



This document sets forth the general requirements for authors interested in contributing to the **2026 World Conference on Packaging**, which will be hosted by **Hunan University of Technology** in Zhuzhou, China, **June 8–12, 2026**. It provides an overview of the process, expectations, and responsibilities associated with submitting an abstract or paper for consideration.

The conference is committed to ensuring that all submissions are evaluated fairly, consistently, and in alignment with the goals of advancing packaging science, technology, and education worldwide. Authors are expected to prepare their work with a high standard of quality, clarity, and originality, and to adhere to the guidelines presented in this document.

By following these requirements, contributors help maintain the integrity of the peer review and general submission processes and ensure that the conference program reflects both the academic rigor and practical relevance that are hallmarks of IAPRI events. Authors should therefore review these guidelines thoroughly before preparing their submission.

PAPER AND PRESENTATION REQUIREMENTS

All accepted abstracts, whether submitted to the peer review stream, general stream, or poster session, must be followed by the submission of a full paper. The paper is required to ensure proper documentation and inclusion in the official conference proceedings.

In addition, all accepted authors are required to deliver an oral presentation of their work during the conference. This includes poster session authors, who must prepare both a poster display and a short oral Poster Pitch summary of their research. These requirements apply to all categories of acceptance and are intended to ensure consistent quality, comprehensive documentation, and meaningful knowledge exchange during the conference.

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WORLD CONFERENCES ELIGIBILITY AND SCOPE

IAPRI World Conference or Member Conference are hosted by one of the members over alternating even numbered years. World conferences are open to all interested parties to apply to make a presentation while member conferences are only open to IAPRI members.

Submissions are welcome from researchers, academics, students, and professionals whose work is relevant to the themes of the conference. Contributions may be accepted in one of several formats:

-  Peer-reviewed research papers
-  General stream presentations
-  Poster presentations

Only submissions that fall within the scope of the conference and within the following topics will be reviewed:

- Active & intelligent packaging
- Distribution packaging
- Logistics & supply chain
- Packaging design, ergonomics & human factors
- Medical, cosmetic & pharmaceutical packaging
- Packaging for food & agriculture
- Packaging for hazardous & dangerous goods
- Packaging machinery & systems
- Packaging materials
- Packaging sustainability
- Packaging standards & legislation

PEER REVIEW ABSTRACT & PAPER AND GENERAL STREAM ABSTRACT REQUIREMENTS

Abstracts are submitted online via the IAPRI Proposal Submission Portal for all formats of presentations. Here is the link: [Submit 2026 Abstract](#)

Peer Review Managed by Packaging Technology and Science (PTS)

Submission to the peer review stream is a 2-step process.

Step 1: All Authors also should submit an abstract (300-500 words) through this online submission tool and indicate that the submission is for the peer-review stream. The Scientific committee will evaluate its fitness to the peer-review stream and provide authors with recommendations regarding further steps.

Step 2: If the abstract is accepted as fit for PTS submission, the authors are required to submit the full manuscript following PTS Journal Instructions at:

<https://onlinelibrary.wiley.com/page/journal/10991522/homepage/forauthors.html>

Authors should select the IAPRI Special Issue when submitting the manuscript to PTS.

Papers submitted through the Peer-Review Stream will be published in Packaging Technology and Science, respecting the journal's editorial policies.

General Stream abstracts for oral and poster presentations



Authors do not need to be concerned with formatting requirements for general stream abstracts, as all submissions are entered directly into the online proposal system, which standardizes the presentation format. Here is the link: [Submit 2026 Abstract](#)

PEER REVIEW ABSTRACT & PAPER AND GENERAL STREAM ABSTRACT DEADLINES

Peer-Review Stream Deadlines

- Abstract Submission to IAPRI: Opens October 15th Firm Closing November 15th
- Full Paper Submission to PTS: January 15th
- Paper Acceptance Notification from PTS will be on a rolling basis

General Stream Deadlines

- Abstract Submission: Opens November 15th, Firm Closing January 15th
- Abstract Acceptance Notification (on a rolling basis): by February 28th
- Full Paper Deadline: May 22nd

The following information is provided for a manuscript for peer review, or an abstract for a non-peer review contribution (oral presentation or poster) for the style for each type of presentation.

PROCEDURE FOR ABSTRACT REVIEW AND PRESENTATION SELECTION BY SCIENTIFIC COMMITTEE

At the beginning of the application process, you will be asked the following questions regarding your proposed technical presentation. Your answers will aid a **review panel of three reviewers** from the **Scientific Committee** to evaluate your submission for **clarity, relevance, scientific merit, and fit with the conference theme**.

- What is the main objective of the research or project?
(Purpose: Helps reviewers evaluate relevance and clarity of goals.)
- What technical methods or approaches were used?
(Purpose: Helps assess technical rigor and sound methodology.)
- What are the primary findings or results?
(Purpose: Ensures there is actual data, insight, or analysis to share.)
- How does this work contribute new knowledge or insight and what is its possible impact?
(Purpose: Supports scoring for originality and contribution to packaging research and education.)
- What stage is the work at (e.g., completed research, pilot, early findings)?
(Purpose: Helps the reviewer determine suitability for presentation.)
- How does the work align with the theme of the conference:
(Purpose: Helps reviewers assess strategic fit with the conference theme.)
- What is novel, innovative, or unique about your research or project?
(Purpose: Allows reviewers to score originality and contribution to the field.)

These questions are organized to align with common review criteria such as **technical rigor, originality, relevance to the association, potential impact, and presentation quality**.



SCIENTIFIC COMMITTEE REVIEW PROCESS

All submissions will be reviewed according to the selected stream. Abstracts submitted to the general stream undergo a review by selected members of the IAPRI Scientific Committee based on originality, scientific quality, innovation, and significance to the research community. Abstracts may be submitted for oral or poster presentations. The Committee reserves the right to assign final presentation type in the best interest of the program. However, the Committee will accommodate as many oral presentations as the conference schedule permits.

The category chair first determines if the subject fits in the IAPRI category as indicated on the submission form and if it fits in the field of packaging. If necessary, they can discuss the issue with the reviewers whom they plan to send it to for review or ask other reviewers to give their opinion. If necessary, contact the submitter to ask to them to make the relation with packaging clearer. Otherwise, the submission can be rejected.

If this is a general stream or poster presentation and accepted by the chair, then it is assigned to 2-3 reviewers for review and scoring. The reviewer can also recommend that the submitter be contacted about the possibility of changing the paper to the peer review stream process.

