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APPENDICES

Appendix A Predicted Mole Fraction

Table A1 Predicted mole fraction at 300°C

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0000	0.0387	0.0000	0.0000
0.0005	0.0384	0.0001	0.0003
0.0010	0.0380	0.0003	0.0005
0.0015	0.0377	0.0004	0.0008
0.0020	0.0373	0.0005	0.0011
0.0025	0.0370	0.0007	0.0013
0.0030	0.0366	0.0008	0.0016
0.0035	0.0363	0.0009	0.0018
0.0040	0.0360	0.0011	0.0021
0.0045	0.0356	0.0012	0.0023
0.0050	0.0353	0.0013	0.0026
0.0055	0.0350	0.0014	0.0028
0.0060	0.0346	0.0016	0.0031
0.0065	0.0343	0.0017	0.0033
0.0070	0.0340	0.0018	0.0036
0.0075	0.0337	0.0019	0.0038
0.0080	0.0333	0.0020	0.0041
0.0085	0.0330	0.0022	0.0043
0.0090	0.0327	0.0023	0.0045
0.0095	0.0324	0.0024	0.0048
0.0100	0.0321	0.0025	0.0050
0.0105	0.0318	0.0026	0.0052
0.0110	0.0315	0.0028	0.0055
0.0115	0.0312	0.0029	0.0057
0.0120	0.0309	0.0030	0.0059
0.0125	0.0306	0.0031	0.0061
0.0130	0.0303	0.0032	0.0064
0.0135	0.0300	0.0033	0.0066
0.0140	0.0297	0.0034	0.0068
0.0145	0.0294	0.0035	0.0070
0.0150	0.0291	0.0037	0.0072

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0155	0.0288	0.0038	0.0075
0.0160	0.0285	0.0039	0.0077
0.0165	0.0283	0.0040	0.0079
0.0170	0.0280	0.0041	0.0081
0.0175	0.0277	0.0042	0.0083
0.0180	0.0274	0.0043	0.0085
0.0185	0.0271	0.0044	0.0087
0.0190	0.0269	0.0045	0.0089
0.0195	0.0266	0.0046	0.0091
0.02	0.0263	0.0047	0.0093
0.0205	0.0261	0.0048	0.0095
0.021	0.0258	0.0049	0.0097
0.0215	0.0256	0.0050	0.0099
0.022	0.0253	0.0051	0.0101
0.0225	0.0250	0.0052	0.0103
0.023	0.0248	0.0053	0.0105
0.0235	0.0245	0.0054	0.0107
0.024	0.0243	0.0055	0.0109
0.0245	0.0240	0.0056	0.0111
0.025	0.0238	0.0057	0.0112
0.0255	0.0236	0.0058	0.0114
0.026	0.0233	0.0058	0.0116
0.0265	0.0231	0.0059	0.0118
0.027	0.0228	0.0060	0.0120
0.0275	0.0226	0.0061	0.0121
0.028	0.0224	0.0062	0.0123
0.0285	0.0221	0.0063	0.0125
0.029	0.0219	0.0064	0.0127
0.0295	0.0217	0.0065	0.0128
0.03	0.0215	0.0065	0.0130

Table A2 Predicted mole fraction at 285°C

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0000	0.0387	0.0000	0.0000
0.0005	0.0383	0.0002	0.0003
0.0010	0.0378	0.0004	0.0007
0.0015	0.0373	0.0005	0.0010
0.0020	0.0368	0.0007	0.0014
0.0025	0.0364	0.0009	0.0017
0.0030	0.0359	0.0011	0.0020
0.0035	0.0355	0.0012	0.0024
0.0040	0.0350	0.0014	0.0027
0.0045	0.0346	0.0016	0.0030
0.0050	0.0341	0.0017	0.0033
0.0055	0.0337	0.0019	0.0037
0.0060	0.0333	0.0020	0.0040
0.0065	0.0328	0.0022	0.0043
0.0070	0.0324	0.0024	0.0046
0.0075	0.0320	0.0025	0.0049
0.0080	0.0316	0.0027	0.0052
0.0085	0.0312	0.0028	0.0055
0.0090	0.0308	0.0030	0.0058
0.0095	0.0304	0.0031	0.0061
0.0100	0.0300	0.0033	0.0064
0.0105	0.0296	0.0034	0.0067
0.0110	0.0292	0.0036	0.0069
0.0115	0.0288	0.0037	0.0072
0.0120	0.0284	0.0039	0.0075
0.0125	0.0280	0.0040	0.0078
0.0130	0.0277	0.0041	0.0080
0.0135	0.0273	0.0043	0.0083
0.0140	0.0269	0.0044	0.0086
0.0145	0.0266	0.0046	0.0088
0.0150	0.0262	0.0047	0.0091
0.0155	0.0259	0.0048	0.0094
0.0160	0.0255	0.0050	0.0096
0.0165	0.0252	0.0051	0.0099
0.0170	0.0248	0.0052	0.0101

