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Process optimization and modeling of microencapsulated phase change material using response surface methodology

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HIGHLIGHTS

- Microcapsules of phase change materials containing paraffin wax and polystyrene have been made.
- Response surface methodology (RSM) was implemented for statistical design and analysis.
- Two models were derived for the prediction of melting latent heat and particle size.
- The microcapsules were characterized by SEM, PSD, DSC, and TGA analyses.
- This study showed that RSM could be applied for modeling and optimization of the system.

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ABSTRACT

Microcapsules containing paraffin wax as cores and polystyrene as shells were prepared by suspension polymerization technique. The influence of four experimental factors, including percentage of initiator/styrene mass ratio (BPO/St wt.%), paraffin wax/styrene mass ratio (PCM/St), percentage of stabilizer/styrene mass ratio (PVP/St wt.%), and water/styrene mass ratio (H_2O/St), on microcapsules properties were investigated. Each factor was in five levels. Response surface methodology (RSM) was implemented for statistical design and analysis of experiments and process modeling. Two mathematical models were derived for prediction of melting latent heat of microcapsules and their average particle size. Analysis of variance showed that PCM/St mass ratio was the most significant factor affecting melting latent heat of parameters, while average particle size is affected by PVP/St wt.% and H_2O/St mass ratio. In process optimization, maximum values of melting latent heat were achieved as 148.5 J/g. Using BPO/St wt.% of 2.18%, PCM/St mass ratio of 1.94, PVP/St wt.% of 8.84%, and H_2O/St mass ratio of 11.67, encapsulation ratio of 78.5% were obtained.

1. Introduction

Microencapsulation of phase change materials (PCMs) is an effective way of enhancing their thermal conductivity and preventing leakage and possible interaction with the surrounding during the melting process. PCMs with a melting point ranging from −10 °C to 80 °C can be microencapsulated [1]. Paraffin waxes are widely used as core material in microencapsulated PCMs (MEPCMs) due to their high latent heat of fusion and availability in a large temperature range. They are also less expensive compared to the other types of PCMs [2].

There are several chemical and physical methods used for the production of microcapsules, which Jamekhorshid et al. [3] went through them completely. Suspension polymerization technique is a chemical method which can encapsulate non-polar PCMs such as paraffin waxes. In this method, droplets of water immiscible reaction mixture are formed through vigorous agitation of the mixture and dissolution of stabilizers in the aqueous continuous phase. Then, polymerization is initiated at the desired temperature until completion.

Polystyrene [4,5], polymethyl methacrylate [6,7], and styrene/methyl methacrylate [8] are the most common shell materials used in this technique [9]. Sánchez et al. [4] successfully encapsulated different non-polar PCMs such as PRS® paraffin wax, tetradecane, Rubitherm®RT27, Rubitherm®RT20, and nonadecane with polystyrene shell.

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Table 1
The level of variables in CCD.

Variable	Low axial ($-\alpha = -2$)	Low factorial (-1)	Center (0)	High factorial ($+1$)	High axial ($+\alpha = +2$)
A: % BPO/St (wt.%)	1	1.75	2.5	3.25	4
B: PCM/St (wt./wt.)	0.2	0.65	1.1	1.55	2
C: % PVP/St (wt.%)	3	5.25	7.5	9.75	12
D: H_2O/St (wt./wt.)	3	5.25	7.5	9.75	12

The latent heat of the MEPCMs depends on the amount of PCM encapsulated; and the application of microcapsules would affected by their size. For those reasons, it is interesting to know how the experimental conditions affect the amount of PCM encapsulated and also the microcapsules size. Some efforts were devoted to enhance the thermal energy storage capacity of the produced microcapsules. Influence of operating conditions such as reaction temperature, stirring rate, and mass ratio of PRS® paraffin wax to styrene on the thermal storage capacity, particle size distribution and morphology of produced particles via suspension polymerization technique were investigated by Sánchez et al. [10]. They also used the Shirasu porous glass (SPG) for production of microcapsules and investigated the effect of different parameters on the particle size distribution and thermal energy storage of microcapsules [11].

To the best of our knowledge there is no research that investigated the influence of material compositions on the thermal energy storage capacity and diameter of particles prepared by suspension polymerization technique. Response surface methodology (RSM) was applied to study the effect of material compositions. A collection of mathematical and statistical techniques are used in RSM to explore the relationships between independent variables and response variables [12].

