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Pyrolysis kinetic behaviour and TG-FTIR-GC–MS analysis of Coronavirus Face Masks

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ABSTRACT

In the times of Covid-19, face masks are considered to be the main source of protection against the virus that reduces its spread. These masks are classified as single-use medical products with a very short service life, estimated at few days, hence millions of contaminated masks are generated daily in the form of hazardous materials, what requires to develop a safe method to dispose of them, especially since some of them are loaded with viruses. 3-ply face masks (3PFM) represent the major fraction of this waste and are composed mainly from polypropylene and melt blown filter with high content of volatile substances (96.6 wt.%), what makes pyrolysis treatment an emerging technology that could be used to dispose of face masks and convert them into energy products. In this context, this work aims to study pyrolysis kinetic behaviour and TG-FTIR-GC–MS analysis of 3PFM. The research started with analysis of 3PFM using elemental analysis, proximate analysis, and compositional analyses. Afterwards, TG-FTIR system was used to study the thermal and chemical decomposition of 3PFM analyzed at different heating rates: 5, 10, 15, 20, 25, and 30 °C/min. The GC/MS system was used to observe the synthesized volatile products at the maximum decomposition temperatures. After that, isoconversional methods, the advanced nonlinear integral isoconversional method, and the iterative linear integral isoconversional method were used to determine the activation energies of mask pyrolysis, while the distributed activation energy model and the independent parallel reactions kinetic model were used to fit TGA and DTG curves with deviations below <1. The TGA-DTG results showed that 3PFM can decompose in three different periods with a total weight loss of 95 % and maximum decomposition in the range 405–510 °C, while the FTIR spectra and GC-MS analysis exhibited that –C=H (aromatic and aliphatic) and 2,4-Dimethyl-1-heptene (28–43 % based on heating rate) represented the major compounds in the released volatile components. Finally, Vyazovkin and the iterative linear integral isoconversional methods gave activation energies almost similar to that obtained by the KAS isoconversional method.

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1. Introduction

After the World Health Organization had declared that the coronavirus (Covid-19) is a global epidemic [1], face masks have become the first prevention measure used to limit the spread of the virus, and the masks have become one of the basic necessities of daily life, similarly to mobile phones, clothes, etc. [2]. Therefore, the countries were quick to buy and store large batches of face masks as they were getting ready for any circumstances [3]. Also, the decision-makers and legislators started to enact laws and make wearing of masks mandatory in the closed gatherings and such places as transport, restaurants and shops, taking the social distancing into account [4,5]. As the time was passing, designers rushed to create and introduce different forms of face masks for all social classes and markets [6,7]. Among these types, the mask of N95 type proved its high efficiency in terms of protection and ease of breathing and wearing [8–10]. However, due to the economic reasons, 3-ply face masks (3PFM) are widely used as a meaningful alternative for N95 mask at present [11]. Also, this type of masks (3PFM) is characterized by cheap price, perfect filtration capacity, hypoallergenic feature, very low breathing resistance, resistance to fluids, and antiviral

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function [12]. 3PFM is composed of three layers of vertically arranged folds: non-woven fabric made from Polypropylene (PP: two layers) and melt blown filter to ensure prevention of virus transmission, as shown in Fig. 1.

Despite all these advantages, these masks have a short service life of only several days, which leads to generation of a huge amount of waste [13]. Therefore, disinfection and sterilization for reuse and non-certified manufacturing was suggested instead of disposal, thus decreasing the amount of generated face masks waste [14]. However, 3PFM is not washable and the washing process leads to increase in the mesh size of the washed masks, thus affecting negatively their performance and giving the possibility to transmit the virus [15]. Even washable masks produce a lot of microfibers during the washing process and these elements are classified as pollutant elements [16–18]. All these issues represent a major obstacle for reuse of the masks and they must be disposed safely, especially since some of them may be loaded with the virus, which increases the possibility of a negative impact, especially as the research has shown that the virus can stay on surfaces for a long time [19]. Depending on their use, these wastes can be classified as medical violations, and they must be collected and disposed of safely to avoid the infection; however, this is not the case with the masks [20]. Based on the above, now disposal of the used masks can be divided into two groups: masks produced in the medical sector (workers in hospitals and isolation units) and masks produced by ordinary people [21]. The first group is disposed of as medical waste, and the second group, unfortunately, is collected as solid waste, hence foreshadowing serious consequences [22]. Therefore, decision-makers have to develop a safe collection system for these masks (the end life of masks), for example, to establish special boxes in specific places for their collection. In order to motivate decision-makers to do so, some techniques must be devised to recycle these masks and turn them into secondary or energy materials [23].

