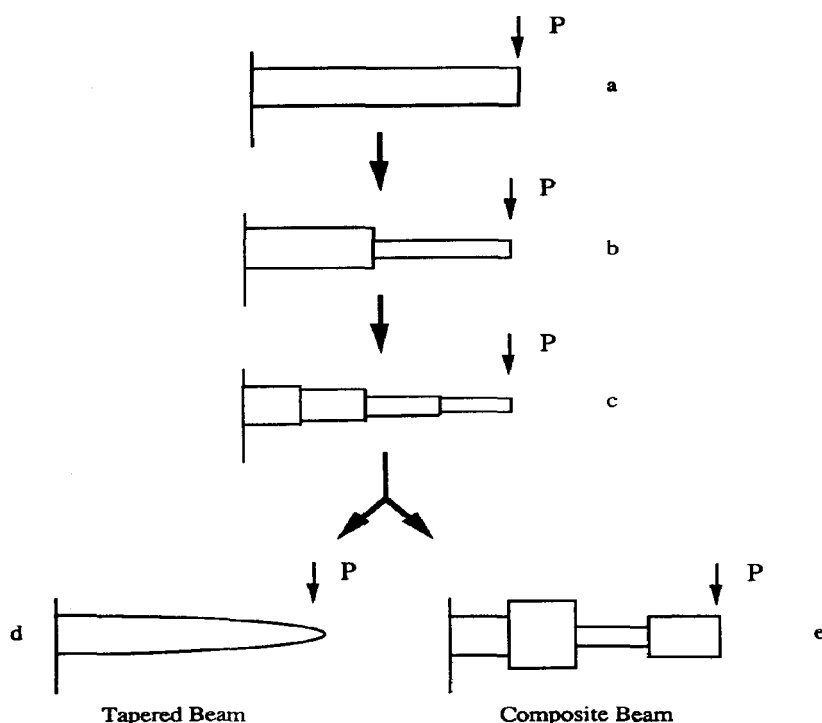


Fig. 2. Optimally directed solutions of beam under flexural load.

the form of the composite beam of Fig. 2e (assuming such bonds could be manufactured).

3. EXAMPLE: INVENTING AN INNOVATIVE REACTOR SYSTEM

The 1stPRINCE design methodology is applied here in the chemical engineering domain for a reactor design problem. Consider a reactor system with maximum reactant conversion and total reactor volume below a prespecified upper limit. The reaction of interest is $A \rightarrow B$, with first-order, constant density kinetics.

This design problem, shown in Fig. 3, is formulated as an optimization problem, where the exiting reactant concentration is minimized subject to the well-mixed reactor design equation and non-negative and maximum total volume constraints. As formulated, this reactor design captures only a subset of the considerations involved in this complex problem. A more complete formulation would involve reactor manufacturing and control system costs, reaction byproduct separation and recycling costs. The optimal reactor volume and conversion would be determined simultaneously rather than fixing the

maximum volume. The simplified formulation is used only to demonstrate the ability of 1stPRINCE to appropriately expand the design space and innovate, but the more complex problem could also be considered. The primitive prototype is given by:

$$\begin{aligned} &\text{minimize } C_{A1}, \\ &\text{subject to } \frac{C_{A0}}{C_{A1}} = 1 + k \frac{V_1}{v_0}, \quad (h_1) \\ &\quad V_1 \geq 0, \quad (g_1) \\ &\quad V_1 \leq V_{\max}, \quad (g_2) \end{aligned}$$

where

C_{A0} = inlet concentration of species A (mol l^{-1}),
 C_{A1} = outlet concentration of species A (mol l^{-1}),
 k = reaction rate constant (s^{-1}),
 v_0 = volumetric feed rate (l s^{-1}),
 V_1 = reactor volume (l),
 V_{\max} = maximum allowable reactor volume (l).

Volume is specified as a dimensional variable. The dimensional variable specification is the *only* domain knowledge input to 1stPRINCE. Qualitative optimization is initially performed by means of monotonicity analysis, which involves determining the possible sets of active constraints for the optimal solution. For ease of presentation, a monotonicity analysis can be demonstrated in tabular form, with the design variables placed in the columns and the objective and constraints placed in the rows. In Table 1 the equality constraint is denoted by " h_1 " and the inequality

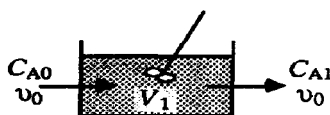


Fig. 3. A constant density reaction in a mixed reaction.

