

# Modelling the Fate of Per- and Polyfluoroalkyl Substances in the North- and Baltic Sea

## Emission and Transport

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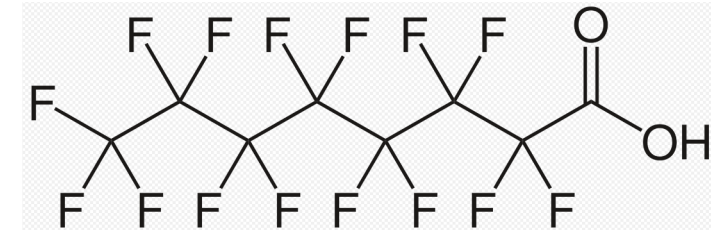
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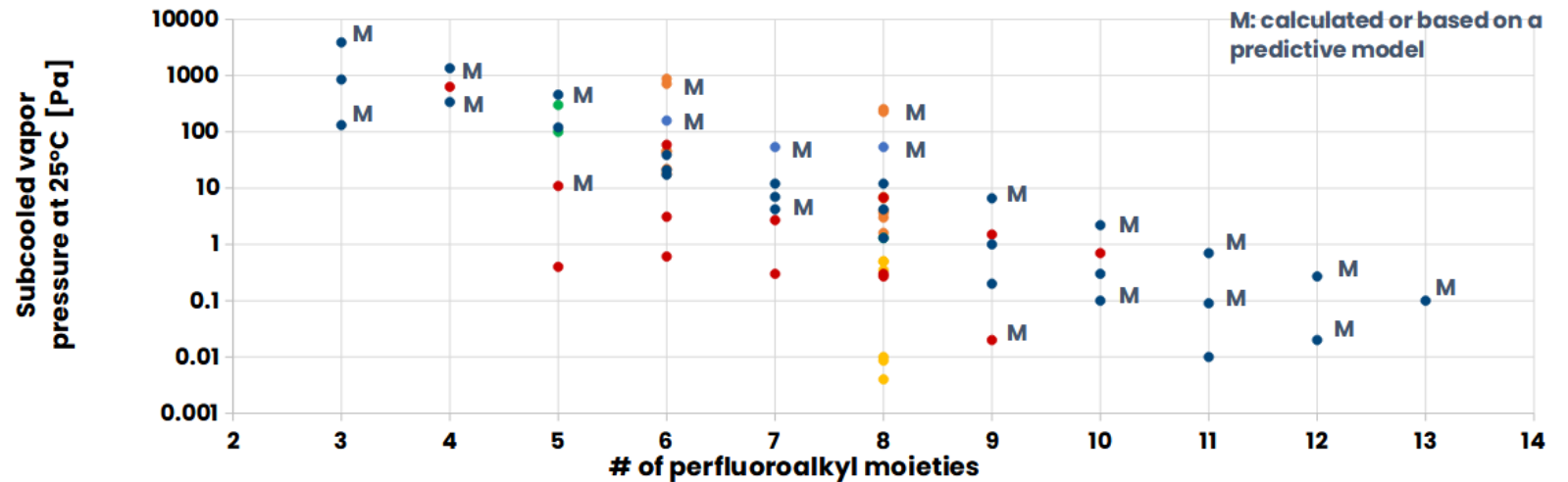
# Per- and Polyfluorinated Alkyl Substances (PFAS)

- **Over 4700** different substances
- **Applications**  
repellents, coatings, flame retardants heat transfer fluids, etc.
- **Persistent, bioaccumulative, toxic**
- **Adverse health effects** (include but are not limited to)  
infertility, complications during pregnancy and birth, liver damage, kidney and testicular cancer, immune suppressing, thyroid damage
- **Uncertainty**  
of physical properties complicates transport modeling and risk assessment