2. Experimental

2.1. Materials and preparation of Coronavirus Face Masks

Because of their advantages listed in the previous section, 3-ply face masks (3PFM) were used as a raw material in the present research. The mask samples used in the present research were collected from the pharmacy in Kaunas. According to the data sheet, the selected sample has the size of 17.5cm × 9.5cm and total weight of 2.7 g [42]. The mask rope was removed from the main body. Afterwards, the main body of the face mask was cut into small pieces and then milled into fine particles using an electric grinder, as shown in Fig. 2A, thus resulting in decreased resistance to heat transfer during the thermal treatment using a pyrolysis process. Finally, all gases and chemicals used in pyrolysis experiments conducted with the help of TGA-TG-FTIR-GC-MS system. Also, pyrolysis kinetics of face masks were studied using model-free methods at different heating rates. DAEM and IPR were used to fit TGA and DTG curves. Finally, the formulated volatile components were observed using FTIR and GC-MS analysis.

2.2. Design of the research experiments

The experiments were designed in five stages: a) characterization of the face mask against Covid 19, using elemental, proximate, and composition analysis, b) thermogravimetric analysis (TGA-DTG) of the face mask, d) determination of the function groups and chemical composition analysis, and g) FTIR analysis and GC-MS analysis.

![Fig. 1. (A) Image of 3-ply face mask and (B) construction of 3-ply face masks.](image-url)
compounds of the synthesized volatile products using FTIR and GC/MS, c) study of pyrolysis kinetic of 3PFM using the model-free methods, the advanced nonlinear integral isoinvconversional method, and the iterative linear integral isoinvconversional method based on the TGA results, d) fitting to TGA and DTG curves using DAEM and IPR, respectively. All these stages and their conditions are illustrated in Fig. 2.

2.3. Characterization of Coronavirus Face Masks

Fourier-transform infrared spectroscopy (FTIR) was used to check the chemical structure of the milled face mask sample. The elemental analysis (Perkin Elmer 2400 CHN Elemental Analyser) was employed to measure carbon (C), hydrogen (H), nitrogen, oxygen (O) and sulphur (S) content in the milled face mask sample, while moisture, volatile matter, fixed carbon, and ash in the milled face mask sample were determined using the proximate analysis according to E1756-01, E872-82, and E1755-01 ASTM standard methods [43]. The concentration of fixed carbon content was calculated by difference. Also, the compositional analyses were performed to measure the percentage of hemicellulose, cellulose, and lignin contents in the milled face mask sample. Lignin and holocellulose contents were determined according to Technical Association of Pulp and Paper Industry TAPPI T222 standard method [44]. Finally, all measurements were conducted on three replicates, then taking the average to improve the accuracy of the final results.

2.4. Thermogravimetric measurements

The thermal decomposition experiments of 3PFM were carried out using the thermogravimetric analyser (TGA; model: STA449 F3; NETZSCH, Selb, Germany) in nitrogen (N2) atmosphere. The experiments were conducted on 8-10 mg from the tested samples with N2 flow rate: 60 ml min⁻¹ in the range from 30 to 900 °C and heating rates: 5-30 · °C min⁻¹. The obtained results were recorded using the TGA analyser in the form of mass loss with the help of Pyris software, then fitting TGA curves in the form of mass loss versus pyrolysis temperatures. The DTG curves at each heating rate were determined to estimate the maximum thermal decomposition peaks, temperatures, and their location. It is worth mentioning that DTG curves were estimated through numerical derivation of the obtained TGA data, then plotting the DTG curves at each heating rate.

