Extended Pooling Problem with the Summer Time (EPA) Complex Emissions Constraints

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Results and Discussion

Table 1: Overview of the Three Case Studies

	Topology							# Variables		# Nonlinear Terms	
	I	J	K	L	$\lVert T_X \rVert$	$\lVert T_Y \rVert$	$\lVert T_Z \rVert$	Contin	Binary	Bilinear Only	All
Case 1	7	2	11	1	4	2	8	214	30	62	108
Case 2	14	3	11	3	10	9	12	331	45	111	180
Case 3	14	10	11	5	14	50	40	1104	150	410	640

Table 1 displays the complexity of the three extended EPA pooling problem test cases [Misener and Floudas, 2009, Misener et al., 2010]. The parameters relevant to the test cases are recorded in Appendices B – D. The feed stocks represent the characteristics of intermediate stocks leaving the processing units of a refinery. Each feed stock is estimated to have a market value based on its composition. Transportation considerations normally require additives to be mixed into gasoline at a distribution station (*e.g.,* ethanol is rarely transported by pipeline with other gasoline components), but the test cases described in this study simplify the problem by assuming that additives are blended into final products at the refinery.

Table 2: Emissions Limits of the Three Case Studies

	$\mathrm{VOC}_{j,\mathrm{MAX}}$ $(\frac{\mathrm{mg}}{\mathrm{mile}})$	$\mathrm{NOX}_{j,\mathrm{MAX}}$ $(\frac{\mathrm{mg}}{\mathrm{mile}})$	$\mathrm{TOX}_{j,\mathrm{MAX}}$ $(\frac{\mathrm{mg}}{\mathrm{mile}})$
Case 1	1200	1300	90
Case 2	1700	1400	95
Case 3	1600	1300	95

The emissions limits for the three test cases are listed in Table 2. These three test cases, assume that the emissions limits are identical for all products, but the complexity of the problems would not change if each product was given a different target emissions level. Further, each of the three test cases assumes that the refineries are blending products during the summer. Compared to the summer model, the winter time EPA Complex Emissions Model would eliminate the non-exhaust volatile organic and non-exhaust benzene

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equations and fix RVP [40CFR80.45, 2007]. The difference between Region 1 and 2 is only a change in parameters (see Appendix A), so these test cases consider both the Region 1 and 2 cases. Figures 1 – 3 list some of the key flow rates in the best-found upper bound for each topology in Region 1.

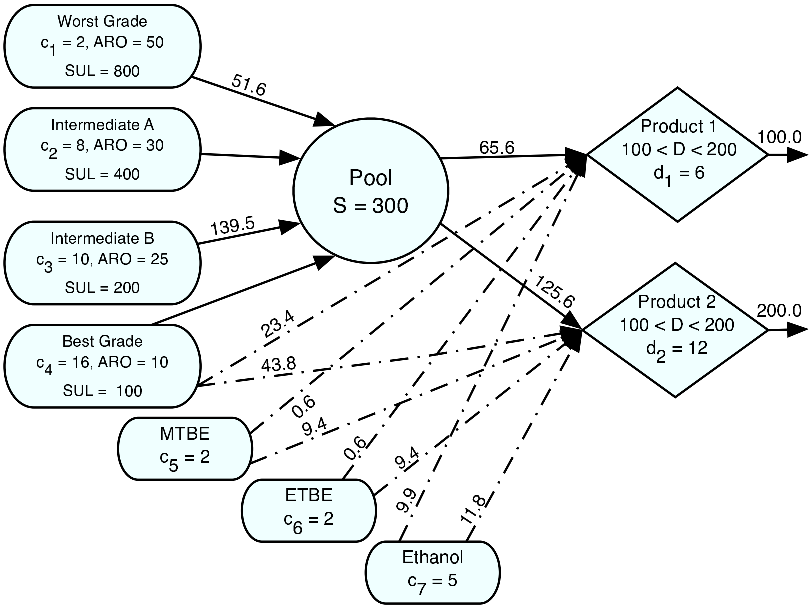

Figure 1: Best Upper Bound found for Region 1 Test Case 1 ($z_p = -2.794 \times 10^2$)