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0175	0.0245	0.0053	0.0104
0.0180	0.0242	0.0055	0.0106
0.0185	0.0238	0.0056	0.0108
0.0190	0.0235	0.0057	0.0111
0.0195	0.0232	0.0058	0.0113
0.0200	0.0229	0.0060	0.0115
0.0205	0.0226	0.0061	0.0118
0.0210	0.0223	0.0062	0.0120
0.0215	0.0219	0.0063	0.0122
0.0220	0.0216	0.0064	0.0124
0.0225	0.0213	0.0065	0.0127
0.0230	0.0211	0.0066	0.0129
0.0235	0.0208	0.0068	0.0131
0.0240	0.0205	0.0069	0.0133
0.0245	0.0202	0.0070	0.0135
0.0250	0.0199	0.0071	0.0137
0.0255	0.0196	0.0072	0.0139
0.0260	0.0194	0.0073	0.0141
0.0265	0.0191	0.0074	0.0143
0.0270	0.0188	0.0075	0.0145
0.0275	0.0186	0.0076	0.0147
0.0280	0.0183	0.0077	0.0149
0.0285	0.0180	0.0078	0.0151
0.0290	0.0178	0.0079	0.0153
0.0295	0.0175	0.0080	0.0155
0.0300	0.0173	0.0081	0.0157

Table A3 Predicted mole fraction at 270°C

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0000	0.0387	0.0000	0.0000
0.0005	0.0381	0.0002	0.0005
0.0010	0.0375	0.0005	0.0009
0.0015	0.0368	0.0007	0.0013
0.0020	0.0362	0.0009	0.0018
0.0025	0.0356	0.0012	0.0022

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0030	0.0350	0.0014	0.0026
0.0035	0.0344	0.0016	0.0031
0.0040	0.0338	0.0018	0.0035
0.0045	0.0332	0.0021	0.0039
0.0050	0.0326	0.0023	0.0043
0.0055	0.0321	0.0025	0.0047
0.0060	0.0315	0.0027	0.0051
0.0065	0.0310	0.0029	0.0055
0.0070	0.0304	0.0031	0.0058
0.0075	0.0299	0.0033	0.0062
0.0080	0.0294	0.0035	0.0066
0.0085	0.0289	0.0037	0.0070
0.0090	0.0283	0.0039	0.0073
0.0095	0.0278	0.0041	0.0077
0.0100	0.0273	0.0042	0.0080
0.0105	0.0269	0.0044	0.0084
0.0110	0.0264	0.0046	0.0087
0.0115	0.0259	0.0048	0.0090
0.0120	0.0254	0.0050	0.0094
0.0125	0.0250	0.0051	0.0097
0.0130	0.0245	0.0053	0.0100
0.0135	0.0241	0.0055	0.0103
0.0140	0.0237	0.0056	0.0106
0.0145	0.0232	0.0058	0.0110
0.0150	0.0228	0.0059	0.0113
0.0155	0.0224	0.0061	0.0116
0.0160	0.0220	0.0063	0.0118
0.0165	0.0216	0.0064	0.0121
0.0170	0.0212	0.0066	0.0124
0.0175	0.0208	0.0067	0.0127
0.0180	0.0204	0.0069	0.0130
0.0185	0.0200	0.0070	0.0132
0.0190	0.0196	0.0071	0.0135
0.0195	0.0193	0.0073	0.0138
0.0200	0.0189	0.0074	0.0140
0.0205	0.0186	0.0075	0.0143
0.0210	0.0182	0.0077	0.0145
0.0215	0.0179	0.0078	0.0148
0.0220	0.0175	0.0079	0.0150