If the submission is for peer review, then one reviewer is assigned who is capable and willing to be part of the PTS reviewer panel if the reviewer scores the submission high enough and moves it to the next stage.

The Scientific Committee members will review and score each abstract according to the following process.

Step 1: Read Submitter's Responses

At the beginning of the application process, you will be asked the following questions regarding your proposed technical presentation. Your answers will aid a review panel of three reviewers from the Scientific Committee to evaluate your submission for clarity, relevance, scientific merit, and fit with the conference theme.

- What is the main objective of the research or project?

(Purpose: Helps reviewers evaluate relevance and clarity of goals.)

- What technical methods or approaches were used?

(Purpose: Helps assess technical rigor and sound methodology.)

- What are the primary findings or results?

(Purpose: Ensures there is actual data, insight, or analysis to share.)

- How does this work contribute new knowledge or insight and what is its possible impact?

(Purpose: Supports scoring for originality and contribution to packaging research and education.)

- What stage is the work at (e.g., completed research, pilot, early findings)?

(Purpose: Helps the reviewer determine suitability for presentation.)

- How does the work align with the theme of the conference:

(Purpose: Helps reviewers assess strategic fit with the conference theme.)



- What is novel, innovative, or unique about your research or project?

(Purpose: Allows reviewers to score originality and contribution to the field.)

This gives context for the evaluation and helps to evaluate your submission for **clarity, relevance, scientific merit, and fit with the conference goals**. The questions are organized to align with common review criteria such as **technical rigor, originality, relevance to the association, potential impact, and presentation quality**.

Step 2: Checking Abstract Content

Confirming the abstract includes:

- A clear, specific title
- An introduction and stated objectives
- Methods used
- Results with main findings (quantitative data if available)
- No vague statements such as “results will be discussed”

Step 3: Apply Review Criteria

Evaluate whether the submission is:

- Original and innovative
- Scientifically rigorous
- Relevant to packaging and the chosen IAPRI topic
- Significant to the research community
- Of potential industry relevance
- Well written and clearly organized

Step 4: Score the Abstract (0–5)

At the beginning of the application process, you will be asked the following questions regarding your proposed technical presentation. Your answers will aid a **review panel of three reviewers** from the **Scientific Committee** to evaluate your submission for **clarity, relevance, scientific merit, and fit with the conference theme**.

- What is the main objective of the research or project.
(Purpose: Helps reviewers evaluate relevance and clarity of goals.)
- What technical methods or approaches were used?
(Purpose: Helps assess technical rigor and sound methodology.)
- What are the primary findings or results?
(Purpose: Ensures there is actual data, insight, or analysis to share.)
- How does this work contribute new knowledge or insight and what is its possible impact?
(Purpose: Supports scoring for originality and contribution to packaging research and education.)
- What stage is the work at (e.g., completed research, pilot, early findings)?
(Purpose: Helps the reviewer determine suitability for presentation.)



- How does the work align with the theme of the conference:
(Purpose: Helps reviewers assess strategic fit with the conference theme.)
- What is novel, innovative, or unique about your research or project?
(Purpose: Allows reviewers to score originality and contribution to the field.)

These questions are organized to align with common review criteria such as **technical rigor, originality, relevance to the association, potential impact, and presentation quality.**

Submitted abstracts will be evaluated to set of clear, objective criteria that reviewers can use to score abstracts (0–5 scale) for an IAPRI conference, aligned with:

- **Academic quality**
- **Relevance to association activities**
- **Significance to the research community**
- **Industry relevance**

Q1. Scientific and Academic Quality (0–5)

Is the abstract based on sound methodology, clear objectives, and appropriate analysis or experimentation?

- **5** – Outstanding clarity, rigor, originality; methods and findings are well-articulated
- **4** – Strong academic content; clear objectives and well-explained methods
- **3** – Adequate, though may lack detail or originality
- **2** – Some methodological or conceptual weaknesses
- **1** – Poorly explained or flawed academic basis
- **0** – Not applicable or lacking academic merit

Q2. Fit with the Association's Scope and Activities (0–5)

Does the research clearly align with the goals, interests, or strategic focus areas of the association?

- **5** – Central to the association's mission and strategic priorities
- **4** – Strong fit with current initiatives or working groups
- **3** – Moderate relevance, possibly tangential
- **2** – Limited connection to association interests
- **1** – Weak alignment
- **0** – Not aligned at all

Q3. Significance to the Packaging Research Community (0–5)

Will this research advance knowledge, inspire further investigation, or fill an important gap?

- **5** – High impact; likely to influence ongoing or future research
 - **4** – Valuable contribution; strong interest to researchers
 - **3** – Modest contribution or incremental advance
 - **2** – Narrow scope or minimal new knowledge
 - **1** – Very limited relevance
 - **0** – No evident research contribution
-



Q4. Industry Relevance and Practical Application (0–5)

Does the research address real-world packaging challenges or have the potential for implementation?

- **5** – High practical value; clear pathway to application or commercialization
- **4** – Strong potential for industrial interest or collaboration
- **3** – Some application possible; moderate relevance
- **2** – Unclear or limited practical implications
- **1** – Minimal relevance to industry
- **0** – Not applicable to industry

Q5. Overall Clarity and Organization of the Abstract (0–5)

Is the abstract clearly written, logically structured, and understandable to a multidisciplinary audience?

- **5** – Extremely clear and professional
- **4** – Well written with minor issues
- **3** – Understandable but some structural or grammatical weaknesses
- **2** – Difficult to follow or disorganized
- **1** – Poorly written
- **0** – Incomprehensible or missing

Q6. Technical Rigor and Methodology (0–5)

Does the abstract demonstrate appropriate and clearly described methods, sound technical approach, and logical analysis suitable for the research question or problem?

- **5** – Methodology is clearly defined, appropriate, and the abstract shows a strong command of research design and analytical reasoning.
- **4** – The methodology is sound and appropriate with good technical depth.
- **3** – The methodology is generally acceptable, technical reasoning is present but not especially strong.
- **2** – The approach is vague, overly simplistic, or partially inappropriate for the stated objectives.
- **1** – Major methodological weaknesses or significant technical flaws.
- **0** – No methodology provided.

Step 5: Provide Comments & Recommendations

The reviewer is encouraged to add comments and indicate if the requested presentation type (oral/poster) is appropriate. They may suggest resubmission as a poster or recommend rejection. If the work merits consideration for peer review, that will be noted as well.

