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Maleic Anhydride to Succinic Acid Conversion in a Green Hydrogen-Generating Flow Reactor with COSMO-RS Solvent Interaction Modeling

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Succinic acid is an important molecule for polymer and biological applications. Two main methods produce succinic acid: bioreactors using renewable feedstocks and catalytic hydrogenation. Hydrogenation is usually an energy- and cost-intensive process; however, electrolysis can generate hydrogen cheaply and deliver it efficiently. This study utilizes a reactor that can produce and inject electrolytically generated hydrogen to a Pd/C catalyst to hydrogenate maleic anhydride to succinic acid. Excellent conversion and selectivity were achieved at lower temperatures than those reported in the literature, with >99% conversion at ambient conditions. In addition, the interactions between maleic anhydride and various solvents were simulated to determine polarity, affinity, and activity coefficients, with the most compatible solvent being dimethylformamide (DMF) having a simulated activity coefficient of .53.

1. Introduction

Succinic Acid (SA) is an important chemical platform for many biochemical and polymer applications. It has also been used as a nutritional supplement and a food additive. Multiple methods exist for producing succinic acid, but two major systems are the bioreaction of renewable feedstocks and the catalytic hydrogenation of maleic anhydride (MA). While fermentation processes offer multiple benefits for producing succinic acid, poor yields and inefficient separation have been observed (Khunnonkwao et al., 2018). Until these issues are resolved, improving the efficiency and safety of the catalytic hydrogenation process is important. An additional benefit of the catalytic process is the ability to prioritize intermediates, as well as other important chemicals such as γ-butyrolactone (GBL) and tetrahydrofuran (THF). Figure 1 details a pathway for this. Possible pathways exist between these two major routes, but the catalysts and conditions are usually distinct enough that, apart from designed experiments, there is little to no overlap (Herrmann & Emig, 1998; Q. Wang et al., 2024). Hydrogenation of malic acid to succinic acid is thermodynamically unfavored at milder conditions, so the hydrogenation of maleic and fumaric acids is dominant (López Granados et al., 2020).
Noble metal catalysts, which often exhibit excellent selectivity and conversion in hydrogenation processes, are widely used for the conversion of maleic anhydride to succinic acid (Dou et al., 2022; Orozco-Saumell et al., 2022; Q. Wang et al., 2024). Cheaper transition-metal catalysts have been developed, including nickel- and copper-based catalysts (Herrmann & Emig, 1997; H. Wang et al., 2025). Regarding reaction parameters, the succinic acid pathway is temperature and pressure-dependent. Much work has focused on reducing the temperature and pressure requirements for this process, with mild conditions achieved (Guo et al., 2012; Kim et al., 2015). The source of hydrogen used in hydrogenation processes is often a cause for concern, as conventional methods pose several environmental and safety risks.

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To address these concerns, electrolytic hydrogenation is an optimal method for lab-scale experimentation, reducing the safety and environmental impacts of hydrogen production and storage. Scale-up to industrial levels is also possible and is an area of future research (Anand et al., 2025). In this study, a novel reactor that supplies electrolytic hydrogen to a packed bed reactor (PBR) was used to convert maleic anhydride under various conditions. This was done to improve safety, as well as to source the hydrogen more economically and in an environmentally friendly way. Palladium on carbon was used as the catalyst, as it demonstrates the highest selectivity and conversion(Dou et al., 2022; Orozco-Saumell et al., 2022).

