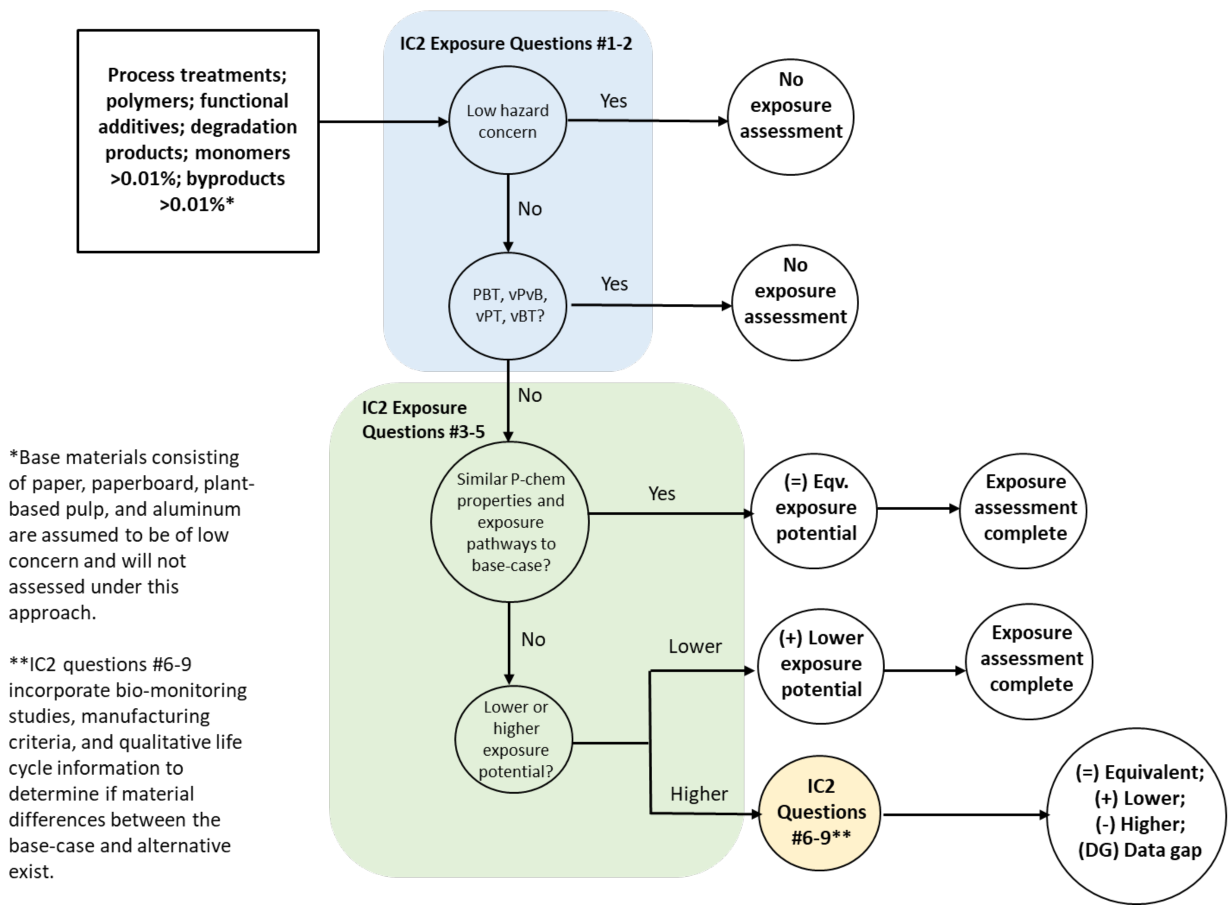
Washington State PFAS in Food Packaging AA – Exposure Assessment Approach & Decision Rules (3-18-2020)

1. Tiered Approach to Comparative Exposure Assessment

The exposure assessment approach for this AA will follow the IC2 Guidelines for a Level 1 Basic Comparative Exposure Assessment (*herein IC2 Guide*), which is a qualitative, property-based approach to characterizing exposure. This approach meets the U.S. National Academy of Sciences (NAS) "Path B" recommendations for comparative exposure assessment. Our approach also incorporates elements of EPA's The Sustainable Futures Interpretative Assistance Document for Assessment of Polymers (2013) (*herein SF Polymer Criteria*) and the Health and Environmental Sciences Institute's (HESI) Sustainable Chemical Alternatives Technical Committee's qualitative comparative approach (*herein HESI Exposure Guidance*) (Greggs W et al. 2018).