Step 6: Select Final Recommendation

The reviewer recommends one of the following five possible actions for the abstract submission.

- Abstract is appropriate for an oral presentation in the General Stream
- Abstract is considered appropriate to move to PTS for peer review status
- This abstract has the potential to become a Peer Reviewed Paper and submitted to PTS
- Abstract is appropriate for a poster presentation



- This abstract is rejected at the presentation level declared in the submission

Once all assigned reviewers have scored the abstract it moves to the next stage and is finalized by the conference host administrator. Then papers need to be created.

AUTHOR GUIDELINES WHEN SUBMITTING A PEER REVIEW PAPER TO PTS

Peer-reviewed stream submissions accepted by the Scientific Committee must follow the process indicated below and submit a full paper to John Wiley & Sons Ltd.'s publication Packaging Technology & Science for their review and acceptance. For acceptance for publication by Packaging Technology & Science (PTS), the research should demonstrate significant novelty and significance at the theoretical, methodological, material, or application levels. They encourage authors to emphasize the innovative, or scientifically significant aspects of their research in their manuscripts. To ensure your work meets the high standards expected by PTS, IAPRI suggests that you follow these guidelines carefully.

1. Originality and Novel Contribution

- Your paper must present new insights, data, or applications that advance knowledge in the field.
- Work that is a duplicate of previously published material will not be considered.
- Clearly identify the research gap your study addresses and explain the innovation in your approach or findings.

2. Scientific Rigor and Methodology

- State your research question or hypothesis clearly.
- Provide a complete description of the methods so the study can be replicated.
- Use appropriate experimental design, controls, and statistical analysis.
- Present your results honestly; selective reporting, fabrication, or falsification are grounds for rejection.

3. Relevance and Significance

- Position your work within current literature and practice.
- Demonstrate its significance to packaging science and related industries.
- Highlight the theoretical, technological, or practical impact of your findings.

4. Paper Structure and Clarity

- Review the Manuscript Style, Reference Style, and other information at:
<https://onlinelibrary.wiley.com/page/journal/10991522/homepage/ForAuthors.html>
- Organize your paper according to scholarly convention:
 - **Title** – precise and informative.
 - **Abstract** – 300–500 words summarizing aims, methods, results, and conclusions.
 - **Introduction** – background, literature review, and statement of objectives.
 - **Methods** – detailed procedures and materials for reproducibility.
 - **Results** – clearly presented findings with appropriate tables and figures.
 - **Discussion** – interpretation, relation to previous studies, limitations, and implications.
 - **Conclusion** – concise summary of contributions and future research directions.
- Use clear, concise, and professional English throughout.



- Reference Style

<https://onlinelibrary.wiley.com/page/journal/10991522/homepage/ForAuthors.html>

5. Data Quality and Analysis

- Ensure the dataset is adequate to support your conclusions.
 - Present figures and tables that are clear, correctly labeled, and accompanied by explanatory captions.
 - Provide analysis that explains the meaning and implications of the data rather than only describing it.
 - Avoid overstating conclusions beyond what your data supports.
-

6. Ethical Standards

- Disclose funding sources and potential conflicts of interest.
 - Acknowledge collaborators and contributions appropriately.
 - Share data or materials openly when required by PTS policy.
-

7. References and Scholarship

- Provide a comprehensive and current literature review.
- Cite prior work accurately and fairly.
- Follow the required referencing style of PTS.

<https://onlinelibrary.wiley.com/page/journal/10991522/homepage/ForAuthors.html>

- Avoid plagiarism and excessive self-citation.
-

8. Technical Quality and Presentation

- Prepare all graphics, tables, and images at publishable quality.
- Ensure consistent terminology, abbreviations, and units of measure.
- Proofread carefully for grammar, spelling, and formatting errors.
- Format your manuscript according to PTS requirements.

<https://onlinelibrary.wiley.com/page/journal/10991522/homepage/ForAuthors.html>

9. Critical Discussion and Impact

- Address the limitations of your study honestly.
 - Suggest how the results may be applied in research, education, or industry practice.
 - Explain the contribution of your work to the packaging community and future research opportunities.
-

10. Readiness for Peer Review

- Submit only a polished, complete manuscript. Drafts will not be accepted.
 - Be prepared to revise your paper based on reviewer feedback.
 - Understand that not all submissions are accepted; peer review is selective and designed to uphold the highest standards of quality.
-

✦ *By following these guidelines, authors help ensure their work is of true peer-reviewed quality and makes a valuable contribution to the global body of packaging research.*



GENERAL STREAM CONFERENCE RESEARCH PAPER REQUIREMENTS

Research presentation submissions approved by the IAPRI Scientific Committee will result in the author's preparing full 4-8 page papers for the conference which must be submitted by the deadline and will be published in the conference proceedings.

English language is required, and it is important to use, a coherent writing style and readable sentences. The paper shall include the following content that follows the prescribe lengths:

Title and Author Information:

A clear and concise title that reflects the main topic of the research.

Authors' names with affiliation.

Abstract (300-500 words):

Provide a summary of the research problem/s, objective, methodology, key findings, and implications.

Keywords (3-5 keywords):

List relevant keywords that describe the subject matter of your research. Avoid repeating words of the title and buzz words.

Suggested Lengths: For use with these section headings.

1. Introduction (approximately 1/2 page):

Clearly state the research problem or question related to packaging and the objective of the published work.

Provide context for the research.

Explain the significance of the study.

Summarize relevant literature and prior research related to packaging.

Highlight gaps or controversies in the existing knowledge.

Explain how your research addresses or contributes to these gaps.

2. Methodology (approximately 1 page):

Describe the research methods employed in the study.

Explain the data collection and analysis processes.

Justify the chosen methodology and address any limitations.

In general, the methodology section should be precise enough for another research group to reproduce the study.

3. Results (approximately 1-2 pages):

Present the primary findings of your packaging research.

Use tables, figures, or diagrams to illustrate key data.

Include any statistical analysis if applicable.

4. Discussion (approximately 1-2 pages):

Interpret the results in the context of the research question and objectives.

Discuss the implications of the findings for the packaging industry or related fields.

Address any limitations encountered during the research.

Suggest areas for further research in packaging.

The result and discussion section can be joined if the authors consider it more effective.



5. Conclusion (approximately 1/2 page):

Explain how the study and its findings have answered the scientific question or hypothesis set down in the introduction.

Emphasize the significance of the research in the field of packaging.

Offer a concise closing statement.

