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Characterization and synthesis of methyl lactate through esterification reaction under supercritical state of carbon dioxide

Kirti Bhushan Zare* **and Manisha Tanver**
Dr. D.Y. Patil Institute of Engineering Management and Research, Pune, MS, India
kaprekirti07@gmail.com

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Abstract

Optimization of Methyl lactate has been done through two factorial methods, to learn various effective factors such as temperature, pressure, mole ratio for obtain higher conversion. Esterification reactions were carried out under supercritical state of cabondioxide. Optimize condition is formed at 1:8 mole ratio, 110^{0}C temperature and 6 hours.

Keywords: Optimization, Esterification reaction, supercritical CO_2, Methyl lactate, Calcium carbonate.

Introduction

Fischer esterification reactions take place when carboxylic acid is mixed with alcohol in presences of acid catalyst esterification reaction where present in equilibrium state. As alcohol present in large excesses, it used for solvents. In present article two factorial methods are used to find out optimum condition of product. Methyl lactate is also called as methyl ester of lactic acid. Methyl lactate is mixture of methanol and lactic acid.

Methyl lactate is ester of lactate compounds that are measured as nontoxic and readily biodegradable[1]. The application areas for methyl lactate is production of lacquers and drops. Ester is compound resulting from an acid. The ester is contains one –OH group which is substituted by an –O–alkyl group[2]. Ester is more volatile than the same molecular weight carboxylic acid[3].

Supercritical carbon dioxide is a fluid condition of carbon dioxide, where it is kept at its critical temperature and severe pressurized or above. Supercritical CO_2 is becoming an important commercial and industrial solvent due to its low toxicity and environmental impact, due to its role in chemical extraction.

Due to the relatively low temperature of the reaction and the CO_2 stabilization, more compounds are poorly or not sold. In addition, the replacement of many extracted compounds in CO_2 varies with pressure[4]. It used in Electro physical carbon absorption reaction of para-isobutyl benzyl to ibuprofen[5].

Supercritical carbon dioxide has various applications. Supercritical carbon dioxide in agriculture is used to remove pesticides and metals. It is used in Venus planets as possible solvent to support organic movement. Supercritical carbon dioxide is naturally refrigerant. There is number of application of coz as co-solvents, so in the present articles we had maintained supercritical is at 31^{0}C and 73 bar. It is worthwhile, that among many polar organic compounds used widely for this purpose are certainly methanol, ethanol, and propanol[6]. Carbon-based esters having wide application in chemical field for production of perfumery, aromas, medicines, plasticizers, diluters and intermediates. Methyllactate is lactate measured as nontoxic, highly and readily biodegradable[6].

Methyl lactate is used in pharmaceutical and cosmetic industries. It is also used as solvents into lacquers, nitrocellulose and polyvinyl compounds. Methyl lactate is water solvable and prepared by esterification reaction.

There are four basis methods for prepare methyl ester as follows: i. Lactic acid and alcohol antigen with estrotic reaction, ii. Reaction of 2-Hydroxypropanoic acid and alcohol through Transesterification reaction, iii. Conversion of methyl lactate into esters through alcohol, iv. metal lactate and alkyl halide reaction.

Therefore, recovery and recycling of alkali metal is possible to form a pollution-free process for the synthesis of pure methyl lactate[7]. Polymers include synthetic equipment production, pesticide preparation, and plastic formation. Their production requires very pure monomeric lactic acid[8]. Lactoyalactic acid is also both acid and alcohol, and hence the formation of intermolecular ester can continue, resulting in the formation of atoms containing three or more milk-acid components and it is possible to create highly high-molecular polymer[9].

Methodology

A mole ratio of 1:8 of calcium lactate and methanol has been taken into reactor. Pressurized CO_2 into rector four-five times to achieve carbon dioxide into liquid formed. After that keep reactor at room temperature to attain supercritical condition. The reaction mixture heated to formed product .Then samples has been taken for analysis.

