Energy Efficient Catalytic Reaction and Production of Cumene

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Sandia National Laboratories

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Abstract

Alkylation reactions of benzene with propylene using zeolites were studied for their affinity for cumene production. The current process for the production of cumene involves heating corrosive acid catalysts, cooling, transporting, and distillation. This study focused on the reaction of products in a static one-pot vessel using non-corrosive zeolite catalysts, working towards a more efficient one-step process with a potentially large energy savings. A series of experiments were conducted to find the best reaction conditions yielding the highest production of cumene. The experiments looked at cumene formation amounts in two different reaction vessels that had different physical traits. Different zeolites, temperatures, mixing speeds, and amounts of reactants were also investigated to find their affects on the amount of cumene produced. Quantitative analysis of product mixture was performed by gas chromatography. Mass spectroscopy was also utilized to observe the gas phase components during the alkylation process.

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Introduction

Production of cumene is a major petrochemical product used as feedstock for production of phenol and acetone.[1] Most of the current cumene plant production processes utilize a patented supported phosphoric acid catalyst,[2] with a few using a Friedel-Crafts reaction with aluminum trichloride.[3] Both of these processes generate problems with corrosion and contamination, providing an impetus for the recent exploration of recyclable zeolite catalysts.

The usage of large-pore zeolites for the alkylation of benzene has become preferred, as it does not form significant quantities of n-propyl benzene as the medium-pore zeolites do. The first catalytic alkylation experiments over β-Zeolite, a large-pore zeolite, utilized isopropanol,[4] whereas later experiments began utilizing propene.[5,6] Optimization of the zeolites and their acidities, as well as experimental conditions of the reaction, are still being done to most effectively produce cumene.

The current study compares different reactants and their efficiency for producing cumene. Four different zeolites [β-Zeolite (300:1[Si:Al ratio]), β-Zeolite (25:1), H-Zeolite-Y (4:1), H-Zeolite-Y (30:1)] were studied with many different experimental conditions. Variable conditions included different concentrations of propylene (14.5% and 33.3% in N_2), different mixing rates, and different reaction vessels ("T" reactor and pot reactor) resulting in 21 experiments (see Appendix 1). The experiments carried out in this study are meant to direct the transformation of the current process for producing cumene. This investigation's particular interest is in finding the most efficient combination of hydrocarbon mixtures and catalysts in order to develop an energy efficient method of producing cumene. At this point, results are presented, though some questions remain to be worked out regarding reproducibility, and discussed regarding optimization of cumene production. The study is part of a larger Sandia investigation into optimized catalytic reactions and separations.[7-9]

Experimental

Materials and Equipment

Zeolite materials used in the reactions were readily obtained from commercial sources, these are: β-Zeolite (300:1), β-Zeolite (75:1), β-Zeolite (25:1), H-Zeolite-Y (4:1), H-Zeolite-Y (30:1). Benzene (Aldrich, 99+%) was used without further purification. The alkylating agent, propylene (14.5 and 33.3%) in nitrogen gas was purchased premixed from TriGas. To aid in the determination of an optimum reactor design, two styles were used, run and results compared. The first set of experiments was conducted in a "T" reactor with an internal volume of 60 cc. This reactor was designed and built in this summer program. It was constructed from 1" VCR fittings (a tee and straight extension) with a gas valve and a 1" VCR plug that was bored out to hold ~10 cc of reactants. The "T" reactor scheme is shown in Figure 1 below. The vessel was held with tongs and wrapped with heat tape and aluminum foil to ensure even heating. A variable autotransformer, or Variac, supplied the power for the heat tape. Thermocouples monitored the temperature at two locations.
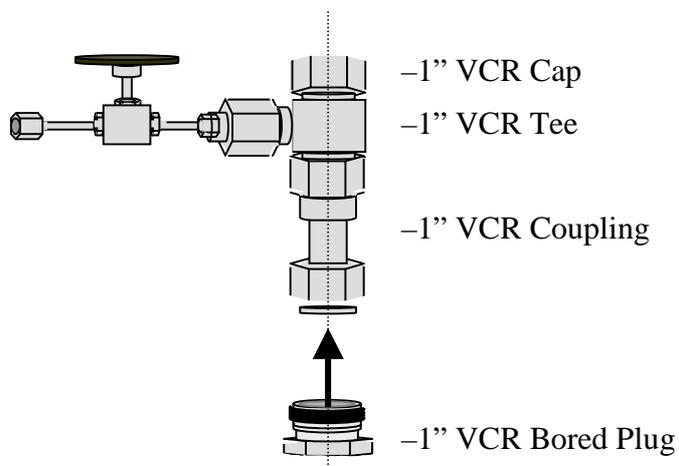
Figure 1. "T" Reactor Schematic.