6. References

Author Last Name First Initial Middle Initial. Title in sentence case. Abbreviated Journal Title in Title Case. Year; Volume (Issue#): PP-PP. doi: ##

Book: Author's last name Initials. Book Title: Subtitle. Publisher; Year.

Journal: Author last name Initials. Article title. Journal Name. Year; Volume (Issue): Page range. doi or URL.

Reference style. AMA – American Medical Association.

All references should be numbered consecutively in order of appearance and should be as complete as possible. In text citations should cite references in consecutive order using Arabic superscript numerals.

Use a 10-point font, single-spaced.

7. Acknowledgments (optional):

Figures

- Provide informative captions for all figures, placed below the figure.
- Reference figures with the text (e.g., "figure 1 shows...")
- Number figures sequentially (e.g., Figure 1, Figure 2).
- Ensure figures are of high quality and legible.

Tables

- Use tables for presenting data when appropriate.
- Reference tables with the text (e.g., "table 1 shows...")
- Number tables sequentially (e.g., Table 1, Table 2).
- Provide clear titles below each table.
- Ensure tables are well-organized and easy to read.

Equations

- Use Equation Editor or a similar tool for mathematical symbols and equations.
- Number equations sequentially in parentheses (e.g., (1), (2)).

Language

- Use clear and concise English language.
- Proofread and edit for grammar and spelling errors.
- Avoid using jargon or overly technical language without explanation.

Submission

- Submit papers in PDF format.
- Submit your paper electronically through the conference host requirements.



Influence of Molecular Weight and Shape on Diffusion Coefficients of Small Molecules in Polyethylene Terephthalate

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Abstract: In this study, the diffusion coefficients of 13 kinds of small molecules with molecular weights ranging from 32 to 339 g.mol⁻¹ in amorphous PET are calculated based on molecular dynamics (MD) simulation. The results suggest that diffusion coefficient of migrant depends not only the molecular weight but also the shape of migrant molecules. Further, the free volume of polymer matrix is calculated using Connolly surface method. The results show that some small free volume cavities conjoin together and form the larger cavities which facilitate the diffusion of migrant molecules in polymer matrix. The diffusion trajectories suggest that the molecules in first class move actively, but the molecules in class third class move limitedly and the movement mobility of molecules in second class is between that of first class and third class. The diffusion trajectories of small molecules strongly depend on the shape and molecular weight of migrant molecules, which is consistent with the diffusion coefficients.

Keywords: molecular dynamics simulation; diffusion coefficient; molecular weight; molecular shape

Introduction

Polyethylene terephthalate (PET) is a kind of excellent barrier material and has been widely used in food packaging engineering. A number of low-molecular-weight substances might migrate from the material into the food when PET packaging material contacts food. Diffusion coefficient is very important for migration models, which represents the migration rate and determines the process of migration dynamics. The experimental determination of the diffusion coefficient is very difficult. The literature has reported a series of sophisticated models for theoretical estimation of diffusion coefficients^[1-4], however for non-polyolefin polymers such as PET, it seems not as reliable.

A computer simulation technique based on classical mechanics provides a new way to study the diffusion process. Over the last twenty years the molecular dynamics (MD) simulation technique on the basis of classical molecular mechanics has been widely used for the investigation of diffusion of small molecules in polymers^[5-12]. Pavel and Shanks^[9] applied the MD simulation technique to study the diffusion of oxygen and carbon dioxide in bulk amorphous PET and related aromatic polyesters and focused on the influence of free volume, temperature and number of aromatic rings on diffusion coefficients. Hahn and Mooney^[10] investigated phenol diffusion in bisphenol-A-polycarbonate by means of MD simulation and obtained an approximate Arrhenius behavior for the diffusion coefficient. Li et al^[11] used MD simulation to calculate the diffusion coefficients of small molecules with molecular weights ranging from 16.04 (methane) to 452.50 (fluocinolone acetonide) Daltons in four amorphous polymers and compared with the experiments in literatures. These studies provided results which agree qualitatively with

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experimental observations and suggested that MD simulation technique may be useful in obtaining relative diffusion coefficient. It has been recognized that in general the larger molecular weight, the lower its diffusion coefficient.

Methodology

However, a precise understanding is lacking for the influence of changes in molecular structure, such as size and shape of molecules, on the diffusion coefficient. For example, at a given molecular weight, linear molecules would diffuse faster than others, spherical molecules being the slowest.

Using MD simulations technique, we decided to measure diffusion coefficients of molecules selected on the basis of their molecular structure and functional groups, including compounds up to molecular weight 339 g/mol. The object of this paper is to reveal the influence of molecular weight and shape of molecules on diffusion.

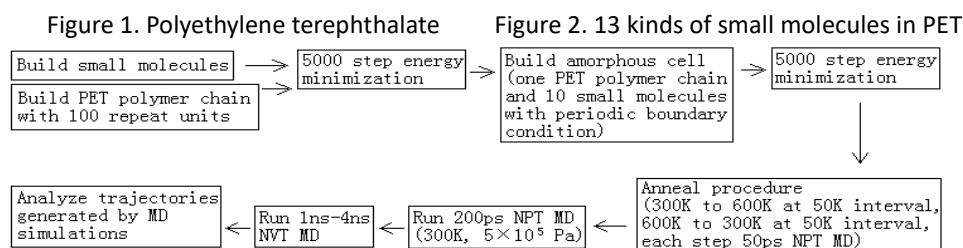
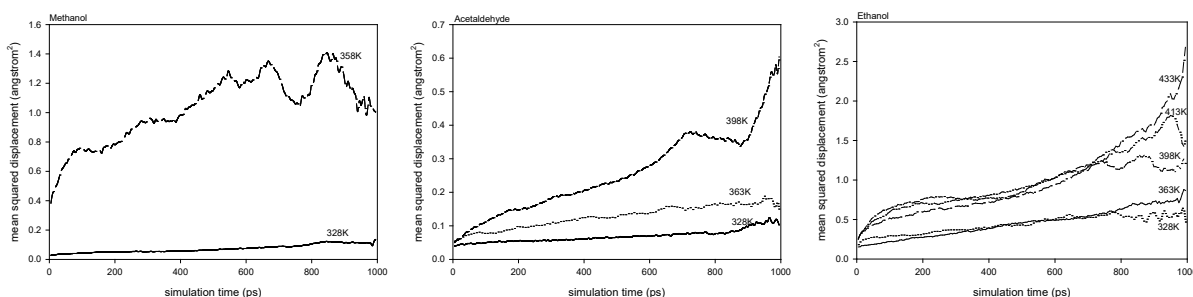


Figure 3. Schematic figure of MD simulation

The structure of PET is shown in Figure 1, and the structures of 13 kinds of small molecules with molecular weights ranging from 32 to 339 g.mol⁻¹ in PET are shown in Figure 2. The model building and simulation procedure are similar to the authors' previous studies^[13-15]. Here, the schematic figure of MD simulation is only given in Figure 3, and the details can refer to the references^[13-15]. When the final NVT (the number of molecules N , volume V and temperature T of the system are kept constant) MD simulation is completed, the atomic trajectory is recorded every 5 ps for the subsequent analysis.

