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Structured Process Optimization Problems

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Abstract

Successive Quadratic Programming (SQP) has been the method of choice for the solution of nonlinear programming problems. For the solution of large problems with SQP based codes, the combinatorial complexity associated with active set methods for the treatment of inequalities has been a bottleneck in exploiting the problem structure. In this paper, we examine the merits of incorporating an interior point method within an SQP framework and the significant computational savings are demonstrated on problems drawn from optimal control. We also provide a novel intepretation of the popularly used predictor-corrector interior point method using the principles of reduced Hessian SQP (rSQP).

INTRODUCTION

With the widespread use of Successive Quadratic Programming (SQP) for process optimization in design, operations and control, a variety of different implementations and strategies have been developed for this algorithm. One important benefit for SQP is its ability to be modified in order to take advantage of a particular problem structure. This is especially important for large, sparse systems that include problems in parameter estimation [1], multiperiod optimization and model predictive control.

However, one hurdle in exploiting the problem structure is an efficient strategy for treating inequality constraints in the QP subproblem. Here, while most of the commonly used QP codes use active set strategies, it has been observed that they can become combinatorially expensive for large problems. A popular alternative has been to explore interior point methods. Previous studies in the application of interior point strategies to SQP have shown considerable promise for these strategies (Morales and Sargent [8], Kyriakopoulou and Kalitventzeff [6]). However, it is especially advantageous when applied to SQP strategies that exploit the structure of the optimality conditions (without inequality constraints).

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To develop this approach, we incorporate the characteristics of the well studied Mehrotra [7] predictor-corrector method, which is a path following algorithm within an SQP framework for the solution of nonlinear programming problems. The method could be used in a full space or reduced space for solving large QP problems. Moreover, it has been tested on a battery of literature examples (e.g., the netlib test set) that involve LPs, QPs and LCPs. In addition, this interior point scheme has been coupled to efficient sparse decomposition strategies that can be modified to take advantage of a particular problem structure.

In this study, we consider a class of optimal control problems that have this characteristic. These problems arise in dynamic state and parameter estimation and in model predictive control. This approach is demonstrated on a wide range of structured optimization problems between 10000 and 100000 variables. Applications are drawn from optimal control and nonlinear model predictive control for the Tennessee Eastman problem.

DEVELOPMENTS IN INTERIOR POINT METHODS

Ever since the publication of the landmark paper by Karmarkar [5] in 1984, interior point methods have been an active research area in the optimization community. The 1990s have seen the emergence of ***primal dual methods*** as an important class of interior point algorithms from a computational as well as a theoretical standpoint. Below, the concept behind primal-dual methods is explained considering a linear program (LP) (1) and its dual (2).

$$min\ c^T x, \qquad s.t.\ Ax = b,\ x \geq 0 \tag{1}$$

$$max\ b^T \lambda, \qquad s.t.\ A^T\lambda + s = c,\ s \geq 0 \tag{2}$$

Primal-dual methods solve the optimality conditions (3) of the problem (1),(2) by applying variants of the Newton's method. Various methods differ in the way the search directions are generated and step lengths are enforced to ensure nonnegativity of x,s.

$$Ax = b$$
$$A^T\lambda + s = 0$$

$$x_i s_i = 0$$
$$(x, s) \geq 0 \tag{3}$$

The monograph by Wright [10] gives an excellent description of primal- dual interior point methods. The extension to nonlinear problems is however nontrivial and has been receiving considerable attention recently.