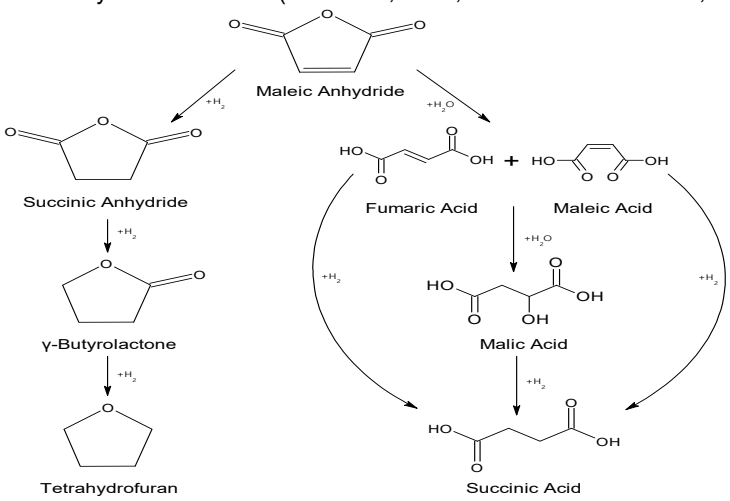

Figure 1: General Reaction Pathways for Maleic Anhydride Hydrogenation

2. Methodology

2.1 Materials

The materials used in this research were as follows: ACS-grade Acetone was purchased from bulk supplies held by the Missouri University of Science and Technology Department of Chemistry. Maleic anhydride was purchased from Fisher Scientific (Fair Lawn, NJ, USA). Fumaric acid, maleic acid, malic acid, and succinic acid for standards and DMSO-d6 for NMR testing were purchased from Fisher Scientific in Fair Lawn, NJ, USA. The H-Cube-compatible 10% Pd/C catalyst cartridge was purchased from ThalesNano (Budapest, Hungary).

2.2 Procedure

Maleic Anhydride was dissolved in a 50:50 vol% solution of water and acetone to hydrolyze to maleic acid. This solution was then fed into a ThalesNano H-Cube Mini Plus Hydrogenation reactor operated under predetermined temperatures, pressures, and flow rates. The reactor was primed with a 50:50 (v/v) water-ethanol solution before and after each experiment. After collection, the sample was then dried in a vacuum oven for 48 hours before analysis. Three samples were taken for each experiment. Table 1 contains the tested temperatures, pressures, and flow rates. For the samples prepared at 0 barg, pressure excursions up to 15 barg were experienced. This is most likely due to shifting of the catalyst within the cartridge, and the manufacturer has confirmed that the pressure excursions are normal with operation.

Table 1: Experimental Conditions

Label	Initial MA Conc. (M)	Temperature (°C)	Pressure (barg)	Flow Rate (ml/min)	Catalyst
A	0.18	50	0*	0.5	10% Pd/C
B	0.18	50	30	0.5	10% Pd/C
C	0.18	21	0*	0.5	10% Pd/C
D	0.18	21	30	0.5	10% Pd/C

2.3 Analytical Techniques

Nuclear magnetic resonance (NMR) spectroscopy was conducted with a Magritek Spinsolve Carbon benchtop NMR Spectrometer. Analysis was performed using Magritek Spinsolve software. After drying, samples were dissolved in 600 µl of DMSO-d6 before NMR analysis.

2.4 COSMO-RS Computational Methodology

COSMO-RS calculations were performed using the COSMO-RS module of the Amsterdam Modeling Suite (AMS, SCM). Molecular structures were geometry-optimized using DFT at the BP86/TZP level, followed by COSMO calculations to generate the surface charge-density distributions and sigma profiles. The lowest-energy conformer of each compound was used. Calculations were conducted at 298.15 K. Maleic anhydride was treated as an infinitely dilute solute in each pure solvent, and the corresponding activity coefficients were calculated to evaluate solvent–solute affinity.