## PFOA



## Perfluorooctanoic acid

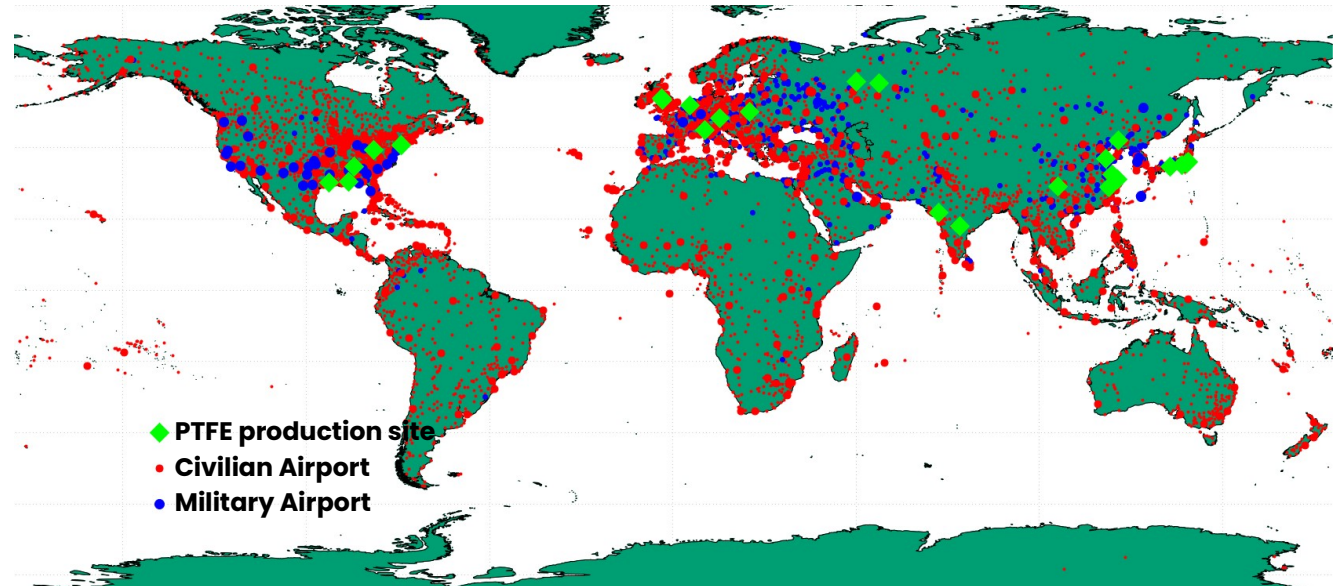
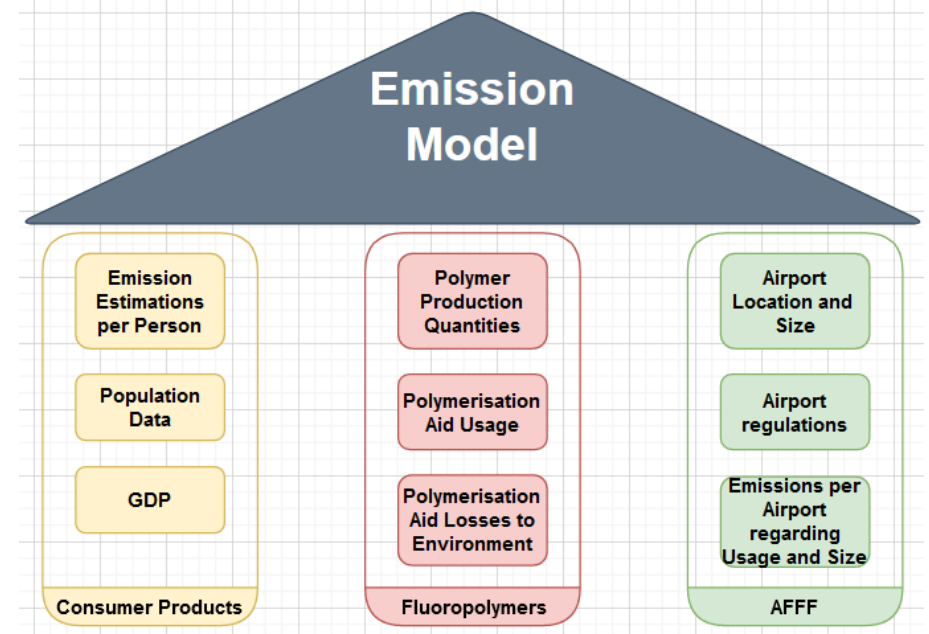