Nonlinear programing problems

Consider the nonlinear programming problem

$$\begin{aligned} min \quad & f(z) \\ s.t. \quad & g(z) = 0 \\ & h(z) \leq 0 \end{aligned} \tag{4}$$

Bounds on variables are not explicitly treated in (4) as they are a special case of the inequality constraints. The SQP method for solving (4) solves the following QP subproblem (5) at the current point z_k to generate a search direction x_k.

$$\begin{aligned} min \quad & c(z_k)^T x + \frac{1}{2} x^T Q x \\ s.t. \quad & g(z_k) + Ax = 0 \\ & h(z_k) + Cx \leq 0 \end{aligned} \tag{5}$$

$c = \nabla f$, Q is the Hessian of the Lagrangian or a positive definite approximation to it, $A = \nabla g^T$ and $C = \nabla h^T$. Expressing the constants in each subproblem on the right hand side and introducing slack variables s, (5) can be written as

$$\begin{aligned} min \quad & c^T x + \frac{1}{2} x^T Q x \\ s.t. \quad & Ax = b \\ & Cx + s = d \\ & s \geq 0 \end{aligned} \tag{6}$$

The optimality conditions of (6) are given by (7)-(11).

$$Qx + A^T \lambda + C^T \nu + c = 0 \tag{7}$$
$$Ax = b \tag{8}$$
$$Cx + s = d \tag{9}$$
$$SVe = 0 \tag{10}$$
$$(s, \nu) \geq 0 \tag{11}$$

λ and ν are the multipliers of the equalities and inequalities respectively. S and V are diagonal matrices of s and ν.

This system of equations could be solved iteratively by applying Newton's method to a linearization of (7)-(10) and carrying out a line search to enforce the nonnegativity constraints (11). However, this could result in some of the components of (s, ν) from getting too close to the boundary of the nonnegative orthant, and subsequent iterates making little progress towards the solution. This limitation has given rise to the concept of what is known as the *central path* in interior point literature. It is an arc which keeps the iterates biased towards the interior of the nonnegative region $(s, \nu) > 0$, following which forces all the complementarity pairs to converge at a similar rate. The *complementarity gap* μ is a measure of the average value of the products $s_i \nu_i$ and is defined as:

$$\mu = s^T \nu / n \tag{12}$$

A typical strategy used to keep the iterates in the interior is to replace (10) with (13) where $0 \leq \sigma \leq 1$ is a parameter.

$$SVe = \sigma \mu e \tag{13}$$

$\sigma = 1$ corresponds to a pure centering direction, *ie.* moving all the pairwise products to the current average value μ. On the other hand, $\sigma = 0$ gives a standard Newton step. Various *path following methods* differ in the way the search direction is modified and σ is chosen. In the following section we will adapt it to an SQP framework and provide a novel, intuitive interpretation of this procedure in this context.

INTERIOR POINT SQP

SQP has been the method of choice for the solution of nonlinear programming problems. The superlinear convergence properties and the ability to exploit the problem structure have been well studied by many researchers in the past decade. For process engineering problems, in the absence of inequality constraints, various decomposition strategies can be applied to greatly improve the efficiency for large scale problems. On the other hand, application of active set strategies to the imposition of inequality constraints can make these problems much more expensive to solve. The motivation to incorporate an interior point strategy within an SQP framework arises from this handicap of the active set strategies. We would like to integrate the interior point method and SQP in such a way that we still retain fast linear performance as well as the structured decomposition.

To develop this approach, we apply certain characteristics of the well studied Mehrotra [7] predictor-corrector algorithm. Each Mehrotra iterate solves an affine scaling *predictor* step (14) and a *corrector* step (15) alternately. r_1, r_2, r_3 are the residuals of the equations at the current point. The predictor step helps in reducing the complementarity gap and centering is accomplished through the corrector step which also incorporates a second order correction term.

$$\begin{bmatrix} Q & A^T & C^T & 0 \\ A & 0 & 0 & 0 \\ C & 0 & 0 & I \\ 0 & 0 & S & V \end{bmatrix} \begin{bmatrix} \Delta x^p \\ \Delta \lambda^p \\ \Delta \nu^p \\ \Delta s^p \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ SVe \end{bmatrix} \tag{14}$$

$$\begin{bmatrix} Q & A^T & C^T & 0 \\ A & 0 & 0 & 0 \\ C & 0 & 0 & I \\ 0 & 0 & S & V \end{bmatrix} \begin{bmatrix} \Delta x^c \\ \Delta \lambda^c \\ \Delta \nu^c \\ \Delta s^c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \sigma \mu e - \Delta S_p \Delta V_p e \end{bmatrix} \tag{15}$$