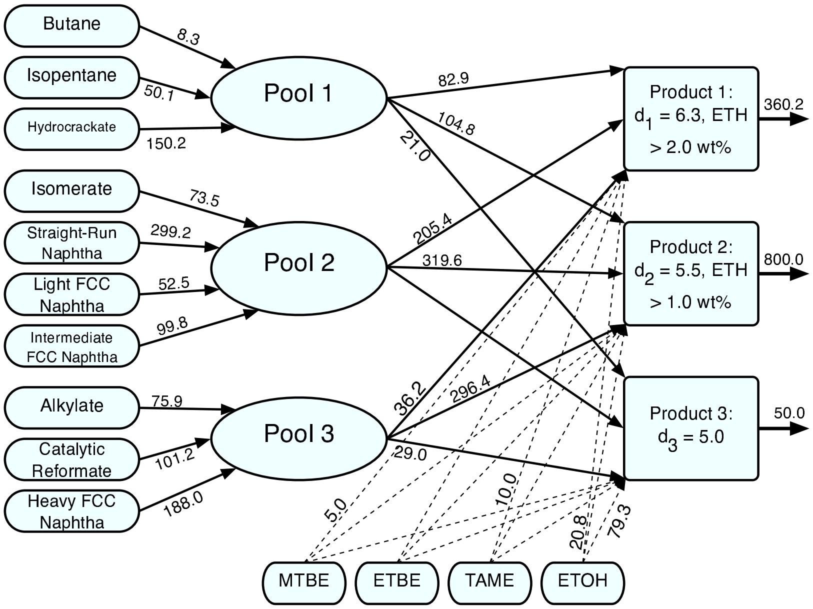

Figure 2: Best Upper Bound found for Region 1 Test Case 2 ($z_p = -4.567 \times 10^3$)

In Misener and Floudas [2009], we describe solving these test cases on a Linux workstation with an Intel Core 2 Quad processor containing four 2.83 GHz cores. The optimization process was written in C++

and run serially using CPLEX Version 11.0 [ILOG, 2007] for the node relaxations and MINOS Version 5.51 [Murtagh et al., 2004] for the local upper bounding solves. Table 3 lists the results of the optimization runs. There are few nodes in the branch-and-bound trees because the underestimators we developed in Misener et al. [2010] tightly relax the problem.

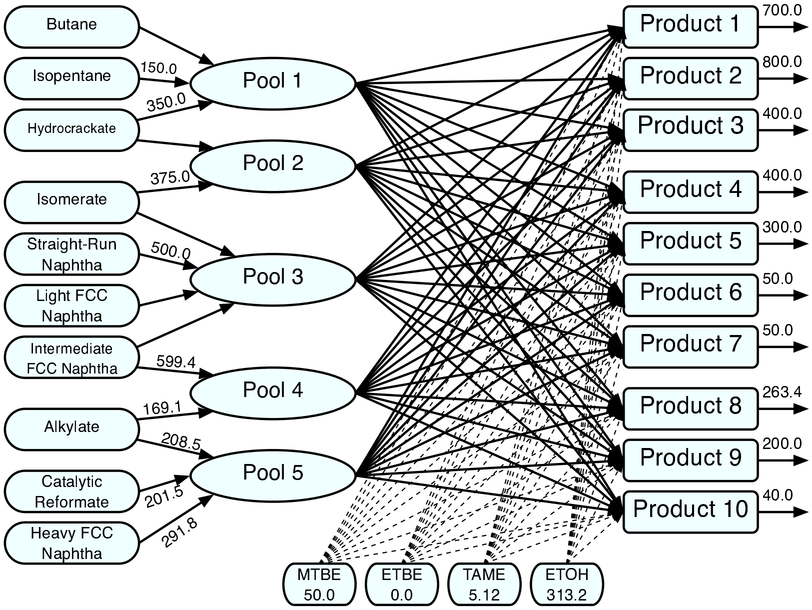

Figure 3: Best Upper Bound found for Region 1 Test Case 3 ($z_p = -1.490 \times 10^4$)

