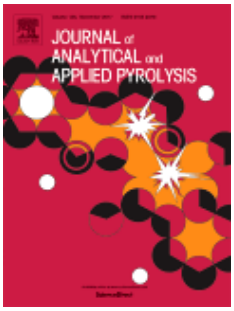
JOURNAL OF ANALYTICAL AND APPLIED PYROLYSIS

AUTHOR INFORMATION PACK

TABLE OF CONTENTS



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DESCRIPTION

The international *Journal of Analytical and Applied Pyrolysis* is devoted to the publication of qualitative and quantitative results relating to:

- **Controlled pyrolysis** (thermal degradation, thermolysis) of chemical materials, including synthetic and natural macromolecules as well as lower molecular weight chemicals.

- Fundamental studies of **pyrolysis processes** by chemical, physical and physicochemical methods.

- Studies of pyrolysis **reaction kinetics**, energetics, and mechanisms.

- Technical developments and new instrumentation for pyrolysis techniques in combination with chromatographic or spectroscopic **methods**.

- **Analytical pyrolysis**, namely the characterization of a material by chemical degradation reactions induced by thermal energy or by thermally assisted decomposition reactions.

- Environmental, geochemical, biological, medical, and forensic applications of **analytical pyrolysis**.

- Pyrolysis investigations of **energy**-related problems, looking for relationships between pyrolysis conditions and product characteristics (i.e. fossil/synthetic fuels, biomass derivatives, thermal catalytic products, coal liquefaction products).

- Automation, optimization and standardization of pyrolysis **techniques**.

- **Computer** handling and **processing** of pyrolysis **data**, including library filing and retrieval techniques, and computer matching and advanced pattern recognition techniques.

- Studies in **high temperature chemistry** of synthesis and decomposition reactions.

- **Applied pyrolysis**, i.e. the use of pyrolysis methods, including thermal cracking, catalytic cracking, hydrothermal treatments, in the disposal of waste materials, in exploiting biomass resources, in fossil fuel transformations for the production of energy, valuable chemicals or engineering materials.

The Journal does not consider studies based solely on:

- thermal analysis, unless combined with the chemical characterisation of the thermal degradation products (e.g. TG-MS, TG-FTIR);

- chemical activation for the synthesis of activated carbons;

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

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

- combustion, incineration, unless specifically related to the pyrolysis process.

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

The international *Journal of Analytical and Applied Pyrolysis* is devoted to the publication of qualitative and quantitative results relating to:
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- Fundamental studies of **pyrolysis processes** by chemical, physical and physicochemical methods.
- Studies of pyrolysis **reaction kinetics** , energetics, and mechanisms.
- Environmental, geochemical, biological, medical, and forensic applications of analytical pyrolysis;
- Technical developments and new instrumentation for pyrolysis techniques in combination with chromatographic or spectroscopic **methods** .
- **Analytical pyrolysis** , namely the characterization of a material by chemical degradation reactions induced by thermal energy or by thermally assisted decomposition reactions.
- Environmental, geochemical, biological, medical, and forensic applications of **analytical pyrolysis** .
- Pyrolysis investigations of **energy** -related problems, looking for relationships between pyrolysis conditions and product characteristics (i.e. fossil/synthetic fuels, biomass derivatives, thermal catalytic products, coal liquefaction products).
- Automation, optimization and standardization of pyrolysis **techniques** .
- **Computer** handling and **processing** of pyrolysis **data** , including library filing and retrieval techniques, and computer matching and advanced pattern recognition techniques.
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- thermal analysis, unless combined with the chemical characterisation of the thermal degradation products (e.g. TG-MS, TG-FTIR);
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- theoretical studies, kinetic modelling etc. which are not complemented/validated with experimental data;
- combustion, incineration, unless specifically related to the pyrolysis process.

Types of contributions

The *Journal of Analytical and Applied Pyrolysis* publishes research papers, reviews and short communications. Research papers and reviews which cover any topics within the scope of the Journal are welcomed. Authors of reviews may want to check with one of the Editors prior to submission to make sure that the topic is appropriate for the Journal. Three categories of short communications may be considered. First, brief articles describing significant new pyrolysis concepts or applications may be submitted. For these the author(s) generally wishes to establish priority or seek rapid feedback from other investigators. It is usually expected that such articles will be followed by a full paper. Second, comments on papers that have appeared in the Journal may be submitted. In this case, the author(s) of the work being discussed will ordinarily be allowed to reply. Third, editorial reports of various kinds will be considered. These may include comments
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State the objectives of the work and provide an adequate background, avoiding a detailed literature survey or a summary of the results.

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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.

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Results should be clear and concise.

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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.

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

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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.

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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 ? lines. Where resolution into ?1-?2 doublets occurs, the identification of the d spacing for each line as d?1, d?2 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.

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[2] W. Strunk Jr., E.B. White, The Elements of Style, fourth ed., Longman, New York, 2000.
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[3] G.R. Mettam, L.B. Adams, How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), Introduction to the Electronic Age, E-Publishing Inc., New York, 2009, pp. 281–304.
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[4] Cancer Research UK, Cancer statistics reports for the UK. http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/, 2003 (accessed 13 March 2003).
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length *l*; metre: m
mass *m* kilogram kg; gram g
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*; m3; 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); 10-6μ (micro); 10-9 n (nano); 10-12 p (pico); 10-15 f (femto); 10-18 a (atta)

10 da (deca); 102 h (hecto); 103 k (kilo); 106 M (mega); 109 G (giga); 1012 T (tera); 1015P (peta); 1018 E (exa)

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