To interpret the predictor-corrector method, let us pose the subproblem (6) as (16) with the optimality conditions (7)-(9) as constraints. Note that the complementarity constraint is different from (10) and (13).

$$\begin{aligned} min \quad & f(q) \\ s.t. \quad & Qx + A^T\lambda + C^T\nu + c = 0 \\ & Ax = b \\ & Cx + s = d \\ & SVe = qe \end{aligned} \tag{16}$$

Since (16) has just 1 degree of freedom (q), consider the iterative solution of (16) in the context of a reduced Hessian SQP framework [3]. Linearization of the constraints give:

$$\begin{bmatrix} Q & A^T & C^T & 0 & 0 \\ A & 0 & 0 & 0 & 0 \\ C & 0 & 0 & I & 0 \\ 0 & 0 & S & V & -e \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \\ \Delta s \\ \Delta q \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ S_k V_k e - q_k e \end{bmatrix} \tag{17}$$

Following the analysis in [3] it could be shown that

$$\Delta q = -f'(q)/f''(q) \tag{18}$$

The null space and range space steps are given by (19) and (20).

$$\begin{bmatrix} Q & A^T & C^T & 0 \\ A & 0 & 0 & 0 \\ C & 0 & 0 & I \\ 0 & 0 & S & V \end{bmatrix} \begin{bmatrix} \Delta x^z \\ \Delta \lambda^z \\ \Delta \nu^z \\ \Delta s^z \end{bmatrix} = - \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{f'(q)}{f''(q)} e \end{bmatrix} \tag{19}$$

$$\begin{bmatrix} Q & A^T & C^T & 0 \\ A & 0 & 0 & 0 \\ C & 0 & 0 & I \\ 0 & 0 & S & V \end{bmatrix} \begin{bmatrix} \Delta x^y \\ \Delta \lambda^y \\ \Delta \nu^y \\ \Delta s^y \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ S_k V_k e - q_k e \end{bmatrix} \tag{20}$$

We choose $f(q) = \frac{1}{K} q^K$ where K is a constant. Then,

$$\frac{f'}{f''} = \frac{q}{K-1} \tag{21}$$

Define c as in (22). For $c \to 0, K \to 2$. (21) reduces to (23).

$$K = \frac{2-c}{1-c} \tag{22}$$

$$\frac{f'}{f''} = (1-c)q \tag{23}$$

Combining the null and range space steps and from (23) we get

$$\begin{bmatrix} Q & A^T & C^T & 0 \\ A & 0 & 0 & 0 \\ C & 0 & 0 & I \\ 0 & 0 & S & V \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \\ \Delta s \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ S_k V_k e - c q_k e \end{bmatrix} \tag{24}$$

A second order correction on the constraints is then applied to the step obtained from (24). It is important to note that on the right hand side of (24) we have obtained the term $cq_k e$, which does the centering and keeps the iterates in the interior of the nonnegative orthant. Compare this term with (13) with $q_k = \mu$ and $c = \sigma$. Note that for $c = 0$ we get an affine scaling step (14). Hence, by an appropriate choice of the objective function, we have a framework which incorporates the characteristics of the concept of centering in interior point methods within an SQP method for the solution of nonlinear programming problems. This procedure could be implemented within a full space or a reduced space method and the strong theoretical and superlinear convergence properties which have been developed for these methods should apply in this case as well. We will henceforth refer to this framework as ISQP.