Table 3: Branch & Bound Optimization of the Three Test Cases

	Region	Root Node Relaxation	# Nodes	Termination			CPU Time (s)
				Lower Bnd	Upper Bnd	% Gap	
Case 1	1	-4.731×10^2	7	-2.808×10^2	-2.794×10^2	0.5	4.6
	2	-4.731×10^2	7	-2.818×10^2	-2.808×10^2	0.5	4.5
Case 2	1	-4.598×10^3	9	-4.587×10^3	-4.567×10^3	0.4	292
	2	-4.598×10^3	9	-4.588×10^3	-4.567×10^3	0.5	263
Case 3	1	-1.500×10^4	11	-1.498×10^4	-1.490×10^4	0.5	5274
	2	-1.500×10^4	1	-1.500×10^4	-1.496×10^4	0.2	411

Comparison with Commercial Solvers

Because the global optimization results in Table 3 correspond to the relaxation developed in Misener et al. [2010] rather than a direct solve of the nonlinear model presented here, we have tested the full model on an array of commercial solvers: DICOPT, BARON, SBB, and AlphaECP. The reader should be advised that the algorithm we present in Misener et al. [2010] is specialized for EPA pooling applications and therefore may perform more favorably than pre-packaged software. Table 4 only displays results using BARON and SBB. After some experimentation with appropriate options, we were unable to solve any of the problems with DICOPT. We had difficulty with the AlphaECP solver taking much longer than its allotted time and we were therefore only able to address the small case study with AlphaECP. SBB does not find rigorous lower bounds and therefore terminates at suboptimal points (SBB reports feasible solutions that are up to 48% different from the optimum recorded in Table 3). BARON is able to approach the small and medium size test cases. The CPU times for Case 2 are 10-fold larger than those in Misener et al. [2010]. For Case 3, BARON exhibits a gap greater than 100% after 10 CPU hours.

Table 4: Specialized Relaxations versus Commercial Software

		Region	Lower Bound	Upper Bound	% Gap	CPU Time (s)
Misener et al. [2010]	Case 1	1	-2.808×10^2	-2.794×10^2	0.5	4.6
		2	-2.818×10^2	-2.808×10^2	0.5	4.5
	Case 2	1	-4.587×10^3	-4.567×10^3	0.4	292
		2	-4.588×10^3	-4.567×10^3	0.5	263
	Case 3	1	-1.498×10^4	-1.490×10^4	0.5	5274
		2	-1.500×10^4	-1.496×10^4	0.2	411
BARON	Case 1	1	-2.822×10^2	-2.808×10^2	0.5	7.2
		2	-2.822×10^2	-2.808×10^2	0.5	7.6
	Case 2	1	-4.590×10^4	-4.567×10^4	0.5	2327.9
		2	-4.590×10^4	-4.567×10^4	0.5	2328.9
	Case 3	1	-1.500×10^4	-1.674×10^2	> 100	36000
		2	-1.500×10^4	-1.674×10^2	> 100	36000
SBB	Case 1	1	–	-2.808×10^2	–	0.4
		2	–	-2.808×10^2	–	0.3
	Case 2	1	–	-4.269×10^3	–	1.3
		2	–	-4.269×10^3	–	1.2
	Case 3	1	–	-1.066×10^4	–	100.4
		2	–	-7.798×10^3	–	96.4

References

40CFR80.45. Code of Federal Regulations: Complex emissions model, 2007. http://www.gpoaccess.gov/cfr/retrieve.html.

C. E. Gounaris and C. A. Floudas. Formulation and relaxation of an extended pooling problem. In *2007 AIChE Annual Meeting*, Salt Lake City, Utah, 2007. AIChE.

ILOG. CPLEX. http://www.ilog.com/products/cplex/, 2007. Version 11.0.0.

B. A. Murtagh, M. A. Saunders, W. Murray, M. A. Saunders, P. E. Gill, R. Raman, and E. Kalvelagen. MINOS. http://www.gams.com/dd/docs/solvers/minos.pdf, 2004.

R. Misener and C. A. Floudas. Advances for the pooling problem: Modeling, global optimization, and computational studies. *Applied and Computational Mathematics*, 8(1):3 – 22, 2009.

R. Misener, C. E. Gounaris, and C. A. Floudas. Mathematical Modeling and Global Optimization of Large-Scale Extended Pooling Problems with the (EPA) Complex Emissions Constraints. *Comput. Chem. Eng.*, In Press, 2010.