# PFOA / PFOS Emission Inventory “POPE”

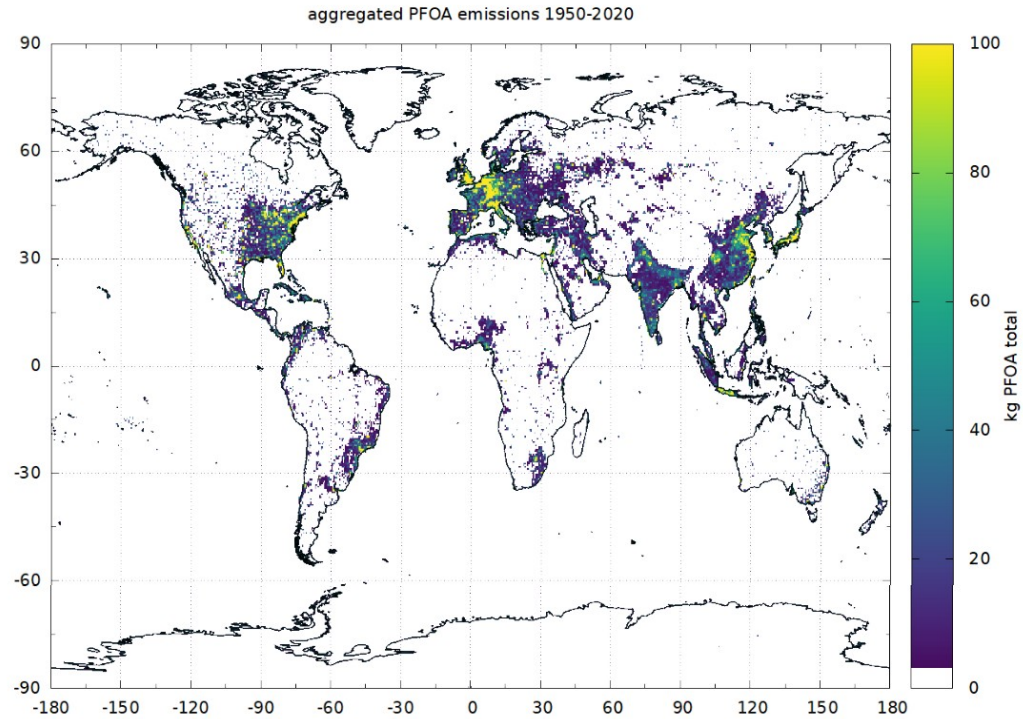
- Global, Gridded, 0.5° x 0.5° resolution
- Annual
- Covers the time span 1951-2020
- Includes the emissions to water and air by:
  - fluoropolymer production
  - aqueous film forming foams
  - PFOA / PFOS containing products
- In agreement with known global Inventories (Wang et al. 2014, Prevedourous et al. 2006...)