Results

The mean-squared displacement (MSD) curves for long times are obtained by analyzing the atomic trajectories. MSD curves for 13 kinds of small molecules in PET at different temperatures are shown in Figure 4.



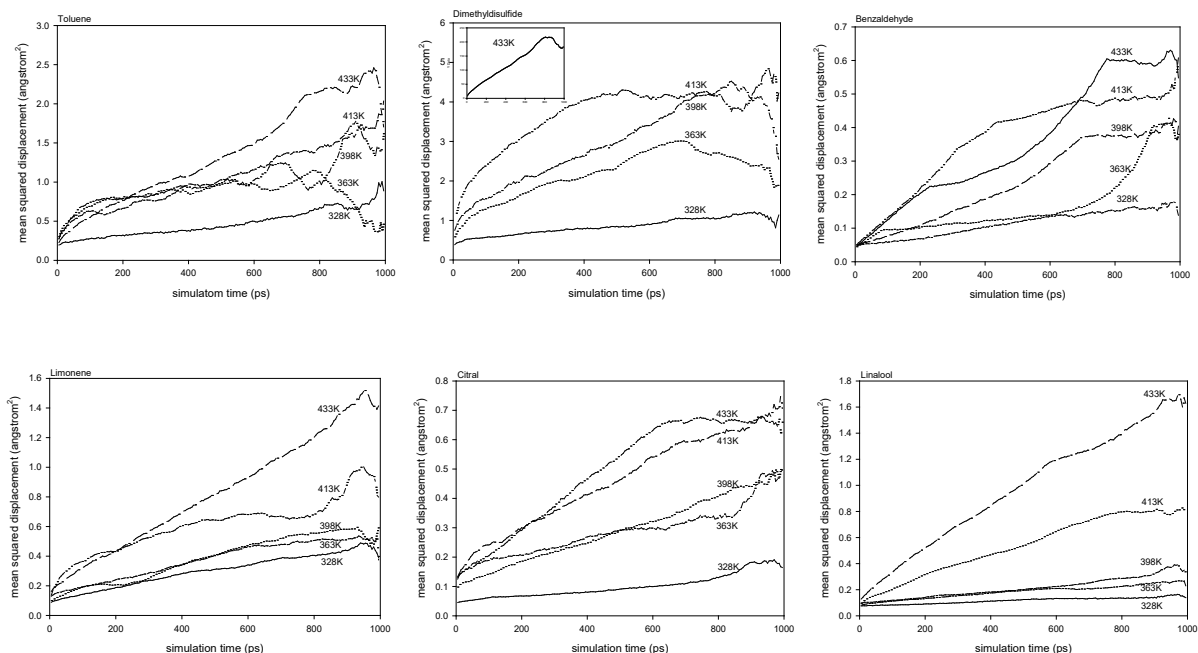


Figure 4 MSD curves for small molecules in PET at different temperatures

It can be observed from Figure 4 that the MSD curves for m-Xylene, limonene, linalool and tetracosane at five temperatures are almost linear, but for other molecules the curves are not satisfactorily linear. In order to obtain perfect linear MSD curves, longer simulation times are required. This may be results from the stronger interactions between the small molecules and the polymer matrix, such as hydrogen bond.

3.1 Diffusion Coefficients

The glass transition temperatures T_g of pure and amorphous PET are about 80°C and 65°C, respectively. Above T_g , polymer segmental motions occur, whereas below T_g , they are frozen. Diffusion of small molecules in a rubbery polymer can be safely calculated by employing MD simulation and invoking the Einstein relation. In this paper, simulation temperatures are all above the T_g of amorphous PET except for one temperature 328K. The diffusion coefficients of small molecules in PET are calculated from the slope of the linear fitting of MSD curves by Einstein relation. The simulated diffusion coefficients are listed in Table 1.



Table 1. Simulated diffusion coefficients (cm²/s) of 13 kinds of small molecules

Molecules	No	Molecular weight	328K	363K	398K	413K	433K
Methanol	1	32	1.33E-09	8.06E-09			
Acetaldehyde	2	44	7.32E-10	1.61E-09	6.02E-09		
Ethanol	3	46	5.89E-09	5.92E-09	1.07E-08	1.09E-08	1.57E-08
Toluene	4	92	1.52E-09	2.30E-09	2.32E-09	2.45E-09	7.31E-09
Dimethyl disulfide	5	94	1.15E-08	5.05E-08	6.57E-08	1.00E-07	4.06E-06
Benzaldehyde	6	106	1.01E-10	1.16E-10	1.07E-09	2.44E-09	3.88E-09
m-Xylene	7	106	2.59E-10	1.21E-09	3.19E-09	8.85E-09	6.41E-08
Ethyl-butylate	8	116	3.17E-09	5.01E-09	9.55E-09	1.03E-08	1.15E-08
Chloroform	9	119	7.83E-09	8.28E-09	3.78E-08	3.10E-08	6.37E-08
Limonene	10	136	4.17E-09	4.26E-09	4.39E-09	4.75E-09	2.19E-08
Chitral	11	152	1.58E-09	1.12E-09	3.53E-09	8.21E-09	9.06E-09
Linalool	12	154	1.31E-10	1.43E-10	1.48E-10	5.73E-10	8.95E-09
Tetracosane	13	339	2.52E-09	6.33E-09	1.07E-08	1.13E-08	1.66E-06

Reynier^[16-17] defined three different diffusion behaviors: (1) diffusion behavior is the same as that of linear alkanes with the same molecular weight; (2) diffusion behavior is lower than that of linear alkanes with the same molecular weight; (3) intermediate behavior. Molecules behaving as the first class diffusion behavior are linear or approximately linear molecules, the second class molecules are spherical molecules, and the third class molecules have both linear parts and spherical parts. Linear molecules diffuse faster than spherical molecules with the same molecular weight, which has been confirmed. According to the classification, 13 small molecules studied in this paper can be divided such that molecules 1, 2, 3, 5, 8 and 13 belong to the first class, molecules 4, 6, 7 and 9 the second class, and molecules 10, 11, 12 the third class. For molecules 1, 2 and 3, three linear molecules and smallest molecules in this paper, the diffusions are relative to their structures of linear molecules, and the diffusion coefficients by simulation are very close to their corresponding theoretical predictions and experimental values^[18]. The molecules 4 and 5, with almost similar molecular weight, have quite different diffusion coefficients and the diffusion of the molecule 5 is much faster than that of the molecule 4 because the molecule 5 is a linear one and the molecule 4 is a spherical one. The molecules 6 and 7 are observed to have almost the same diffusion coefficients, which is probably because they have the same molecular weight and similar shape (spherical molecule). This case also occurs among molecules 10, 11 and 12. The molecular 13, in spite of the largest molecular weight, doesn't show the smallest diffusion coefficient because it is linear alkane and diffuses faster.

