CHAPTER V

OPTIMIZATION OF AN ALKYLATION PROCESS

5.1 Alkylation Process

The principle of alkylation as it applies to motor fuel production involves the combination of an isoparffin, usually iso-butane, with an olefin such as propylene, butylene, or amylene. The resulting product is a high-octane gasoline component with very desirable stability properties.

5.2 Process Description

The conventional sulfuric acid akylation [3], [4], [25], [26], which is illustrated in Fig 5.1 is described here.The olefin feed, recycle isobutane and acid are contacted in a reaction system. The heat of reaction is removed by a refrigeration section. The reactor effluent is treated and fractionated to separate and recover the recycle isobutane and the alkylate product. Propane and butane which are present in the feed as diluents are rejected.

5.3 Problem Formulation

5.3.1 Description of model variables

The variables in this problem are as follows

Z(1) - Olefin feed rate (barrel/day).

Z(2) - Isobutane recycle rate (barrel/day).

Z(3) - Fresh acid addition rate (thounsands of pounds/day).

Z(4) - Alkylate product rate (barrel/day).

Z(5) - Make-up isobutane rate (barrel/day).

Z(6) - Spent acid strength (wt %).

Z(7) - Motor octane number. (-)

Z(8) - External isobutane-to-olefin ratio. (-)

Z(9) - Acid dilution factor, ADF. (-)

Z(10) - F-4 performance. (-)

5.3.2 The mathematical model

The objective is to maximize the profit f(Z) and the scaled mathematical model to be optimized is as follows [4].

$$\text{Maximize } f(Z) = 0.63Z(4)Z(7) - 5.04Z(1) - 3.36Z(5) - 0.035Z(2) - Z(3)$$

subject to

h(1) : Relation between alkylate yield and external isobutane ratio

$$h(1) = Z(4) - Z(1)(1.12 + 0.1316Z(8) - 0.006667Z^2(8)) = 0$$

h(2) : Definition of external isobutane ratio

$$h(2) = Z(2) + Z(5) - Z(1)Z(8) = 0$$

h(3) : Volumetric balance around reactor.

$$h(3) = 1.22Z(4) - Z(1) - Z(5) = 0$$

h(4) : Acid usage based on alkylate product, acid dilution factor and acid strength.

$$h(4) = Z(6)Z(4)Z(9) - 1000Z(3)(98 - Z(6)) = 0$$

h(5) : Relationship between F-4 performance and acid dilution factor.

$$h(5) = 35.82 - 0.222Z(10) - Z(9) = 0$$

h(6) : Relationship between octane number and F-4 performance.

$h(6) = -133+3Z(7)-Z(10) = 0$

h(7) : Octane number based on volumetric external isobutane-to-olefin ratio and acid strength.

$h(7) = 86.35+1.098Z(8)-0.038Z^2(8)-0.325(Z(6)-89)-Z(7) = 0$

5.4 Result of Optimization

All the results given in Table 5.1 came from the same starting point (SP1). The value of the objective function obtained by the GRG (Generalized Reduced Gradient) method was better than Rangaiah's Muliplier Method [16] and Luus and Jakola's Random search Technique [27] though it was lower than Vinante's Muliplier Method [17]. However the GRG method satisfied all the constraints more accurately than Vinante's.

In Table 5.2, an arbitrary starting point (SP2) as well as the optimum point of Rangaiah's (SP3) is used as starting points. It was found that the GRG method reached the same optimum point as when SP1 was used. Thus it was resonable to conclude that a global optimum had been obtained.

5.5 Conclusions

With respect to the above alkylation process, it has been demonstrated the GRG method performed better than the method of multiplier and the random search technique. Using the same starting point as that used by [3], [17], [16], [27]as well as the optimum point given by [16] and an arbitrary starting point, the GRG method yielded identical results that are superior either in the satisfaction of the equality constraints and/slash or in the value of the objective function.

Thus it is reasonable to expect that the GRG algorithm will be quite an effective and robust method for solving numerous chemical engineering optimization problems.

Table 5.1 Summary of the results of the alkylation process problem as optimized with the GRG algorithm and the methods of [17], [16] and [27].