**“POPE” is available for Download  
at the ECCAD database**  
[www.eccad3.sedoo.fr](http://www.eccad3.sedoo.fr)

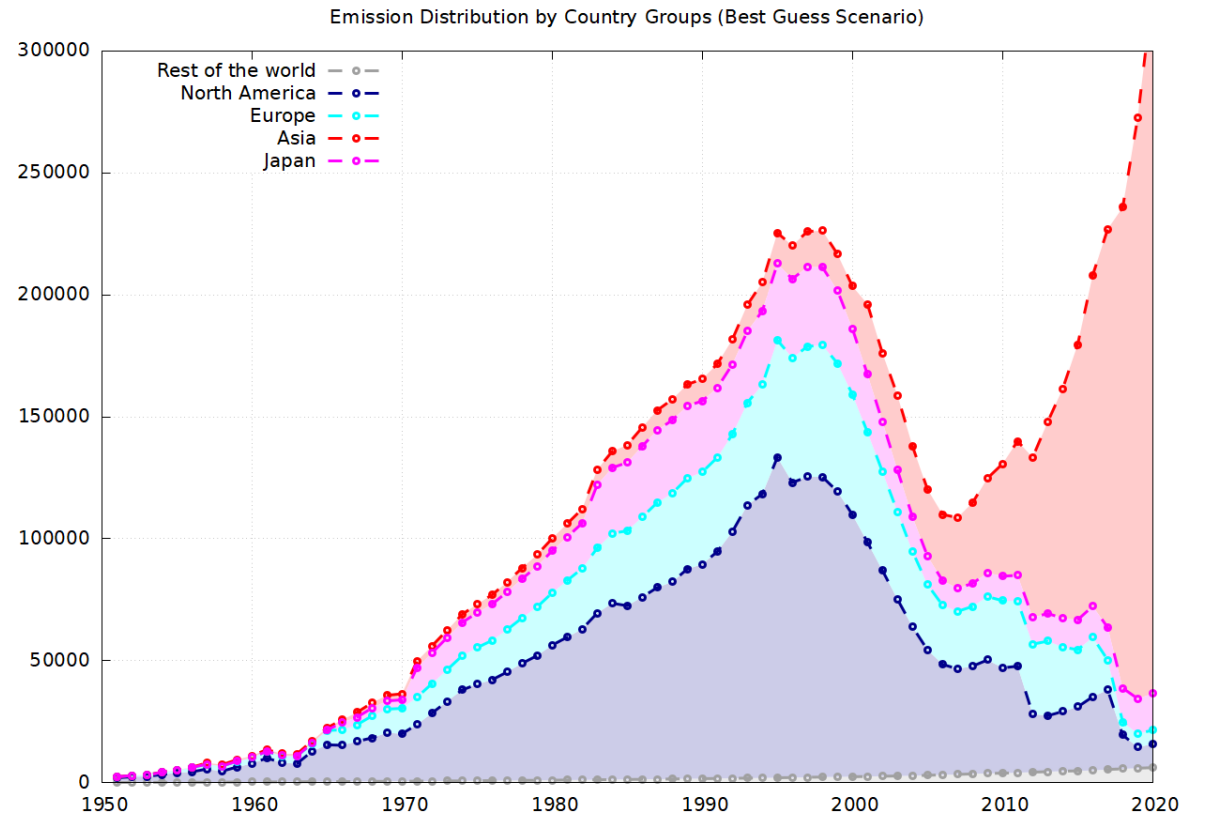


# Total emissions worldwide



**“POPE” is available for Download  
at the ECCAD database**