2.5. Chemical analysis of the formulated chemical compounds

In order to determine the functional groups and chemical structure of the synthesized compounds at each heating rate, TG-FTIR was used. The analysis was conducted on the formulated compounds at the maximum decomposition temperatures in the ranges from 300 to 400 °C based on the DTG results and heating rates. Meanwhile, the thermogravimetry-gas chromatography–mass spectrometry (TG–GC–MS, Thermo Scientific ISQ™ single quadrupole GC–MS) was used to determine the identified and quantified chemical compounds of the synthesized volatile products at the maximum decomposition temperatures. The GC–MS analyses were performed using a laboratory set-up consisting of an Automation Autoinjector™ system connected with Thermogravimetric analyser to collect the obtained gases, then examine the chemical composition of the obtained compounds in the range of 30–600 m/s using GC–MS (Shimadzu GC-2010). The measurements were carried out in the following analytical conditions for the micro GC: sample pump time (20 s), column setting (Argon ≥99.999 %, 20 psi, 100 °C, and 130 s), inject time (30 ms), injector temperature (90 °C), TCD temperature (70 °C), and data rate (50 Hz) [45].

2.6. Pyrolysis kinetics of 3-ply face masks

2.6.1. Model-free methods

Although 3PFM are composed of three layers as explained before (including, polypropylene and melt blown filter), the DTG results in Section 3.3 showed that all layers decompose together at significant peak, which indicates that face mask waste pyrolysis can be considered as a single reaction and model-free methods (including, Friedman method, Flynn-Wall-Ozawa method, and Kissinger-Akahira-Sunose method) could estimate activation energy (Ea) without any mathematical assumptions. In case of this kind of waste, the conversion rate (X) and conversion rate (dX/dt) can be described using Eqs. (1),(2) and the rate constant k(T) can be expressed using the Arrhenius Law (Eq. (3)).

\[
X = \frac{\text{Initial mass} - \text{Astantaneous mass}}{\text{Initial mass} - \text{Final mass}}
\]  

(1)
\[
\frac{dX}{dt} = \frac{dX}{dT} = k(T)f(X)
\]  
(2)

\[k(T) = Ae^{-Ea/RT}
\]
(3)

where \(f(X)\), \(T\), \(k(T)\), \(A\), \(E\), and \(R\) are different conversion function, absolute temperature (K), and the rate constant, pre-exponential factor (\(\text{min}^{-1}\)), apparent activation energy (kJ/mol), and gas constant (J \(\text{mol}^{-1} \cdot \text{K}^{-1}\)), respectively.

By merging Eqs. (2) and (3) and adding the linear heating rate \(\beta (dT/\, dt)\), the new formula can be developed, as shown in Eq. (4), while Eq. (5) shows the final formula after rearrangement. It is worth mentioning that \(f(Ea/RT)\) term in Eq. (5) does not have an exact solution and, thus Kissinger, Kissinger-Akahira-Sunose (Eq. (6)), Flynn-Wall-Ozawa (Eq. (7)), and Friedman formulations (Eq. (8)) were used to determine this term as shown in Table 1. Regarding the nonlinear integral isoconversional (Vyazovkin) and iterative linear integral isoconversional (Cai) models, these models can be used to calculate activation energies numerically using Eqs. (10),(11). The algorithms were built using MATLAB software and all formulas can be found here [38,39].

\[
\frac{dX}{dt} = k(T)f(X) - \frac{A}{\beta} \beta f(X)
\]  
(4)

\[\ln \left(\frac{\beta}{T^2}\right) = \left(\ln \left(\frac{AR}{Ea}\right) + \ln\left(n[1 - X_m^{1-n}]^n\right)\right) - \frac{Ea}{RT}\]
(5)

2.6.2. Distributed activation energy model (DAEM)

DAEM was used in the present research to calculate both activation energy and pre-exponential factor. DAEM model can be described using Eq. (12), while \(Ea\) and \(A\) can be calculated by plotting of \(\ln(\beta / T^2)\) versus \(1/T\) curves [40]. It is worth mentioning that this kind of modelling needs initial guesses of reaction mechanisms to estimate the kinetic parameters accurately in minimum running time, therefore the average action energy resulting from free-methods was used as an initial guess for DAEM and fine-tuned kinetic parameters. Also, this model can be used to verify the TGA experimental data with theoretical data.

\[
\ln \left(\frac{\beta}{T^2}\right) = \ln \left(\frac{AR}{Ea}\right) + 0.6075 \frac{Ea}{RT}
\]  
(12)

