Optimized Space Shuttle First Stage Guidance Targets

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Abstract

This paper describes the optimization of Space Shuttle First Stage Open-Loop Guidance targets for mission STS-49 using Sequential Simplex Optimization. A subsequent Central Composite Design experiment was conducted to model the response surface in the region of the optimum.

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Section 1

Introduction

The system this project will study is a software simulation of the powered-flight portion of a Space Shuttle ascent trajectory. Figure 1.1 illustrates a nominal trajectory profile and Figure 1.2 illustrates the various components of a mission.

Powered flight starts at Solid Rocket Booster (SRB) ignition and ends at Space Shuttle Main Engine (SSME) cut-off (MECO). A typical powered flight trajectory lasts 508 seconds (8 minutes, 28 seconds) from lift-off to MECO commanded. The experiment will focus on the first part of the flight, from lift-off to SRB separation (the first 2 minutes, 4 seconds of powered flight). This phase of flight is called “first stage,” and the separation of the SRBs from the orbiter and External Tank (ET) is called “staging.”

Shuttle First Stage starts at SRB ignition. The vehicle maintains an attitude hold (vertical pitch) until clear of the tower, for about 6 seconds. At this point Single-Axis Roll (SAR) maneuver is commanded to steer the vehicle to a heads-down attitude and a pitch/yaw direction optimum for the target orbital inclination for the mission. For STS-49 the target orbital inclination is 28.45 degrees, which is ($\approx$) the latitude of Kennedy Space Center (KSC). Therefore the commanded yaw at SAR is about 90°. The commanded pitch is designed to minimize aero forces, moments on the aerosurfaces (elevons and body flap) and ET heating. SAR pitch is usually around 65°. Engine throttle is also commanded at SAR initiation from 100% to the first design level, either 100% or 104% rated power level.

The vehicle continues flying the First Stage guidance pitch/yaw design profile (continuing a heads-down roll attitude of 180°) until maximum dynamic pressure is reached. At this point the engines are throttled back to (usually) 67% until the dynamic pressure begins to fall. The engines are then throttled back up to 104% for the remainder of First Stage.

The first part of the experiment will determine the region of the optimum First Stage guidance targets by using sequential simplex optimization. A subsequent central composite design experiment will be conducted to model the region around the optimum. During actual flight the shuttle hardware may malfunction and induce a variance in, among other things, the guidance targets. A description of the response surface around the optimum targets can be used by real-time flight support personnel to gauge how these anomalies effect performance. If it is determined that performance has been impacted to the point where a minimum orbit (referred to as an Abort-to-Orbit, or ATO call) cannot be reached then an RTLS (Return to Launch Site) or TAL (Transoceanic Landing) abort is declared and the shuttle changes targeting to either land back at KSC or at one of the landing sites in Europe or Africa.

