JOURNAL OF ANALYTICAL AND APPLIED PYROLYSIS

AUTHOR INFORMATION PACK

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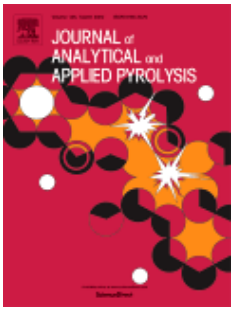

ISSN: 0165-2370

DESCRIPTION

The *Journal of Analytical and Applied Pyrolysis* (JAAP) is devoted to the publication of papers dealing with innovative applications of pyrolysis processes, the characterization of products related to pyrolysis reactions, and investigations of reaction mechanism. To be considered by JAAP, a manuscript should present significant progress in these topics. The novelty must be satisfactorily argued in the cover letter. A manuscript with a cover letter to the editor not addressing the novelty is likely to be rejected without review.

More specifically, the Scope of the Journal includes:

Fundamental pyrolysis researchon chemical substances and materials comprising:
- experimental studies of pyrolysis reactions such as chemical mechanism and kinetic investigations; this includes preparative pyrolysis methods for the synthesis of novel compounds and mechanisms of high temperature reactions;
- computational and theoretical studies of reaction mechanism, kinetics, and thermodynamics are acceptable, provided they are directly related to experimental data, either new or previously published, but they must be described adequately in the paper;
- computational processing of pyrolysis data, such as advanced pattern recognition and principal component analysis and other multivariate analyses.

Analytical pyrolysis, i.e. the characterization of a material in inert atmosphere by thermally induced degradation reactions;
- exploring chemical composition and structure of materials by revealing thermal and chemical decomposition reactions leading to products fully identified by chemical and spectroscopic methods;
- applications of analytical pyrolysis in environmental, biological, medical, forensic, cultural heritage, food, geochemical, polymer, and materials science;
- new instrumentation and new analytical methods using pyrolysis reactions or to unravel the chemical composition of pyrolysis products.

Applied pyrolysis dealing with the development of pyrolysis processes for producing valuable chemicals and/or energy carriers (gas, liquid, solid or electricity) and/or materials from fossil or renewable feedstock or waste, the recycling of materials, and the disposal of toxic substances. The manuscript must discuss the relationships between pyrolysis conditions and product characteristics. This topic includes:

- various feedstock (fossil fuels, biomass, wastes, polymers, etc.) and the co-processing of different feedstock;

- various thermal processes (slow and fast pyrolysis, torrefaction, carbonization, high pressure pyrolysis, catalytic pyrolysis, deoxygenation, hydropyrolysis, solvent liquefaction).

The combination of a pyrolysis process with other types of treatment (mechanical, biological, or chemical) or materials characterization is within the scope of the journal only if the main focus of the manuscript is the pyrolysis process. Integrated processes combining pyrolysis reactors and products purification are welcome, if different pyrolysis conditions are studied. The computational modeling of pyrolysis reactors or processes should be related to experimental data, either new or previously published, but they must be described adequately in the paper.

The pyrolysis conditions should be described thoroughly (residence times of solid and vapors, temperature distributions, etc.). The pyrolysis products must be chemically characterized. Catalysts should be physically and chemically characterized before reaction, and, when feasible analysis of catalysts after reaction is also desirable. While this may not always be possible, at least qualitative assessments should be made.

The investigation of pyrolysis of a new feedstock or material with conventional methods, but without new development of the pyrolysis process is not sufficiently novel to be considered by JAAP.

Review articles are invited by the Editors but may also be proposed in writing to the Review Editor. The subject of review articles should be broad enough to appeal to a wide range of readers. Discussion should be concise, but adequate. More detailed discussion may be appropriate in some cases. It is expected that reviews should be critical rather than just catalogs of published data. They should include the most important, recent advances in the topic, whereas papers of low scientific significance should be given very limited coverage.

Out of the scope of JAAP

The Journal does not consider studies based on:

- the activation of carbons and characterization of activated carbons;

- thermal analysis, mass yields without characterization of the pyrolysis products by chemical and spectroscopic methods;

- characterization and application of pyrolysis products, unless clearly related to/aimed at understanding the influence/details of pyrolysis processes and conditions;

- theoretical studies, kinetic modelling etc. which are not complemented with or validated by experimental data

- combustion, gasification or incineration unless specifically related to the interplay between pyrolysis and oxidation reactions.

