1. How good do models have to be?

Initially the regulator needs to know if there is a possible health risk as assessed by a screening model using worst case assumptions (e.g. no metabolism in the plant and all pollutant ultimately available for plant uptake). If a potential health risk is indicated, then site specific data can be collected and input into the model to refine the worst case assumptions. This approach is believed to be preferable to going to a more complex model, for which the parameters and processes may not have been validated. (This will be a single chemical approach).

- Two orders of magnitude useful
- One order of magnitude target
- High uncertainty in some processes my have little impact on endpoint (tiered approach)
- Over-estimation more desirable than under-estimation

Modelling approach

- The modelling approach needs to address the whole suite of potential pollutants. Transport to plant components would be related to physico-chemical properties e.g. non ionised compounds of log Kow <0 and weak acids are likely to undergo phloem transport to sink tissues e.g. fruits and tubers. All compounds with log Kow upto 4 would undergo xylem transport i.e. transfer from root to shoot. Where the chemical's log Kow > 4, soil adhesion to the plant and partitioning into the roots will be the dominant processes. Ensure categories are identical to matrix below
- Further experiments maybe required on some ionisable chemicals e.g. PFOS a strong acid.

2. Modelling approach

- Uptake processes are dynamic, but steady state solution maybe reasonable.
- Desorption from soil not thought to be a rate limiting step where steady state conditions have been achieved. Assume desorption in equilibrium, ignore processes such as hysterisis. More complex model may include such processes, but would we would need data to include this. Likely to have more impact in compunds log Kow > 4.
- Chromatography in stem occurs but does not require extra modelling.
- Favour developing one core model. Transport should not vary too much between crops, metabolism may however.
- Model construction and screening approach shown below.

The Matrix Solution

Pathways vs. Chemicals

Pathway/ Process	Root Uptake (external adsorption only)	Translocation in xylem to roots and leaves	Translocation in xylem to fruit	Translocation in phloem	Soil particle adhesion	Soil vapour via atmosphere to leaf
Relevant Phys/Chem Property Range	3 < log Kow < 5	Log Kow <3.5	Log Kow <3.5	Log Kow <0	Log Kow >3	5 < log Koa < 8 (guess) Henry's Law constant $>10^{-3}$
Relevant Chemical Charge State	Neutral and positively charged compounds	Neutral compounds and weak acids/bases in their neutral form	Neutral and charged compounds	Neutral and weak acids, including metabolites of root absorbed compounds (weak acids and glycosylated compounds)	Neutral and positively charged compounds	Neutral compounds.

The Matrix Solution

Crops & Modeling

Pathway/ Process	Root Uptake	Translocation in xylem to roots / leaves	Translocation in xylem to fruit	Translocation in phloem	Soil particle adhesion*	Soil vapour via air to leaf
Relevant Crop Type	Root veg. Tuber	Fruit Leafy vegetables Root veg.	Fruit	Tubers (for metabolites) Fruit	Roots Tubers Low growing fruits Leafy veg.	Leafy veg. Canopy specific, eg. ‘plastic agriculture’.
Recommended Modeling Approach	Diffusion-limited partitioning taking into account physico-chemical properties of root, chemical	Root uptake followed by mass flow in xylem with steady state partitioning to other plant parts.	Mass flow in xylem with partitioning in stem, with sink term at end of transport pathway (fruit). Loss from fruit.	Mass flow (e.g. ~0.01x xylem flow. dry weight mass balance) Metabolism, rate of entry into phloem, transport through phloem.	Empirical factors for soil mass loading, if possible crop specific (1% of dry weight assumed)	Soil air conc, dilution factor, diffusion from air to leaf (resistance model)
Estimated Uncertainty	1 oom	2 oom	2 oom	3 oom	1 oom	2 oom

Footnote

- Background/atmospheric deposition may have large impact and increase levels beyond guidance value. Soil value alone doesn’t provide this information. Direct deposition would need to be included in a model.
- Growth dilution effect will be Kow dependent, as consequence of low mass flow from soil for compounds with log Kow > 4.
- Processed cereals although large part of diet undergo lots of processing and dilution so data may not be necessary.
- Possible exception zucchini. Observed to accumulate some POPs.

3. Metabolism

- Many metabolites sequestered, but some also mobile within the plant.
- Many metabolites (e.g. glycosylated) less toxic, probably can be ignored in first tier risk assessment
- Metabolic rates can be highly species specific
- First (coarse) cut may be to estimate from human/mammal metabolism data
- Need for models that describe metabolite formation and accumulation in plants, test relevance with existing data
- Exclusion of metabolism may be conservative. This assumes metabolites less toxic, true in the majority of cases.
- Where data is available a metabolic rate could be included.

4. Data variability

- Need clear definitions of parameters used in models.
- Guidelines required for data used in the validation and calibration of models, eg. TSCFs. This will require plant and chemical specialists.
- Field validation – targetted measurements necessary (e.g. soil pore water), but only after establishing key processes to be captured in models.