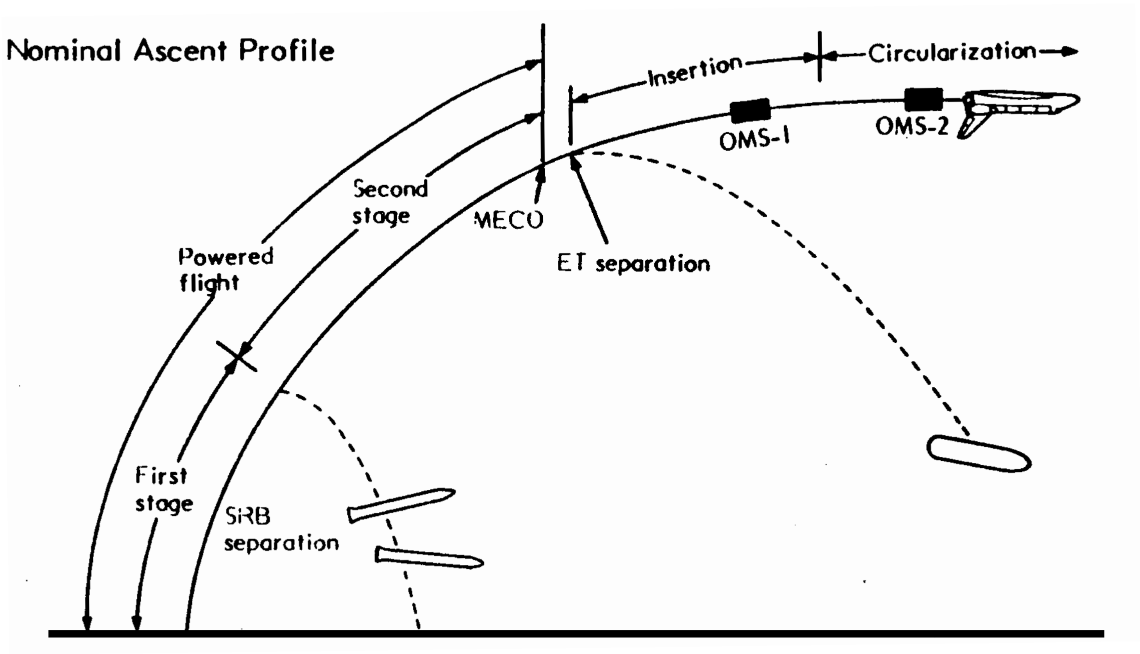

Figure 1.1: Space Shuttle Ascent Trajectory Profile

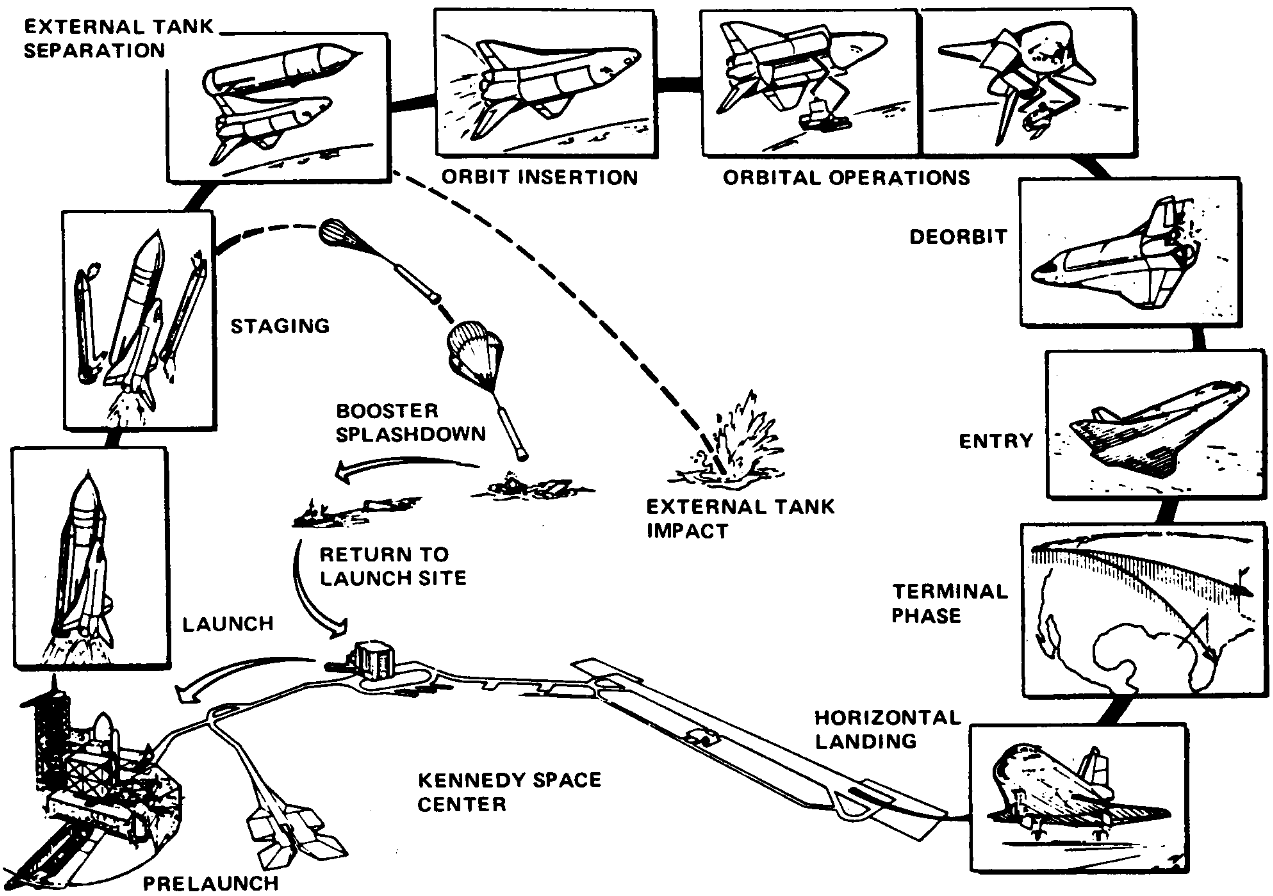

Figure 1.2: Components of a Space Shuttle Mission

Section 2

Background

First stage uses a maneuver called Single Axis Roll (SAR), starting at about 6 seconds after lift-off, to put the vehicle into the proper orientation (heads down—roll angle $180°$) and direction. Figure 2.1 illustrates the shuttle roll, pitch and yaw directions and axes. Also during first stage the engine throttle level is reduced to keep the vehicle from travelling too fast in the low atmosphere. It is during this throttle-down period the the vehicle experiences maximum aerodynamic pressure on the aerosurfaces. The equation for dynamic pressure is

$$\underline{q} = \frac{1}{2}\rho(r)\ v^2$$

where $\underline{q}$ (referred to as QBar) is the dynamic pressure, ρ is the atmosphere density (a function of altitude r) and v is the aerodynamic reference speed of the vehicle. The throttle-down time is reached when the vehicle approaches maximum dynamic pressure and the time to throttle the engines back up is the time when $\underline{q}$ begins to decrease.

The three factors for the study are SAR pitch & yaw angles and the engine throttle-up time. The principle response to be measured is the weight of the vehicle at main engine cut-off (MECO). The optimum trajectory will burn the smallest amount of fuel, and therefore the MECO weight can be used to gauge the steering performance. This experiment will therefore attempt to maximize the vehicle weight at MECO.

There are several other responses which are actually constraints on the vehicle trajectory. These responses (constraints) will be scaled using desirability functions and normed together to obtain a net constraint response. The net constraint response will range from 0 to 1. The normed results of the desirability functions will be multiplied by the MECO weight to obtain a single response which the simplex algorithm will maximize.

The desirability functions scale the constraints using exponential decay from the optimum, illustrated in Figure 2.2. Exponential functions were used since for large deltas from the optimum the exponential will return a small, non-zero value. Choosing a desirability function that returns zero for certain constraints yields a net response of zero and this tells the simplex algorithm very little. Two responses far from the optimum may not be equally "bad" but two zero results appear that way. Using exponential functions gives the simplex a non-zero result which is used to guide the progress to the optimum.

The constraints to be implemented in this study are as follows:

Throttle-Altitude Constraint. A minimum throttle level, as a function of altitude, is required to avoid loss of SSME efficiency. This loss is caused by separation of exhaust gases at the engine nozzle lip from the nozzle. The loss of efficiency reduces engine thrust and may induce high side loads on the engine bells, potentially resulting