A comparison of this approach to that of Mehrotra [7] for the solution of LPs and Linear Complementarity Problems (LCPs) would be of interest. Mehrotra's approach is two-pronged as explained at the beginning of this section. It does not consider the centering term $\sigma\mu_k e$ in the predictor step. In the implementations of this method, the centering parameter is chosen adaptively and incorporated along with the second order correction term in the corrector step. Testing of the performace of ISQP and Mehrotra's method on the LP test problems from the Netlib directory gave similar performances in terms of number of iterations as seen in Table 1. The number of iterations for different values of c for the ISQP approach are also shown. α in the third column corresponds to the fractional line search step taken in the penultimate iteration. Since the objective of this paper is to look at structured process optimization problems, we consider more of such examples in the following section.

Problem	Var/Ineq/Eq	ISQP/c values			PC
		.01	.01(1-α)	.005	
recipe	180/275/90	13	13	13	14
sierra	2036/4771/528	24	23	24	24
80bau3b	9799/15047/498	65	57	58	57

Table 1: Number of iterations of ISQP and Mehrotra predictor-corrector on LP test problems

EXAMPLES

In this section, we consider two examples. The first is an optimal control problem which demonstrates that the number of iterations in interior point and active set methods could differ by orders of magnitude for a large number of time steps. The second example is the Tennessee Eastman challenge problem [4].

An important aspect of optimal control and dynamic optimization problems that causes difficulties is the presence of inequality constraints. Inequalities in these problems arise from safety considerations as well as physical limitations upon the control input. In the formulation the number of inequalities grows with the number of time steps. As a result the worst case scenario of an active set approach could considerably slow the solution time. Interior point methods hold promise not only because they tend to converge in a fixed number of iterations, but also because of their structure. Unlike active set methods, interior point formulations have a fixed structure that is sparse and almost block diagonal. Because of this sparse fixed structure and the block diagonal form, sparse linear algebra solvers should be very efficient.

Example 1: Illustrative Optimal Control Problem

In the test problems we considered, active set methods generally require a number of iterations that grows superlinearly with the size of the problem, whereas with interior point methods, the number of iterations is constant independent of the number of time steps. As an example, we compare the performance of the following quadratic optimal control problem:

$$\begin{aligned} \min \quad & \int_0^1 (2x_1^2(t) + x_2^2(t) + 6u^2(t))dt + 2x_1^2(1) + x_2^2(1) \\ s.t. \quad & x_1'(t) = x_2(t) \\ & x_2'(t) = -x_1(t) + u(t) \\ & -1 \leq u(t) \leq 1 \\ & x_1(0) = 15 \\ & x_2(0) = 5 \end{aligned} \tag{25}$$

This problem has a control profile which is at its bounds for about half of the time horizon as seen in figure 1. In figure 2 we compare the number of iterations for ISQP, and two active set based codes, MINOS and QPSOL. As seen from the figure, the number of iterations for MINOS and QPSOL increase with the number of time steps (active constraints), whereas the interior point method keeps at a constant 6 iterations.

Example 2: Model Predictive Control of the Tennessee Eastman Reactor

At each time step of a Model Predictive Control(MPC) algorithm an optimal control problem of output horizon, n_y, and input horizon n_u must be solved. Consequently any MPC algorithm must have an efficient means of solving the optimal control problem. The efficiency is critical with the Tennessee Eastman Reactor because of its inherent nonlinearity. Solutions of optimal control problems possessing nonlinear differential algebraic models requires a Newton method to iterate to the final solution. Consequently the solution of the linearized optimal control problem must be efficient. It was the goal of this example to investigate the viability of using interior point techniques for a simultaneous approach to solving the nonlinear optimal control problem.