The second set of experiments was conducted in a standard 420cc stainless steel Parr pressure reactor. The reactor consists of a bottom pot, a lid, and collar. The lid includes a stirrer powered by electric motor, thermocouple, pressure release, gas valve, and optional pressure gauge. The collar consists of two semi-circular steel pieces that hold the top and bottom pot together using six 9/16" screws. Figure 2 below shows the pot reactor details. The heat source is a Parr pressure reactor heat sleeve that hugs the bottom pot while the reactor is held by a stand. Thermocouple and stirrer are both monitored and powered by a Parr 4843 power source. Aluminum foil was used to wrap the top of the reaction vessel to help evenly heat the top. Figure 3 below shows the whole pot reactor assemblage.
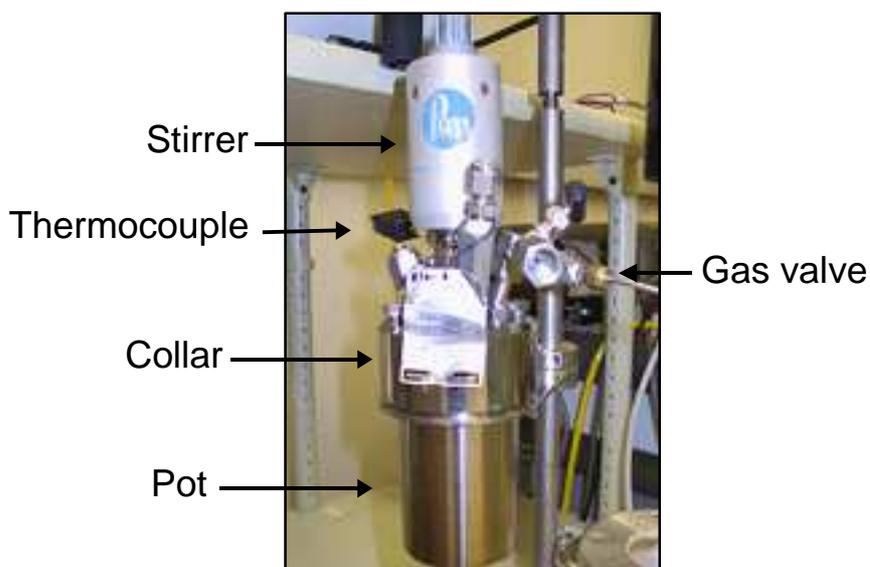
Figure 2. Picture of the Parr pot reactor.
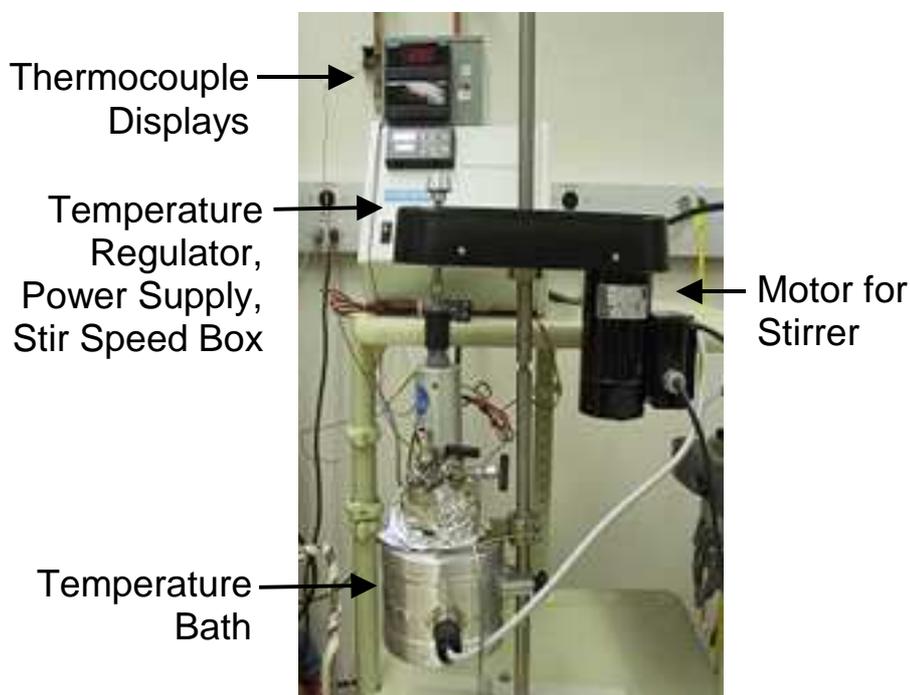
Figure 3. Picture of the pot reactor assembly.

Reaction products were analyzed by gas chromatography (GC), (Hewlett Packard Gas Chromatograph-Model 5890A) using a Bentone 34/DNDP SCOT (50' x 0.02") capillary column from Supelco. The column was predetermined to be selective for reactants and products with this study. A flame ionization detector was used to detect and quantify the amount of products in each sample.

Procedures

The investigation has been divided into three parts. Part I compared the two different reactors and their affect on cumene production. Part II examines the effect of different reactants on cumene production. Part III uses the Mass Spectrometer to study products and reactants as a function of time, and what side-products are produced during the reaction.

Part I: Comparison of Different Reactors

For both reactor vessels, a similar procedure was followed to run a reaction. Each zeolite catalyst was weighed on a Mettler digital balance and then added to the well of the reactor. A volumetric pipette was used to measure benzene and was added to the well. All "T" reactor experiments required 40 mg of zeolite and 2 ml of benzene; the pot reactor ran with 100mg of zeolite and 5 ml of benzene. The volumes of the reactors are approximately 60 cc and 225 cc for the "T" and pot reactors, respectively. This combination of reactants in these reactor volumes results in equivalent molar ratios of benzene to propylene in the reactors. The "T" reactor was screwed in tightly, placed in tongs, and wrapped with heat tape and aluminum foil to ensure even heating. Propylene in N_2 was filled to a pressure of 120 psig and 80 psig, for the "T" and pot reactors, respectively, after the reactors reached 80°C. The reactors were allowed to typically stay for one hour at the reaction temperature, and then quenched with an ice water bath and

allowed to cool until reaching approximately 30°C. Completed reactions were vented to atmospheric pressure into an exhaust vent and taken to a hood where the sample was extracted.

The solution that was left in the bottom of the well was poured into a funnel, which emptied into a syringe with a 0.22 μm filter on the end. The liquid was then filtered and emptied into a 25 ml graduated cylinder. The well and reactor inner surfaces were rinsed with hexane and filtered into the cylinder. The funnel and syringe were also rinsed and filtered. The product and rinse were totaled up to 10 or 25 ml, for the "T" and pot reactors, respectively, and stirred with a pipette until there was no visible separation of products. A pipette was used to extract the solution from the half way full point, put into a sample vial, sealed with Parafilm, and stored in a refrigerator until gas chromatography could be performed. The products were all quantitatively analyzed by gas chromatography (GC).

Part II: Comparison of Different Reactions on Cumene Production

A set of controlled experiments was performed to test the reproducibility of experiments, therefore enabling a comparison of results from the previous study to this study. Data set DT-39-70B (β-Zeolite (75:1), 150°C, stirrer on 3/5 speed) was the control standard based on a high cumene production with good selectivity. This control standard was performed on the pot reactor, and products were analyzed on the GC.

The procedure and sample extraction is the same as listed above for the pot reactor. A matrix of different zeolites [β-Zeolite (300:1), β-Zeolite (25:1), H-Zeolite-Y (4:1), H-Zeolite-Y (30:1)], temperatures (125°C, 150°C, 175°C, 200°C), stirring rates (1/5 speed and 3/5 speed), and amounts of propylene (14.5%, 33.3%) were the variables for this study.