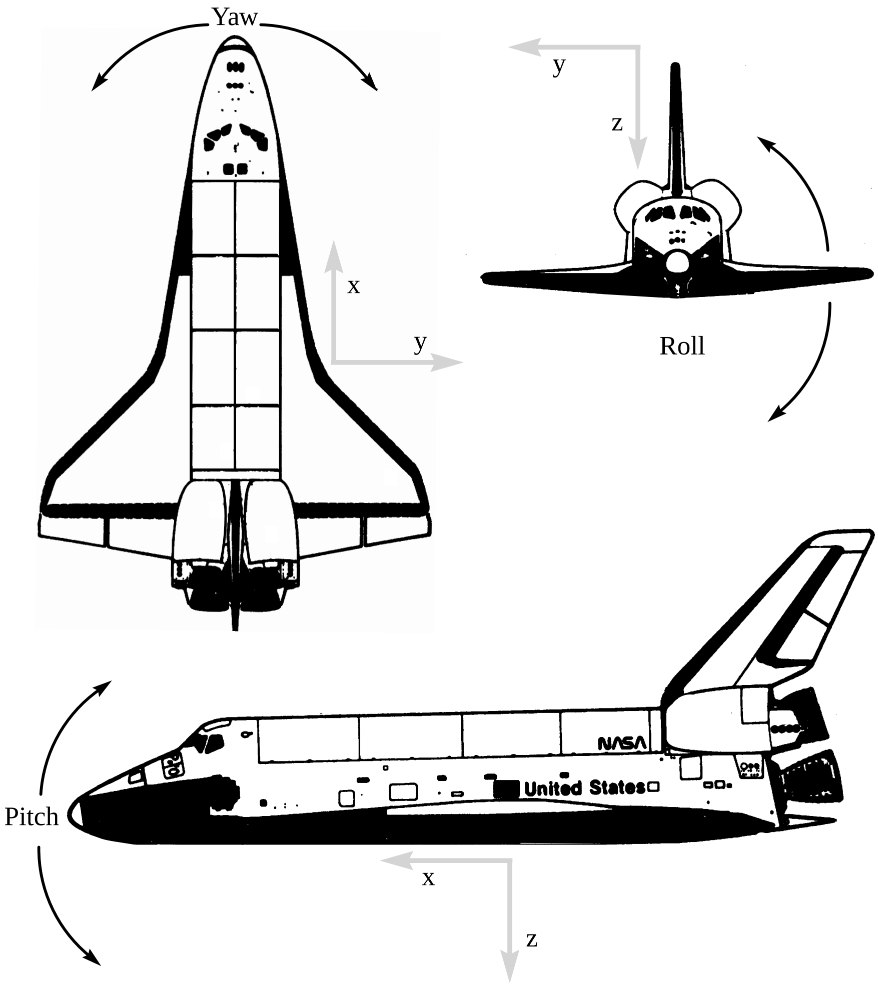

Figure 2.1: Shuttle Roll, Pitch and Yaw Attitude

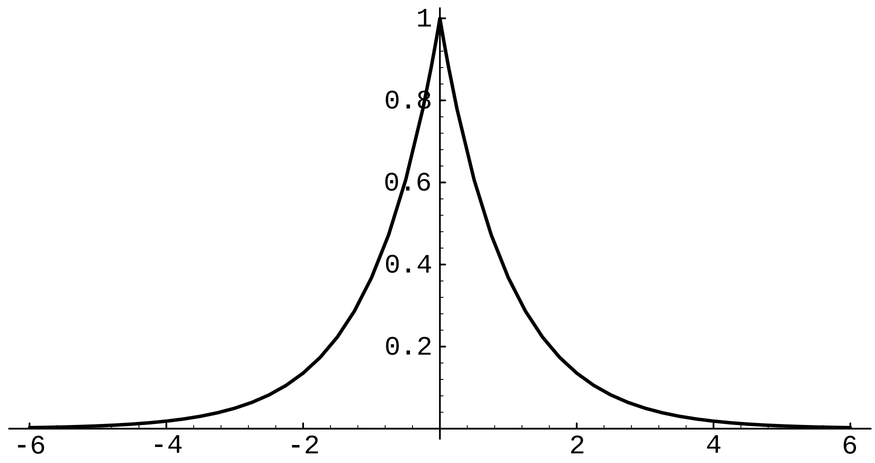

Figure 2.2: Exponential Decay

in engine bell collision and nozzle damage. The engine throttle percent is constrained above a minimum and is illustrated in Figure 2.3.

Yaw Discontinuity at PEG Guidance Convergence. This constraint deals with the amount of corrective steering that second stage guidance (closed-loop Powered Explicit Guidance (PEG)) must command to bring the trajectory back toward the MECO targets. Closed-loop guidance is where navigation feeds back to guidance actual position, velocity and attitude so guidance can steer to specific targets in the sky. Open-loop guidance is used in first stage which flies a velocity/attitude profile (if you're going this fast, then you should have this roll, pitch and yaw attitude). Second-stage steering to take out a yaw discontinuity means spending fuel to change direction. This spent fuel degrades performance. The magnitude of the performance degradation can be approximated as the arc length between the actual and desired velocity vectors, or $|\vec{v}|\theta$, where θ is the angle in radians of the yaw discontinuity.

The yaw discontinuity is minimized by an optimum SAR yaw angle. This is the first factor in the experiment.

Early Dynamic Pressure Overshoot. Reference Figure 2.4. The SSME throttles can be changed at a maximum rate of 10%/second. If dynamic pressure is building too fast then when the maximum dynamic pressure is reached the finite throttle-down time required will be insufficient to prevent a (short) maximum dynamic pressure exceedence. A typical throttle-down change is from 104% to 67% rated thrust and requires about 4 seconds to complete. The slope of the dynamic pressure curve in the "early QBar" region must be shallow enough to just reach the maximum dynamic pressure limit as the engines are finishing throttling back. The early dynamic pressure overshoot is adjusted by varying the SAR pitch. A lower pitch (more horizontal attitude) applies more of the engine thrust force to increasing speed and less to gaining altitude. SAR pitch is the second factor in the experiment.

Late Dynamic Pressure Overshoot. Reference Figure 2.5. The late dynamic pressure constraint results from the dynamic pressure falling off due to decreased atmospheric density as the vehicle gains altitude. At this time the SSMEs are throttling at 67%. When the pressure begins to drop the engines can be throttled back up to 104%, again at a rate of 10%/second. Throttling up too early would, again, cause a maximum dynamic pressure exceedence. The earliest time the engines can be throttled back up is the third factor in the experiment.

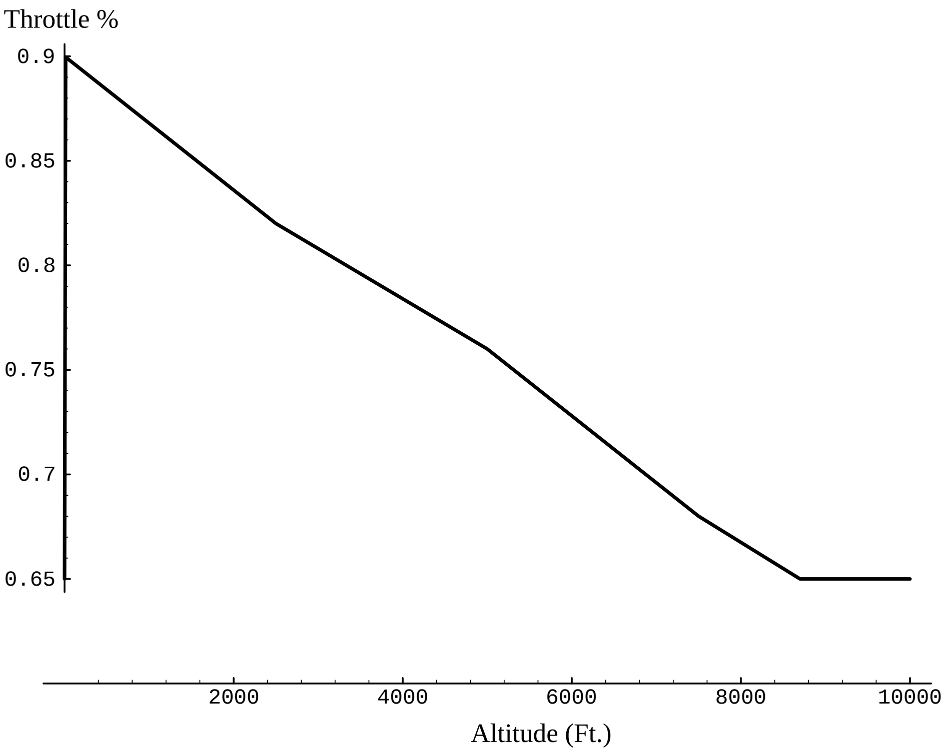

Figure 2.3: Throttle-Altitude Constraint Line

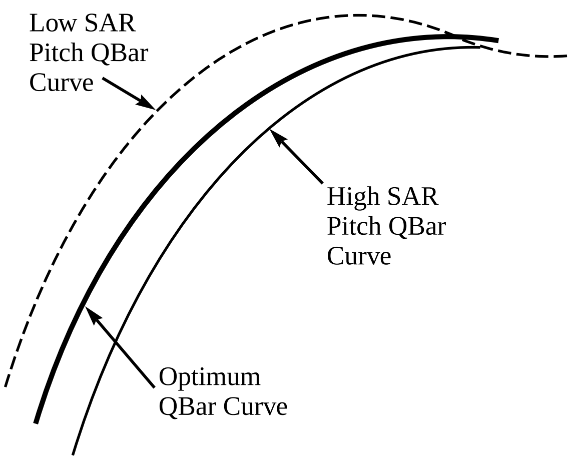

Figure 2.4: Early Maximum Dynamic Pressure (QBar) Region

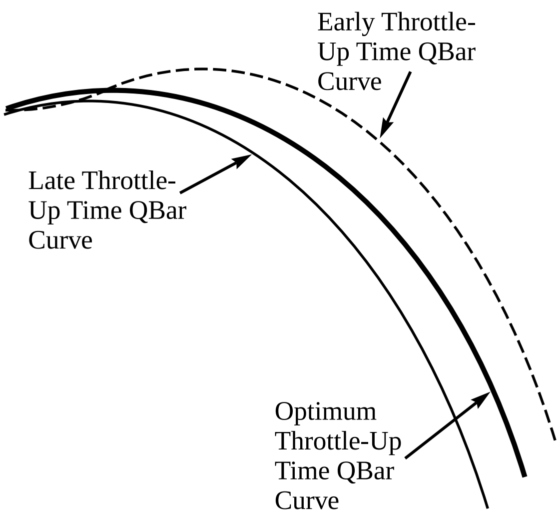

Figure 2.5: Late Maximum Dynamic Pressure (QBar) Region

Section 3

Simplex Optimization

The region of the optimum for the three factors was determined using a variable-sized sequential simplex. The initial simplex vertexes spanned the factor space and was generated using the corner initial simplex algorithm. There are four initial vertexes equal to the number of factors plus 1.