2.6.3. Independent Parallel Reactions Kinetic Model (IPR)

According to the IPR model, main pseudo components are degraded individually and simultaneously in the form of more independent parallel reactions. Based on the data sheet, the face mask used in the present research contains more than two pseudo components, including PP and filter paper. However, the DTG curves in Section 3.2 show only one visible peak resulting from simultaneous decomposition of all pseudo components in a single reaction. The linear combination of the overall rates of conversion of partial reactions after considering the mass of each subcomponents \((c_i)\) can be described using Eq. (13) [41].

\[
\frac{dm}{dt} = -(m_0 - m) \sum_{i=1}^{3} C_i \frac{dX_i}{dt}
\]
(13)

where \(n_0\) \(\beta\), \(T\), \(R\), \(C_i\), and \(dm/\, dt\) are apparent reaction order of each subcomponent \(i\), time, temperature, and the universal gas constant, and the mass fraction of each of three subcomponents, and the rate of mass loss, respectively.

The algorithm in Matlab® code coupled with the gradient-based minimization function fmincon of Matlab® was built to determine the optimal parameters \((Ea, A, C_i)\) that are able to minimize Dev. of DTG (Derivative Thermogravimetry (DTG) objective function) as an objective function using Eq. (14). Finally, the deviation (Dev.%)) between the theoretical and experimental DTG curves was evaluated for all heating rates using Eq. (15).

\[
\text{Dev.(%)} = \frac{100\sqrt{\text{F.O.DTG}(Z - N)}}{\text{max}[(dm/\, dt)]}
\]  
(14)

where \(Z\) and \(N\) are the number of data points and the number of parameters employed in the model, respectively.

3. Results and discussion

3.1. Chemical structure of the milled face mask

FTIR spectroscopy (FTIR, Vertex70 spectrometer) was used to determine functional groups and chemical structure of 3PFM. As shown in FTIR spectra (Fig. 3), the milled sample contains only one sharp peak at 3004 cm\(^{-1}\) characteristic to the associated –OH groups and this main functional group refers to Polypropylene non-woven fabrics [47]. Also, other distributed weak peaks appeared at 2950 cm\(^{-1}\) because of C–H present in CH2OH group; these peaks are typically the peak of filter paper [48]. It is worth mentioning that because of low concentration of melt blown filter in the milled sample, these peaks are characterized by low intensity.
3.2. Basic properties of 3-ply face mask

Table 2 shows the ultimate, proximate analyses, and compositional analyses of the milled face mask. As shown in the table, carbon (C) and hydrogen (H) represent the major elements in the tested sample with average concentration of 84.71 wt.% and 14.35 wt.%, respectively. This strong presence of carbon indicates that face mask can be regarded as a promising source of carbon precursor. Also, it was noted that sulphur (S) and nitrogen (N) were almost completely absent; their concentration was estimated at < 0.01 wt.%. This ensures that no toxic emissions (e.g., SO₂ and NOₓ) are produced during pyrolysis treatment at large scale [49]. With regard to the proximate measurements, the analysis showed that the face mask contains a huge amount of volatile matter up to ~97 wt.% with little ash content with average value of 3.28 wt.%. This high volatile matter content contributes to conversion process and increase in heating value of the synthesized fuel. In addition, ash content acts as a catalyst leading to changed reactivity of the substances to be activated and increased quality and amount of the formulated oil. Finally, the compositional analysis shows that the tested sample is rich in cellulose and hemicellulose components, what contributes to the conversion process and higher energy yield [50].

3.3. TGA-DTG data analysis

Fig. 4 shows TGA-DTG profiles of 3PFM in the ranges from 25 to 900 °C and different heating rates in the scope of 5, 10, 15, 20, 25, and 30 °C. According to TGA results (Fig. 4A), the face mask can decompose in three stages at all different heating rates. Three stages are within the temperature scopes of 50–404 °C, 405–510 °C, and 511–900 °C. The first and last decomposition stages (Y1 and Y3) represent minor degradation regions due to moisture evaporation (~1 wt.%) and char devolatilization/decomposition (~5 wt.%), respectively [51], while the second stage represents (Y2) the main and major decomposition region of the tested sample with weight loss of ~95 % due to the decomposition of organic materials, including polypropylene and melt blown filter [52, 53]. Meanwhile, the DTG curves (Fig. 4B) showed that all components of the tested face mask had decomposed at a single degradation peak even when the heating rates changed. However, the intensity of this peak and maximum degradation temperature increased gradually from 448 to 476 °C. This shifting in the decomposition peak and increase in maximum degradation temperature were caused by increase in heating rates leading to increase in heat generation and heat flux transfers between the surroundings of the tested mask and their internal moroclaur, thus accelerating the degradation process and complete decomposition of all the mask’s compounds in short time [54].