The IC2 Guide organizes the Basic Comparative Exposure Assessment via a series of questions that will be addressed and documented. The questions assess readily available data to identify whether material differences exist between the chemical of concern and potential alternatives. If the properties and potential pathways are similar, additional evaluation is not necessary and the decision rules are applied. If there are material differences, then additional evaluation will be conducted by addressing questions related to biomonitoring data, manufacturing criteria, or lifecycle information. Figure 1 provides an illustration of this approach and how the decision rules are incorporated.

IC2 Basic Comparative Exposure Approach for PFAS in Food Packaging AA



2. IC2 Level 1 Exposure Assessment Methodology

- **Question #1:**
  1. Has the alternative been evaluated for hazard and determined to be of low concern (e.g. GS Benchmark 3 or 4)?
  - The exposure assessment will be applied to the candidate alternatives (process treatments only), polymers, functional additives, degradation products, and monomers and byproducts present at >0.01% that have been fully screened by the Level 2 Hazard Assessment and deemed to be of moderate concern.
  - Substances that are concluded to be of low concern under the Tiered Approach to Hazard Assessment will not undergo a comparative exposure assessment.
  - Base materials consisting of paper, paperboard, plant-based pulp, and aluminum are assumed to be of low concern and will not be assessed under this approach.

- **Question #2:**
  2. Does the alternative have persistence, bioaccumulative, and/or toxic properties of concern?
  - Highly persistent and/or highly bioaccumulative and/or toxic alternatives (vPvB, vPT, vBT, PBT) will be removed from consideration and will not undergo exposure assessment.

- **Question #3:**
  3. Are the chemical properties for the chemical of concern and alternative materially similar? Or do material differences exist?
  - Pertinent properties will be assessed and evaluated using the endpoint criteria in the IC2 Guide with some additional endpoints supplemented by the **HESI Exposure Guidance**, summarized in Table 1.

Table 1. IC2 Level 1 & and HESI Exposure Related Properties

Property	Reason	Guidelines (NAS, 2014)
Volatility/ vapor pressure	Volatility/vapor pressure influence how likely the chemical is to be found in the air or how likely it is to enter the body	>10-8 mmHg; considered likely to found in the air. > 10-4 mmHg; considered to be more likely to enter the body.
Molecular weight	Generally, as molecular weight and size increase, bioavailability decreases (leading to a lower toxicity potential)	>1,000 amu is less likely to be bioavailable
Solubility in water	Generally, a chemical that is highly soluble in water will have more bioavailability and toxicity. In addition, water soluble chemicals are more likely to be found water bodies and precipitation.	<1 ppb generally have lower water solubility
Log Kow	The log of the water-octanol coefficient (Log Kow), is an indicator of potential for bioaccumulation, as well as bioavailability.	<5 for mammals <4 for aquatic species

Boiling point	The boiling point helps to determine if the chemical will be a liquid or gas at a certain temperature.	<25 C will be a gas at room temperature
Melting point	The melting point will determine if the chemical will be a solid or liquid at a certain temperature.	<25 C will be a liquid at room temperature
Density/ specific gravity	Has implications for where the chemical might partition when with other liquids or gases.	
pH	A measure of free hydrogen. Has implication for water solubility and potential damage to cells.	For certain products, a pH of >2 and <11.5 is safest for eyes and skin (Safer Choice 2015)
Corrosivity	Associated with the ability to gradually destroy materials by chemical reaction.	GHS criteria used to determine level of concern. Typically, the more extreme the pH (either high or low), the more likelihood of corrosivity issues whether it be to the eye, skin, respiratory system, etc. Typical pH values used are approximately below 3 and above 10. Review GHS criteria for more details.
Environmental Partitioning	A measure of how easily molecules or salts will break apart in under certain conditions (primarily in solution)	The higher the constant (Kd), the more likely the molecules or salts will break apart.
Use characteristics (binding properties) or synergistic effects	Other properties that can help determine the state of the chemical in the environment and biological compartments or interactions with other chemicals found in the environment.	The acid dissociation constant (pKa) is used to help identify availability of chemicals to bind to one another. pKas of concern typically range between < 3 (acid) and > 11 (bases). Synergistic effects identify how other chemicals may impact availability of the chemical of concern. For example, dimethyl sulfoxide (DMSO) easily enters skin. Chemicals dissolved in DMSO can be more biologically available than chemicals dissolved in other solvents.
Property	**Reason**	**HESI Exposure Guidance**
Particle size	Addresses inhalation exposure related to particulates.	Likely to penetrate the alveolar region <10 µm; Likely to enter the nose or mouth and penetrate the tracheo-alveolar region ≥10 and ≤100 µm; Not likely to be inhaled >100 µm Inhalable fraction (in mg/kg) - Firm granules, flakes, or pellets: ≤100; Granules, flakes, or pellets: 100–500; Course dust: 501–2000; Fine dust: >2000–5000; Extremely fine and light powder: >5000
Volatility (Henry's Law Constant)	Henry's Law Constant is used to estimate the potential to volatilize from water surfaces.	Very volatile from water: $>10^{-1}$; Volatile from water: 10^{-1} to 10^{-3}; Moderately volatile: 10^{-3} to 10^{-5};