Results and discussion

In the design of experiments, eight run has been carried out by two factorial methods for optimization. The three variables remained measured for optimization.

Whereas, A: Molar ratio (Calcium lactate: Methanol), B: Reaction temperature ($^{\circ}$C) C: Time (hour).

Table-1: Optimization of Methyl Lactate

Molar Ratio	Temp(^{0}C)	Time (hour)	%Formation
1:2	95	6	80
1:2	95	4	70
1:2	110	6	72
1:2	110	4	76
1:6	98	6	79
1:6	98	4	71
1:6	110	6	65
1:8	110	6	88

After optimization, sample was analyzed through Coulometric titration, Liquid chromatography–mass spectrometry.

Table-2: Calibration curve of Methyl lactate.

Cont. of Methyl lactate	Cont. of Isopropanol	Cont. of methyl Lactate (%)	Area of methyl lactate
0.0177	9.9016	0.17844	2710.7
0.1022	9.9914	1.01	27812

Firstly standard has been prepared with concentration of methyl lactate and isopropanol. Then Plot concentration vs. area of methyl lactate as shown in Figure-1 similarly different area of methyl lactate were obtained from eight batches fitted in Figure-1.

From ideal gas law, at low pressure, real gasses behave like perfect gases.

PV = NRT

Where, P=Pressure, V=Volume, N=Number of moles, R=Universal gas constant, T= Temperature.

As increase into pressure temperature also increase, hence different Behavior of methanol and Carbon dioxide with different temperature and pressure.

Table-3: Behavior of Carbon dioxides.

Temperature(^{o}c)	Pressure(bar)
50	25
100	30
150	40
200	45
250	50
300	52

Temperature and pressure profile of carbon dioxide, at different values of temperature with acquired value of pressure.

Table-4: The different temperature has been taken for calculating pressure.

Temperature(^{o}C)	Pressure(bar)
120	2
140	3
160	3.5
180	4
200	4.5
220	5

As increase in temperature of methanol pressures also increases, which profile has been shown in Figure-3.

Conclusion

We had done optimization of methyl lactate through esterification reaction. In this processes eco-friendly route were followed for preparing metal salts. Accordingly our results it was observed pressure and temperature condition of carbon dioxide is directly proportionally to production of methyl esters. Whereas presences of moisture into reactant decreases efficiency of methyl lactate.

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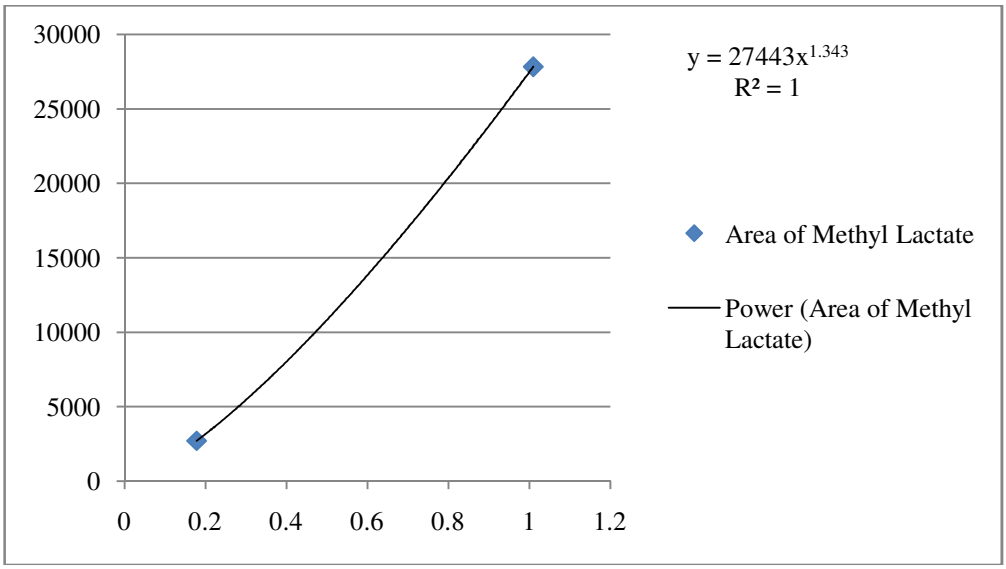

Figure-1: Calibration Curves for Methyl Lactate.