3.2 Free Volume

Polymer matrix consists of the occupied volume and free volume. The volume which is not occupied by the matrix atoms is usually defined as "free volume". Free volume plays an important role in the diffusion behavior of small molecules in the polymers. The calculation of free volume adapts the Connolly surfaces methods. The Connolly surface is calculated when the probe molecule with the radius rolling over the Vander Waals surface, and the free volume is defined as the volume on the side of the Connolly surface without atoms. The morphology of free volume is shown in Figure 5.

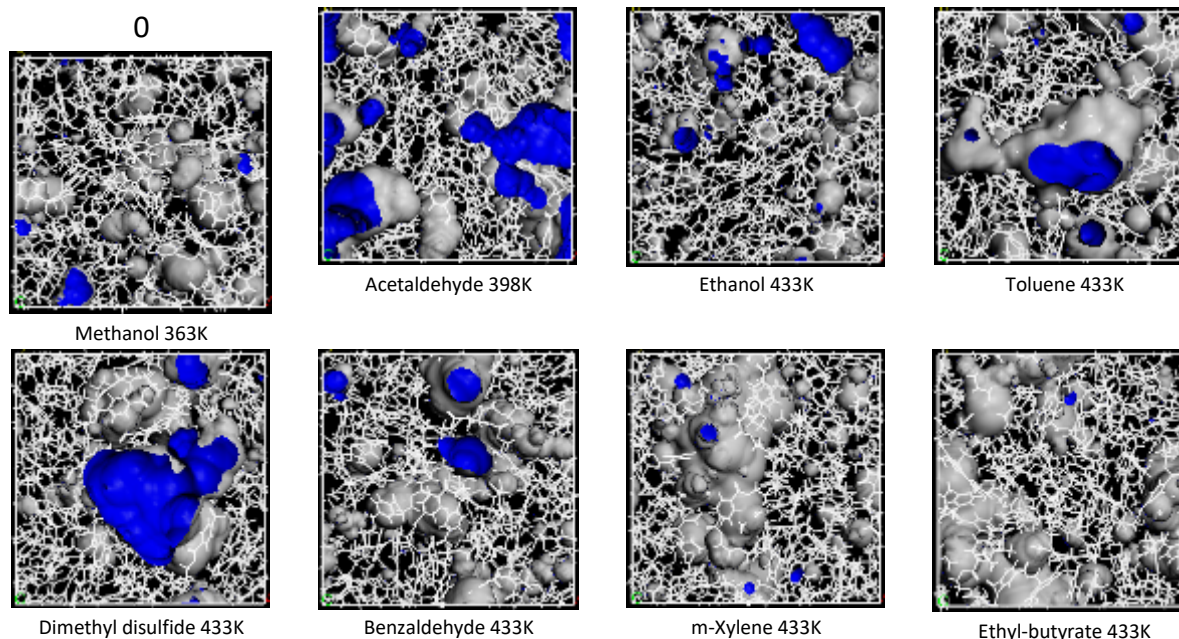


Figure 5. The simulated morphology of free volume: “blue” for high-energy surface and “gray” for low-energy surface of free volume (to reduce the size of the file, some pictures have been taken out)

Figure 6 Diffusion trajectories of migrant molecules in packing models during 1ns MD simulation

Discussion

The simulated morphology consists of many different shapes and size free volume cavities, and these free volume cavities are mutually connected. Some of them are connected to flaky area, such as Acetaldehyde, Toluene, Dimethyl disulfide, Limonene, Linalool. When small molecules move into the flaky free volume cavities, they tend to move forward rather than coming back and forth, which is available to diffuse from one cavity to another cavity of free volume. The movement of migrant molecules strongly depends on two aspects. One is the properties of free volume, such as the shapes, size, and amount of free volume. Another is temporary channels between adjacent cavities in the polymer matrix. The frequency of temporary channels forming is determined by the mobility of polymer segment. The channel changes faster when the segment moves faster. With the segment movement, some smaller cavities of free volume have more chance to conjoin one larger cavity enough to accommodate the migrant molecule. At the same time the migrant molecule uses temporary channels to diffuse from one cavity to another cavity.

Figure 6 shows the diffusion trajectories of migrant molecules during 1ns MD simulation. The diffusion trajectories of small molecules show the difference of species. The movement trajectories of molecules 1, 2, 3, 5, 8 and 13 distribute very widely, which suggests that the movements of these molecules in polymer are very vigorous. The movement trajectories of small molecules 4, 6, 7 and 9 overlap densely, which suggests that the movements of these molecules in polymer are not vigorous. The movement trajectories of molecules 10, 11, 12 are between those of the first class and the second class and have a wide range of distribution with some overlap. The diffusion trajectory strongly depends on the molecular shape and weight, which is consistent with the simulated diffusion coefficient.



Conclusion

The diffusion coefficients of 13 kinds of small molecules with molecular weights ranging from 32 to 339 g/mol in amorphous PET are calculated based on molecular dynamics simulation. The results suggest that diffusion coefficient of migrant depends not only its molecular weight but also its molecular shape. Connolly surface method is used to calculate free volume of polymer matrix. The results show that some small free volume cavities conjoin together and form the larger cavities which exactly accommodate migrant molecules. Thus, it facilitates the diffusion of migrant molecules in polymer matrix. The diffusion trajectories suggest that the molecules in first class move actively, but the molecules in third class move limitedly. The movement mobility of molecules in second class is between that of first class and third class. The diffusion trajectory of small molecules strongly depends on the shape and molecular weight, which is consistent with the simulated diffusion coefficient.