The Tennessee Eastman challenge problem was originally presented by Downs and Vogel [4]. In this paper the authors describe the process, present a black box simulator, and purposely gave no model. The model of the Tennessee Eastman Plant used in this example was taken from the work of Ricker and Lee [9]. Since the whole Tennessee plant has 26 differential equations, 83 algebraic constraints and 323 variables, this example confines its scope to the control of the unstable reactor. The reactor is a jacketed CSTR,two phase system, with the reaction dynamics occurring in the vapor phase. The DAE model of 8 differential and 28 algebraic equations is given in the Appendix. With the inlet vapor compositions, $y_{i,6}$, down stream pressure, P_s, activity coefficients, $\gamma_{i,r}$, vapor pressure P_i^{sat}, and parameters α_i and β_7 fixed there are 38 variables. Tight control of this reactor is nec-

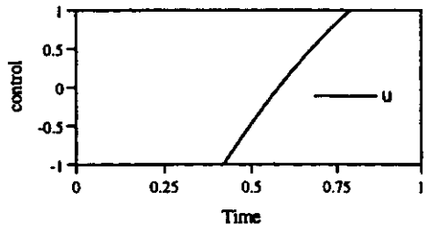

Figure 1: Control profile for problem (25).

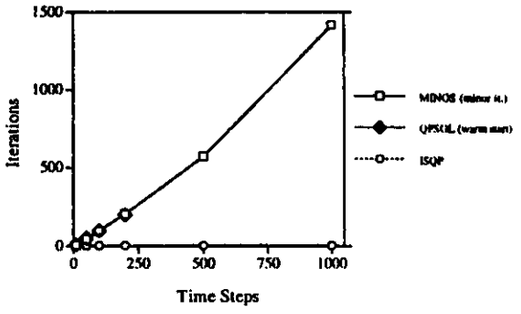

Figure 2: Number of iterations for ISQP, MINOS and QPSOL for problem (25).

essary because there exists a tendency for the pressure to increase exponentially. The presence of this unstable mode can cause problems with stable integration due to the accumulation of round off error. In order to guarantee stable integration an implicit Runge-Kutta/collocation method is needed as well as an addition of an endpoint constraint on the unstable mode, pressure. The endpoint constraint changes the problem from an unstable initial value problem to a stable two point boundary value problem(BVP)[2]. The solution of the BVP is trivial when a simultaneous approach is used where as sequential strategies require multiple shooting techniques to handle ill conditioning.

The differential system was discretized using collocation on finite elements. The finite elements were chosen to be equally spaced with a length value of 6 minutes. The step lengths for model predictive controller were chosen to have this same time span. Within each finite element two collocation points were used. As a result the discretized system contains 110 variables and 108 equality constraints per time step. It is important to note that the number of variables takes into consideration the fact that the control variables reactor temperature, T_r, and inlet feed flow rate, F_6, are constant throughout the finite element.

No.	Variable	Min.	Max	Δ Max.
1	F_6 (kmol/hr)	800	2200	20
2	T_r ($^\circ K$)	388	401	2
3	V_{Lr} (M^3)	2	30	1.0
4	P_r (kPa)	P_s	2900	-

Table 2: Operational Constraints

The optimal control problem also imposed 14 inequality constraints per time step. They involve maximum and minimum bounds as well as rate of change bounds on the inputs, F_6 and T_r,and the outputs, V_{Lr} and P_r. The values are given in Table 2. The control variable V_{Lr} represents the reactor volume and P_r, the reactor pressure. The lower bound on P_r forces the reactor pressure to be higher than the downstream pressure. During the control horizon,the first n_u steps, the rate of change is given by the table values while for the remaining $n_y - n_u$ steps the change is set equal to zero. The remaining constraints of the optimal control problem include the initial conditions on the differential variables. The objective function is given by (26).

The nonlinear system was solved using SQP with the Hessian approximated by the second derivative of the objective. The QP subproblems were solved using the augmented equation form which is obtained by reducing (24) to the space of primal variables, equality multipliers, and inequality multipliers by substitution of the slacks by the relation $\Delta s = -V^{-1}S\Delta\nu$. The resulting system takes the form (27), where $r_4 = r_3 + V^{-1}S(SVe - cqe)$.