Variable	Lower Bound	Upper Bound	Starting Point	Multiplier		Random Search Technique [27]	GRG Method
				Vinante's [17]	Rangaiah's [16]		
Z(1)	0.0	2.000	1.745	1.623	1.698	1.728	1.7289
Z(2)	0.0	1.600	1.200	1.568	1.582	1.600	1.600
Z(3)	0.0	1.200	1.100	0.312	0.54	0.984	.419
Z(4)	0.0	5.000	3.048	2.963	3.031	3.056	3.056
Z(5)	0.0	2.000	1.974	1.992	2.000	2.000	2.000
Z(6)	0.85	0.93	0.892	0.851	0.901	0.906	0.85
Z(7)	0.90	0.95	0.928	0.950	0.950	0.942	0.949
Z(8)	3.00	12.000	8.100	10.889	10.49	10.41	10.41
Z(9)	0.0	4.000	3.600	1.590	1.56	2.61	2.10
Z(10)	1.450	1.620	1.450	1.533	1.535	1.496	1.518
Objective Function ($/day)			0.792	1.9997	1.768	1.162	1.872

Table 5.2 Summary of the results of the alkylation process problem as optimized with the GRG algorithm using an arbitary starting point and the optimum point of [16].

Variable	Lower Bound	Upper Bound	Starting point		GRG Method
			SP2 arbitrary	SP3 optimum of [16]	
Z(1)	0.0	2.000	1.902	1.698	1.7289
Z(2)	0.0	1.600	1.440	1.582	1.600
Z(3)	0.0	1.200	0.462	0.54	.419
Z(4)	0.0	5.000	2.751	3.031	3.056
Z(5)	0.0	2.000	1.800	2.000	2.000
Z(6)	0.85	0.93	0.93	0.901	0.85
Z(7)	0.90	0.95	0.90	0.950	0.949
Z(8)	3.00	12.000	9.370	10.49	10.41
Z(9)	0.0	4.000	2.311	1.56	2.10
Z(10)	1.450	1.620	1.450	1.535	1.518
Objective Function ($/day)			-1.002	1.768	1.8722

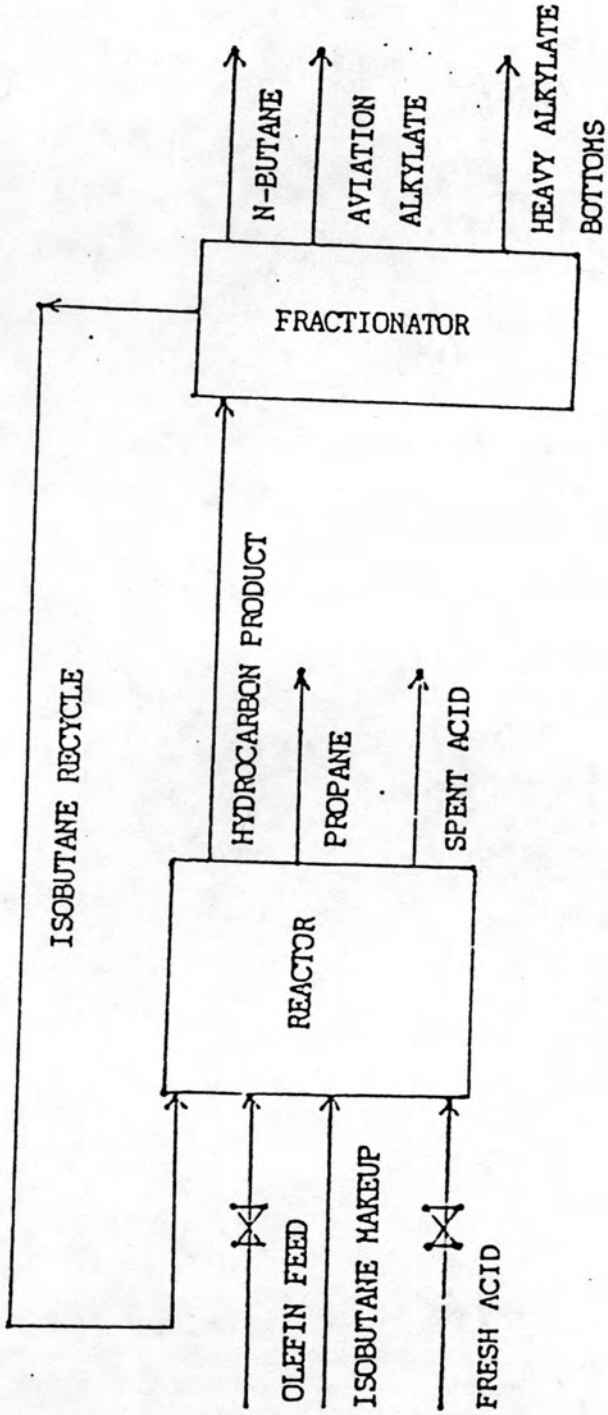

Fig 5.1 Simplified Alkylation Process Flow Diagram