References

- [1] Limm W, Hollifield HC. Modeling of additive diffusion in polyolefins. Food additives and contaminants 1996; 13(8), pp. 949-967.
- [2] Piringer OG. Evaluation of plastics for food packaging. Food Additives and Contaminants 1994; 11(2), pp. 221-230.
- [3] Brandsch J, Mercea P, Ruter M, Tosa V, Piringer OG. Migration modeling as a tool for quality assurance of food packaging. Food Additives and Contaminants 2002; 19(Suppl.), pp. 29-41.
- [4] Helmorth E. Stochastic modeling of migration from polyolefins. Journal of the Science of Food and Agriculture 2005; 85(6), pp. 909-916.
- [5] Takeuchi H, Okazaki K. Molecular dynamics simulation of simple gas molecules in polymers. II. Effect of free volume distribution. Journal of chemical physics 1990; 93, pp. 9042-9048.
- [6] Gee RH, Boyd RH. Small penetrant diffusion in polybutadiene: a molecular dynamics simulation study. Polymer 1995; 36(7), pp. 1435-1440.
- [7] Hofmann D, Ulbrich J, Fritsch D, Paul D. Molecular modeling simulation of gas transport in amorphous polyimide and poly (amide imide) membrane materials. Polymer 1996; 37(21), pp. 4773-4785.
- [8] polyethylene terephthalate. Packaging Technology and Science 2010; 23, pp. 457-469
- [9] Reynier A, Dole P, Humbel S, Feigenbaum A. Diffusion coefficients of additives in polymers. I. Correlation with geometric parameters. Journal of Applied Polymer Science 2001; **82**, pp. 2422-2433.
- [10] Reynier A, Dole P, Feigenbaum A. Additive diffusion coefficients in polyolefins. II. Effect of swelling and temperature on the D=f(M) correlation. Journal of Applied Polymer Science 2001; **82**, pp. 2434-2443.
- [11] Begley TH, Castle L, Feigenbaum A, et al. Evaluation of migration models that might be used in support of regulations for food-contact plastics. Food Additives and Contaminants 2005; 22, pp. 73-90.

Acknowledgments:

The authors want to thank Reliable Packaging Research for their sponsorship of this research project.



IAPRI CONFERENCE POSTER RESEARCH PAPER GUIDE

Here's a **structured guide** for authors preparing a **4-page companion paper** that accompanies their **poster submission**. This short paper helps attendees understand the research project in greater depth than the poster alone can provide, while remaining concise and accessible.

Guide for Writing a 4-Page Paper to Accompany a Poster Presentation

Purpose of the Paper

This paper is not a full journal article. Instead, it is a structured summary of the work behind your poster that allows conference attendees (and later readers of the proceedings) to:

- Understand the project's context, goals, and methods.
- Review key findings in more detail than the poster allows.
- Identify applications, relevance, and next steps.
- Contact you or follow up for collaboration.

1. Paper Format

- **Length:** Maximum 4 pages (including figures, tables, and references).
- **Font & Spacing:** Calibri or similar, 11–12 pt, 1.15–1.5 spacing.
- **Margins:** Standard (2.5 cm or 1 inch on all sides).
- **Structure:** Organized with headings (see below).
- **Figures & Tables:** High quality, numbered, with captions.
- **References:** Keep concise, use consistent citation style (e.g., APA, IEEE, or conference standard).

2. Recommended Structure

A. Title and Authors

- Same as poster title.
- Full author names, affiliations, and contact email.

B. Abstract (150–200 words)

- A short, stand-alone summary.
- Include: purpose, methods, main results, and key implications for packaging research.
- Avoid jargon—aim for clarity.

C. Introduction (0.5–1 page)

- Define the problem or challenge in packaging research.
- Provide background and context.
- State the gap in knowledge or practice.
- End with **clear research objectives or questions**.

D. Methods / Experimental Approach (1 page)

- Describe **materials, procedures, and experimental setup**.
- Mention standards used (ASTM, ISO, TAPPI, etc.) where relevant.
- Include diagrams, flowcharts, or photos.
- Be concise—avoid excessive technical detail.

E. Results (1–1.5 pages)

- Present findings with clarity.
- Use graphs, tables, and images to communicate effectively.
- Highlight trends, differences, or significant outcomes.



- Include only data essential to support conclusions.

F. Discussion (0.5–1 page)

- Interpret results in relation to research objectives.
- Explain significance for packaging science and practice.
- Address limitations or unexpected findings.

G. Conclusions and Future Work (0.5 page)

- Summarize key insights in **3–4 bullet points**.
- Indicate practical implications (e.g., improved materials, reduced costs, environmental benefits).
- Outline next research steps or application pathways.

H. Acknowledgements Optional

- Credit funding sources, collaborating institutions, and special assistance.

I. References

- 6–10 concise citations of relevant standards, key papers, or prior research.

3. Style Guidelines

- **Write for clarity:** Assume your reader may not specialize in your exact field of packaging research.
- **Be concise:** 4 pages require prioritizing main findings.
- **Visual emphasis:** Figures and tables are preferred over long paragraphs.
- **Professional tone:** Academic but accessible to a mixed audience (academics, industry, government).

4. Checklist for Authors

- ✓ Title matches poster submission
- ✓ Abstract summarizes entire project
- ✓ Problem and objectives are clear
- ✓ Methods described logically and briefly
- ✓ Figures and tables included and explained
- ✓ Results tied directly to objectives
- ✓ Conclusions are evidence-based
- ✓ References formatted consistently

IAPRI CONFERENCE PAPER PUBLICATION

All accepted abstracts and general stream papers will be published, either in printed format or electronically, in an IAPRI handout and distributed to the attendees at the conference.

Peer Reviewed may be published by PTS in either an IAPRI issue or individually in regular issues. In addition, some papers may be considered for possible expansion into a peer review paper for publication by PTS. Authors may be required to sign a copyright transfer or license agreement.



IAPRI CONFERENCE REGISTRATION

At least one author of each accepted submission must register for the conference by the specified deadline. Registration fees and policies will be provided with the registration information. Authors are responsible for their own travel and accommodation expenses. If you do not register as a speaker by the deadline, your presentation may not be included in the conference program.

ETHICAL AND PROFESSIONAL STANDARDS

Authors submitting an abstract for consideration at the IAPRI Research Conference must review and initial below to indicate agreement.

Authors must initial the following Agreement Points for Abstract Submission when submitting your abstract.