Part III: Mass Spectrometer Reaction Monitoring

The control standard reactants (DT-39-70B) were added to the pot reactor and the reactor was assembled. The vacuum chamber of the quadrupole mass spectrometer (RGA-300, Stanford Research Systems) was connected up to the reactor vessel by use of crushed-capillary leak. The leak rate of the capillary was small enough as to not significantly effect the pressure in the reactor over the reaction time. After 80°C had been reached and the propene/nitrogen gas was introduced into the system, the mass spectrometer started collecting data. The reaction was allowed to run for 2.5 hours. Signal intensity vs. time for the representative cation masses of interest was continuously recorded, these were at m/z = 28 (nitrogen), 41 (propylene), 78 (benzene), 105 (cumene), and 147 (diisopropylbenzene). The complete analog mass spectrum was then also recorded at the end of the reaction time. No significant reaction byproducts were observed in the analog spectra. Signal intensity vs. time is proportional to each of the relative concentrations of reactants and products in the system with time.

Results

Part I: Comparison of Different Reactors

Extensive experiments have been performed utilizing the pot reactor, with several experiments done using the "T" reactor for efficiency comparisons. The Appendix tables A-1 and A-2 contain the summary of all reactions performed using the "T" reactor the pot reactor, respectively. Some values are left blank due to lack of a reliable standard being run prior to GC

data acquisition. From this data, comparing their relative yields of and selectivity for cumene can show the effectiveness of the two reactors. This is shown in Figure 4, the relative cumene yield is calculated from the standard-calibrated gram yield of cumene divided by the theoretical maximum yield (0.960 and 0.384 grams for the pot and "T" reactors, respectively) based on the weight of benzene added, as limited by the propylene molar ratio (1/7), and scaled by molecular weight ratio (120/78, cumene/benzene). The percent selectivity was calculated directly from the GC results, where the assumption was that the sensitivities of cumene were the same as both the 1,3- and 1,4-diisopropylbenzene byproducts. This assumption will be confirmed at a later date.
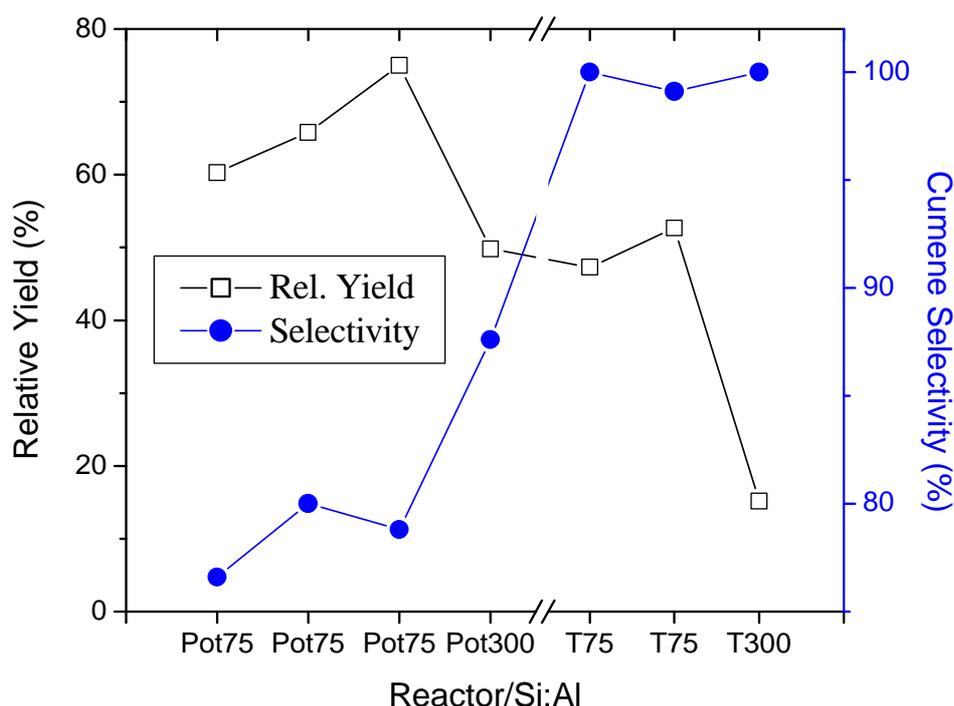
Figure 4. Comparison of the efficiency of the pot reactor with the "T" reactor; relative yields and selectivity for cumene shown for several reactions run at 150°C with two different H$^+$-form β-zeolites (75:1 and 300:1 Si:Al ratios).

In each reactor the relative activity for cumene production is shown to be greater with the higher Aluminum content (75:1, more acidic). Selectivity, however, is decreased with these higher yields. The "T" reactor shows less ability to generate high cumene yields, but has excellent selectivity characteristics, all three reactions had >99%. As with all other reactor reactions performed, the only byproduct observed was the diisopropylbenzenes (DIPB).

Part II: Comparison of Different Reactions on Cumene Production

Extensive comparison of the production yield and selectivity for cumene was performed through a series of four zeolites: β-zeolite (H$^+$-form), H-Zeolite-Y, MCM-22, and Engelhard (Grade F-24). For β-zeolite and H-Z-Y zeolite different acidity ranges were tested by varying the Si:Al ratio. Every zeolite reaction was performed at four (4) temperatures: 125, 150, 175 and 200°C. All reactions were run at temperature for 1 hour.

Of primary importance were the measure of cumene production (in grams) and its relative selectivity versus other side-products. The maximum possible cumene yield for the 7:1 benzene to propylene molar ratio reactions is 0.960 grams, 0.336 grams for the 20:1 ratio. For all reactions studied there were no benzene-derived side-products except for diisopropylbenzenes (DIPB). Based upon the GC measurement of relative amounts of cumene to DIPB, assuming identical instrument response levels, the percent value of selectivity was obtained. The following graphs summarize some of the better reaction results from the β-zeolite series Si:Al = 25:1, 75:1, and 300:1 (Figs. Figure 5–Figure 7). Open black data markers represent cumene yield while the filled blue markers are the selectivity. Some of the experiments were repeated and shown as initial data (circles) and repeat data (squares).

Figure 5. Results from two separate pot reactor experiments running the H-form of β-zeolite (25:1) in a 7:1 (benzene:propylene) molar ratio. Initial data (○) show no trends, but the recent data (□) indicates increased activity with temperature with loss of some selectivity.