A Reformulated Gasoline Parameters

Table 5: Coefficients

Coefficient	Region 1	Region 2
α_1^V	1226.9	1063.3
α_2^V	-353.4	-300.8
α_3^V	31.8	27.0
α^{POM}	0.003355	
α_1^{NB}	1.7502	1.5210
α_2^{NB}	-0.6031	-0.5161
α_3^{NB}	-0.0403	-0.0352
α_4^{NB}	0.0738	0.0628
α_5^{NB}	0.0116	0.0100
α_6^{NB}	-0.0026	-0.0022
α_7^{NB}	-0.0010	-0.0009

Table 6: Weighting Factors

Constant	Emitter 1 ($e = 1$)	Emitter 2 ($e = 2$)
w_e^V	0.444	0.556
w_e^N	0.738	0.262
w_e^T	0.444	0.556

Table 7: Baseline emission values

	Summer ($\frac{\text{mg}}{\text{mile}}$)	Winter ($\frac{\text{mg}}{\text{mile}}$)
VOC(b)	907.00	1341.00
NOX(b)	1340.00	1540.00
BENZ(b)	53.54	77.62
ACET(b)	4.44	7.25
FORM(b)	9.70	15.34
BUTA(b)	9.38	15.84

Table 8: Normal ($e = 1$) and high ($e = 2$) emitter values

	Summer		Winter	
	$e = 1$	$e = 2$	$e = 1$	$e = 2$
$e^{v_e(b)}$	0.0621	0.1038	0.0579	0.0971
$e^{n_e(b)}$	1.6438	0.8353	1.6664	0.8420
$e^{b_e(b)}$	3.5308	5.8617	3.0231	5.6183
$e^{f_e(b)}$	0.3403	0.2550	0.3542	0.2439
$e^{a_e(b)}$	0.4715	0.3337	0.4862	0.3441
$e^{d_e(b)}$	0.2600	0.4995	0.2688	0.5382

Table 9: Constant Coefficients

Constant	Emitter 1 ($e = 1$)	Emitter 2 ($e = 2$)
$c_{e,1}^{V}$	-0.003641	-0.003626
$c_{e,2}^{V}$	0.0005219	-0.000054
$c_{e,3}^{V}$	0.0289749	0.043295
$c_{e,4}^{V}$	-0.01447	-0.013504
$c_{e,5}^{V}$	-0.068624	-0.062327
$c_{e,6}^{V}$	0.0323712	0.0282042
$c_{e,7}^{V}$	-0.002858	-0.002858
$c_{e,8}^{V}$	0.0001072	0.000106
$c_{e,9}^{V}$	0.0004087	0.000408
$c_{e,10}^{V}$	-0.0003481	-0.000287
$c_{e,1}^{N}$	0.0018571	-0.00913
$c_{e,2}^{N}$	0.0006921	0.000252
$c_{e,3}^{N}$	0.0090744	-0.01397
$c_{e,4}^{N}$	0.000931	0.000931
$c_{e,5}^{N}$	0.000846	-0.00401
$c_{e,6}^{N}$	0.0083632	0.007097
$c_{e,7}^{N}$	-0.002774	-0.00276
$c_{e,8}^{N}$	-0.000000663	0.0
$c_{e,9}^{N}$	-0.000119	-0.00007995
$c_{e,10}^{N}$	0.0003665	0.0003665
$c_{e,1}^{BE}$	0.0	-0.096047
$c_{e,2}^{BE}$	0.0006197	0.000337
$c_{e,3}^{BE}$	-0.003376	0.011251
$c_{e,4}^{BE}$	0.02655	0.011882
$c_{e,5}^{BE}$	0.22239	0.222318
$c_{e,1}^{F}$	-0.010226	-0.010226
$c_{e,2}^{F}$	-0.007166	-0.007166
$c_{e,3}^{F}$	0.0	-0.031352
$c_{e,4}^{F}$	0.0462131	0.0462131
$c_{e,1}^{A}$	0.0002631	0.0002627
$c_{e,2}^{A}$	0.039786	0.0
$c_{e,3}^{A}$	-0.012172	-0.012157
$c_{e,4}^{A}$	-0.005525	-0.005548
$c_{e,5}^{A}$	-0.009594	-0.05598
$c_{e,6}^{A}$	0.31658	0.3164665
$c_{e,7}^{A}$	0.24925	0.2493259
$c_{e,1}^{BU}$	0.0	-0.060771
$c_{e,2}^{BU}$	0.0001552	0.0
$c_{e,3}^{BU}$	-0.007253	-0.007311
$c_{e,4}^{BU}$	-0.014866	-0.008052
$c_{e,5}^{BU}$	-0.004005	-0.004005
$c_{e,6}^{BU}$	0.028235	0.043696

B Case Study 1 Parameters

This case study was taken from Gounaris and Floudas [2007]. The singular pool has capacity $S_1 = 300$.