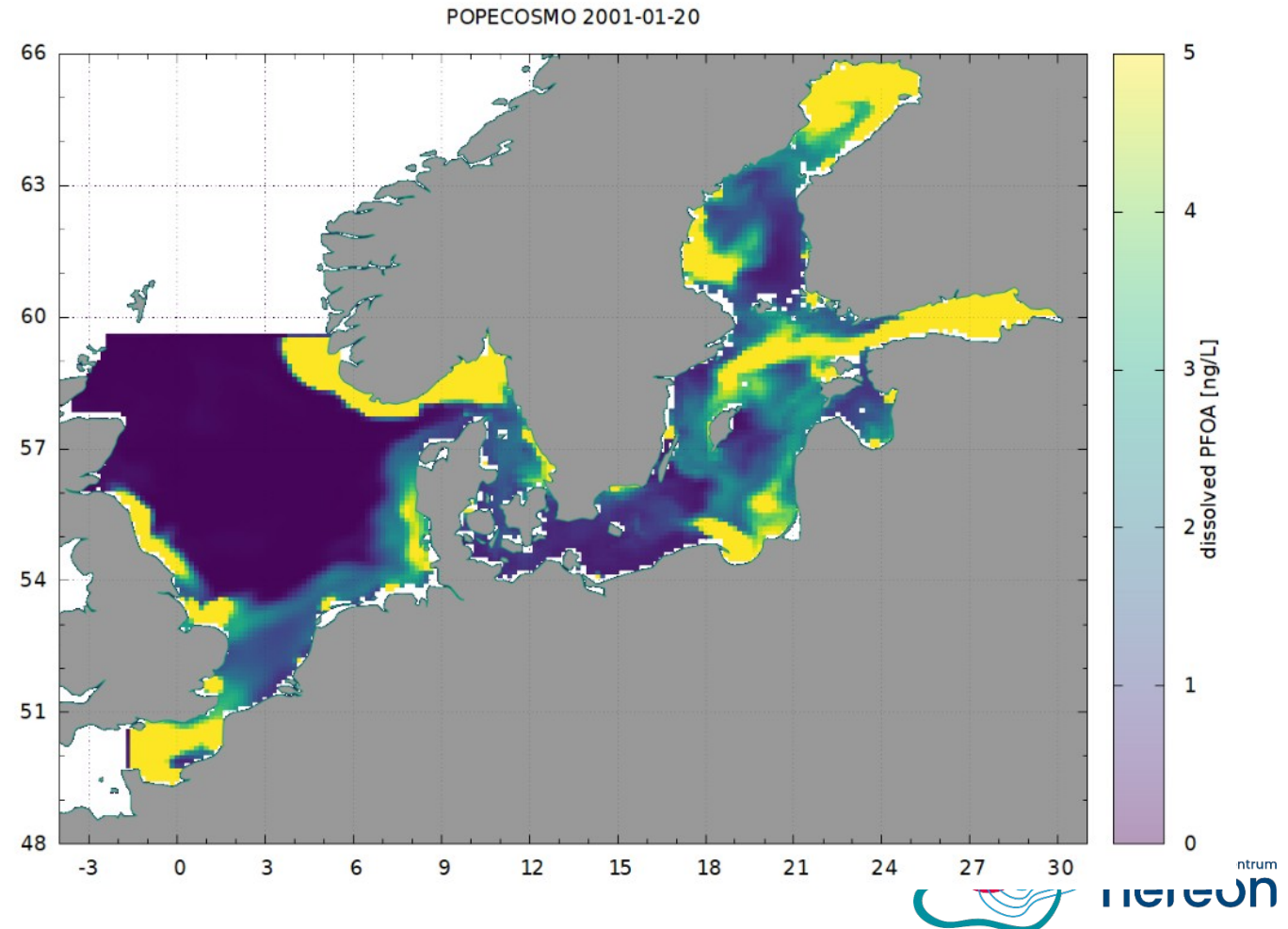
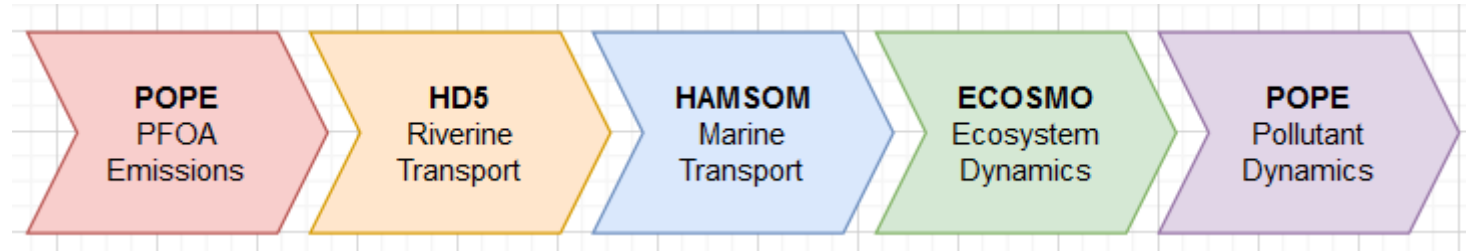
[www.eccad3.sedoo.fr](http://www.eccad3.sedoo.fr)



# Transport model POPE

- Domain: North- and Baltic Sea
- Resolution:  $6' \times 10'$  ( $\sim 10$  km)