AUDIENCE

Analytical Chemists; Researchers involved in Chromatography, Mass Spectrometry, and Polymer Science; Geochemists, Technologists in Plastic and Rubber Industries; Bacteriologists; Food and Medical Chemists.

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INTRODUCTION

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BEFORE YOU BEGIN

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Introduction

State the objectives of the work and provide an adequate background, avoiding a detailed literature survey or a summary of the results.

Material and methods

Provide sufficient details to allow the work to be reproduced by an independent researcher. Methods that are already published should be summarized, and indicated by a reference. If quoting directly from a previously published method, use quotation marks and also cite the source. Any modifications to existing methods should also be described.

Results
Results should be clear and concise.

Discussion
This should explore the significance of the results of the work, not repeat them. A combined Results and Discussion section is often appropriate. Avoid extensive citations and discussion of published literature.

Conclusions
The main conclusions of the study may be presented in a short Conclusions section, which may stand alone or form a subsection of a Discussion or Results and Discussion section.

Appendices
If there is more than one appendix, they should be identified as A, B, etc. Formulae and equations in appendices should be given separate numbering: Eq. (A.1), Eq. (A.2), etc.; in a subsequent appendix, Eq. (B.1) and so on. Similarly for tables and figures: Table A.1; Fig. A.1, etc.

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Abstract

A concise and factual abstract is required. The abstract should state briefly the purpose of the research, the principal results and major conclusions. An abstract is often presented separately from the article, so it must be able to stand alone. For this reason, References should be avoided, but if essential, then cite the author(s) and year(s). Also, non-standard or uncommon abbreviations should be avoided, but if essential they must be defined at their first mention in the abstract itself.

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Immediately after the abstract, provide a maximum of 6 keywords, using American spelling and avoiding general and plural terms and multiple concepts (avoid, for example, 'and', 'of'). Be sparing with abbreviations: only abbreviations firmly established in the field may be eligible. These keywords will be used for indexing purposes.

Acknowledgements
Collate acknowledgements in a separate section at the end of the article before the references and do not, therefore, include them on the title page, as a footnote to the title or otherwise. List here those individuals who provided help during the research (e.g., providing language help, writing assistance or proof reading the article, etc.).

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List funding sources in this standard way to facilitate compliance to funder's requirements:

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Nomenclature and units
As default the international system of units (SI) should be used (see the IUPAC *Green Book*). If other units are used, give their equivalent value in the SI unit at the first mention (e.g. 1 kcal = 4.184 kJ). Basic SI units and other accepted metric nomenclature are given in the section "Quantities and units".

Authors are urged to consult the IUPAC 'color books' of chemical nomenclature: *Chemical Terminology* (Gold Book), *Nomenclature of Organic Chemistry* (Blue Book), *Nomenclature of Inorganic Chemistry* (Red Book), *Analytical Nomenclature* (Orange Book) and *Compendium of Polymer Terminology and Nomenclature* (Purple Book).

Contributions which report mass spectrometric results should follow the IUPAC recommendations for analytical pyrolysis: Pure Appl. Chem. 65 (1993) 2405; for GC-MS: K. K. Murray et al. Pure Appl. Chem. 85 (2013) 1515, and py-GC-MS: IUPAC Orange Book.

Symbols, formulae and equations should be written with care, capitals and lower case letters being distinguished where necessary. Particular care should be taken in typing mathematical expressions containing superscripts and subscripts, and in proof-reading such equations. Unusual symbols employed for the first time should be defined by name in the left-hand margin. Acronyms and abbreviations require definition when first used, and they should not be used in the title, abstract, or highlights, except if widely known such as GC-MS, NMR, FTIR etc. Abbreviations for long chemical names (e.g. DMSO, EDTA, TBAH) are useful, especially in equations, tables or figures, but uncommon abbreviations and acronyms should not be used in the title, abstract, conclusion, or highlights.

Significant figures: avoid numbers with too many digits. The number of significant figures should be consistent with the precision of the data.