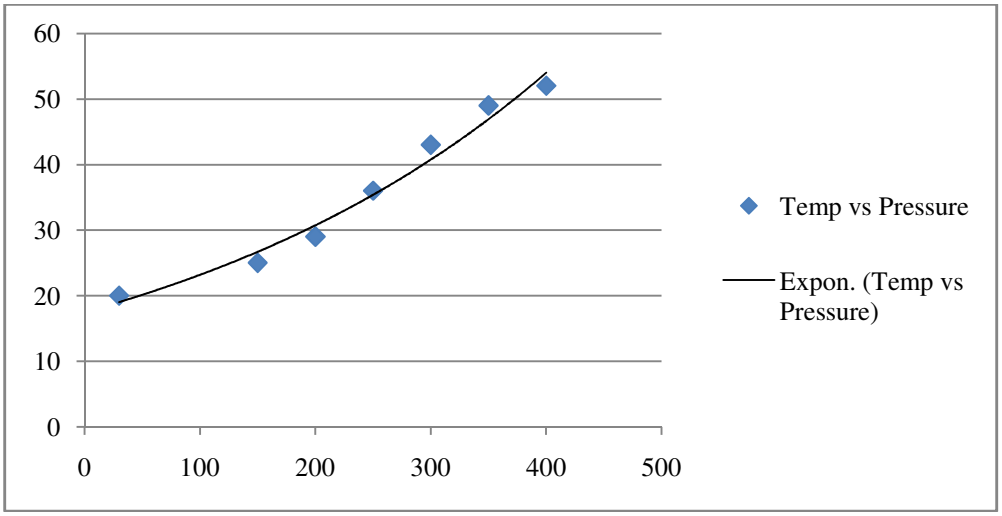

Figure-2: Temperature vs. pressure profile of CO_2.

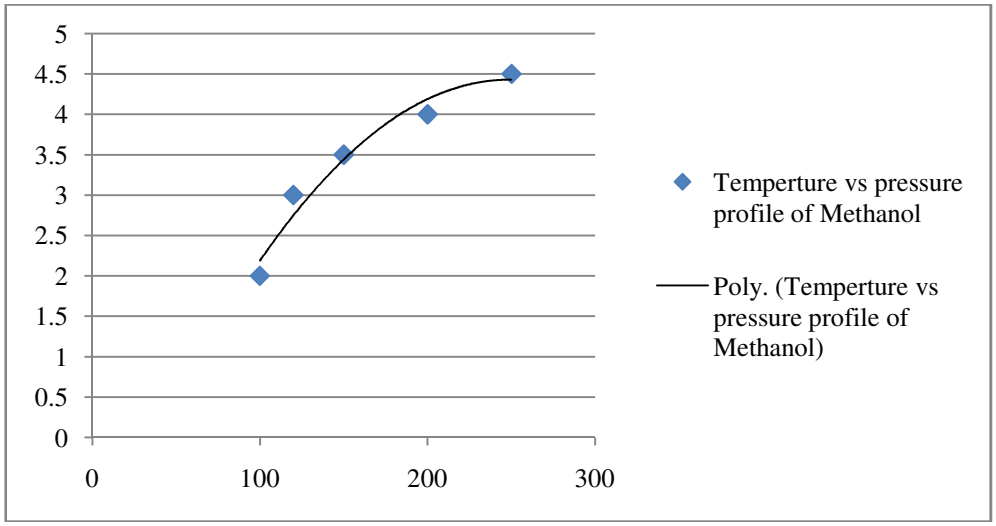

Figure-3: Temperature vs. pressure profile of Methanol.

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