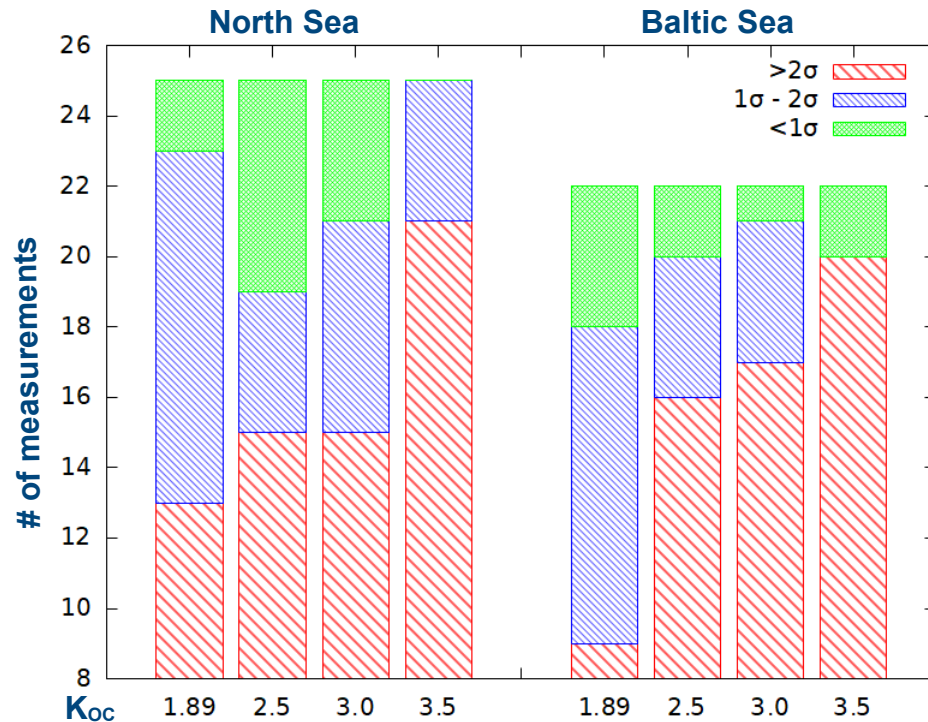
- **Sources:**
  - Rivers
  - Air-sea-exchange
  - **Remineralization**
- **Sinks:**
  - Photolytic Degradation
  - Losses to Atlantic and Arctic Ocean
  - **Sedimentation**



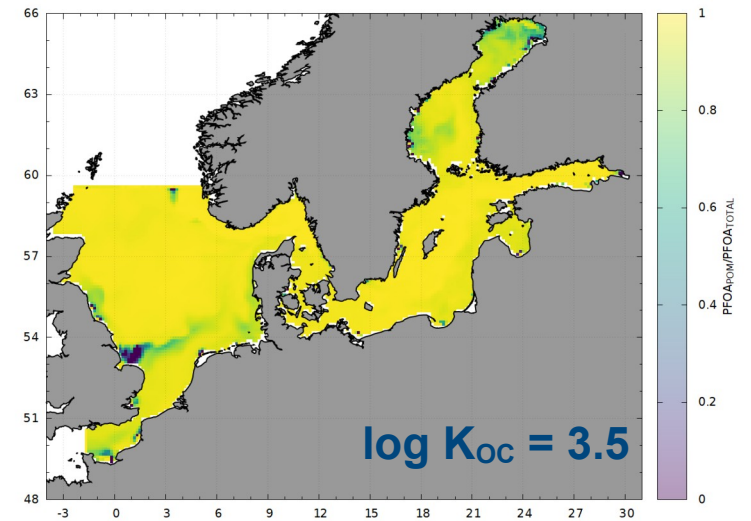
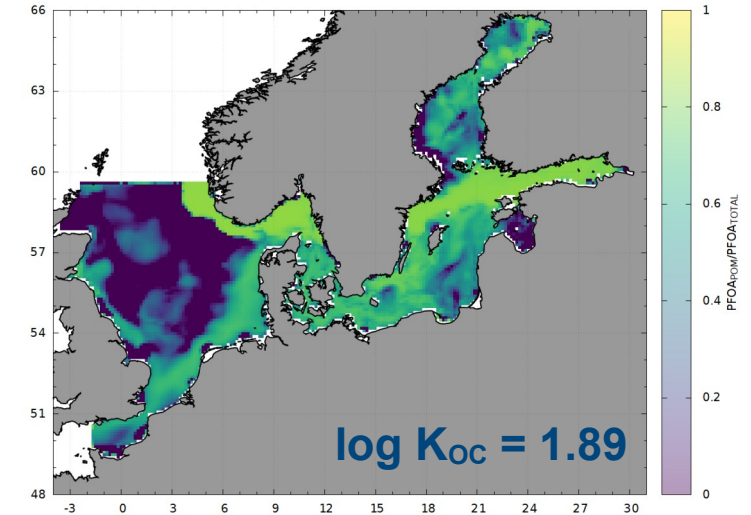