3.4. Mechanism of 3-ply face mask’s pyrolysis

As mentioned before, 3PFM are composed of many compounds, thus making their thermal degradation using pyrolysis treatment so complicated. In order to understand the pyrolysis mechanism of the face mask and overcome this complexity, this section was developed. The pyrolysis mechanism was explained based on the thermogravimetric results, particularly at a heating rate of 30 °C/min, which is considered an optimum condition leading to the highest yield of volatile compounds, as shown in the next sections. According to the TGA profile, the decomposition of the face mask started with evaporation of moisture up to 130 °C and elimination of the textile materials, including virus. The researchers stressed specifically that the virus can be eliminated at the temperature up to 100 °C [14]. As the reaction temperature increased, the detangled element between the milled particles was removed and the friction-mechanical bonds between the mask’s fabric were dismantled and converted into individual microparticles (around 280 °C) in the form of debris and damaged micro particles [43]. These particles contained a lot of damages in form of scratches, cracks, and notches on their surface resulting from the pre-treatment process using milling process, thus leading to decrease in crystallinity of these particles, which helped to accelerate decomposition of carbohydrates in organic components into sugar molecules at the applied high temperature. Then penetration of the produced heat flux inside the damaged particles followed, breaking Van der Waals, hydrogen, β-1,4-glycosidic bonds of cellulose, lignin, and hemicellulose molecules, forming small molecules and some amorphous regions up to 420 °C [55]. As the temperature increased, small molecules of hydrocarbon decomposed into liquid and gas pyrolysis products up to 510 °C, then formulating char devolatilization/decomposition in the last region in the form of soft black solid residues in the end of the reaction [52].

3.5. Chemical analysis of the synthesized chemical compounds

The formulated chemical compounds at the maximum decomposition temperatures derived from DTG results of 3PFM were examined using FTIR coupled with TG for all heating rate ranges 5–30 °C/min. The observation process using 2–3D FTIR analysis was performed for the compounds that had been synthesized in the ranges from 448 to 476 °C (based on the DTG results). Fig. 5 displays 2–3D FTIR spectra of the degraded samples at different heating rates. As shown in 2D FTIR analysis, all tested samples had almost the same features, particularly three main peaks at 3000 cm⁻¹, 1500 cm⁻¹, and 600 - 1000 cm⁻¹ (fingerprint zone) assigned to -C (aromatic and aliphatic), N-O group, and aromatic compound, respectively [51]. It was noted that, as heating rates increased, the percentage and absorbance of -C (aromatic and aliphatic) compounds increased significantly as a result of the generated heat flux, which led to increased heat penetration inside of the tested samples, followed by decomposition of all the complex organic molecules into aromatic and aliphatic compounds [55,56]. Also, it was observed that as heating rates increased, the disturbance peaks disappeared from FTIR 3D spectra, what indicates that whole organic components were converted into energy and chemical products. These results agree with the calculated activation energy in the following sections, which showed that the highest activation energies were achieved at higher heating rates. Finally, in order to determine the main composition and yield of the formulated products, GC was used in the next section for that purpose.

3.6. Chemical analysis of the synthesized chemical compounds using GC–MS

Fig. 6 shows GC–MS analysis of the milled face mask at different heating rates (5–30 °C/min). GC–MS analysis showed that the formulated products were composed of several chemical compounds, including pentane, 2,4-Dimethyl-1-heptene, 2-Acetylcyclopentanone, etc. Also, it was noted that 2,4-Dimethyl-1-heptene represented the major compound in the released volatile products and the yield of this
Fig. 4. A) TGA and B) DTG analysis of the milled 3-ply face mask at different heating rates.

Fig. 5. 2-3DFTIR analysis of the decomposed 3-ply face mask at different heating rates.