Table 10: Cost (c_i) and Availability (A_i^L & A_i^U) of Feed i

	i						
	1	2	3	4	5	6	7
c_i	2	8	10	16	2	2	5
A_i^L	50	0	0	0	0	0	0
A_i^U	400	200	200	100	10	10	50

Table 11: Price (d_j) and Demand (D_j^L & D_j^U) of Product j

j	d_j	D_j^L	D_j^U
1	6	100	200
2	12	100	200

Table 12: Quality Bounds k on Product j ($P_{j,k}^L$ & $P_{j,k}^U$) and Quality k of Raw Material i ($C_{i,k}$)

	k										
	1	2	3	4	5	6	7	8	9	10	11
$P_{1,k}^L$	0.3	50	6.4	30	70	0.0	0.0	0	0.1	0.1	0.1
$P_{2,k}^L$	0.3	50	6.4	30	70	0.0	0.0	0	0.1	0.1	0.1
$P_{1,k}^U$	4.0	500	10.0	70	100	30	2.0	25	4.0	4.0	4.0
$P_{2,k}^U$	4.0	250	8.0	60	85	25	0.5	10	4.0	4.0	4.0
$C_{1,k}$	0.1	800	6.0	20	70	50	0.0	10	0	0	0
$C_{2,k}$	0.2	400	8.8	60	85	30	0.8	15	0	0	0
$C_{3,k}$	0.4	200	8.0	55	80	25	1.0	15	0	0	0
$C_{4,k}$	0.7	100	8.0	50	75	10	0.2	5	0	0	0
$C_{5,k}$	18.15	0	8.4	100	100	0	0.0	0	18.15	0	0
$C_{6,k}$	15.66	0	8.0	100	100	0	0.0	0	0	15.66	0
$C_{7,k}$	34.73	0	9.6	100	100	0	0.0	0	0	0	34.73

Table 13: Connectivity of each Feed i to the Pools l and Products j

	i						
	1	2	3	4	5	6	7
l	l1	l1	l1	l1			
j				j1 – j10	j1 – j10	j1 – j10	j1 – j10

C Case Study 2 Parameters

Table 14: Quality k of Raw Material i ($C_{i,k}$)

	k										
	1	2	3	4	5	6	7	8	9	10	11
$C_{1,k}$	0.00	0	60.0	100	100	0.0	0	0	0.00	0.00	0.00
$C_{2,k}$	0.00	0	21.0	100	100	0.0	0	0	0.00	0.00	0.00
$C_{3,k}$	0.00	0	7.4	50	95	0.0	0	0	0.00	0.00	0.00
$C_{4,k}$	0.00	50	10.0	100	100	0.0	0	0	0.00	0.00	0.00
$C_{5,k}$	0.00	100	9.0	70	100	7.5	2	37	0.00	0.00	0.00
$C_{6,k}$	0.00	15	3.4	60	85	3.2	0	12	0.00	0.00	0.00
$C_{7,k}$	0.00	200	10.2	85	100	10.0	1	60	0.00	0.00	0.00
$C_{8,k}$	0.00	400	8.2	45	80	35.0	3	20	0.00	0.00	0.00
$C_{9,k}$	0.00	700	2.1	15	60	65.0	4	15	0.00	0.00	0.00
$C_{10,k}$	0.00	10	7.4	30	70	60.0	5	3	0.00	0.00	0.00
$C_{11,k}$	18.15	0	8.8	100	100	0.0	0	0	18.15	0.00	0.00
$C_{12,k}$	15.66	0	5.7	95	100	0.0	0	0	0.00	15.66	0.00
$C_{13,k}$	15.66	0	2.7	70	100	0.0	0	0	0.00	0.00	0.00
$C_{14,k}$	34.73	0	23.0	100	100	0.0	0	0	0.00	0.00	34.73