$$\begin{aligned} min \quad & \sum_{i=1}^{n_y} 0.034(P_r(i) - P_r^{ss})^2 + 0.6(F_7(i) - F_7^{ss})^2 \\ & + \sum_{j=1}^{n_u} 0.2\Delta F_6(j)^2 + 0.4\Delta T_r(j)^2 \end{aligned} \tag{26}$$

$$\begin{bmatrix} Q & A^T & C^T \\ A & 0 & 0 \\ C & 0 & -V^{-1}S \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta\nu \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_4 \end{bmatrix} \tag{27}$$

The system can also be restructured by time steps to yield an almost block diagonal system(ABD) as illustrated by the reordered matrix.

$$\begin{bmatrix} Q_1 & A_1^T & C_1^T & 0 & & & & & & \\ A_1 & 0 & 0 & \bar{A}_1 & & & & & & \\ C_1 & 0 & w_1 & \bar{C}_1 & & & & & & \\ 0 & \bar{A}_1^T & \bar{C}_1^T & Q_2 & A_2^T & C_1^T & 0 & & & \\ & & & A_2 & 0 & 0 & \bar{A}_2 & & & \\ & & & C_2 & 0 & w_2 & \bar{C}_2 & & & \\ & & & 0 & \bar{A}_2^T & \bar{C}_2^T & \ddots & & & \\ & & & & & & & Q_n & A_n^T & C_n^T \\ & & & & & & & A_n & 0 & 0 \\ & & & & & & & C_n & 0 & w_n \end{bmatrix}$$

Where

$$w_i = -V_i^{-1}S_i$$

Both the almost block diagonal system and the original ordered system forms were used for simulation studies. The simulation studies also compared the speed of both the sparse symmetric solver MA27 and unsymmetric solver MA28 from Harwell. In the solution of the nonlinear optimal control problem the initial point was chosen close to the steady state values. As a result relatively few Newton iterations were required. The input horizon for all cases was chosen to be 4. For all of the simulations the number of Newton iterations were the same. The number of interior point iterations for each simulation only varied by one or two. The results for a Mehrotra predictor-corrector implementation and ISQP are given in Table 3. This table also gives information about the problem size including the number of primal variables, equality constraints, inequality constraints, the number of active inequalities at the solution as well as the total cpu time in seconds that it took to solve the nonlinear optimal control problem. Table 4 illustrates the time per iteration for all of the simulations. The results show that the MA28 implementations were faster than the MA27 versions. However, MA27 cpu times appeared to grow linearly with problem size while MA28s did not. The simulations also show that the sparse solvers were unable to take advantage of the almost block diagonal ordering. The use of a sparse multifrontal algorithm,

N_y	Var/Eq/Ineq/Act	Time	Newt/PC/ISQP
10	1100/1081/140/24	8.1	2/16/17
20	2200/2161/280/64	54.0	4/39/38
40	4400/4321/560/144	178.2	3/31/36
80	8800/8641/1120/304	566.7	3/33/36
160	17600/17281/2240/624	1462	3/31/30

Table 3: Problem size, cpu seconds and iterations using MA28 and original ordering with Mehrotra predictor-corrector and ISQP implementations

N_y	Time MA28	Time MA28-ABD	Time MA27	Time MA27-ABD
10	0.51	0.77	2.31	2.40
20	1.39	1.90	4.64	4.71
40	5.75	6.02	9.99	12.68
80	17.17	16.79	23.13	24.99
160	47.17	46.83	50.67	62.38

Table 4: Time per interior point iteration for MA28, MA28 ABD Ordering, MA27 and MA27 ABD ordering

such as MA42, is expected to take advantage of the ADB structure and provide improved cpu times.

As is typical of interior point algorithms the number of iterations required to solve the quadratic programming problems is independent of the number of inequalities in the problem. In fact the simulation examples revealed that approximately 10 interior point iterations are required per QP. The benefit of using interior point techniques becomes evident when the simulation with an output horizon of 160 time steps is examined. In that problem the solution has 624 active constraints. If an active set method using the typical one constraint at a time technique were used the solution would require at least 624 iterations! Keeping this in mind, the 33 iterations taken by the interior point technique to solve the whole problem seems trivial. Thus, interior point techniques provide great promise for the solution of problems with a large number of inequality constraints.