		Slightly volatile: 10^{-5} to 10^{-5}; Nonvolatile: $<10^{-7}$
$LogK_{oc}$	Addresses the potential to migrate in soil which could lead to groundwater contamination.	Very strong sorption, negligible migration: >4.5; Strong sorption, negligible to slow migration: 3.5–4.4; Moderate sorption, slow migration: 2.5–3.4; Low sorption, moderate migration: 1.5–2.4; Negligible sorption, rapid migration: <1.5
Bioaccumulation	Considers the potential for the target chemical to accumulate in organisms.	BCF/LogBCF or BAF/LogBAF: Very high: >5000 (>3.7); High: 5000 to 1000 (3.7 to 3); Moderate: <1000 to 100 (<3 to 2); Low: <100 (<2)
Persistence	Addresses the potential for the target chemical to persist in environmental media.	Half-life in days: Very high: >180 (air: >2); High: 60–180; Moderate: <60 to ≥16; Low: <16 or pass ready biodegradability test not including the 10-d window; Very low: pass biodegradability test with 10-d window
Property	**Reason**	**Approach**
Other	Ecology will evaluate any other available, or relevant data that could inform the potential for exposure.	Where applicable, Ecology will apply established criteria from authoritative sources such as GHS or approaches applied in previous Ecology assessments. Professional judgment may be applied and will be accompanied by adequate justification.

Polymers with low molecular weight (MW <1000; SF Category 1) are expected to be bioavailable and will be evaluated using the same methods and approaches as for discrete substances, including the evaluation of any experimental physical property data or reliable estimation methods (read across, QSAR models, etc). The Sustainable Futures Interpretative Assistance Document for Assessment of Polymers (2013) (*herein SF Polymer Criteria*) will be used to address the special considerations associated with evaluating polymers with high MW (MW >1000; SF Category 2 & 3). Many of these substances are of variable composition and lack adequate data sets, making it difficult to evaluate their physicochemical properties. Various approaches for assessing physical/chemical properties are summarized in the SF Polymer Criteria. In cases where the data set for an endpoint contains limited or conflicting data, a weight of evidence (WoE) approach may be used. Endpoint characterizations based on WoE will be supported by adequate justification.

- **Question #4:**
  4. *Compare exposure pathways between the chemical of concern and the alternative(s). [Are there material differences?]*
     - This question addresses the potential for ingestion, inhalation, and dermal exposures related to the use and disposal of the chemical of concern and the candidate alternatives.

- The comparison will encompass any relevant media and biota related to human and environmental exposures.

3. Comparative Exposure Decision Rules

- **Question #5:**

5. *Are there substantive differences between the chemical of concern and the possible alternatives that are likely to increase exposure concerns for the any of the alternatives?*
    - After populating the assessment template (Appendix 1), the overall comparison of the proposed alternative to the chemical of concern will be conducted and the decision rules in Table 2 will be applied.
    - Rationale for the relevance parameters, the key parameters driving the conclusion, uncertainties and data gaps will be written in a brief discussion.