Figure 6. Results from two separate pot reactor experiments running the H-form of β-zeolite (75:1) in a 7:1 (benzene:propylene) and 20:1 molar ratios. Initial 7:1 data (○) show a correlation between yield and selectivity. Recent 7:1 experiment at 150ºC (□) demonstrates a reasonable repeatability. The 20:1 data are shown with triangles (Δ).
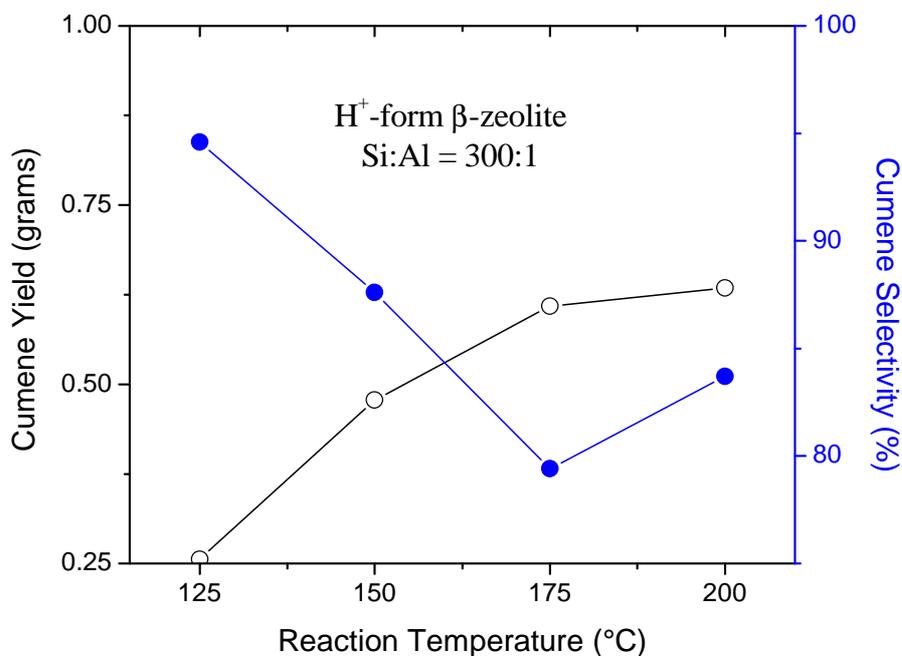
Figure 7. Results from pot reactor experiments running the H-form of β-zeolite (300:1) in a 7:1 (benzene:propylene) molar ratio. Correlation between yield and reaction temperature is observed.

Very high yields are seen with the two most acidic β-zeolites (25:1 and 75:1), whereas higher temperatures are required to obtain a good cumene yield with the 300:1 β-zeolite. Quite different results of the selectivity were obtained between the two different experiments on β-zeolite 25:1, as seen from Figure 5. The recent experiments indicate quite good cumene selectivity of ~90% (i.e. low DIPB production), while the initial results showed poor selectivity of around 60%. The reasons for this discrepancy are as yet unknown and will be further investigated.

Experiments with H-Zeolite-Y (4:1), summarized in Figure 8 below, indicate a relatively low yield when compared to the β-zeolites, around half of the predicted maximum yield. Also, a disparity of product selectivity is seen between the two sets of experiments, though both experiments show a similar trend of minimal change in selectivity over reaction temperatures. Initial data indicate ~50% selectivity, while recent data are around 75%.

Results from the MCM-22 and Englehard F-24 zeolites are not presented in this section because of their low yields and small data sets. This data has been included in the Appendix.