Vertex	Pitch	Yaw	Throttle-Up Time
1	65.0	85.0	50.0
2	80.0	85.0	50.0
3	65.0	95.0	50.0
4	65.0	85.0	65.0

Variable-size simplex was used since the system is a software simulation. Different combinations of factors may command the Shuttle to fly a trajectory which exceeds some tolerance, and this would cause the program to abort. This, however, is the worst that can happen (no equipment will be at risk) and therefore we can push the limits. A principal goal of this project was to explore a wide region of the factor space to answer the question: Are there several optimum points in the response surface? What we expected to find is that there is only one optimum, and this is what the results show.

The data was generated at Rockwell Space Operations Company using the Simulation of Rocket Trajectories (SORT) program. Software scripts were developed to run the experiment without modification to SORT. Figure 3.1 illustrates the flow of data and the various scripts and programs. The output of these scripts is a listing of vertexes similar to the results listed in the Chapters 3 and 4 exercises in the Sequential Simplex Optimization text. The approach to the region of the optimum is best illustrated by three 2-dimension plots (Figures 3.2, 3.3 and 3.4). Each picture is looking down one axis. Combining the data into a 3-dimensional plot cluttered the approach to optimum progress since the initial simplex spanned the factor space. The simplex algorithm required about 28 iterations to arrive in the region of the optimum. The algorithm was allowed to run on to investigate how close the simplex could get to the optimum point. The cut-off criteria was a difference in responses from the best to worst vertexes of less than 50. The The algorithm terminated with final vertexes of

Vertex	Pitch	Yaw	Throttle-Up Time
1	66.4958	90.1981	55.3355
2	66.4944	90.1961	55.3470
3	66.4956	90.1987	55.3312
4	66.4936	90.1966	55.3540

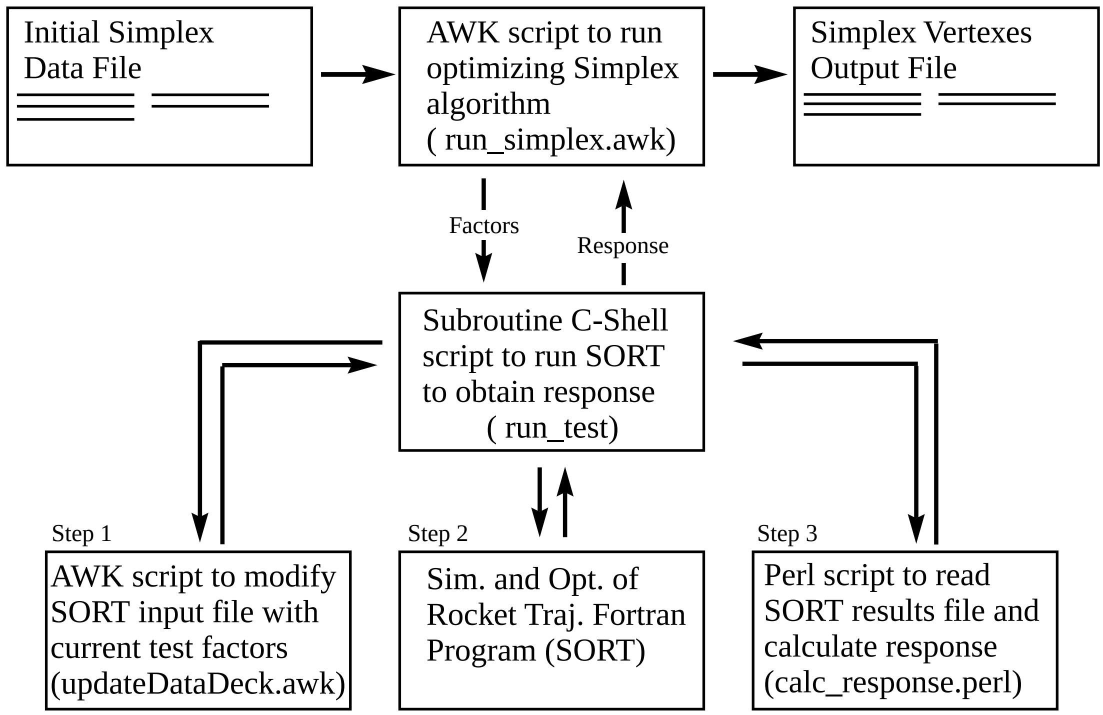

Figure 3.1: Rockwell Software Scripts and Programs

These values compare, to the second rounded decimal place, with the SORT program's single-factor-at-a-time optimization results. The center point used in the central composite design in the next section is a rounded average of the final simplex vertexes.