Table 2. Decision Rules for IC2 Comparative Exposure Assessment

Exposure Determination	Score[1]	Assessment Complete?
The potential exposure is likely to be equivalent to the chemical of concern	=	Yes
The potential exposure of the alternative is likely to be lower than the chemical of concern	+	Yes
The potential exposure of the alternative is likely to be higher than the chemical of concern	-	No, proceed to Question #6
Data Gap[2]	DG	Yes

1. Based on the example template IC2 Guide pg 112
2. Only applied if initial comparison suggests higher exposure potential and there are insufficient data to address questions 6-9

- **Questions #6-9** of the IC2 Guide will be addressed if initial comparison suggests the alternative has higher exposure potential. These questions aim to clarify and confirm whether a higher exposure concern is justified. Should the assessment proceed to this level, the IC2 Guidance will be followed exactly. All conclusions will be justified with adequate documentation.
    - **Question #6** requires the identification of any available bio- or environmental monitoring studies.
    - **Question #7** considers manufacturing criteria to evaluate exposure concern
    - **Question #8** considers qualitative life cycle aspects to evaluate exposure concern
    - **Question #9** considers whether there are sufficient data to evaluate exposure or if exposure should be considered a critical data gap.

Comparative exposure outcomes will be generated for the process treatment or polymer as well as functional additives; degradation products; residual monomers >0.01%; and byproducts >0.01%

IC2 Comparative Exposure Outcomes for PFAS in Food Packaging AA

Comparative Exposure Outcomes
Process Treatments or Polymers*; Functional additives; degradation products; monomers >0.01%; byproducts >0.01%
= : Equivalent exposure potential
+ : Lower exposure potential
- : Higher exposure potential

* Active ingredient that is contributing oil and grease repellency to the product.

4. Data Needs (For Stakeholders)

SRC will work with stakeholders interested in sharing relevant exposure data that can be incorporated in this assessment. In general, data needs for characterizing exposure includes:

1. Ingredient physical chemistry properties, as identified in Table 1
    a. OR, substance identification or details that support adequate estimation of physical-chemical properties using QSAR's models
2. Unpublished studies on disposal considerations or environmental fate pathways
3. If additional evaluations are needed to address Questions #6-9, information related to
    a. bio- or environmental monitoring
    b. manufacturing criteria
    c. lifecycle

References:

A Framework to guide Selection of Chemical Alternatives, National Resource Council of the National Academy of Sciences, 2014, 280 pages.

Greggs W. et al. 2018. Qualitative approach to comparative exposure in alternatives assessment. Integrated Environmental Assessment and Management. *IEAM* June 8, 2018. Available at: https://setac.onlinelibrary.wiley.com/doi/full/10.1002/ieam.4070

Appendix 1 – Template for the qualitative exposure assessment*

	Property	Positive	Minus	Equal	Not enough data
Compare physicochemical properties between the chemical of concern and alternative.					
Brief summary comparing the properties between the chemical of concern and candidate alternative	Volatility/ vapor pressure				
	Molecular weight				
	Solubility in water				
	Log Kow				
	Boiling point				
	Melting point				
	Density/ specific gravity				
	pH				
	Corrosivity				
	Environmental Partitioning				
	Use characteristics (binding properties) or synergistic effects				
Consider other inherent chemical properties of the alternative relevant to exposure.					
Brief summary comparing the properties between the chemical of concern and candidate alternative	Particle size				
	Volatility (Henry's Law Constant)				
	$LogK_{oc}$				
	Other relevant data such as sewage treatment plant removal				
	Bioaccumulation				
	Persistence				
Compare human exposure pathways between the chemical of concern and alternative.					
Brief summary comparing the exposure pathways between the chemical of concern and candidate alternative	Ingestion				
	Inhalation				
	Dermal				
Compare ecological exposure pathways between the chemical of concern and alternative.					
Brief summary comparing the exposure pathways between the chemical of concern and candidate alternative	Terrestrial media				
	Terrestrial biota				
	Aquatic media				
	Aquatic biota				
	Atmospheric media				
	Disposal/End of life				
Has the alternative been found in bio or environmental monitoring studies? [If required]		Yes	No	NA	NA
Compare the manufacturing criteria for the chemical of concern and alternative. *[If required]*					
	Manufacturing process				
Compare the product life cycle on a qualitative basis. *[If required]*					
	Manufacture				
	Transportation/storage				
	Use				
	End-of-life				
	Other				
Conclusion: Are there material differences between the chemical of concern and the candidate alternative?					
Brief summary of findings					

*Based on IC2 Guide pg 112