Fig. 6. GC-MS analysis of the decomposed 3-ply face mask at different heating rates.
The compound increased significantly with increase of the heating rate from 32.13 % at 5 °C/min to 41.86 % at 5 °C/min due to the significant increase in the generated heat flux. The strong presence of these GC compounds confirms that the obtained products from the pyrolysis of the face mask were typical energy products [57, 58]. Also, it was noted that carbon dioxide compounds responsible for formation of char fraction were not observed, and these results agree with TGA, thus confirming that the decomposed sample does not have char [55]. The synthesized chemical compounds with their respective peak areas at the specified conditions are illustrated in Table 1S. Finally, the formulated pyrolysis compounds can be used in many applications related to chemicals, pharmaceuticals, energy, etc. Therefore, the pyrolysis treatment can be considered as a promising strategy to dispose of face masks and convert them into energy products, especially at high heating rates.

3.7. Kinetic analysis of face mask pyrolysis

3.7.1. Activation energy for the entire pyrolysis process

Activation energy for the entire pyrolysis process of 3PFM was estimated using Kissinger model, and fitting thoroughly the linear relationship between \( \ln(\beta/ T_m^2) \) versus \( 1/T \) and the slope of this curve represented by the slope of \(-Ea/R \) (\( R = 8.31 \text{ JK}^{-1} \text{ mol}^{-1} \)). Fig. 7A shows the fitted curve of Kissinger method and the determined Ea, where the linear slope is represented by \(-Ea/RT_m\) and Ea was determined by 269.51 kJ mol\(^{-1}\). In the literature, several researches have been developed to estimate Ea of pyrolysis of fabric rich in polymer, such as Patnaik et al. [33], Zhu et al. [35], Miranda et al. [34] and Ea for these fractions were estimated at 192, 167, 186 kJ/mol, respectively [33–35], which means that the face mask can produce Ea higher than non-woven plastics, ramie fabric wastes, and textile wastes by 29, 38, and 31 %, respectively. This is due to the fact that the feedstocks used in the current study were composed of several components, including non-woven fabric, melt blown filter, and non-woven fabric, and each component has a different Ea [11,12]. However, all these components were decomposed together in a single reaction (as shown in the DTG analysis) and the obtained Ea represent the summation of Ea of all these components, that is why the pyrolysis of 3-PLY face mask gave higher activation energy compared to other feedstocks [33,34]. Also, Ea was improved as a result of high purity of face mask, its uniform chemical composition and size, and smaller crystallinity, which led to digestibility of the face mask and its conversion into energy components.

3.7.2. Estimation of activation energies for the entire conversion zone

On the other hand, FWO, KAS, Friedman routes were used to determine Ea over the range of conversion rate from 10 to 90 % estimated by the slope of \(-Ea/R \) (\( R = 8.31 \text{ JK}^{-1} \text{ mol}^{-1} \)) from a straight line of plotting of \( \ln(\beta/ T_2) \) versus 1000/T (FWO), \( \ln(\beta) \) versus 1/T (KAS), and \( \ln(dx/dt) \) versus 1/T (Friedman). The slope of these fitting curves represented by \(-Ea/RT_m\) and -1.0516Ea/R (FWO), whereas Ea values were determined numerically in the case of Vyazovkin and Cai methods as shown above in Table 1. Fig. 7B–D shows the plot curves. It is clear that KAS and FWO plots have almost similar trend in the form of parallel straight lines with very small variations in the whole conversion range, especially with the progressing conversion rate within the range of 0.3–0.9 as a result of generation of more simultaneous reactions in the lower conversion region [59]. Meanwhile, in case of Friedman, the linear plot was more accurate and all fitting lines were matched together up to 70 % in conversion, whereas at 0.8 and 0.9 they showed a big variation as a result of more unstable radicals joined simultaneously in the highest conversion region [60]. Based on these results, FWO, KAS, and Friedman models are valid methods to simulate the reaction mechanism of the face mask in the main conversion zone (0.2 to 0.7) and these results agree with the results listed in the literature.