3. Results and Discussion

3.1 NMR Results

Figure 2 shows the characteristic ^{1}H NMR chemical shift results for the conditions in Table 1. The teal line is the spectra for the solution, which exhibits major peaks at 10.3, 6.1, and 2.4 ppm, corresponding to hydroxyl, vinyl alcohol, and methyl groups. Notably, there is no significant peak around 7.0 ppm, which is indicative of maleic anhydride. This shows that hydrolysis of the maleic anhydride to maleic acid is achieved with >99% conversion. The solution is therefore comprised mostly of maleic acid. The other spectra show a major peak at 2.2, with a weak broad peak between that shifts between 7-12 ppm. Various weak peaks are also present at 3.9, 3.7, 3.5, 1.3, 1.2, and 1.0. The peaks in the range of 1-3 are related to unsaturated alkyl groups, while the weak broad peak is related to hydroxyl groups which can show up differently due to the solvent, concentration, and magnetic field strength. Apart from the hydroxyl groups, there is no significant peak at 7.0, or 6.0, which indicates that there is little to no maleic anhydride or maleic acid present, and that conversion is very high. Succinic acid conventionally has a strong peak at 2.4 and a very weak and broad peak around 12. Shifting of the peak due to the lower concentration and magnetic field strength could result in the alkyl peak showing up at 2.2 and the hydroxyl peak showing across a broad range. Addition of the area of all the peaks not related to these were less than 1% of the total area, therefore conversion to succinic acid is >99%.

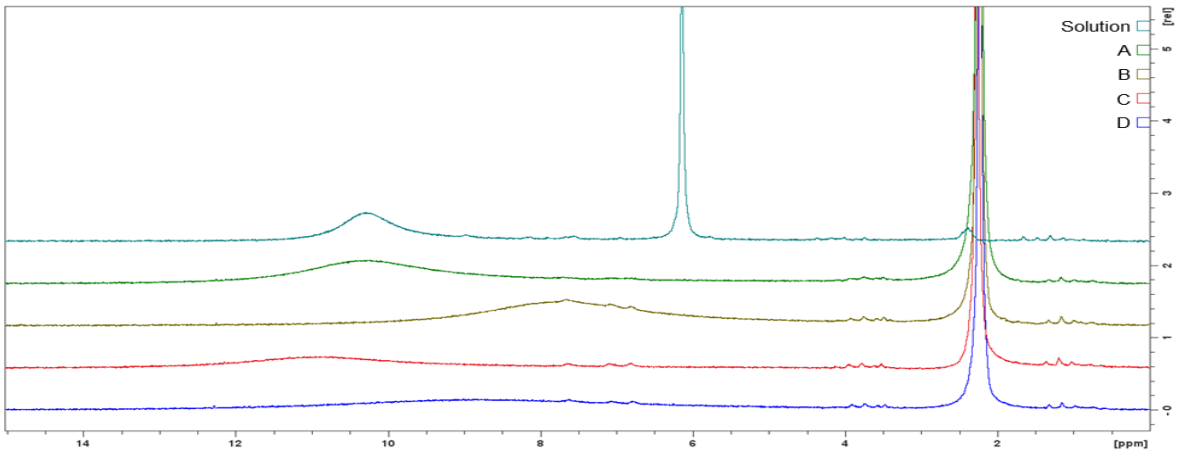

Figure 2: Characteristic NMR Spectra of: MA Solution (Teal; Solution), 50 °C 30 bar (Green; A), 50 °C 0 bar (Brown; B), 21 °C 30 bar (Red; C), and 21 °C 0 bar (Blue; D)

3.2 Sigma Profile Analysis of Maleic Anhydride and Selected Solvents

The sigma profile, p(σ), describes the distribution of surface charge densities on a molecule and provides insight into the polarity and hydrogen-bonding characteristics of each solvent (Figure 3).
The central region around σ = 0 e/Å² represents nonpolar molecular surface area, while the negative and positive σ regions represent polar surface segments associated with hydrogen-bond acceptor and hydrogen-bond donor behavior, respectively. The sigma profiles of the selected solvents show clear differences in polarity and interaction potential with maleic anhydride. Maleic anhydride contains highly polar anhydride oxygen atoms, which behave mainly as hydrogen-bond acceptor sites. Therefore, solvents with strong polar surface distributions and suitable complementary interaction regions are expected to better stabilize maleic anhydride in solution. Polar aprotic solvents such as DMF, acetone, acetonitrile, dioxane, γ-butyrolactone, and tetrahydrofuran show favorable surface charge distributions because they provide strong dipolar interactions without forming highly self-associated hydrogen-bonding networks. These characteristics allow them to interact