Table 1. Monotonicity table representing the objective and the constraints for the reactor design (first iteration) with g_1 inactive

(a) Unresolved table			(b) Volume constrained from above		
	C_{A1}	V_1		C_{A1}	V_1
Minimize C_{A1}	+		Minimize C_{A1}	+	
$(h_1) \frac{C_{A0}}{C_{A1}} = 1 + k \frac{V_1}{v_0}$?	?	$(h_1) \frac{C_{A0}}{C_{A1}} \leq 1 + k \frac{V_1}{v_0}$	-	-
$(g_1) V_1 \geq 0$		-	$(g_1) V_1 \geq 0$		-
$(g_2) V_1 \leq V_{\max}$		+	$(g_2) V_1 \leq V_{\max}$		+

constraints are denoted by " g_1 " and " g_2 ". Inequality constraints bound the allowable increase or decrease for the corresponding variables. The direction of that bound is given by the sign of the partial derivative of a constraint with respect to each variable when the constraint is represented in the negative null form (Papalambros and Wilde, 1988). The direction of monotonicity of equation constraints is not known *a priori*, so question marks are placed in the appropriate columns of Table 1a. Equality constraints can be written as a set of two inequality constraints, only one of which can be active.

Within a monotonicity table the rules of monotonicity are summarized by the following steps of interpretation:

1. The objective function is always relevant.
2. Each variable column must have at least a "+" and a "-" or otherwise no entries.

An equality constraint is always active, but not necessarily significant (*relevant*) in bonding an optimization problem. Irrelevant constraints can be ignored without affecting the final solution; in optimization theory the corresponding Lagrange multipliers are zero.

Applying the above steps to the unresolved Table 1a, we deduce Table 1b. Constraint h_1 must be active as an inequality constraint of the direction shown in Table 1b, to balance the increase of C_{A1} in the objective function. This also introduces a "-" in the column for V_1 , requiring that constraint g_2 becomes active to avoid an unbounded increase of the reactor volume. Note that " \leq " and " \geq " are used to denote inequalities which emanate from relevant equality or active inequality constraints.

The monotonicity table (1b) is uniquely and properly bounded and constraint g_2 is active. The optimal value of the outlet concentration C_{A1} is determined

symbolically by backsubstituting the active constraints into the objective function, giving the constraint-bound solution:

$$(C_{A1})_{\min} = C_{A0} / \left(1 + k \frac{V_{\max}}{v_0} \right). \quad (4)$$

The designer can either accept the proposed design, or attempt to improve it by employing the principle of DVE. The only dimensional variable in this problem is the reactor volume V_1 , which becomes a *candidate critical variable* and is expanded. Two separate reactors are created with volumes V_{11} and V_{12} , as shown in Fig. 4. The design and non-negative reactor volume constraints (h_1 and g_1 of Table 1b) are distributed to the individual reactors. The total volume constraint (g_2 of Table 1b) now applies to the sum of the individual reactor volumes. The resulting problem formulation is shown in Table 2. Note the creation of the new variables C_{A11} , C_{A12} , V_{11} and V_{12} which did not exist in the original formulation. The notation $x_{m \dots n0}$ denotes a variable x in region o which is derived from region n , ..., which is derived from region m . For example, C_{A12} denotes the exiting concentration from region 2, which is derived from region 1 of the previous design.

Again the monotonicity table is properly bounded and the value of the outlet concentration C_{A2} is determined by backsubstituting the active constraints into the objective function:

$$C_{A12} = C_{A0} / \left(\left(1 + k \frac{V_{11}}{v_0} \right) \left(1 + k \frac{V_{\max} - V_{11}}{v_0} \right) \right). \quad (5)$$

In this iteration there is one *degree-of-freedom* in V_{11} . To establish the optimal value of C_{A12} , the partial derivative of the above expression with respect to V_{11} is equated to zero:

$$\frac{\partial C_{A12}}{\partial V_{11}} = 0 \Rightarrow V_{11} = V_{12} = \frac{V_{\max}}{2}$$

and

$$(C_{A12})_{\min} = C_{A0} / \left(\left(1 + k \frac{V_{\max}}{2v_0} \right)^2 \right). \quad (6)$$

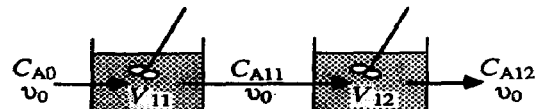


Fig. 4. Reactor system configuration during the second iteration.

