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Predicting Specific Mechanical Energy (SME) in Composite Compounding Process: An Analysis of Area Under Graph Base Selection Effects

Haniffah Wan Hussin[1], Khalina Abdan[1,2], Salit M. Sapuan[1,3*], E. S. Bakar[1,4]

1 Makmal Biokomposit, Institut Perhutanan Tropika Dan Produk Hutan (INTROP), 43400 UPM Serdang, Selangor, Malaysia
2 Jabatan Kejuruteraan Biologi dan Pertanian, Fakulti Kejuruteraan, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia
3 Jabatan Kejuruteraan Mekanikal dan Pembuatan, Fakulti Kejuruteraan, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia
4 Fakulti Perhutanan, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia

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ABSTRACT

This study investigates the Specific Mechanical Energy (SME) of compounding processes, a crucial parameter in polymer composite manufacturing. SME can be derived from the area under the torque-time graph. However, when comparing different compounding processes, the basis for calculating this area, either on a same time basis or a same torque basis, can vary, potentially influencing the accuracy of SME prediction. This study aimed to evaluate the impact of this basis selection on the predictability of SME, using a regression equation and the data fitness value (R^2). We calculated the area under the graph from 28 composite compounding processes, examining the overall SME as compounding progressed and SME for specific segments of the torque-time graph. Our main finding reveals that using the same torque basis consistently yields better R2 values than the same time basis. Specifically, R^2 values improved for overall SME when analyzed with the same torque basis, whereas no improvement was observed with the same time basis. For segments of the area under the graph, the same time basis produced unreliable R^2 values, while the same torque basis resulted in highly reliable R^2 values exceeding 0.999. In conclusion, for compounding Polypropylene (PP)/kenaf core composites, the most effective and reliable method for comparing SME is using the same torque basis, particularly for analyzing specific area segments under the torque-time graph. This approach ensures greater predictability and accuracy in understanding the energy input during the compounding process.

Keywords:
Specific Mechanical Energy, Regression, Homogeneous

1. Introduction

An internal mixer is commonly used to prepare lab-scale thermoplastic composites. Various researchers have conducted studies of the mixing behaviour of polymers or composites through the

* *Corresponding author.*
E-mail address: sapuan@upm.edu.my(Salit M. Sapuan)

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torque generated by an internal mixer [1–9]. Most of the presented papers use torque-time graphs to describe reactions that took place during mixing. It is well-established in polymer processing that torque-time graphs provide valuable insights into the mixing behavior and material transformations within an internal mixer, such as molar mass variation, viscosity, and interaction between materials of the compound [10].

Torque-time graphs can be further analyzed to find energy transmitted to the material during processing. Energy transmitted to a specific amount of material is presented as Specific Mechanical Energy (SME) using Equation (1).

$$SME = \frac{\omega}{m}\int_{t1}^{t2} C\ (t)dt \tag{1}$$

where C(t) is torque during processing between t_1 and t_2; $\int_{t1}^{t2} C(t)dt$ is the area under the graph between t_1 and t_2. c is rotational speed, and m is sample mass; both ω and m are fixed throughout the experiment; thus, they become constants for the Equation.

As a dependent variable, the value of SME is influenced by the area under the graph. However, the area under the graph is a product of two independent variables, torque and time. To compare several replications, the parameters that determine the area under the graph must be the same for all replications. Normally, the time parameter, i.e., the limits of the integral (t1 and t2) in Equation (1), is selected as a common factor for comparison between replications. The starting point for compounding, t=0, was usually chosen at the fiber insertion stage, as shown in Figure 1. Beyond this point, the shape of the fiber insertion graph varies between replications due to the manual insertion of fiber. After all the fibers were inserted, the torque gradually decreased towards a constant torque in the homogenization stage.