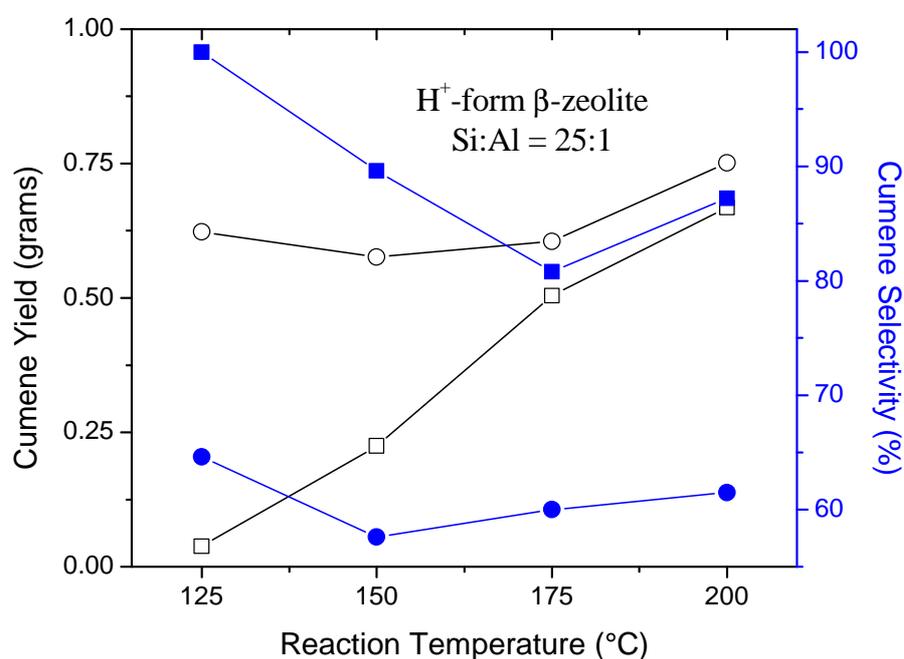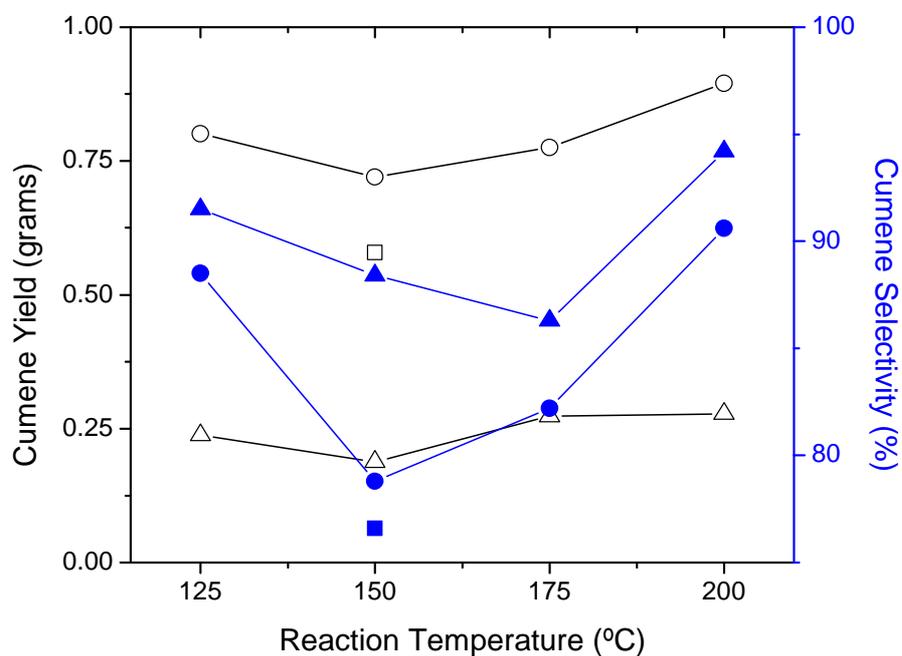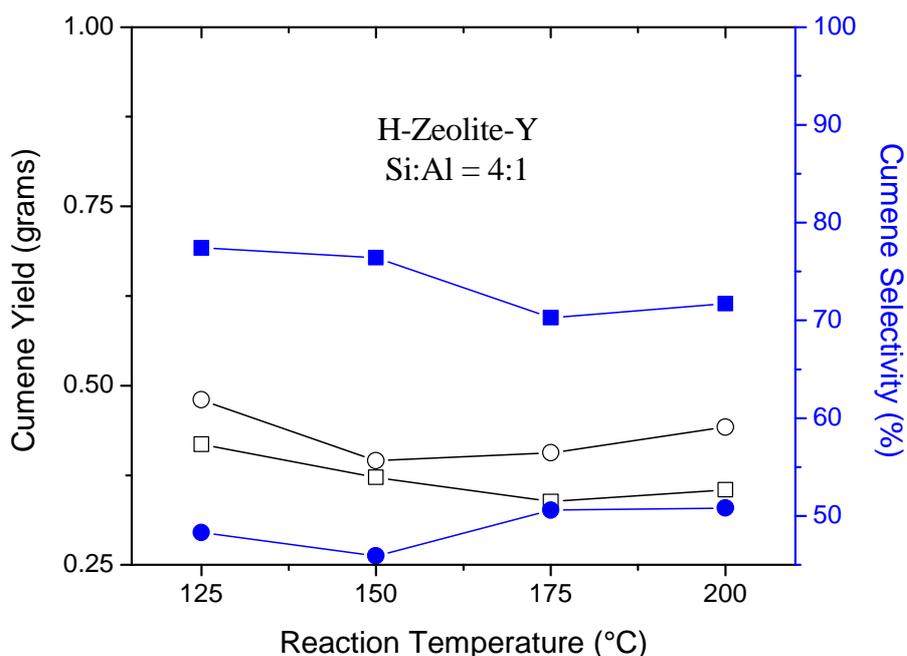**Figure 8.** Results from two separate pot reactor experiments running the H-Zeolite-Y (4:1) in a 7:1 (benzene:propylene) molar ratio. Initial data (○) show a slight correlation between yield and selectivity. Recent experiments (□) indicate a much higher selectivity for cumene that initial observed.

Part III: Mass Spectrometer Reaction Monitoring

The residual gas analyzer mass spectrometer was utilized in order to monitor the catalytic reaction in real time. This may allow for the determination of the optimal reaction time, e.g. when the cumene production has peaked and/or before the formation of impurities. In order to do this monitoring, each molecular species had a mass/charge (m/z) ion selected to represent its relative pressure. An m/z of 78 was easily selected to represent benzene, as this parent mass ion

is quite strong and there will be little direct overlap from heavier hydrocarbons. The fragmentation of benzene and cumene needed to be considered when selecting its representative ion. Standard spectra from the *Registry of Mass Spectral Data*[10] show propylene with very prominent ion peaks at $m/z = 39$ and 41. Benzene, however, is known to have a notable peak at $m/z = 39$ (~10%). This was confirmed experimentally by analog mass spectra taken from the pot reactor containing only benzene as compared to after being filled with the propylene/nitrogen mix. These two spectra are compared in Figure 9, confirming that $m/z = 41$ is indeed the best representation for propylene. Of interest too in this graph is the high amount of $m/z = 32$ signal, the source of which must be oxygen from the 14.5% propylene in nitrogen mixture. Tri-Gas may have generated the mixture with air instead of nitrogen. Standard spectra also confirmed m/z of 105 as being the major ion generated from cumene. The side product DIPB has a small overlap with this cumene signal; standard spectra show all the DIPB isomers have $m/z = 147$ as the highest ion population.
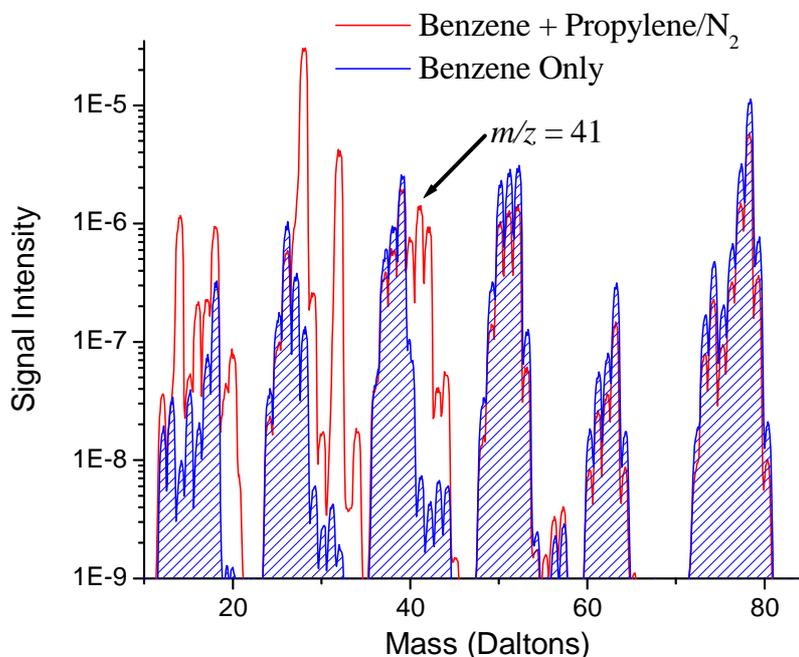
Figure 9. Analog mass spectrum from the pot reactor filled with benzene and residual air only (filled tracing) as compared to after pressurizing with 14.5% propylene in N_2. Demonstrates the most unique propylene peak is at $m/z = 41$.