Table 2. Monotonicity table for the second iteration with g_{11} and g_{12} inactive

	C_{A11}	C_{A12}	V_{11}	V_{12}
Minimize C_{A12}		+		
$(h_{11}) \frac{C_{A0}}{C_{A11}} \leq 1 + k \frac{V_{11}}{v_0}$	-		-	
$(h_{12}) \frac{C_{A11}}{C_{A12}} \leq 1 + k \frac{V_{12}}{v_0}$	+	-		-
$(g_{11}) V_{11} \geq 0$			-	
$(g_{12}) V_{12} \geq 0$				-
$(g_2) V_{11} + V_{12} \leq V_{\max}$			+	+

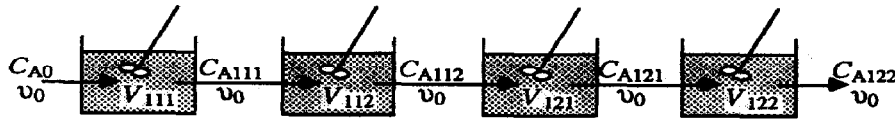


Fig. 5. Reactor system configuration during the third iteration.

This new design has *new features* and satisfies our definition of innovation. It remains to determine whether the optimal outlet concentration of the new design (two separate reactors, each with volume $V_{\max}/2$), is lower than that of the original design of one reactor with volume V_{\max} . Equation (7) compares the outlet concentrations of the one reactor and the other two reactor designs:

$$\begin{aligned} \frac{(C_{A12})_{\min}}{(C_{A1})_{\min}} &= \frac{1 + k \frac{V_{\max}}{v_0}}{\left(1 + k \frac{V_{\max}}{2v_0}\right)^2} \\ &= \frac{1 + k \frac{V_{\max}}{v_0}}{1 + k \frac{V_{\max}}{v_0} + \left(j \frac{V_{\max}}{2v_0}\right)^2} < 1. \end{aligned} \quad (7)$$

Therefore the new design outperforms the original design. The improvement in performance results from the ability of 1stPRINCE to form a new design by creating new variables and providing additional *degrees-of-freedom*. This result demonstrates that the reactor volume is indeed a critical variable in this design problem. As with the previous iteration, the designer can accept the above design or search for a better design. By searching for a better design, 1stPRINCE applies DVE again and creates two reactors out of each reactor, resulting in a total of four independent reactors in series, as shown in Fig. 5. The problem formulation is shown in Table 3.

The monotonicity table is properly bounded and the value of the outlet concentration C_{A122} , is determined by backsubstitution into the objective function:

$$\begin{aligned} C_{A122} &= C_{A0} \left/ \left(1 + k \frac{V_{111}}{v_0}\right) \left(1 + k \frac{V_{112}}{v_0}\right) \right. \\ &\quad \left. \left(1 + k \frac{V_{121}}{v_0}\right) \left(1 + k \frac{V_{122}}{v_0}\right) \right. \end{aligned} \quad (8)$$

Three *degrees-of-freedom*, associated with the reactor volume, have been created in this iteration. The optimal value of C_{A122} is determined by equating the partial derivatives with respect to the three independent volumes to zero:

$$\begin{aligned} \frac{\partial C_{A122}}{\partial V_{111}} = \frac{\partial C_{A122}}{\partial V_{112}} = \frac{\partial C_{A122}}{\partial V_{121}} &= 0 \Rightarrow V_{111} \\ &= V_{112} = V_{121} = V_{122} = \frac{V_{\max}}{4}, \end{aligned}$$

giving

$$(C_{A122})_{\min} = C_{A0} \left/ \left(1 + k \frac{V_{\max}}{4v_0}\right)^4 \right. \quad (9)$$

$(C_{A122})_{\min}$ is always smaller than $(C_{A12})_{\min}$, indicating that this design outperforms the previous one. Again 1stPRINCE has been able to innovate by expanding the design space.

The design equality constraints h_{ij} , and the maximum allowable volume inequality constraint g_2 , remain active across all three iterations. Similarly, the non-negative volume constraints g_{1ij} , remain inactive. These trends are recognized and these constraints are declared *inductively active* and *inductively inactive*, respectively. The methodology proposes the limit of infinitely many and differentially small mixed reactors in series:

$$\begin{aligned} \lim_{N \rightarrow \infty} [(C_{A121} \dots 2_N)_{\min}] \\ &= \lim_{N \rightarrow \infty} \left[C_{A0} \left/ \left(1 + k \frac{V_{\max}}{(2^N)v_0}\right)^{(2^N)} \right] \right. \\ &= C_{A0} / \exp\left(k \frac{V_{\max}}{v_0}\right) \Rightarrow \frac{C_{A0}}{(C_{A1})_{\text{new reactor}}} \\ &= \exp\left(k \frac{V_{\max}}{v_0}\right). \end{aligned} \quad (10)$$