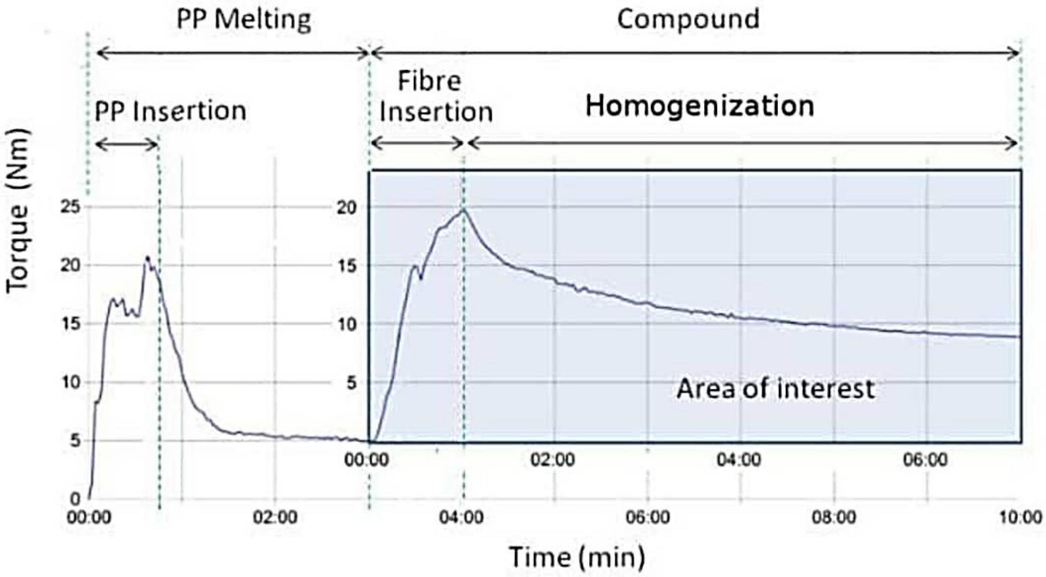

Fig. 1. Typical torque time graph produced by internal mixer for compounding PP/kenaf core composites in this study. Axis x and y were adjusted to the beginning of the compounding process

Constant flow of fiber into the mixing chamber is impossible due to fiber blockage at the chamber entrance, physical pushing of fiber to break the blockage, and release of gaseous due to fiber exposure to heat. Manual insertion of fiber usually took place less than 2 minutes after initial fiber insertion. To overcome the inconsistency problem of the fiber insertion process, the area under the graph is divided into segments so that a segment with fiber insertion stage is excluded from the analysis. However, this study's approach includes the fiber insertion stage to evaluate the performance of the regression equation as the compounding process progresses.

As previously mentioned, the area under the graph can also be determined by selecting torque as a reference to compare SME between replications. Therefore, this study explores the possibility of using torque as a limit of integration to forecast SME values. Changes in the limits of the integral require a modification of Equation (1) so that the limits of the integral are based on torque. The new formula is presented in Equation (2).

$$SME = \frac{\omega}{m}\int_{t\ when\ \tau 1}^{t\ when\ \tau 2} C\ (t)dt \tag{2}$$

where τ_1 and τ_2 are fixed torque values.

Regression analysis is very important as a forecasting tool in physical science, where precise data and a constant relationship are established [1-13]. Given the established relationship between area under the graph and SME as in Equations (1) and (2), R^2 (coefficient of determination) can be used as an indicator to validate the performance of a model in forecasting [14-15]. An R^2 value close to 1.0 is good for forecasting , as all the data are fitted on the regression equation.

The study aimed to compare the effects of integral limits selection on the R^2 values of the SME regression equation. The integral limit selections are based on the time of compounding (fixed time basis) and the torque applied to composites during the compounding process (fixed torque basis).

2. Materials

Kenaf core fiber size less than 40 micrometers was used as the fiber. Kenaf core fibers were heat-treated at temperatures 103, 165, 175, 185, 195 and 205°C in a normal atmosphere to produce variations in processing.

Polypropylene (brand Titan Pro grade 6331 with a melt flow index of 14) was used as a matrix for the composite.

3. Methodology

3.1 Compounding process

This study compounded 16g of kenaf core and 24g of polypropylene to produce a polypropylene/kenaf core composite with 40% fiber loading. The compounding process was replicated 4 times for every treated fiber using a Brabender Plastogram internal mixer (Germany), with a Plastograph EC drive unit and a W 50 EHT mixer. The rotational speed and temperature for the compounding process were 60 rpm and 175°C, respectively.

The compounding process comprises three distinct stages: polymer melting, fiber insertion, and homogenization, as illustrated in Figure 1. In the initial stage, polypropylene (PP) was introduced into the mixing chamber and heated until a uniform melt was achieved, indicated by a stable torque reading. The second stage marks the focal point of this study, where kenaf core fiber was manually fed into the chamber. The graph axes were adjusted to exclude torque and time data associated with PP melting to isolate this phase, as shown in Figure 1. During fiber addition, external force was applied to disrupt fiber bridging and clogging at the chamber entrance, thereby ensuring consistent material flow into the mixer. In the final stage, once all fibers were inserted, a 5 kg weight was placed to seal the entrance, maintaining closed conditions until the compounding process was complete.