efficiently with the anhydride group of maleic anhydride. In contrast, water and alcohols show strong polar profiles due to their hydrogen-bonding capacity; however, their strong solvent–solvent hydrogen bonding can reduce their ability to solvate maleic anhydride effectively. Dissolution in these solvents requires disruption of the existing hydrogen-bond network, which creates an energetic penalty. This explains why protic solvents, especially water and higher alcohols, are predicted to be less favorable for dissolving maleic anhydride compared with polar aprotic solvents.

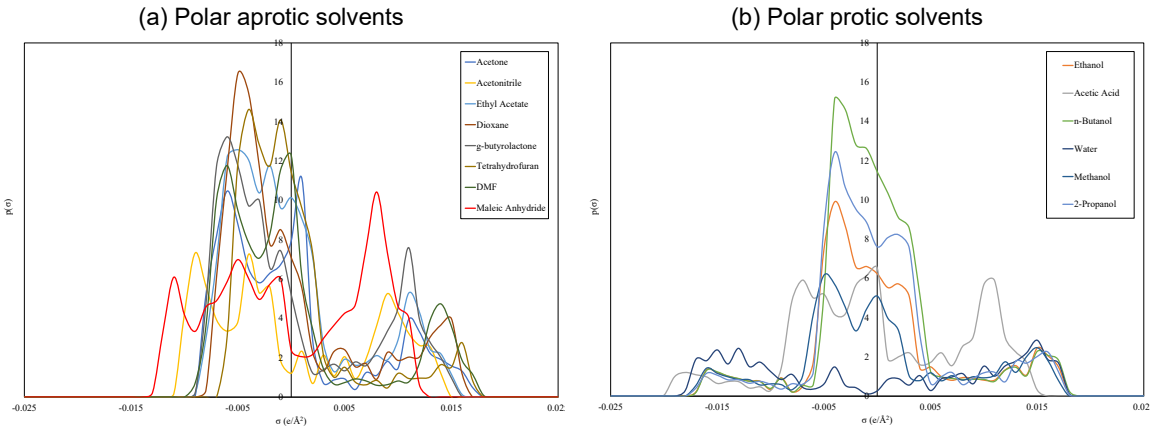

Figure 3: Sigma profile for maleic anhydride and the solvents

3.3 Activity Coefficient Analysis of Maleic Anhydride in Selected Solvents

The activity coefficients in Table 2 quantify the thermodynamic compatibility between maleic anhydride and each solvent, with lower values indicating stronger solute–solvent affinity and more favorable dissolution.

Table 2. Activity coefficients of maleic anhydride dissolution in the solvents.

Solute	Solvent	Activity Coefficient
Maleic Anhydride	Acetone	0.7141433
	Ethanol	5.86777322
	Acetic Acid	2.62001875
	Ethyl	1.1169528
	Propanol	5.35859647
	Butanol	7.37962702
	Water	225.74254
	Dioxane	0.77646906
	γ-butyrolactone	0.62683214
	Tetrahydrofuran	1.15698868
	Methanol	5.1547364
	DMF	0.53147812
	Acetonitrile	0.73824377

DMF shows the strongest predicted affinity, with an activity coefficient of 0.531, followed by γ-butyrolactone and tetrahydrofuran (0.627), acetone (0.714), acetonitrile (0.738), and dioxane (0.776). These results indicate that polar aprotic solvents provide the most favorable environment for dissolving maleic anhydride. Ethyl acetate shows nearly ideal behavior (1.117), while acetic acid is less favorable (2.620). Alcohols exhibit substantially higher activity coefficients, including methanol (5.155), 2-propanol (5.359), ethanol (5.868), and n-butanol (7.380), indicating weaker compatibility. Water has by far the highest activity coefficient (225.743), demonstrating extremely poor thermodynamic compatibility, and is further unsuitable because maleic anhydride can hydrolyze to maleic acid. The activity coefficient results are consistent with the sigma profile, sigma potential, and surface charge density analyses, confirming that polar aprotic solvents, particularly DMF, γ-butyrolactone,

tetrahydrofuran, acetone, acetonitrile, and dioxane, are the most suitable candidates for dissolving maleic anhydride without hydrolysis occurring.