Mathematical Formulae
Please submit math equations as editable text and not as images. Present simple formulae in line with normal text where possible and use the solidus (/) instead of a horizontal line for small fractional terms, e.g., X/Y. In principle, variables are to be presented in italics. Powers of e are often more conveniently denoted by exp. Equations that have to be displayed separately from the text should be numbered consecutively and referred to explicitly in the text.

Chemical Formulae
Should be drawn in ChemDraw format with standard bond lengths and angles. The standard settings are:
Chain angle: 120 degrees
Bond spacing: 18% of length
Bond length: 0.508 cm (14.4 pt)
Bold width: 0.071 cm (2 pt)
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Margin width: 0.056 cm (1.6 pt)
Hash spacing: 0.088 cm (2.5 pt)
Captions: Arial 10 pt
Atom labels: Arial 10 pt or Helvetica 12 pt.
Bond angles and length: "fixed" is recommended.

Other drawing programs such as Isis/Draw, ChemSketch and MarvinSketch may be used as long as the same or similar settings are used and the overall visual impression remains the same. Computer-generated calculated structures should not replace ChemDraw structures in reaction schemes, equations and figures but may be used in separate figures, when details of the calculated structures are discussed in the text. In such cases annotation with essential bond lengths and angles will be helpful. Calculated structures which are not discussed in the text may be presented in the Supplementary material.

Pyrolysis Experiments
Drawings or illustrations of pyrolysis apparatus are welcome, except if they are commonly known and commercially available. However, even if there is little novelty, details of the apparatus may be of interest, and in such cases the information should be placed in the Supplementary material. In all cases apparatus should be described in sufficient detail to allow others to repeat the experiments.

Pyrolysis temperatures should be recorded with reasonable accuracy, e.g. 535 oC, not 534.63 oC, unless extreme accuracy is documented (see 'Significant figures' above). The method used for determining heating rates should be defined, and the rates should be realistic; for example, a heating rate of 100 oC/s is unrealistic for many compounds. For reactors, comments should be made on the distribution of temperatures.

The methods of pressure measurement should be presented (sensors type, calibration range, etc.), as applicable.

The residence times of solids and vapors and the temperature gradients for gas-phase sections should be given or estimated even for micro-pyrolysis experiments. The methods of gas/vapor sampling (length and temperature of heated lines, volume of sampling loop for GC, direct injection through molecular beam or capillary lines, adsorption followed by desorption conditions, etc.), vapour condensation system (temperatures, volumes, etc.), and liquid sampling (e.g. from the condenser to the vial) should be presented in detail.

Compound Characterization
Stable, *new* organic compounds synthesized or isolated from pyrolysis reactions should be characterized in the usual way, i.e. by 1H and 13C NMR spectroscopy, IR spectroscopy, mass spectrometry and elemental analysis (tolerance 0.4%), and evidence for homogeneity should be given. If elemental analysis is not reported, copies of the 1H and 13C NMR should be provided in the Supplementary material. If high resolution mass spectral measurements are reported, the full low resolution mass spectra, with relative abundances, should be reported too. Melting points for solids should be given.

When *known* compounds are identified by py-GC-MS methods, the experimental procedure should be described fully, and adequate references to libraries of GC and/or MS data used in the characterization should be given. Methods used to measure yields should be described, clear distinctions between relative and absolute yields must be made, and information of experimental errors in percentages of products must be given. For example, relative yields should not simply be read off the instrument and reported as e.g. 21.89%, 47.31%, etc for single-run experiments with no information on precision. Representative gas chromatograms and mass spectra should be published as Supplementary material with sufficient detail to enable other researchers to duplicate the results.

Concerning analysis of liquids, details of sample preparation (filtration, dilution, type of solvent(s), etc.) and storage (vial type, temperature and time) should be given.

The method for liquid chromatography should be presented: injection volume, column type and reference, solvent(s) gradient and flow-rate(s), temperature of the column, conditions for the detectors (notably ionization conditions for MS).

Calibration methods used for all analytical methods must be specified: the authors should indicate the standards used (concentration, etc.), response factors (in Supplementary material), and volumes of internal standards, if used. Internal calibration is preferred to external calibration for the quantification of liquid products from pyrolysis reactions.

Information on transient compounds or reactive intermediates that cannot be isolated in pure form may be given, but it is important to explicitly distinguish between stable and unstable compounds.