The objective of this work was to apply statistical methods to investigate the effects of experimental factors, including percentage of initiator/styrene mass ratio, paraffin wax/styrene mass ratio, percentage of stabilizer/styrene mass ratio, and water/styrene mass ratio on particles characteristics (diameter and thermal energy storage capacity). Central composite design (CCD), which is an experimental design useful in RSM for building a second order model for the response variables, was employed to evaluate the coefficients of quadratic mathematical models for the optimization of process. Consequently, the proper material compositions for suspension polymerization process were evaluated to obtain PCM microcapsules with the maximum thermal energy storage capacity.

2. Materials and methods

2.1. Materials

Styrene was of synthesis grade (Merck Chemical) and used as monomer for forming the microcapsule shell. Styrene was washed twice with 5 wt.% NaOH solution to remove the inhibitor. Then it was washed again with distilled water for four times to ensure that sodium hydroxide is completely removed. In each washing stage, styrene and water were separated from each other in a decanter.

Paraffin wax was of extra pure grade and used as PCM. Benzoyl peroxide (BPO) of synthesis grade (Merck Chemical) was used as initiator. Polyvinylpyrrolidone (PVP) of reagent grade (Merck Chemical) was used as stabilizer agent. Methanol was of extra pure grade and used to pour the samples.

2.2. Preparation

PCM microcapsules containing paraffin wax were prepared by suspension polymerization technique in a 1 L double-jacketed glass reactor equipped with a Rushton turbine stirrer with six vertical blades.

Table 2
Experimental plan of polymerization tests and obtained results.

No.	A		B		C		D		Latent heat of fusion [J/g]	Average diameter [μm]
	Coded	Actual	Coded	Actual	Coded	Actual	Coded	Actual		
1	−1	1.75	−1	0.65	−1	5.25	−1	5.25	80.7	245
2	+1	3.25	−1	0.65	−1	5.25	−1	5.25	45.5	381
3	−1	1.75	+1	1.55	−1	5.25	−1	5.25	135.1	225
4	+1	3.25	+1	1.55	−1	5.25	−1	5.25	145.8	330
5	−1	1.75	−1	0.65	+1	9.75	−1	5.25	52.3	313
6	+1	3.25	−1	0.65	+1	9.75	−1	5.25	71.2	245
7	−1	1.75	+1	1.55	+1	9.75	−1	5.25	124.7	194
8	+1	3.25	+1	1.55	+1	9.75	−1	5.25	113.4	216
9	−1	1.75	−1	0.65	−1	5.25	+1	9.75	72.3	260
10	+1	3.25	−1	0.65	−1	5.25	+1	9.75	50.2	269
11	−1	1.75	+1	1.55	−1	5.25	+1	9.75	134.5	260
12	+1	3.25	+1	1.55	−1	5.25	+1	9.75	86.2	223
13	−1	1.75	−1	0.65	+1	9.75	+1	9.75	89	177
14	+1	3.25	−1	0.65	+1	9.75	+1	9.75	76.9	101
15	−1	1.75	+1	1.55	+1	9.75	+1	9.75	132.1	187
16	+1	3.25	+1	1.55	+1	9.75	+1	9.75	104.5	196
17	−2	1	0	1.1	0	7.5	0	7.5	81.2	295
18	+2	4	0	1.1	0	7.5	0	7.5	103	166
19	0	2.5	−2	0.2	0	7.5	0	7.5	22.3	241
20	0	2.5	+2	2	0	7.5	0	7.5	136.4	231
21	0	2.5	0	1.1	−2	3	0	7.5	86.7	264
22	0	2.5	0	1.1	+2	12	0	7.5	106	188
23	0	2.5	0	1.1	0	7.5	−2	3	142.1	307
24	0	2.5	0	1.1	0	7.5	+2	12	137.3	189
25	0	2.5	0	1.1	0	7.5	0	7.5	97	259
26	0	2.5	0	1.1	0	7.5	0	7.5	87.3	248
27	0	2.5	0	1.1	0	7.5	0	7.5	102.3	265
28	0	2.5	0	1.1	0	7.5	0	7.5	93.7	252