Table 3. Monotonicity table for the third iteration with g_{111} , g_{112} , g_{121} and g_{122} inactive

	C_{A111}	C_{A112}	C_{A121}	C_{A122}	V_{111}	V_{112}	V_{121}	V_{122}
Minimize C_{A122}				+				
$(h_{111}) \frac{C_{A0}}{C_{A111}} \leq 1 + k \frac{V_{111}}{v_0}$	—				—			
$(h_{112}) \frac{C_{A111}}{C_{A112}} \leq 1 + k \frac{V_{112}}{v_0}$	+	—				—		
$(h_{121}) \frac{C_{A111}}{C_{A121}} \leq 1 + k \frac{V_{121}}{v_0}$		+	—				—	
$(h_{122}) \frac{C_{A121}}{C_{A122}} \leq 1 + k \frac{V_{122}}{v_0}$			+	—				—
$(g_{111}) V_{111} \geq 0$					—			
$(g_{112}) V_{112} \geq 0$						—		
$(g_{121}) V_{121} \geq 0$							—	
$(g_{122}) V_{122} \geq 0$								—
$(g_2) \sum V_{ij} \leq V_{\max}$					+	+	+	+

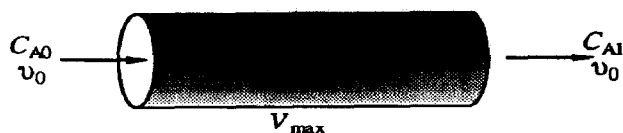


Fig. 6. A plug flow reactor.

where N is the number of reactor volume expansions, creating 2^N separate mixed reactors. The 1stPRINCE methodology has induced a new type of reactor, *using only the knowledge of the mixed reactor design*. The design equation of the new reactor is readily recognized as the *plug flow reactor* design equation for constant density first-order kinetics (Levenspiel, 1972), as shown in Fig. 6.

It is interesting to note that 1stPRINCE has been able to "reinvent" the plug flow reactor without using any heuristics specific to the domain of chemical engineering. The designer is called upon to recognize that for the given reaction kinetics, mixing should be avoided in order to achieve maximum conversion. Other considerations, such as reactor cost, may still favor the mixed reactor, but in this example they have not been captured because they have not been included in the primitive-prototype input model. This information could be modeled in a more complex application.

As expected, application of this methodology to the design of a mixed reactor for a second-order constant density kinetics suggests that a plug flow reactor will outperform a mixed reactor of equal volume. In this case, however, lack of closed form roots when equating the partial derivatives to zero necessitates the use of numerical analysis which the authors have performed for verification but which is omitted from this discussion. For zero-order kinetics, on the other hand, 1stPRINCE notes that the system is indifferent to reactor volume splits, and concludes that volume is not a critical variable.

4. IMPLEMENTATION

The DVE module of the 1stPRINCE methodology has been implemented in Common Lisp and Flavors on a Macintosh II by Cagan (1990). The induction module has been implemented in Franz Lisp and Flavors on Vax-series computers by Cagan and Agogino (1990, 1991). Monotonicity analysis, symbolic algebra and symbolic application of the Karush-Kuhn-Tucker conditions has been implemented in the SYMON/SYMFUNE programs by Choy and Agogino (1986) and Agogino and Almgren (1987). The user must currently input the problem formulation into each module. Because monotonicity analysis is combinatoric, the designer may prune out unwanted paths of reasoning beyond those filtered out by application of the Karush-Kuhn-Tucker conditions and constraint dominance, and the user may also aid the program in complicated symbolic algebra manipulations.

5. CONCLUSION

The 1stPRINCE design methodology uses first principles to perform innovative design in chemical engineering, which until now has had minimal computer-aided support. The approach, in its current state, is applicable to design problems which are posed as optimization problems. More powerful search is attained if the functions involved are monotonic. Since only derivative sign information is needed, only functional relations are required. With the exception of specifying the dimensional variables, these requirements render 1stPRINCE domain independent.

The 1stPRINCE methodology combines fundamental equations, symbolic optimization and search techniques to achieve its task. The methodology has been applied in the mechanical engineering domain to innovate beams and rods. In chemical engineering, 1stPRINCE has been applied to the design of a mixed reactor for maximum conversion of a first-order reaction. Starting from the mixed reactor design equation, the methodology has been able to reinvent the superior design of a plug flow reactor, from first principles and without any domain-specific heuristics.

More complex examples will involve more interplay among performance issues. If, for example, a competing side reaction and economic considerations were modeled, the reactor configuration may have been much different. As more of these issues are addressed, numerical solutions become necessary. The presented methodology could still be used in the development of a design structure in this more complex environment.

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