Finally, the activation energies at all conversion rates (0.1 to 0.9) were determined using Eqs. (7)–(11) and all estimated values of Ea are summarized in Fig. 8. It seems that the estimated values of Ea using the
FWO and Friedman methods have an almost similar trend in all the conversion regions; even the average values have almost the same values, which were estimated at 268.70 kJ mol\(^{-1}\) (FWO) and 280.91 kJ mol\(^{-1}\) (Friedman). Ea estimated using the KAS was smaller in all conversion zones than average Ea estimated at 236.52 kJ mol\(^{-1}\). Friedman approach had higher percentage than 16% (KAS) or 4% (FWO). Also, it is clear that the maximum Ea was achieved at the progressing conversion rate within the range of 0.3–0.7, while the lowest Ea was at low conversion rates in the ranges of 0.1–0.2 and higher conversion rate (0.9) because of simultaneously generated reactions and simultaneous contacting of unstable radicals [60, 61]. This means that thermal decomposition of face masks using pyrolysis process is a complex process and needs a multi-stage reaction mechanism for different components such as lignin, cellulose, hemicelluloses, etc. [62]. Despite the variation in the results, model-free methods serve as a reliable approach to investigate the reaction mechanism of face mask in the major conversion region (0.3 to 0.7). These results agree with the results reported in the literature for waste of similar composition [33–35]. Finally, it seems that the calculated kinetic parameters using nonlinear integral isoconversional were perfectly matched with those obtained by isoconversional methods, especially the KAS method because the points obtained were linear, which means that both models are valid for modeling the pyrolysis kinetics of face masks.

### 3.7.4. Fitting of TGA data using IPR

Based on the data sheet, the face mask contains more than two pseudo components, including PP and filter paper. However, the DTG curves in Section 3.2 reveal only one visible peak resulting from simultaneous decomposition of all pseudo components in a single reaction. IPR was used to verify experimental DTG data and the calculated data by plotting the experimental data. Fig. 10A,B shows the DTG experimental data (solid lines) and calculated (dotted lines) curves of DTG for all heating rates (5–30 °C/min) using Eq. (13). It is clear that the plotting data match completely the DTG experimental data with a very small deviation <1. Based on the IPR model, activation energy and pre-exponential factors were estimated at 265.1504 kJ mol\(^{-1}\) and 3.05E+14, receptivity.

Based on the TG-FTIR-GC–MS results of the face masks in CO2 atmosphere, pyrolysis treatment can be considered as a promising technology to dispose of the face masks and convert them into energy products. Also, model-free methods, DAEM, and IPR models were successful to calculate kinetic parameters and to plot TGA and DTG curves with economic deviations below <1.

### 4. Conclusions

In this work, the authors introduced the pyrolysis treatment using the TG-FTIR-GC–MS system as a safe and economic environment technology to dispose of face masks protecting against Covid 19. The research started with the analysis of the elements and ultimate properties of the face mask, followed by determination of its pyrolysis properties and the synthesized chemical compounds using the TG-FTIR-GC–MS measurements. Afterwards, pyrolysis kinetic parameters

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**Fig. 8.** The apparent activation energy at different conversion rates.

**Fig. 9.** TGA experimental and calculated data at (A) 5–15 °C/min and (B) 5–15 °C/min.
The results showed that the face mask is rich in volatile matter and can decompose in three stages in the range of 360–500 °C (with mass loss of 67–96 %). Meanwhile, the kinetic results showed that average activation energies were estimated at 237 kJ mol⁻¹ (KAS), 268.70 kJ mol⁻¹ (FWO), 280.91 kJ mol⁻¹ (Friedman), 231 kJ mol⁻¹ (Vyzavokin), and 223 kJ mol⁻¹ (Cai), whereas the pre-exponential factor was calculated using DAEM and IPR and estimated at 7.96E + 17 and 3.05E + 14, respectively. On the other hand, the GC-MS results showed that Propene and Furan, 2,4-Dimethyl-1-heptene and Isopropylcyclobutane, etc. were the major compounds in the synthesized pyrolysis products and the intensity of these compounds increased significantly with increase in the heating rates. Based on these results, the pyrolysis treatment can be used as a cleaner and safer industrial solution for face masks that have a high potential to be applied in the renewable energy sector, thus causing less environmental problems.

Author statement

Samy Yousef: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Writing - original draft, Writing - review & editing.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.jaap.2021.105118.

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