3.2 Data extraction

Since the software did not provide raw data of the process, the produced graphs of the compounding process were digitized using Web Plot Digitizer [16]. The areas under the graph were calculated using the trapezium formula based on data produced by Web Plot Digitizer.

3.3 Data analysis

Although the aim is to compare R^2 of the SME regression equation, this study's approach began by analyzing progressive SME, which begins when the fiber is inserted into the compounding processes until the composite becomes homogeneous. Therefore, the calculation for the area under the graph used time as the limit of the integral (fixed time). The lower limit began with t=0 minutes; the upper limits were t=2, 3, 4, 5, and 6 minutes. Similarly, for torque as an integral limit (fixed torque), the lower limit began with t when τ = 0 Nm, and the upper limits were t when τ = 14, 13, 12, 11 and 10 Nm.

Next, the study used a segmented SME approach, excluding external forces applied during the fiber insertion stage. The segments were one-minute intervals for fixed time limits and 1 Nm for fixed torque analysis. Therefore, area under the graph for fixed time limit were calculated for segment with t=2 minutes as the lower limit and t=3 as the upper limit; t=3 minutes as the lower limit and t=4 as the upper limit; t=4 minutes as the lower limit and t=5 as the upper limit; and lastly, t=5 minutes as the lower limit and t=6 as the upper limit.

Segments for fixed torque analysis used t when τ = 14 as the lower limit and t when τ = 13 as the upper limit, t when τ = 13 as the lower limit and t when τ = 12 as the upper limit, t when τ = 12 as the lower limit and t when τ = 11 as the upper limit and lastly t when τ = 11 as the lower limit and t when τ = 10 as the upper limit.

Table 1
An overview of the analysis carried out in this study. Constant parameters were ω = 60 rpm, m = 40 g and barrel temperature = 175 °C

Progressive SME				Segmented SME			
Fixed time (min)		Fixed torque (Nm)		Fixed time (min)		Fixed torque (Nm)	
Lower limit	Upper limit	Lower limit	Upper limit	Lower limit	Upper limit	Lower limit	Upper limit
0	2	0	14	2	3	10	11
0	3	0	13	3	4	11	12
0	4	0	12	4	5	12	13
0	5	0	11	5	6	13	14
0	6	0	10	6			

The linear regression equations between the area under the graph and SME and R-squared values were obtained using Microsoft Excel 2010.

4. Results and Discussions

SME has a linear relationship with the area under the torque graph, as shown by Equation 1. A simple linear regression between SME and torque was produced by fixing the area under the graph based on time compounding.

4.1 *Progressing compounding with fixed time effects on SME*

Results of progressing compounds are presented in Figure 2. Generally, longer compounding periods would produce higher SME as the area under the graph is larger. Therefore, SME for an area under a graph of fixed intervals between 0 and 2 minutes is located in the lowest cluster compared to the other fixed intervals.

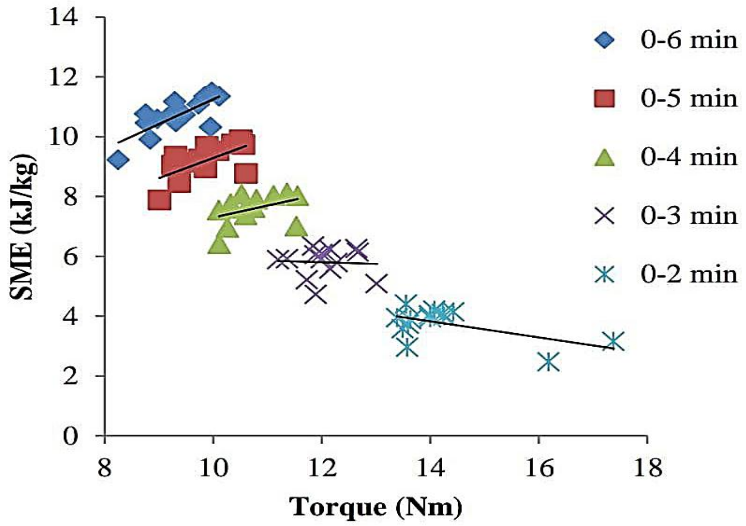

Fig. 2. Relation between SME and torque (fixed time)