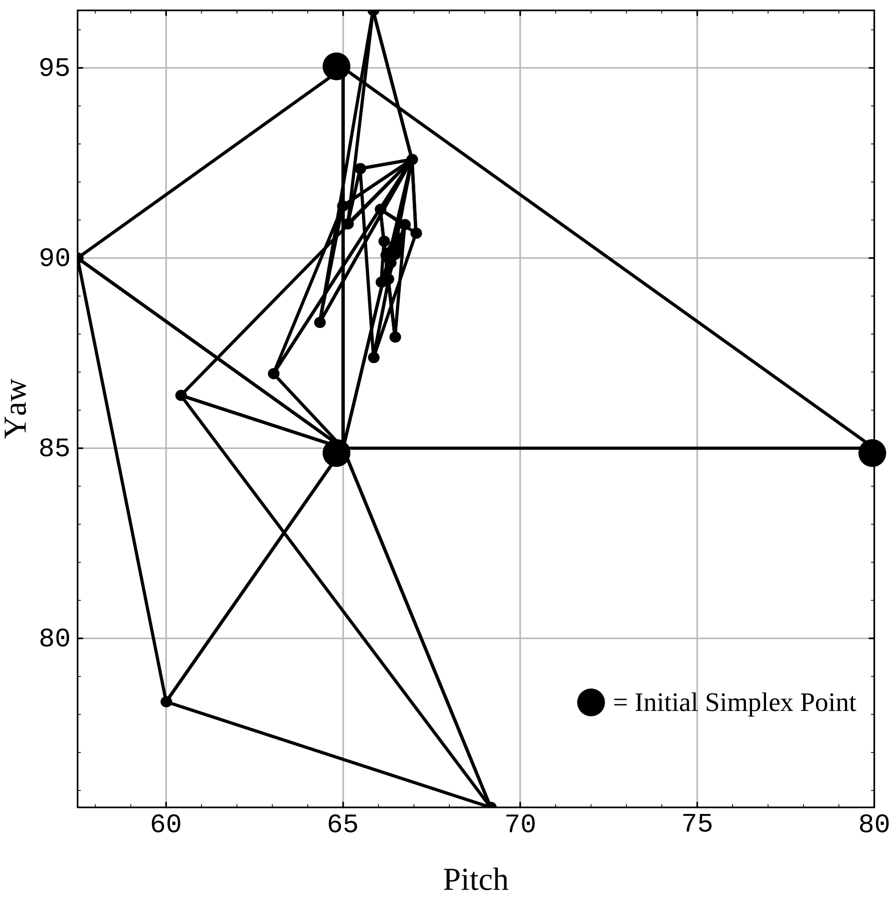

Figure 3.2: Simplex Results Looking Down the Throttle-Up Time Axis

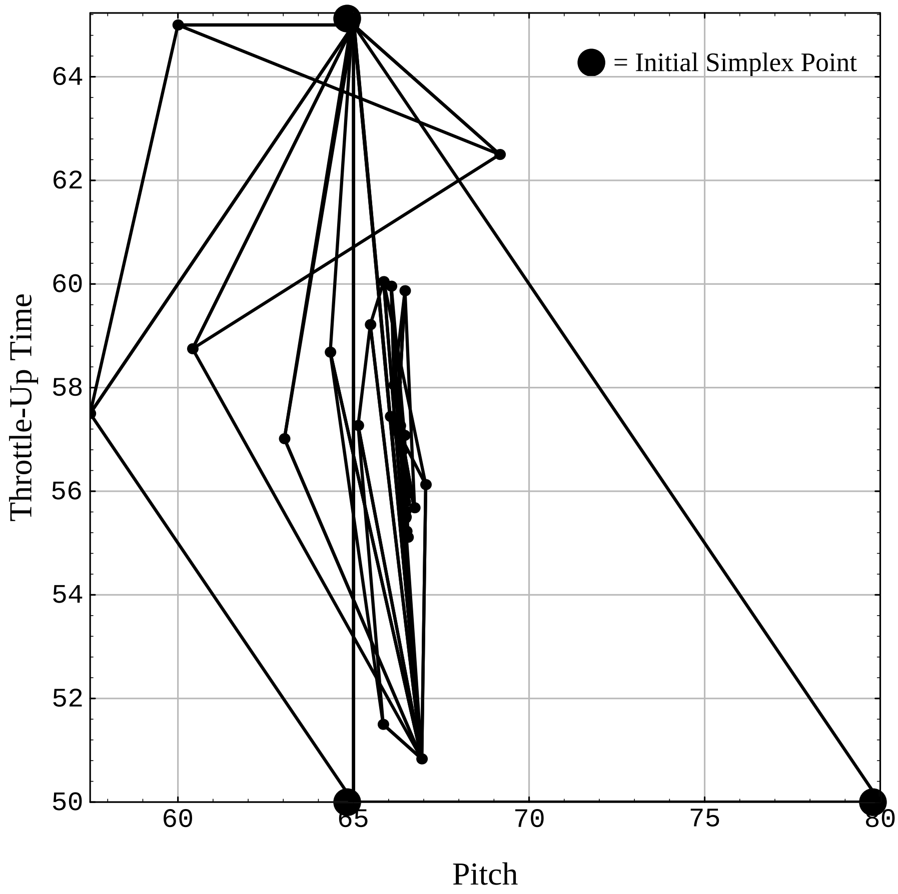

Figure 3.3: Simplex Results Looking Down the Yaw Angle Axis

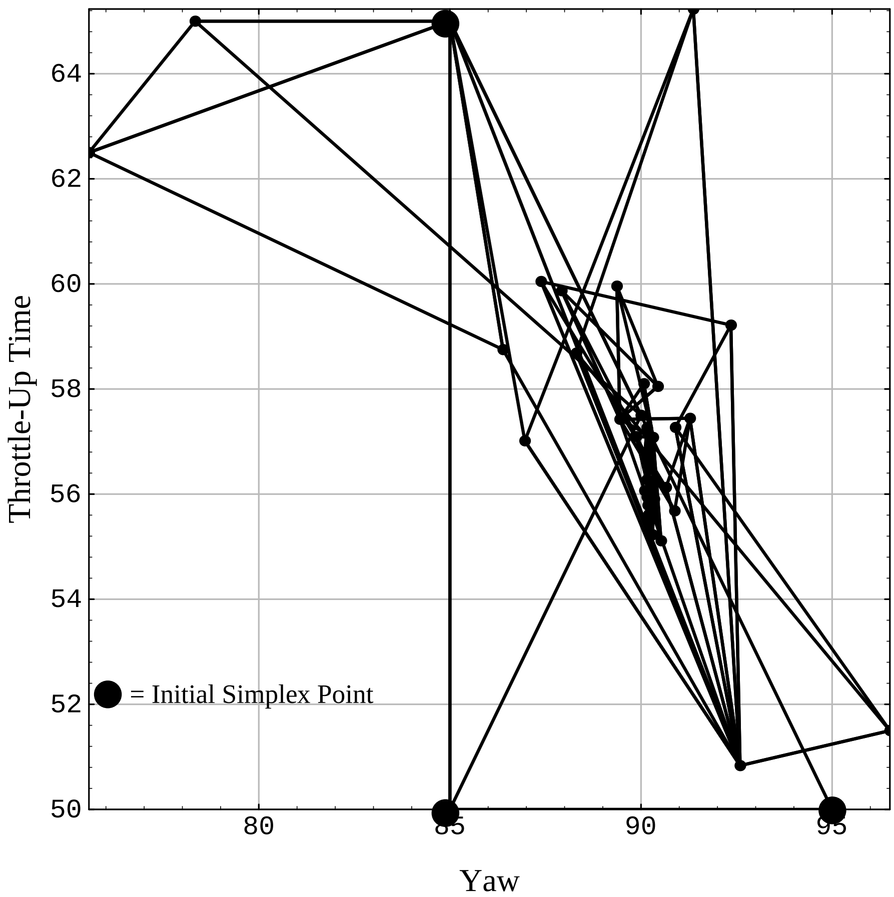

Figure 3.4: Simplex Results Looking Down the Pitch Angle Axis

Section 4

Experimental Design

4.1 Design

The experimental design to model the response surface in the region of the optimum is a circumscribed central composite design. Figure 4.1 illustrates the design in 3-dimensional space. The number of unique design points (f) for the central composite design experiment will be 15, given by

$$2^k + 2k + 1 = 2^3 + 2(3) + 1 = 15$$

with k being the number of factors. With $k = 3$ factors this requires

$$p = \frac{1}{2}(k+1)(k+2) = \frac{1}{2}(3+1)(3+2) = 10$$

parameters in the full second-order polynomial (FSOP) model. The equation to be used to model the response surface is

$$\begin{aligned} y_{1i} &= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_{12} x_{1i} x_{2i} + \\ &\quad \beta_{13} x_{1i} x_{3i} + \beta_{23} x_{2i} x_{3i} + \beta_{11} x_{1i}^2 + \beta_{22} x_{2i}^2 + \beta_{33} x_{3i}^2 + r_{1i} \end{aligned}$$

We replicate the center point twice to test for experimental uncertainty, giving $n = 17$. The degrees-of-freedom (DOF) tree is illustrated in Figure 4.2. The experimental design provides sufficient DOF for lack-of-fit and experimental error.