3.4 Surface Charge Density Distribution of Maleic Anhydride

The surface charge density map of maleic anhydride shows the polar and nonpolar regions on its molecular surface, as shown in Figure 4. The anhydride oxygen atoms create strongly electron-rich regions, shown by the highly polar surface zones around the oxygen-containing functional group. These regions confirm that maleic anhydride behaves primarily as a hydrogen-bond acceptor molecule. The molecule contains no hydroxyl, amine, or other hydrogen-bond donor groups. Therefore, maleic anhydride is not expected to donate hydrogen bonds, but it can accept hydrogen bonds through its carbonyl and bridging oxygen atoms. This structural feature explains why solvents that stabilize electron-rich anhydride oxygen atoms are important for dissolution. The surface charge density also shows that maleic anhydride contains both polar and moderately nonpolar regions. The polar anhydride group dominates the interaction behavior, while the carbon backbone contributes limited nonpolar character. Therefore, an ideal solvent for maleic anhydride should provide sufficient polarity to stabilize the anhydride group while remaining compatible with the organic molecular framework. This balance is best achieved with polar aprotic solvents, which explains their better-predicted solubility performance.

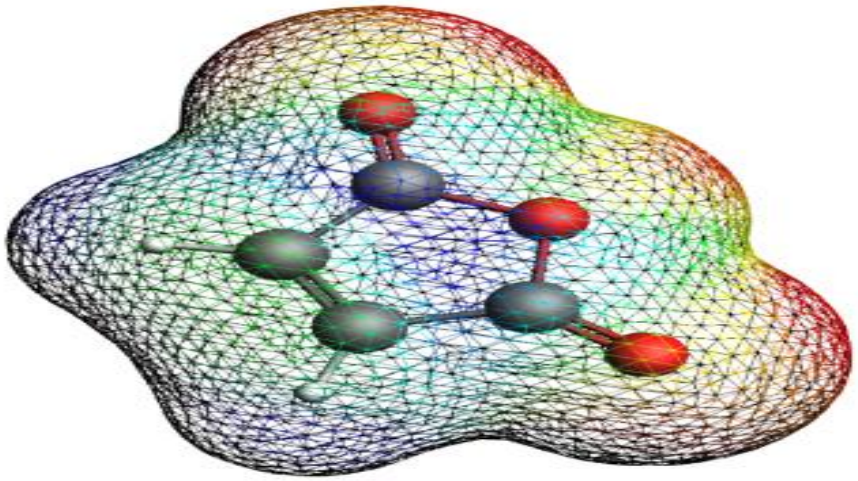

Figure 4. Surface charge density distribution of maleic anhydride

4. Conclusions

Maleic Anhydride is a chemical that contains both polar and non-polar regions. As a result, similarly structured aprotic solvents show the best activity coefficients for forming solutions. The sigma profile of maleic anhydride highlights its polar surface characteristics and its potential interactions with solvents, particularly through the anhydride oxygen atoms. This allows for multiple end products, such as tetrahydrofuran and succinic acid. The conversion of maleic anhydride to succinic acid proceeds via hydrolysis of maleic anhydride to fumaric and maleic acids, which are then hydrogenated to succinic acid. Other mechanisms exist but are thermodynamically unfavorable. The chosen hydrogenation method was electrolysis. This was done to improve process safety and energy efficiency. Experimental results show that at elevated pressures, a Pd/C catalyst enables very high selectivity and conversion at low temperatures, achieving >99% conversion.

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