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0225	0.0172	0.0081	0.0153
0.0230	0.0169	0.0082	0.0155
0.0235	0.0166	0.0083	0.0157
0.0240	0.0163	0.0084	0.0160
0.0245	0.0159	0.0085	0.0162
0.0250	0.0156	0.0087	0.0164
0.0255	0.0153	0.0088	0.0166
0.0260	0.0150	0.0089	0.0168
0.0265	0.0148	0.0090	0.0170
0.0270	0.0145	0.0091	0.0172
0.0275	0.0142	0.0092	0.0174
0.0280	0.0139	0.0093	0.0176
0.0285	0.0137	0.0094	0.0178
0.0290	0.0134	0.0095	0.0180
0.0295	0.0131	0.0096	0.0182
0.0300	0.0129	0.0097	0.0184

Table A4 Predicted mole fraction at 255°C

W/F (hr)	Tetralin	<i>cis</i> -Dec	<i>trans</i> -Dec
0.0000	0.0387	0.0000	0.0000
0.0005	0.0379	0.0003	0.0006
0.0010	0.0371	0.0006	0.0012
0.0015	0.0363	0.0010	0.0018
0.0020	0.0356	0.0013	0.0023
0.0025	0.0348	0.0016	0.0029
0.0030	0.0341	0.0019	0.0034
0.0035	0.0333	0.0022	0.0040
0.0040	0.0326	0.0024	0.0045
0.0045	0.0319	0.0027	0.0050
0.0050	0.0312	0.0030	0.0055
0.0055	0.0305	0.0033	0.0061
0.0060	0.0298	0.0036	0.0066
0.0065	0.0291	0.0038	0.0070
0.0070	0.0285	0.0041	0.0075
0.0075	0.0278	0.0043	0.0080
0.0080	0.0272	0.0046	0.0085

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0085	0.0266	0.0048	0.0089
0.0090	0.0260	0.0051	0.0094
0.0095	0.0254	0.0053	0.0098
0.0100	0.0248	0.0056	0.0103
0.0105	0.0242	0.0058	0.0107
0.0110	0.0236	0.0060	0.0111
0.0115	0.0231	0.0062	0.0115
0.0120	0.0225	0.0065	0.0119
0.0125	0.0220	0.0067	0.0123
0.0130	0.0214	0.0069	0.0127
0.0135	0.0209	0.0071	0.0131
0.0140	0.0204	0.0073	0.0134
0.0145	0.0199	0.0075	0.0138
0.0150	0.0194	0.0077	0.0142
0.0155	0.0190	0.0079	0.0145
0.0160	0.0185	0.0080	0.0148
0.0165	0.0181	0.0082	0.0152
0.0170	0.0176	0.0084	0.0155
0.0175	0.0172	0.0086	0.0158
0.0180	0.0167	0.0087	0.0161
0.0185	0.0163	0.0089	0.0164
0.0190	0.0159	0.0091	0.0167
0.0195	0.0155	0.0092	0.0170
0.0200	0.0151	0.0094	0.0173
0.0205	0.0147	0.0095	0.0176
0.0210	0.0144	0.0097	0.0179
0.0215	0.0140	0.0098	0.0182
0.0220	0.0136	0.0100	0.0184
0.0225	0.0133	0.0101	0.0187
0.0230	0.0130	0.0103	0.0189
0.0235	0.0126	0.0104	0.0192
0.0240	0.0123	0.0105	0.0194
0.0245	0.0120	0.0106	0.0196
0.0250	0.0117	0.0108	0.0199
0.0255	0.0114	0.0109	0.0201
0.0260	0.0111	0.0110	0.0203
0.0265	0.0108	0.0111	0.0205

W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.0270	0.0105	0.0112	0.0207
0.0275	0.0102	0.0113	0.0209
0.0280	0.0099	0.0114	0.0211
0.0285	0.0097	0.0115	0.0213
0.0290	0.0094	0.0116	0.0215
0.0295	0.0092	0.0117	0.0217
0.0300	0.0089	0.0118	0.0219

Appendix B Experimental Mole Fraction

Table B1 Experimental mole fraction at 300 °C

Tetralin flow rate is 3.66 mL/hr (3.55 g/hr).

W (g)	W/F (hr)	Tetralin	cis-Decalin	trans-Decalin
0.02	0.0056	0.0353	0.0015	0.0024
0.04	0.0085	0.0343	0.0020	0.0031
0.05	0.0113	0.0307	0.0035	0.0056
0.06	0.0141	0.0300	0.0036	0.0062
0.07	0.0169	0.0294	0.0041	0.0065
0.08	0.0225	0.0263	0.0052	0.0088
0.1	0.0282	0.0248	0.0061	0.0096

Table B2 Experimental mole fraction at 285 °C

Tetralin flow rate is 3.66 mL/hr (3.55 g/hr).