4.2 Initial Numerical Results

The experimental design matrix is centered about the point $66.5, 90.2, 55.3$ with deltas from this point of $0.4, 0.5, 0.75$ for the cube points and deltas of $0.69282, 0.86603, 1.2990$ (the cube deltas multiplied by $\sqrt{3}$) for the star points. These delta values are small since the simplex optimization results showed that performance was sensitive to small changes from the optimum. The center point has been replicated twice (experiments 16 and 17) to test for purely experimental uncertainty, although since the system is a software simulation we would not expect there to be any. The

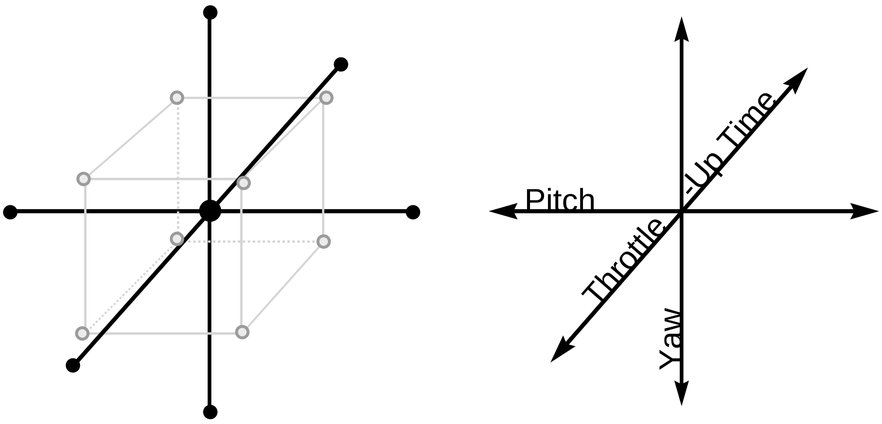

Figure 4.1: Circumscribed Central Composite Design

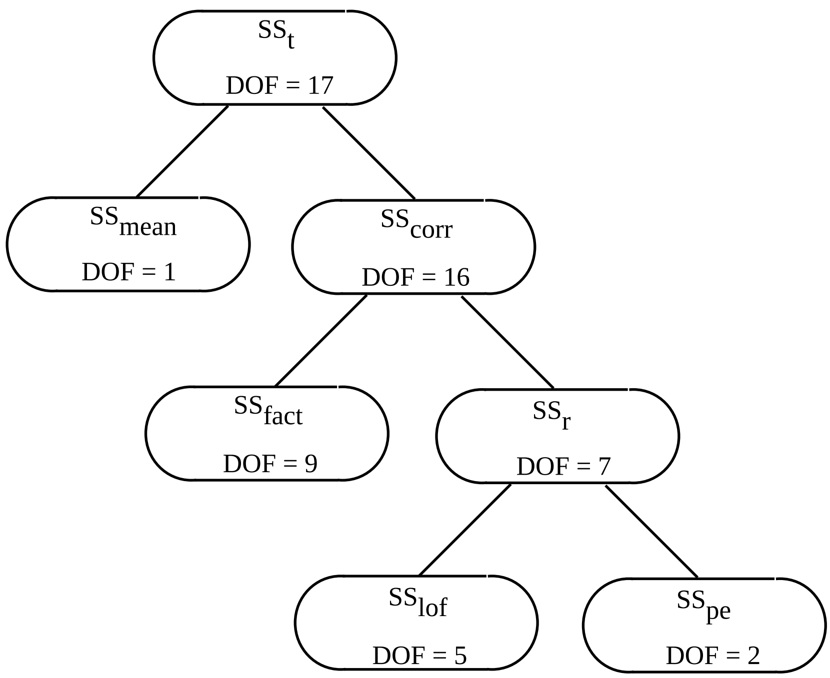

Figure 4.2: Degrees of Freedom Tree

Experiment	Pitch	Yaw	T/U Time	Response
1	66.1000	89.7000	54.5500	232880.1
2	66.9000	89.7000	54.5500	232069.5
3	66.1000	90.7000	54.5500	219418.3
4	66.9000	90.7000	54.5500	242331.8
5	66.1000	89.7000	56.0500	244906.1
6	66.9000	89.7000	56.0500	217924.7
7	66.1000	90.7000	56.0500	230877.5
8	66.9000	90.7000	56.0500	228034.4
9	66.5000	90.2000	55.3000	335680.9
10	65.8072	90.2000	55.3000	187317.1
11	67.1928	90.2000	55.3000	190321.0
12	66.5000	89.3340	55.3000	299621.3
13	66.5000	91.0660	55.3000	297806.8
14	66.5000	90.2000	54.0010	318335.8
15	66.5000	90.2000	56.5990	317414.5
16	66.5000	90.2000	55.3000	335680.9
17	66.5000	90.2000	55.3000	335680.9

Table 4.1: Central Composite Experimental Design Matrix

central composite design matrix is listed in Table 4.1. The first eight experiments are the cube, the next seven are the star points and the last two are the replicated center points.

The matrix of parameter coefficients is generated from the design matrix. A row in the parameter coefficients matrix is calculated as follows:

$$[\,1.0 \quad x_{1i} \quad x_{2i} \quad x_{3i} \quad x_{1i}x_{2i} \quad x_{1i}x_{3i} \quad x_{2i}x_{3i} \quad x_{1i}^2 \quad x_{2i}^2 \quad x_{3i}^2\,]$$

The parameter estimates, confidence and risk percentages are listed in Table 4.2. The parameter estimates, variance/co-variance, F-Ratios and % confidence were calculated using the equations

$$b = (x^T x)^{-1}(x^T y)$$

Parameter	Estimate	% Confidence	Risk
β_0	-2154756353.4	99.6306875	0.3693124
β_1	45114720.273	99.9373255	0.0626744
β_2	12056553.329	89.9224142	10.0775858
β_3	4028041.6390	72.8789230	27.1210770
β_{12}	29913.993061	46.0773747	53.9226253
β_{13}	-21636.401774	49.3621330	50.6378670
β_{23}	-239.77699379	0.7468794	99.2531206
β_{11}	-350503.15185	99.9859076	0.0140923
β_{22}	-77794.013838	96.4070358	3.5929641
β_{33}	-23220.769419	87.4524585	12.5475415