Table 2
Linear regression between SME and torque (fixed time)

Fixed time	Regression equation	R^2
0 - 2	y=-10.76x+303.6	0.32
0 - 3	y=-2.223x+258.7	0.003
0 - 4	y=15.89x+132.8	0.162
0 - 5	y=27.18x+99.68	0.401
0 - 6	y=33.25x+117.5	0.569

In actual processing, a low torque value, i.e., a torque value approaching a constant, can only be achieved toward the end of the compounding process, as shown in Figure 2. Negative gradient values can translate this into linear equations, which cause values in the y-axis to get smaller when values in the x-axis get bigger. Therefore, the regression equation should have a negative gradient as achieved by a fixed duration of 0 to 2 minutes and 0 to 3 minutes (shown in Table 2). However, even with negative gradient values, the R^2 value is very low to validate the regression equation's performance for forecasting SME. Only 32% of data fit into the regression equation of fixed time of 0 to 2 minutes, while only 0.3% of data fit into the regression equation for a fixed time of 0 to 3 minutes.

4.2 Progressing compounding with fixed torque effects on SME

Fig. 3 shows the relation between compounding time and SME; The longer the compounding time, the higher the SME. Generally, data on lower fixed torque produces higher SME; fixed torque of 0 to 10 Nm clustered higher because a longer time was required to achieve 10 Nm compared to the time required to achieve 14 Nm (Refer to Figure 3).

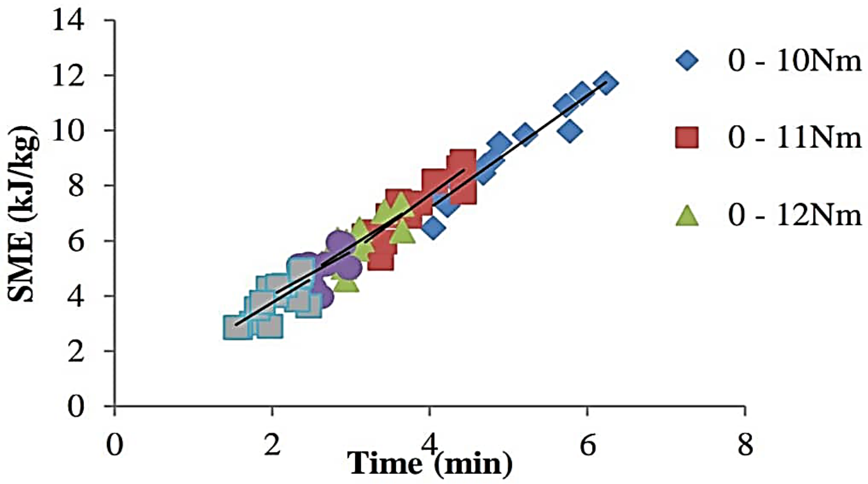

Fig. 3. Relation between SME and time (fixed torque)

All the regression equations have a positive gradient value, which is a valid indication for actual processing conditions. A longer time to achieve fixed torque would produce bigger SME values. However, the coefficient of determination (*R^2*) for fixed torque 0-14, 0-13, 0-12 Nm indicates the regression equation is less reliable for forecasting SME values, shown in Table 3.

Table 3
Linear regression for SME vs time (fix torque)

Fixed Torque	Regression equation	R^2
0 - 10 Nm	y=2.039x-0.968	0.926
0 - 11 Nm	y=2.092x-0.703	0.782
0 - 12 Nm	y=1.813x-0.353	0.57
0 - 13 Nm	y=1.577x+0.873	0.425
0 - 14 Nm	y=1.739x+0.274	0.521

4.3 Segmented compounding with fixed time effects on SME

The area under the graph was segmented into 1-minute intervals throughout the compounding process. The first 2 minutes from the beginning of fiber insertion were omitted to avoid the effect of external forces applied during fiber insertion.

Figure 4 shows that the mechanical energy (SME) applied to the material is higher in the early segment of the compound for breaking cluttered fiber and spreading it equally within the compound. Referring to the x-axis, torque differences tend to approach zero later because torque is approaching a constant at the end of the homogenization stage.