Organometallic and Inorganic Compounds: for new compounds sufficient experimental details must be included to allow another researcher to reproduce the synthesis and characterization. X-ray diffraction may often be the most unambiguous method of structure determination, but because of potential misidentification of atoms, the X-ray diffraction structure alone may not suffice as the only means of characterization. Evidence for elemental constitution must be provided by elemental analysis (e.g. combustion analysis, microprobe analysis), or mass spectrometry. NMR data should be reported for soluble compounds (and where relevant for solids, e.g. char, by solid-state NMR and 2D 1H-13C solid state NMR). IR spectroscopy may be used to support the presence of functional groups, but in most cases IR spectroscopy alone is not sufficient to characterize structures.

Materials
Solid state materials which do not exist in solution may be best characterized by X-ray crystal structure or X-ray powder diffraction (XRD) (see also solid-state NMR above). Elemental analysis (combustion, microprobe) and evidence for homogeneity should also be reported. XRD data should be accompanied by details of the experimental technique, i.e. the source of X-rays, radiation, wavelength, filters or monochromators, camera diameter, the type of X-ray recording, and the technique used for measuring intensities. In cases of unindexed listing of the data, the d spacings of all observed lines should be listed in sequence, together with their relative intensities. If filtered radiation is used, efforts should be made to identify residual β lines. Where resolution into α1-α2 doublets occurs, the identification of the d spacing for each line as dα1, dα2 gives a measure of the quality of the diffraction pattern. When an indexing of the data is electron offered, the observed and calculated 1/d2 values should be listed along with the observed relative intensities (a listing of d spacings is then superfluous), the calculated 1/d2 values to the limit of the data quoted. Where possible and justified by the data, crystal systems should be specified, and possible space groups may be listed. IR spectroscopy may be used to support the presence of functional groups, but in most cases IR spectroscopy alone is not sufficient to characterize materials.

Note that thermal analysis data (TGA etc) without supporting spectroscopic and analytical product characterization are not acceptable.

Biomass, bio-oil, biochar, wastes, coal, etc.: Elemental analysis (C, H, O, N, S as appropriate) and details of organic and mineral content should be provided with full details of the analytical procedure (e.g. combustion analysis, electron microprobe analysis), methods of digestion/mineralisation, inductively coupled plasma (ICP) parameters, XRD, ICP-MS, atomic emission spectroscopy (AES), scanning electron microscopy (SEM) and/or energy dispersive X-ray spectroscopy (SEM-EDS), X-ray powder diffraction (XRD) as appropriate.

Carbohydrates, lignin. In biomass: composition in total carbohydrates (e.g. after hydrolysis) and in lignin (e.g. Klason lignin analysis, etc.) For fossil fuels (coal, crude oil, asphaltenes, pitch, etc.): origin of the resource and method(s) of analysis.

Catalysts: as for other inorganic and organometallic substances; at least XRD and elemental analysis (metal content, composition of the support, etc.) before and after pyrolytic reactions should be provided and when appropriate, coke content after reaction, etc.

Carbons (char, coke, soot, pyrolytic carbon, etc.): NMR, Raman, XPS, and all other spectroscopic methods of analysis are welcome. Full and details of analysis are mandatory.

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time*t*; second s; minute min; hour h
thermodynamic temperature *T*; kelvin K
Celcius temperature *t*,* degree Celcius C
amount of substance *n*; mole mol
molar mass *M*; kg mol^{-1}
concentration (amount) *c*; mol dm^{-3}, mol l^{-1}
molality *m*; mol kg^{-1}
pressure *p*; pascal Pa
energy*E*; joule J
heat *q*, Q; joule J
power, heat flow rate *P*,ø; watt W
volume *V*; m^3; litre l, L
chemical potential (partial molar Gibbs energy) μJ mol^{-1}
viscosity: dynamic η Pa s ; kinematic μ m s^{-1}

Prefixes

10^{-1} d; 10^{-2} c (centi); 10^{-3} m (milli); 10^{-6}μ (micro); 10^{-9} n (nano); 10^{-12} p (pico); 10^{-15} f (femto); 10^{-18} a (atta)

10 da (deca); 10^{2} h (hecto); 10^{3} k (kilo); 10^{6} M (mega); 10^{9} G (giga); 10^{12} T (tera); 10^{15}P (peta); 10^{18} E (exa)

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