Table 4.2: Parameter Estimates

Experiment	Response	Adjusted	Predicted	Residual	LOF	PE
1	232880.1	−14851.344	247872.3	−14992.2	−14992.2	0.0
2	232069.5	−14194.915	248528.7	−16459.2	−16459.2	0.0
3	219418.3	−28103.005	234620.6	−15202.3	−15202.3	0.0
4	242331.8	−3515.381	259208.2	−16876.4	−16876.4	0.0
5	244906.1	−2625.763	260097.9	−15191.8	−15191.8	0.0
6	217924.7	−27933.016	234790.6	−16865.9	−16865.9	0.0
7	230877.5	−16237.089	246486.5	−15609.0	−15609.0	0.0
8	228034.4	−17613.148	245110.5	−17076.1	−17076.1	0.0
9	335680.9	72956.483	335680.1	0.793583	0.793583	0.0
10	187317.1	−94973.265	167750.4	19566.7	19566.7	0.0
11	190321.0	−95596.481	167127.1	23193.9	23193.9	0.0
12	299621.3	15879.863	278603.5	21017.8	21017.8	0.0
13	297806.8	13340.843	276064.5	21742.3	21742.3	0.0
14	318335.8	34582.001	297305.6	21030.2	421030.2	0.0
15	317414.5	32960.639	295684.3	21730.2	21730.2	0.0
16	335680.9	72956.483	335680.1	0.793583	0.793583	0.0
17	335680.9	72956.483	335680.1	0.793583	0.793583	0.0

Table 4.3: Experiment Matrices for Sums of Squares

Source	Sum of Square	Variance	D.F.
Total	1.21764×10^{12}	7.16258×10^{10}	17
Mean	1.1734×10^{12}	1.1734×10^{12}	1
Cor. for Mean	4.42361×10^{10}	2.76475×10^{9}	16
Factors	3.94242×10^{10}	4.38047×10^{9}	9
Residual	4.81184×10^{9}	6.87406×10^{8}	7
Lack of Fit	4.81184×10^{9}	1.20296×10^{9}	5
Pure Error	0.0	0.0	2

Table 4.4: Sums of Squares and Degrees of Freedom

$$
\begin{aligned}
v &= s_r^2 (x^T x)^{-1} \\
\text{FRatio} &= \text{parameter}^{\,2}/\text{variance} \\
\text{Confidence \%} &= \text{CDF[FRatioDistribution}[1, n-p], \text{FRatio}]
\end{aligned}
$$

where FRatioDistribution[] and CDF[] are *Mathematica* functions which calculate the cumulative F-Ratio distribution at the passed-in F-Ratio value.

The sums of squares breakdown are listed in Tables 4.3 and 4.4.

The determination and correlation coefficients are

$$
\begin{aligned}
R^2 &= 0.891224 \\
R &= 0.944046
\end{aligned}
$$

and the Fisher F-Ratios are listed in Table 4.5 The lack of fit F-Ratio is undefined since the SS_{pe} value is 0.

F-Ratio		Estimate	% Confidence	Risk
Fact F(9, 7)	=	6.37247	98.837224	1.162776
LOF F(5, 2)	=	Undefined	—	—

Table 4.5: Fisher F-Ratios

Experiment	Pitch	Yaw	T/U Time	Response
1	-0.57735	-0.57735	-0.57735	-0.38579357
2	0.57735	-0.57735	-0.57735	-0.39672076
3	-0.57735	0.57735	-0.57735	-0.56726371
4	0.57735	0.57735	-0.57735	-0.25838109
5	-0.57735	-0.57735	0.57735	-0.22367855
6	0.57735	-0.57735	0.57735	-0.58739800
7	-0.57735	0.57735	0.57735	-0.41278937
8	0.57735	0.57735	0.57735	-0.45111543
9	0.0	0.0	0.0	1.00000000
10	-1.0	0.0	0.0	-1.00000000
11	1.0	0.0	0.0	-0.95950629
12	0.0	-1.0	0.0	0.51390299
13	0.0	1.0	0.0	0.48944284
14	0.0	0.0	-1.0	0.76618151
15	0.0	0.0	1.0	0.75376204
16	0.0	0.0	0.0	1.00000000
17	0.0	0.0	0.0	1.00000000

Table 4.6: Coded Design and Response Values

4.3 Coded Numerical Results

A subsequent analysis was conducted in a coded factor space to check the results of the experiment. This was prompted by the *Mathematica* error message

```
Inverse::luc:
   Warning: Result for Inverse
     of badly conditioned matrix {<<10>>}
     may contain significant numerical errors.
```

The values in the parameter coefficients matrix for the second-order terms are on the order 10^4. The computations to calculate the matrix inverse, on a 17×17 matrix, can become large. Coding the factor space to a range of ± 1 would remove this concern. The coded design and response values listed in Table 4.6 and was generated with an *AWK* script. The coding ranged the circumscribed points from -1 to $+1$ instead of the cube points, and therefore the cube points have values ± 0.57735 or $\pm \frac{1}{\sqrt{3}}$. This was done both for convenience in the *AWK* script and as a check on the original design matrix.

Running this design and response data set through the regression analysis script yielded the parameter estimates listed in Table 4.7. The non-linear (intercept and second-order) confidence percentages are consistent with the original

Parameter	Estimate	% Confidence	Risk
β_0	0.999997579	99.8248112	0.1751888
β_1	-0.004200589	1.9766585	98.0233415
β_2	-0.017113313	8.0371994	91.9628006
β_3	-0.010928428	5.1388308	94.8611692
β_{12}	0.241952375	46.0773910	53.9226090
β_{13}	-0.262500614	49.3621619	50.6378381
β_{23}	-0.003636693	0.7469511	99.2530489
β_{11}	-2.267956830	99.9859077	0.0140923
β_{22}	-0.786527440	96.4070316	3.5929684
β_{33}	-0.528230801	87.4524596	12.5475404

Table 4.7: Parameter Estimates for Coded Design

confidence percentages. The parameter estimates for β_1, β_2 and β_3 are expected to be zero in the coded space since this is where we centered the coding, and this is reflected in the % confidence values.

Using this coded space has avoided the *Mathematica* matrix inverse warning messages. There is no documentation on what method *Mathematica* uses to calculate the inverse, so working in the coded space is recommended. It is a simple matter to translate the predicted responses back to real space.

4.4 Interpretation of the Results

The parameter coefficient tables show the % confidence results that were expected. The SAR yaw angle does not significantly influence the optimum pitch or throttle-up time, and this is reflected in the β_{12}, β_{13} and definitely in the β_{23} interaction terms. From the descriptions of the constraints in §2 each factor influences a single constraint, but there is little interaction. By the time the second (late) QBar overshoot is encountered any influence from the first QBar overshoot has damped out. The interaction of SAR pitch and throttle-up time (the β_{13} term) can be understood since a large pitch up reduces the duration of exposure to maximum dynamic pressure and therefore influences when the engines can be throttled back up. However, the pitch delta must be large to see the influence, and this is reflected in the % confidence. The other (non-interaction) % confidence values are all high (the lowest is 87.4), which indicates the terms are probably significant.

If we take the partial derivatives with respect to x_1, x_2 and x_3, set each equal to zero and solve the three linear equations simultaneously the result is the optimum pitch, yaw and throttle-up time.

$$\begin{pmatrix} 2\beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & 2\beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & 2\beta_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = - \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}$$

Inserting the numbers and solving for x_1, x_2 and x_3 yields

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 66.49936 \\ 90.19047 \\ 55.28691 \end{pmatrix}$$

These values for SAR pitch (x_1), SAR yaw (x_2) and throttle-up time (x_3) agree with the SORT optimization results to two decimal places in pitch and yaw, and to one decimal place in throttle-up time. The MECO weight (maximum performance) using the optimum guidance targets is on the order of 400 lbs higher (better) than the SORT results.