1. Originality of Work

I confirm that the submitted abstract and proposed paper represent original work and have not been previously published or presented at another conference.

2. Accuracy of Submission

I verify that all information provided in the abstract (title, authors, affiliations, and content) is accurate and complete.

3. Authorship Responsibility

I confirm that all listed co-authors have reviewed the abstract and agree to be named as contributors.

4. Presentation Commitment

If the abstract is accepted, at least one author will register, attend, and present the paper (oral or poster) at the conference.

5. Format & Guidelines Compliance

I agree to prepare the full paper according to IAPRI's formatting and submission requirements within the specified deadlines.

6. Peer Review Process

I understand that the submission is subject to peer review or committee review, and acceptance decisions are final.

7. Proceedings & Publication Rights

I grant IAPRI the non-exclusive right to publish the abstract and accepted paper in the official conference proceedings.

8. Ethical Standards

I affirm that the work complies with accepted research ethics and contains no plagiarism, falsification, or misrepresentation.

9. Permissions & Copyright

I have obtained all necessary permissions for third-party content (e.g., figures, tables, images, or data) used in the submission.

10. Withdrawal Policy

I understand that if I must withdraw my submission, I must notify the conference organizers in writing before the stated deadline.



11. Conference Policies

I agree to abide by all conference policies, including deadlines, code of conduct, and registration/payment requirements.

ORAL PRESENTATION REQUIREMENTS

Accepted authors must present their work in person at the conference. Formats include:

- **Oral PowerPoint presentations:** 20 minutes in length with 5 minutes for Q & A. at the conclusion of the presentation. Sessions must end at 25 minutes to allow time for attendees to move to the next conference session.
- **Poster presentations:** Authors of accepted posters will have the opportunity of giving a short pitch of 3-4 minutes informing people of the poster during a dedicated session informing attendees about the study. They must be present at the poster during the dedicated poster sessions.

At least one author must be present to deliver the presentation.

ORAL PRESENTATION POWERPOINTS

- PowerPoint presentations are needed in **16:9 (widescreen) format**.
- Videos are to be embedded in your PowerPoint slide rather than acquired with external links.

Tips for Creating your PowerPoint Presentation

Body Text:

- Use a font that is easy to read. Arial, Verdana or Calibri tend to be the easiest to read on screens.
- Font should be no smaller than 18pt.
- Align text left. Centered text is harder to read.
- Write in point form, not complete sentences.
- Include 4-5 bullet points per slide.
- Avoid wordiness and clutter: A headline, a few bullet points, maybe an image – anything more than that and you risk losing your audience.

Headings:

- Heading font should be bigger than your body text.

Color:

- Put dark text on a white background. This is easiest to read. If you must use a dark background – for instance, if your institute/company uses a standard template with a dark background – make sure your text is quite light (white, cream, or light grey) and increase the font size.

Images, Charts and Diagrams:

- A chart, diagram or image can often convey much more to your audience than text.
- Don't use low resolutions images as these can appear blurry on the screen.

Slide Timing:

- Anticipate no more than 1-2 slides per minute for your presentation.

For more information about PowerPoint or sample PowerPoint templates please click [here](#).



POSTER DISPLAY INSTRUCTIONS

Poster Size and Orientation

- **Standard Size:** a 36"w × 48"h. or AO (841 mm x 1189 mm) hosts choice
- **Orientation:** Portrait.
- **Margins:** Leave at least ¼ inch margin around all edges to avoid trimming.

Recommended Poster Layout and Required Elements

Title Block

- Clear, concise, and descriptive (avoid excessive jargon).
- Include project focus (e.g., "*Biodegradable Barrier Films for Snack Food Packaging*").
- Font size: ~85–100 pt.

Authors, Affiliations & Conference

- Full names, institutional logos, and contact details (email for corresponding author).
- Presenting author's name underlined.
- Place conference name at top right or left.

Introduction / Background

- **Purpose:** Provide context and why the research matters to packaging science.
- **Content:**
 - Brief overview of the problem or gap in current packaging technology.
 - Relevance to industry, sustainability, or policy.
- **Objectives / Research Questions**
 - Clearly state 1–3 specific objectives.
 - Avoid vague terms—focus on measurable outcomes.
- **Tips:**
 - Use bullet points for clarity.
 - Include 1–2 background images or diagrams.

Methods / Experimental Approach

- Flowcharts, process diagrams, or schematic packaging prototypes work well.
- Include:
 - Materials used (film types, adhesives, machinery).
 - Testing standards followed (e.g., ISTA, ASTM, ISO).
 - Experimental design and variables measured.
- Keep text minimal—use visuals wherever possible.

Results

- Presented in **tables, graphs, or high-resolution images**.
- Highlight:
 - Key quantitative findings.
 - Statistical significance if applicable.
- Use consistent colors and units.

Conclusions

- 3–4 bullet points summarizing the main takeaways.
- State potential applications in packaging industries.
- Mention limitations briefly.



Recommendations, References, & Acknowledgements

- Indicate ongoing experiments, technology scaling, or next research steps.
- Only cite key sources (e.g., standards, foundational studies).
- Funding bodies, collaborators, facilities used
- Use smaller font (20–24 pt).

Visual & Design Guidelines

- **Fonts:**
 - Titles: Arial, Calibri, Helvetica) in large size (85–100 pt).
 - Body text: 24–32 pt, easily readable at 3' distance.
- **Color Scheme:**
 - Limit to 2–3 main colors.
 - High contrast between background and text.
- **Images:**
 - Minimum resolution: 300 dpi.
 - Use diagrams instead of long text descriptions.
- **Flow:**
 - Organize as shown in the Research Poster Template.

3-MINUTE ORAL POSTER PITCH INSTRUCTIONS

- All presentations must be created using Microsoft PowerPoint.
- IAPRI has a Poster Pitch template you can obtain here: [Poster Pitch Template 2026.pptx](#)
 - It is a Google Doc that must be saved as a MS PowerPoint to edit.
- We request that all presentations (i.e. PowerPoint presentation) be emailed to (Email to Be Determined) by (Date to Be Determined). A reminder email will be sent to you closer to the due date.

IMPORTANT SPEAKER DATES

- Speaker Registration Due (acceptance on the program): (Date to Be Determined)
- Speaker Headshot Image Due (Website/App): (Date to Be Determined)
- PowerPoint Presentations Due (widescreen format 16:9): (Date to Be Determined)
- 3 -4 minute Oral Posters Presentations Due: (Date to Be Determined)
- Posters Installed: (Date to Be Determined)