One of the near optimized catalytic reactions was used as the model for continuous monitoring of gas-phase reactants and products. Chosen was the H^+-form β-zeolite (25:1) running at 150ºC with a 7:1 benzene to propylene molar ratio. Figure 10 contains the continuous monitoring plot beginning after the filling of the reactor with the propylene/nitrogen mix. As the pot reactor was initially heated the signals for nitrogen, propylene and benzene all increase as the internal pressure increased. The reaction clearly starts soon after the system is heated, with propylene being quickly consumed and cumene being produced. DIPB signal eventually appears just above the level of noise; both its production and that of cumene cease due to a lack of propylene. It is believed that propylene is completely consumed and that the remaining signal is due to a cumene ion fragment (~3% as compared to main $m/z = 105$ fragment).[10] No appreciable decrease in the benzene signal is observed due to it being in excess and the plot on a log scale.

Confirmation of the molecular identities attributed to the continuous scan mass spectral data was performed by re-running the same reaction and acquiring a complete analog spectrum. These scans were performed at 30 and 60-minute into the reaction interval. Figure 11 shows the resulting spectral areas of interest. The low mass range spectrum (left) demonstrates the dropping of the propylene mass spectral signature, with the 30-minute tracing filled for clarity. The high mass part of the spectrum (right) shows formation of cumene. No DIPB was observed at either of these times the spectra were taken, though other reactor conditions have generated these spectra.
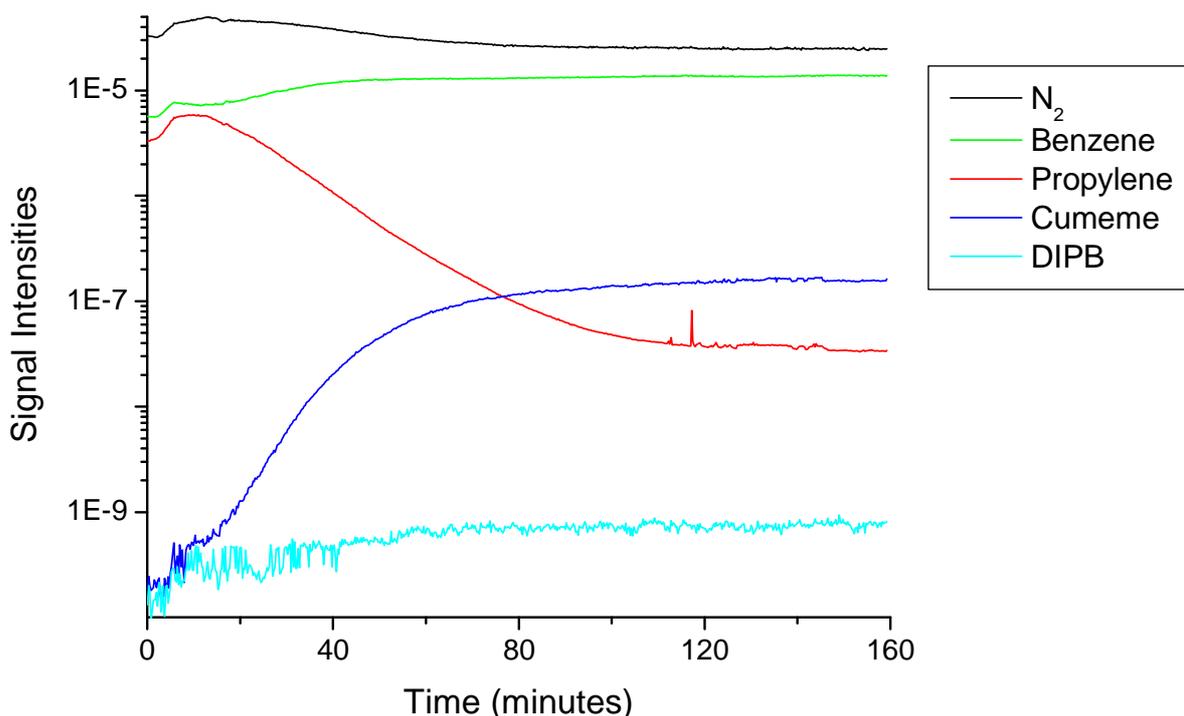
Figure 10. Pressure vs. time plot illustrating the conversion of benzene and propylene into cumene. Very little DIPB side-product is observed with this method. Legend lists species in the same order as seen at 40 minutes.
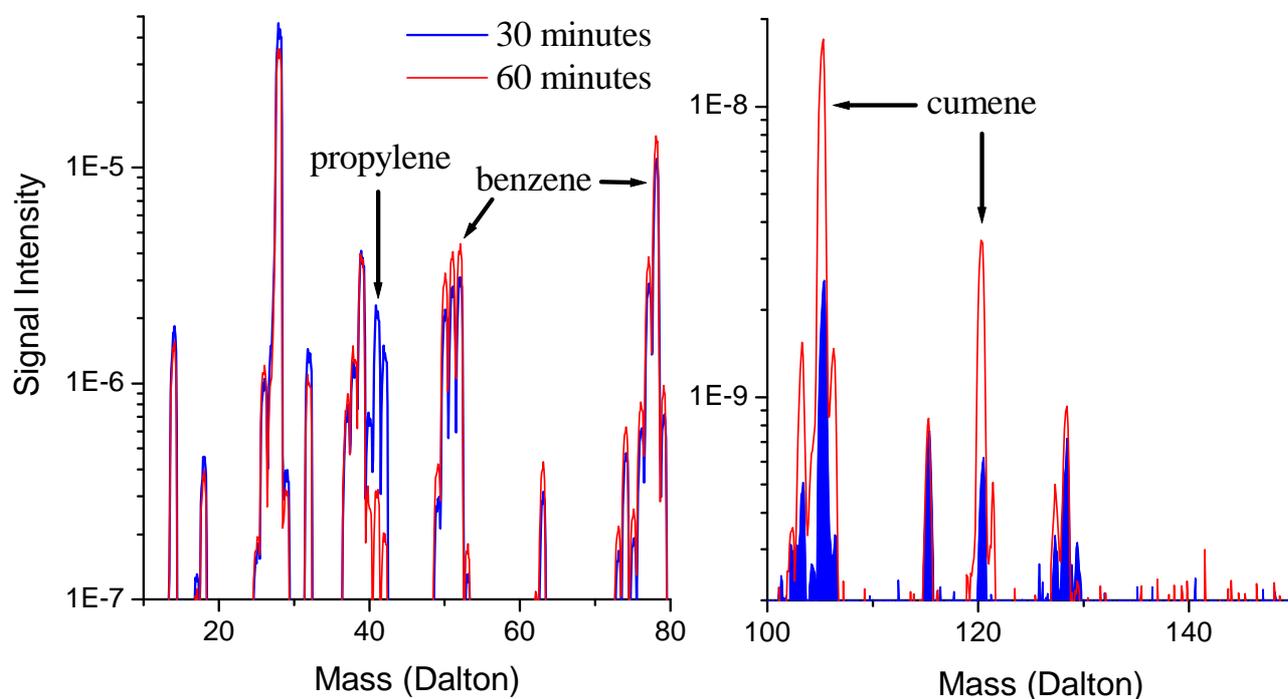
Figure 11. Analog mass spectra taken at 30 and 60 minutes from a 150ºC reaction of H$^+$-form β-zeolite (25:1) in the pot reactor. Creation of cumene and consumption of propylene are most notable.