Table 15: Cost (c_i) and Availability (A_i^L & A_i^U) of Feed i

	i													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
c_i	3.0	2.0	3.5	2.0	1.0	3.0	0.7	0.5	0.3	2.5	7.5	10.5	8.5	5.5
A_i^L	0	0	0	0	0	0	0	10	20	10	0	0	0	0
A_i^U	75	50	75	75	300	150	50	100	200	100	5	10	10	100

Table 16: Capacity S_l of Pool l

	l		
	1	2	3
S_1	400	575	500

Table 17: Price (d_j) and Demand (D_j^L & D_j^U) of Product j

	j		
	1	2	3
d_j	6.3	5.5	5.0
D_j^L	100	0	50
D_j^U	700	800	400

Table 18: Quality Bounds k on Product j ($P^L_{j,k}$ & $P^U_{j,k}$)

	k										
	1	2	3	4	5	6	7	8	9	10	11
$P^L_{1,k}$	0.0	0.0	6.4	30	70	0	0	0	0.0	0.0	2.0
$P^L_{2,k}$	0.0	0.0	6.4	30	70	0	0	0	0.0	0.0	1.0
$P^L_{3,k}$	0.0	0.0	6.4	30	70	0	0	0	0.0	0.0	0.0
$P^U_{1,k}$	3.7	130	10	70	100	50	2	25	3.7	3.7	3.7
$P^U_{2,k}$	3.7	200	10	70	100	50	2	25	3.7	3.7	3.7
$P^U_{3,k}$	3.7	250	10	70	100	50	2	25	3.7	3.7	3.7

Table 19: Connectivity of each Feed i to the Pools l and Products j

	i													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
l	l1	l1	l3	l2	l2	l1	l2	l2	l3	l3				
j											j1 – j10	j1 – j10	j1 – j10	j1 – j10

D Case Study 3 Parameters

The raw material qualities ($C_{i,k}$) are identical in Case Study 2 & 3, so Table 14 records these values.

Table 20: Capacity S_l of Pool l

	l				
	1	2	3	4	5
S_1	900	575	500	800	900

Table 21: Price (d_j) and Demand (D^L_j & D^U_j) of Product j

	j									
	1	2	3	4	5	6	7	8	9	10
d_j	8.0	7.5	6.5	6.0	6.5	5.5	5.0	5.5	5.5	5.0
D^L_j	100	0	50	50	50	50	50	50	100	40
D^U_j	700	800	400	400	300	200	400	300	200	400

Table 22: Cost (c_i) and Availability (A^L_i & A^U_i) of Feed i

	i													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
c_i	3.0	2.0	3.5	2.0	1.0	3.0	0.7	0.5	0.3	2.5	7.5	10.5	8.5	5.5
A^L_i	0	0	0	0	0	0	0	100	50	10	0	0	0	0
A^U_i	175	150	375	375	900	350	250	600	500	200	50	100	100	400

Table 23: Quality Bounds k on Product j ($P^{L}_{j,k}$ & $P^{U}_{j,k}$)

	k										
	1	2	3	4	5	6	7	8	9	10	11
$P^{L}_{1,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	2.0
$P^{L}_{2,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	2.0
$P^{L}_{3,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	2.0
$P^{L}_{4,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	2.0
$P^{L}_{5,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	2.0
$P^{L}_{6,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	1.0
$P^{L}_{7,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	1.0
$P^{L}_{8,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	1.0
$P^{L}_{9,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	1.0
$P^{L}_{10,k}$	0.0	0.0	6.4	30.0	70.0	0.0	0.0	0.0	0.0	0.0	0.0
$P^{U}_{1,k}$	3.7	130	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{2,k}$	3.7	150	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{3,k}$	3.7	170	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{4,k}$	3.7	190	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{5,k}$	3.7	150	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{6,k}$	3.7	150	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{7,k}$	3.7	150	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{8,k}$	3.7	200	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{9,k}$	3.7	200	10	70	100	50	2	25	3.7	3.7	3.7
$P^{U}_{10,k}$	3.7	250	10	70	100	50	2	25	3.7	3.7	3.7

Table 24: Connectivity of each Feed i to the Pools l and Products j

	i													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
l	l1	l1	l4; l5	l2; l3	l3	l1; l2	l3	l3; l4	l5	l5				
j											j1 – j10	j1 – j10	j1 – j10	j1 – j10