Section 5

What Was Learned

The following list summarizes the key points learned from this project.

- Sequential Simplex Design can be used, along with desirability functions, to quickly determine the region of optimum performance for systems. The simplex algorithm can be “wrapped around” existing systems to investigate new ideas, thereby reducing the cost of investigation.
- We now have methods, such as regression analysis, and design criteria, such as replication, which improve experimental design results. If results from a study are presented which show, for example, that the chosen model fits the data exactly, then we now immediately ask “are there degrees of freedom for lack of fit?” We now not only have tools to conduct research but to understand and evaluate research done by others.
- Space Shuttle ascent performance during first stage is optimized by flying commanded SAR pitch/yaw profile of 66.49936, 90.19047 and a throttle-up time of 55.28691.
- The constrained performance response surface has a single optimum, as we expected.
- A detailed study of Space Shuttle guidance and aerodynamic performance has yielded insight into the first stage flight design process.
- Tool manipulation and design for setting up, running, analyzing and reporting results of analysis projects.

Several tools were developed to complete this project at Rockwell. Two of these are anticipated to be used for an upcoming project. The capability to use a simulation as a subroutine will be used to implement multi-case simulations for the new simulation project currently in the verification phase.

The capability to read data from simulation plot files (the *calc_response.perl* script does this) is new and has already been used to write a Unix shell command-line query script. This query can be used to write quick reports of plot data from the command line. Implementing this capability for the simplex study required learning the *Perl* programming language.

Section 6

Conclusion

For most projects a plan of attack is required before work begins. The plan lists techniques, milestones and dates for completion. There has been, however, very little or no instruction as to what these plans contain and how one sets up the experimental design. What is learned from this class, and this project, will fill the void and improve projected and actual results both in terms of time-to-completion and project/resource management.

Appendix A

Regression Analysis Script

The following is a listing of the *Mathematica* script written to generate the regression analysis results. There isn't much error checking built in since the experiment was designed to have DOF for factor effects, residuals, lack-of-fit and experimental error.

```
(* Load in Stat. Package for determination of Confidence % *)
Needs[ "Statistics`NormalDistribution`" ];


SetDirectory[ HomeDirectory[] ];
                (* reset working directory to home dir. *)

SetDirectory[ "school/chemExp" ];
                (* move current directory to Chemical   *)
                (* Experiment subdirectory              *)


(* Read in the Design Matrix here *)
d = ReadList[ "CodedDesign", Number, RecordLists -> True ];


(* Read in the Response Matrix here *)
y = ReadList[ "CodedResults", Number, RecordLists -> True ];


(* Set up the parameter coefficients matrix *)
x = Table[ {     1.0,                    (* b0  parameter *)
                d[[i,1]],               (* b1  parameter *)
                d[[i,2]],               (* b2  parameter *)
                d[[i,3]],               (* b3  parameter *)
                d[[i,1]] * d[[i,2]],    (* b12 parameter *)
                d[[i,1]] * d[[i,3]],    (* b13 parameter *)
                d[[i,2]] * d[[i,3]],    (* b23 parameter *)
```

```
                d[[i,1]] * d[[i,1]],    (* b11 parameter *)
                d[[i,2]] * d[[i,2]],    (* b22 parameter *)
                d[[i,3]] * d[[i,3]]     (* b33 parameter *)
            },
               {i, 1, Length[d] } ];


(* Calculate the parameter estimates matrix *)
If[ Det[ Transpose[x] . x ] == 0,
    {
        Print["Cannot calc. matrix inverse (determinant=0)"];
        Abort[];
    },
    {
        InvXtX = Inverse[ Transpose[x] . x ];
    }
];

b = InvXtX . ( Transpose[x] . y );


(* Set up mean response and estimated response matrices *)
meanY = Sum[ y[[i]], {i, 1, Length[y]} ] / Length[y];
yBar = Table[ meanY, {i, 1, Length[y]} ];
yHat = x . b;



(* A simple loop to calc. the mean replicate responses *)
(* matrix and determine the # of unique design points  *)
(* (f).  There is probably an easier way to do this.   *)

totalCnt = 0;
Jmean = y;

For[ i = 1, i <= Length[d], i++,
    {
        cnt = 0;
        curY = 0;

        For[ j = 1, j <= Length[d], j++,
            {
                If[ d[[i]] == d[[j]],
                    {
                        cnt++;
                        curY = curY + y[[j]];
                    } ];
             }
```

```
        ];

        Jmean[[i]] = N[ curY / cnt ];
        totalCnt = totalCnt + cnt;
    }
]


(* set up the familiar symbols *)
n = Length[y];
p = Length[b];
f = 15; (* OK--my loop didn't work *)


(* Calculate the degrees of freedom values *)
dfTotal = n;
dfMean  = 1;
dfCorr  = n - 1;
dfFact  = p - 1;
dfResid = n - p;
dfLOF   = f - p;
dfPE    = n - f;

(* Calculate the mitrices needed for SS calculations *)
Corr  = y     -  yBar;
Fact  = yHat  -  yBar;
Resid = y     -  yHat;
LOF   = Jmean -  yHat;
PE    = y     -  Jmean;

(* Calculate Sum-of-Squares values *)
SSt    = (Transpose[y]      . y)[[1,1]];
SSmean = (Transpose[yBar]   . yBar)[[1,1]];
SScorr = (Transpose[Corr]   . Corr)[[1,1]];
SSfact = (Transpose[Fact]   . Fact)[[1,1]];
SSres  = (Transpose[Resid]  . Resid)[[1,1]];
SSlof  = (Transpose[LOF]    . LOF)[[1,1]];
SSpe   = (Transpose[PE]     . PE)[[1,1]];


(* Calculate the variance-covariance matrix *)
v = ( SSres / dfResid ) * InvXtX;


(* Calc. the % confidence for the parameter estimates *)
paramC = Table[ CDF[ FRatioDistribution[ 1,dfResid ],
                            b[[i,1]]^2  / v[[i,i]] ],
                 { i, 1, Length[b] } ];
```

```
(* Calc. coefficients of determination and correlation *)

detrCoeff = SSfact / SScorr;
corrCoeff = Sqrt[ detrCoeff ];


(* Calc. Fisher F-Ratios *)
If[ dfFact > 0  &&  SSres > 0  &&  dfResid > 0,
        {
            fisherFact = ( SSfact/dfFact ) / ( SSres/dfResid );
            paramF = CDF[ FRatioDistribution[ dfFact,dfResid ], fisherFact];
        },
        fisherFact = -1.0
];

If[ dfLOF > 0  &&  SSpe > 0  &&  dfPE > 0,
        fisherLOF  = ( SSlof / dfLOF ) / ( SSpe / dfPE ),
        fisherLOF = -1.0
];
```

Appendix B

Additional Data and Scripts

The following two sections are the scripts used and data generated from the simplex optimization and the subsequent central composite design experiment.

BIBLIOGRAPHY

[1] Walters, F., Parker, L., Morgan, S. and Deming, S. *Sequential Simplex Optimization.* CRC Press, 1991.

[2] Wolfram, S. *Mathematica: A System for Doing Mathematics by Computer.* Addison-Wesley, 1991.