W (g)	W/F (hr)	Tetralin	cis-Decalin	trans-Decalin
0.02	0.0056	0.0319	0.0029	0.0048
0.04	0.0085	0.0291	0.0039	0.0071
0.05	0.0113	0.0286	0.0041	0.0074
0.06	0.0141	0.0243	0.0051	0.0113
0.07	0.0169	0.0232	0.0060	0.0116
0.08	0.0225	0.0202	0.0072	0.0138
0.1	0.0282	0.0194	0.0065	0.0154

Table B3 Experimental mole fraction at 270 °C

Tetralin flow rate is 3.66 mL/hr (3.55 g/hr).

W (g)	W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.02	0.0056	0.0309	0.0035	0.0054
0.04	0.0085	0.0284	0.0047	0.0070
0.05	0.0113	0.0274	0.0049	0.0079
0.06	0.0141	0.0222	0.0062	0.0125
0.07	0.0169	0.0199	0.0070	0.0144
0.08	0.0225	0.0148	0.0092	0.0179
0.1	0.0282	0.0147	0.0086	0.0186

Table B4 Experimental mole fraction at 255 °C

Tetralin flow rate is 3.66 mL/hr (3.55 g/hr).

W (g)	W/F (hr)	Tetralin	<i>cis</i> -Decalin	<i>trans</i> -Decalin
0.02	0.0056	0.0061	0.0043	0.0296
0.04	0.0085	0.0076	0.0051	0.0276
0.05	0.0113	0.0087	0.0051	0.0266
0.06	0.0141	0.0116	0.0070	0.0223
0.08	0.0225	0.0186	0.0095	0.0139

Appendix C Calculations of Product Distribution

Tetralin feed = 3.66 ml/hr

$$\begin{aligned} \text{Convert to mole flowrate} &= 3.66 \frac{\text{mL}}{\text{hr}} * 0.97 \frac{\text{g}}{\text{mL}} * \frac{\text{gmol}}{132\text{g}} \\ &= 0.027 \frac{\text{gmol}}{\text{hr}} \end{aligned}$$

Table C1 %Area reported by GC at W/F = 0.0113 hr and temperature of 255 °C

<i>trans</i> -decalin	<i>cis</i> -Decalin	Tetralin
22.05	12.82	64.21

%Area is related to mass composition.

Calculation of mole fraction in liquid

Mole fraction of *trans*-decalin

$$\begin{aligned} &= (22.05/138) / (22.05/138 + 12.82/138 + 64.21/132) \\ &= 0.2162 \end{aligned}$$

Mole fraction of *cis*-decalin

$$\begin{aligned} &= (12.82/138) / (22.05/138 + 12.82/138 + 64.21/132) \\ &= 0.1257 \end{aligned}$$

Mole fraction tetralin

$$\begin{aligned} &= (64.21/132) / (22.05/138 + 12.82/138 + 64.21/132) \\ &= 0.658^1 \end{aligned}$$

Mole flowrates of hydrocarbon

$$\begin{aligned} \text{trans-Decalin} &= 0.2162 * 0.027 \frac{\text{gmol}}{\text{hr}} \\ &= 0.0058 \frac{\text{gmol}}{\text{hr}} \end{aligned}$$

$$cis\text{-Decalin} = 0.1257 * 0.027 \frac{gmol}{hr}$$

$$= 0.0034 \frac{gmol}{hr}$$

$$Tetralin = 0.6581 * 0.027 \frac{gmol}{hr}$$

$$= 0.0178 \frac{gmol}{hr}$$

Mole flowrates of hydrogen

Hydrogen feed flowrates = 250 cm³/min at STP

$$250 \frac{cm^3}{min} * 60 \frac{min}{hr} * \frac{gmol * K}{0.082 * 1000cm^3 * atm} * \frac{1atm}{273K}$$

$$= 0.6701 \frac{gmol}{hr}$$

1 gmol of tetralin reacted with 3 gmol of H₂

$$\text{Hydrogen consumption} = 3 * (0.0058 + 0.0034) = 0.0276 \frac{gmol}{hr}$$

$$\text{Hydrogen remain} = 0.6701 - 0.0276 = 0.6425 \frac{gmol}{hr}$$

Table C2 Mole fraction of total products

Mole	<i>t</i> -Decalin	<i>c</i> -Decalin	Tetralin	Hydrogen	Total
Flowrate (gmole/hr)	0.0058	0.0034	0.0178	0.6425	0.6695
Fraction	0.0087	0.0051	0.0266	0.9600	1

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