The question of whether or not the solution times are fast enough for online model predictive control is debatable. In an online implementation it is reasonable that succeeding time steps will have nearly identical solutions. With such good starting points, the overall number of Newton steps should be small. Taking this into consideration and the fact that the time steps for this problem are 6 minutes long, an output horizon of 20 or 40 time steps could be implementable.

CONCLUSIONS

An intuitive interpretation of the predictor corrector interior point methods using reduced Hessian SQP has been derived in this paper. A framework for the adaptation of a path following primal dual interior point method with an SQP approach has been also been developed. As demonstrated on the example problems, this results in an efficient methodology for the treatment of inequalities while retaining the ability of SQP methods to take advantage of the problem structure at the same time.

Issues related to linear algebra are still under investigation and some of the results using the Harwell subroutines MA28 and MA27 are given in this paper. Detailed study of the linear algebra is planned in the future. Solution of larger examples drawn from dynamic optimization problems in chemical engineering using this methodology is also under consideration.

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Appendix: Model for Example 2

$$
\begin{aligned}
\frac{dN_{A,r}}{dt} &= y_{A,6}F_6 - y_{A,7}F_7 - R_1 - R_2 - \frac{1}{3}R_3 \\
\frac{dN_{B,r}}{dt} &= y_{B,6}F_6 - y_{B,7}F_7 \\
\frac{dN_{C,r}}{dt} &= y_{C,6}F_6 - y_{C,7}F_7 - R_1 - R_2 \\
\frac{dN_{D,r}}{dt} &= y_{D,6}F_6 - y_{D,7}F_7 - R_1 - R_3 \\
\frac{dN_{E,r}}{dt} &= y_{E,6}F_6 - y_{E,7}F_7 - R_2 - \frac{1}{3}R_3 \\
\frac{dN_{F,r}}{dt} &= y_{F,6}F_6 - y_{F,7}F_7 + R_3 \\
\frac{dN_{G,r}}{dt} &= y_{G,6}F_6 - y_{G,7}F_7 + R_1 \\
\frac{dN_{H,r}}{dt} &= y_{H,6}F_6 - y_{H,7}F_7 + R_2
\end{aligned}
$$

$$
\begin{aligned}
x_{i,r} &= \frac{N_{i,r}}{\sum_{i=D}^{H} N_{i,r}} && i = D, E, ..., H \\
y_{i,7} &= \frac{P_{i,r}}{P_r} \qquad i = A, B, ..., H \\
P_r &= \sum_{i=A}^{H} P_{i,r} \\
P_{i,r} &= \frac{N_{i,r} R T_r}{V_{V_r}} && i = A, B, C \\
V_{L_r} &= \sum_{i=D}^{H} \frac{N_{i,r}}{\rho_i} \\
V_{V_r} &= V_r - V_{L_r} \\
P_{i,r} &= \gamma_{i_r} x_{i_r} P_i^{sat} && i = D, E, F, G, H
\end{aligned}
$$

$$
\begin{aligned}
R_1 &= \alpha_1 V_{V_r} exp[44.06 - \frac{42600}{1.987 T_r}] P_{A,r}^{1.08} P_{C,r}^{0.311} P_{D,r}^{0.874} \\
R_2 &= \alpha_2 V_{V_r} exp[10.27 - \frac{19500}{1.987 T_r}] P_{A,r}^{1.15} P_{C,r}^{0.370} P_{E,r}^{1.00} \\
R_3 &= \alpha_3 V_{V_r} exp[59.50 - \frac{59500}{1.987 T_r}] P_{A,r} (0.77 P_{D,r} + P_{E,r}) \\
F_7 &= \beta_7 \frac{5722}{M_7} \sqrt{P_r - P_s}
\end{aligned}
$$