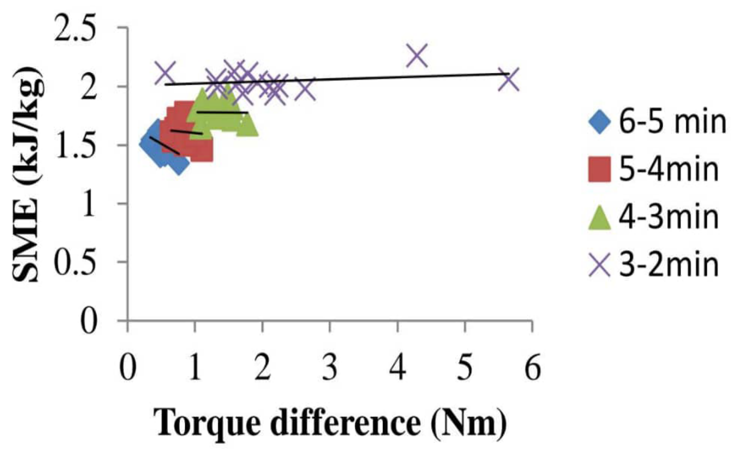

Fig. 4. Relation between SME and torque difference within 1-minute of compounding

Table 4 shows that the regression equation's negative gradient does not comply with the actual compounding, where a higher torque difference produces higher SME. Furthermore, a low value of the coefficient of determination, R^2, indicates poor performance of the regression equation for forecasting purposes.

Table 4
Linear regression for SME vs. torque difference within 1 minute of compounding

Period (min)	Regression equation	R^2
3 - 2	y=0.724x+80.25	0.072
4 - 3	y=-0.213x+71.49	0.000
5 - 4	y=-2.269x+66.44	0.006
6 - 5	y=-13.23x+67.0	0.206

4.4 Segmented compounding with fixed torque effects on SME

Figure 5 shows the value of SME concerning the time it takes for the torque to reduce by 1 Nm. All the data are aligned consistently, and a longer time taken would give a higher SME.

Table 5 shows that the gradient of the regression equation reduced towards the end of the compounding process. This shows the SME near the insertion point is more sensitive toward the compounding duration than toward the end of the compounding process. This indicates a longer time for the torque to reduce by 1 Nm, because more energy was used to disperse and de-clutter the fiber at the early compounding stage compared to the later compounding stage. Moreover, the R^2 indicated that the regression equation is a good forecasting tool at each compounding stage, where almost all data were fitted to the regression equation. The high value of R^2 is possible because the segmented calculation excludes the influence of external forces during the fiber insertion stage.

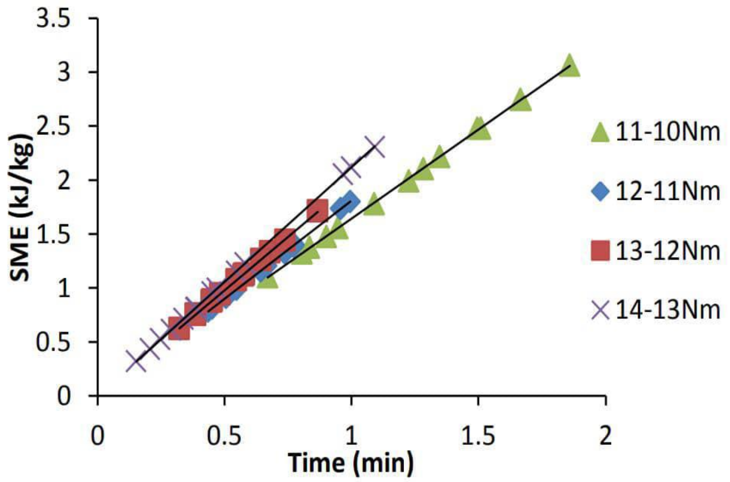

Fig. 5. Relation between SME and time of descending torque

Table 5
Equations and R^2 between SME and time of descending torque

Torque reduction (Nm)	Regression equation	R^2
11 - 10	y=1.648x -0.009	0.998
12 - 11	y=1.818x -0.011	0.999
13 - 12	y=1.980x -0.012	0.997
14 - 13	y=2.117x -0.002	0.999

5. Conclusions

In conclusion, this study found that using a fixed time interval to calculate the Specific Mechanical Energy (SME) from the area under a graph yields inaccurate predictions. Furthermore, including the fiber insertion stage significantly impairs the performance of the regression equation. Therefore, to ensure accurate and comparable SME results across different compounding processes, it is crucial to calculate the area under the graph based solely on the segment of time where torque reduction occurs. This approach effectively excludes the influence of external forces, leading to predictable and replicable SME values.

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