Discussion

The comparison of the two reactor designs has yielded some insight into ways to further optimize the reaction design and conditions. The initial inclination is to feel the "T" reactor did not perform near as well as the pot reactor. The two major differences in the reactors are the lack of a stirring fan and more contained zeolite volume in the "T" reactor's bottom plug. Lack of a fan may slow the catalytic reaction, as the propylene is slower to diffuse to the zeolite surface. In similar fashion, the smaller container for the zeolite in the "T" reactor has less surface exposure, so again the propylene is limited by diffusion into the solid catalyst. These arguments are supported by the 20:1 benzene:propylene results from Figure 6 that indicate an improved selectivity in the pot reactor when less propylene is present; this same trend has been previously observed.[6,11] Also, the lower sample holding volume in the "T" reactor will allow any remaining benzene liquid to remain in direct contact with the zeolite, saturating and creating another diffusion barrier. However, the lower yield was accompanied by a large increase in cumene selectivity (Figure 4) by reduction of DIPB. The "T" reactor may be facilitating the cumene displacement out of the zeolite by its having liquid benzene in contact with the zeolite in the small cup. Given its greater cumene selectivity, further work should be performed on this reactor or a modified zeolite holder placed into the pot reactor.

From all of the pot reactor data, the best results were consistently obtained from the H$^+$-form β-zeolite with a 75:1 Si to Al ratio. Figure 6 demonstrates this, where utilizing either 20:1 or 7:1

benzene to propylene mixtures typically results in >80% selectivity for cumene, with the best yield of approximately 95% at 200ºC reaction with 91% selectivity. A trend seen with all the β-zeolites is that the selectivity profile changes to an increasing selectivity when the reaction gets to its highest temperatures. Perhaps this reflects cumene's ability to desorb more easily at high temperature from the zeolite and allow it to be replaced by the more abundant benzene. Cumene leaving the zeolite, either dissolved in liquid or vaporizing into the gas phase, prevents further alkylation into the DIPB byproduct. Forbearing the appearance of new side reactions, there may exist optimum reaction temperatures over 200ºC.

Comparison to the alkylation results of Siffert et al.[6] show similarity in the ranges of selectivity, but most of our results here do not indicate the temperature effects on yield (their conversion %) they observed. This likely due to their usage of a continuous flowing system as compared to the static volume utilized here. Figure 10 shows that at a 1-hour reaction time >95% of the propylene mass spectral signature has gone. Even our less active reactions may be nearing completion after one hour. Further research is to include the examination of the reaction products at an earlier reaction time-point to improve the sensitivity of cumene yield to reactor variables.

The real-time mass spectral reactor monitoring gives added insight into the heterogeneous catalysis process. When analyzing this data it is important to know that the intensities of the different species cannot be directly compared as they are affected not only by ionization efficiency but also by their vapor pressures. Propylene, having the largest vapor pressure of the organics here, will result in the largest signals followed in descending order by benzene, cumene and DIPB. This being a reason the gas chromatography data of the resulting liquid is used to quantify the components. A close look at the cumene production in Figure 10 indicates a delayed release back into the gas phase while the propylene is quickly absorbed/consumed. This observation, performed at 150ºC, leads credence to the idea proposed above that cumene desorption from the zeolite may be slow when the temperature is < 200ºC.

The analog mass spectra fail to show any appreciable propylene oligomerization, i.e. no increase in C_4–C_6 products, of which hexenes are preferred oligomer products formed from 0.15–0.41%.[12] These and other coke products generated from propene can be readily adsorbed into the zeolite, thereby not seen, and decrease the catalytic efficiency.[6,13]

Conclusion

Production of cumene by the H^+-form β-zeolite, optimally that with a 75:1 Si to Al ratio, has been shown to be efficient under many conditions, with up to 95% yield or 99% selectivity. For this zeolite, optimization of yield occurs with the higher acidity catalysts (75:1 or 25:1) and high temperature, whereas the selectivity is better with less acidic catalysts and either low (125ºC) or high (200ºC) temperatures. Mass spectral component monitoring can show reaction rate information and indicate reaction completion, as well as monitor for side-product formation. This MS monitoring also identified cumene retention was occurring in the β-zeolite, identifying a plausible reason for DIPB production. This cumene retention is reduced in the "T" reactor design by direct saturation in the liquid benzene, resulting in less DIPB formation.

Ongoing research includes (1) use of novel acidified zeolites synthesized at SNL, (2) early reaction monitoring by in-situ mass spectral studies, and (3) improvements in bulk reactor design.

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Appendix

Experimental Results from All Reactions

Table A-1. "T" Reactor Results

Catalyst	Temp (°C)	Initial C_6/C_3 Ratio	% Conversion C_3H_6	C_6H_6	Yield Cumene (grams)	Selectivity (%)
β-Zeolite (300:1)	150	7	72.5	-	0.051	100.0
β-Zeolite (75:1)	150	7	90.2	-	0.159	100.0
β-Zeolite (75:1)	150	7	93.9	-	0.177	99.1

Table A-2. Pot Reactor Results

Catalyst	Temp (°C)	Initial C_6/C_3 Ratio	% Conversion C_3H_6	C_6H_6	Yield Cumene (grams)	Selectivity (%)	Reaction Set [a]
β-Zeolite (25:1)	125	7	79.6	21.7	0.623	64.6	1
β-Zeolite (25:1)	125	7	100		0.038	100.0	2
β-Zeolite (25:1)	150	7	95.1	26.0	0.576	57.6	1
β-Zeolite (25:1)	150	7	100		0.225	89.6	2
β-Zeolite (25:1)	175	7	92.2	24.0	0.605	60.0	1
β-Zeolite (25:1)	175	7	100		0.504	80.8	2
β-Zeolite (25:1)	200	7	91.7	21.6	0.751	61.5	1
β-Zeolite (25:1)	200	7	100		0.668	87.2	2
β-Zeolite (25:1)	75	20	58	23.9	0.096	>90	1
β-Zeolite (25:1)	75	20	99	13.3	0.090	>90	1
β-Zeolite (25:1)	125	20	89	21.7	0.289	>90	1
β-Zeolite (25:1)	150	20	89	18.4	0.233	92.2	1
β-Zeolite (25:1)	150	20	82	17.0	0.223	>90	1
β-Zeolite (25:1)	175	20	95	11.9	0.278	>90	1
β-Zeolite (25:1)	200	20	100	20.9	0.318	93.0	1
β-Zeolite (75:1)	150	**3**	63.3		0.965	71.4	2
β-Zeolite (75:1)	125	7	86.1	22.8	0.801	88.5	1
β-Zeolite (75:1)	150	7	86.1	15.5	0.720	78.8	1
β-Zeolite (75:1)	150	7	100		0.579	76.6	2
β-Zeolite (75:1)	150	7	95.4		0.632	80.0	**3**
β-Zeolite (75:1)	175	7	92.6	20.7	0.775	82.2	1
β-Zeolite (75:1)	200	7	93.7	20.4	0.895	90.6	1
β-Zeolite (75:1)	125	20	84.3	12.9	0.238	91.5	1
β-Zeolite (75:1)	150	20	79.9	10.0	0.188	88.4	1
β-Zeolite (75:1)	175	20	96.5	10.7	0.273	86.3	1
β-Zeolite (75:1)	200	20	93.4	8.3	0.278	94.2	1
β-Zeolite (300:1)	125	7	100		0.256	94.6	2
β-Zeolite (300:1)	150	7	100		0.478	87.6	2
β-Zeolite (300:1)	175	7	100		0.609	79.4	2

β-Zeolite (300:1)	200	7	100		0.634	83.7	2
H-Z-Y (4:1)	125	7	76.2	19.4	0.480	48.3	1
H-Z-Y (4:1)	125	7	94.0		0.418	77.4	2
H-Z-Y (4:1)	150	7	79.3	18.7	0.395	45.9	1
H-Z-Y (4:1)	150	7	98.5		0.372	76.4	2
H-Z-Y (4:1)	175	7	86.4	18.5	0.406	50.6	1
H-Z-Y (4:1)	175	7	90.9		0.338	70.3	2
H-Z-Y (4:1)	200	7	93.3	23.5	0.442	50.8	1
H-Z-Y (4:1)	200	7	89.3		0.355	71.7	2
H-Z-Y (4:1)	125	20	100	12.3	0.207	92.2	1
H-Z-Y (4:1)	150	20	81	6.2	0.178	77.0	1
H-Z-Y (4:1)	175	20	96	16.0	0.233	83.4	1
H-Z-Y (4:1)	200	20	98	13.4	0.260	91.1	1
H-Z-Y (30:1)	125	7	91.8	17.4	0.463	66.6	1
H-Z-Y (30:1)	125	7	89.1	12.9	0.525	58.4	1
H-Z-Y (30:1)	125	7	99.4		0.298	76.7	2
H-Z-Y (30:1)	150	7	98.4		0.400	67.9	2
H-Z-Y (30:1)	175	7	98.4		0.392	62.3	2
H-Z-Y (30:1)	200	7	97.5		0.405	65.1	2
H-Z-Y (60:1)	125	7	79.3	17.6	0.500	68.6	1
H-Z-Y (60:1)	150	7	83.1	11.6	0.480	66.6	1
H-Z-Y (60:1)	175	7	90.4	17.0	0.570	64.0	1
H-Z-Y (60:1)	200	7	94.6	20.6	0.630	58.4	1
MCM-22 (30:1)	150	7	31.7	10.0	0.383	80.5	1
MCM-22 (30:1)	125	20	45.8	5.5	0.131	95.4	1
MCM-22 (30:1)	150	20	89.9	8.6	0.231	83.8	1
MCM-22 (30:1)	175	20	94.6	9.0	0.248	85.2	1
Englehard F-24	150	7	70.8	14.8	0.365	79.5	1
Englehard F-24	125	20	92.9	16.1	0.185	82.4	1
Englehard F-24	150	20	91.1	13.5	0.157	87.2	1
Englehard F-24	175	20	79.0	10.6	0.080	92.5	1
Englehard F-24	200	20	85.0	6.6	0.063	96.5	1

[a] "Reaction Set" refers to who and when the experiment was run and data collected. 1 represent the first reactions run by Dan Trudell; 2 are those run by Stacia Barrow (Summer Intern 2001); 3 are also Stacia but with the stirring mechanism run at a 1/3 slower rate.

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