# Narrowing the range of uncertainty for Physico-chemical properties

- Backwards comparison of model results to measurements for different parameters yields estimation of plausible parameter space
- Example:**  $K_{OC}$  of PFOA
  - typical  $\log K_{OC} = 1.89 - 3.5$  (Higgins, Luthy, Ahrens, Guelfo, Milinovic)



Measurements from Theobald et al. 2011, Nguyen et al. 2017 and Möller et al. 2010



# Thank you

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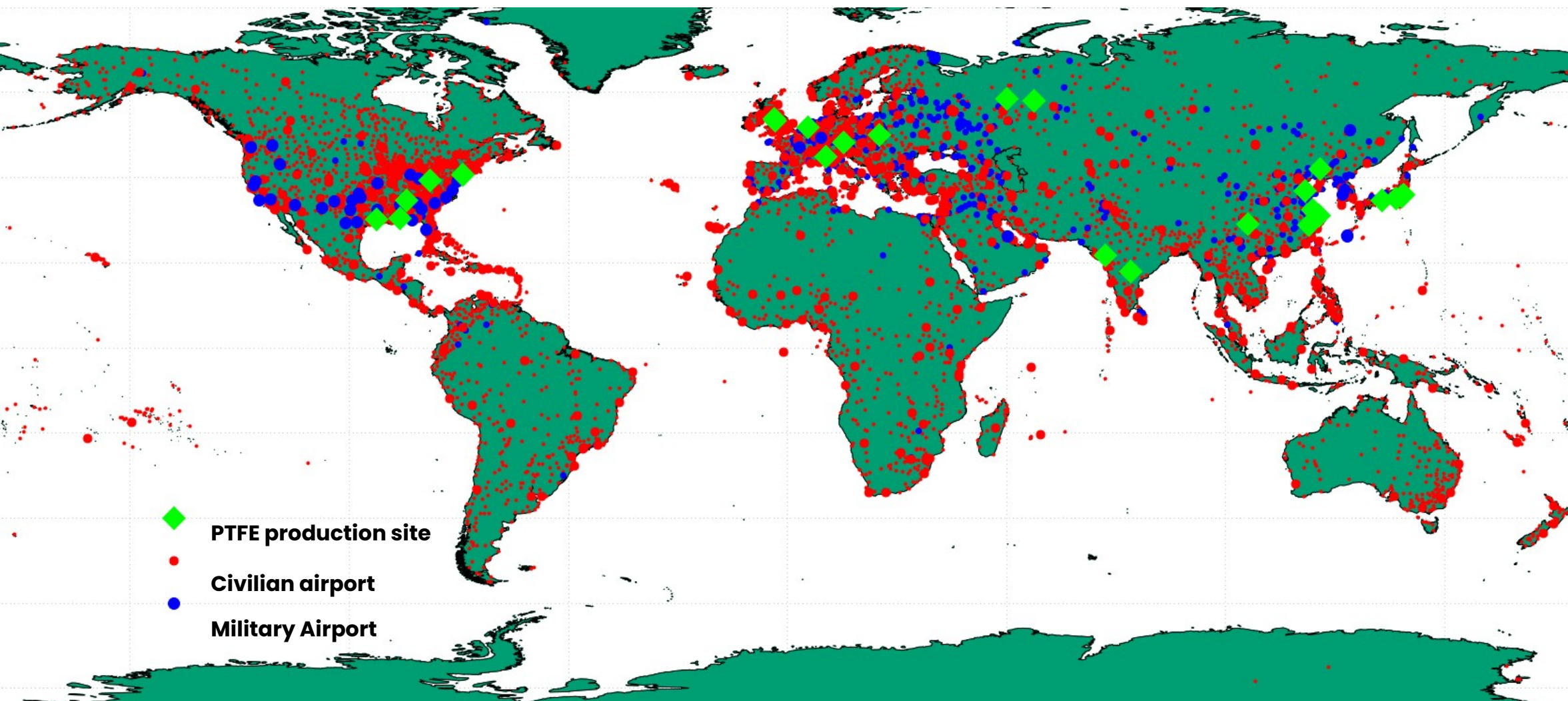
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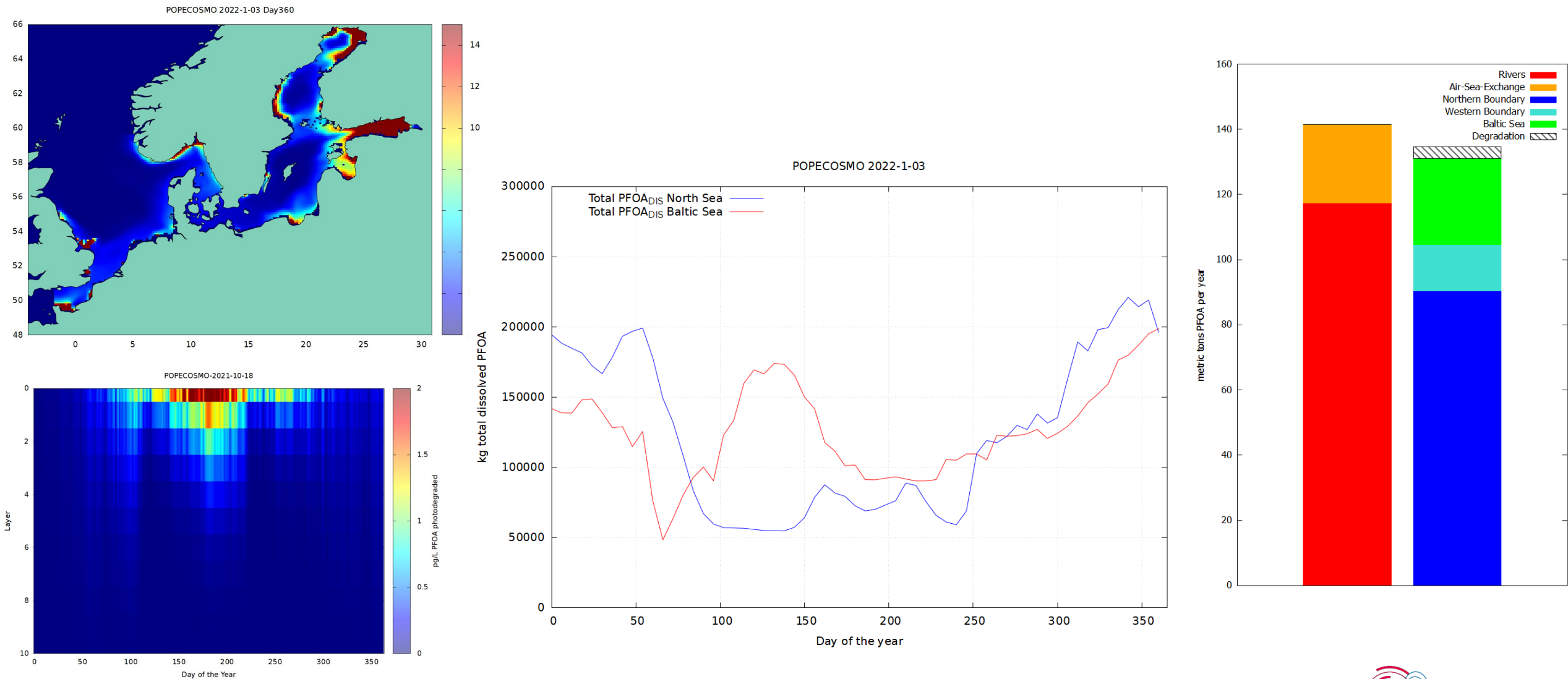
	North Sea (25 measurements)			Baltic Sea (22 measurements)		
log K <sub>OC</sub>	<1σ	1σ - 2σ	>2σ	<1σ	1σ - 2σ	>2σ
1.89	2	10	13	4	9	9
2.5	6	4	15	2	4	16
3	4	6	15	1	4	17
3.5	0	4	21	2	0	20



# Pointsources worldwide



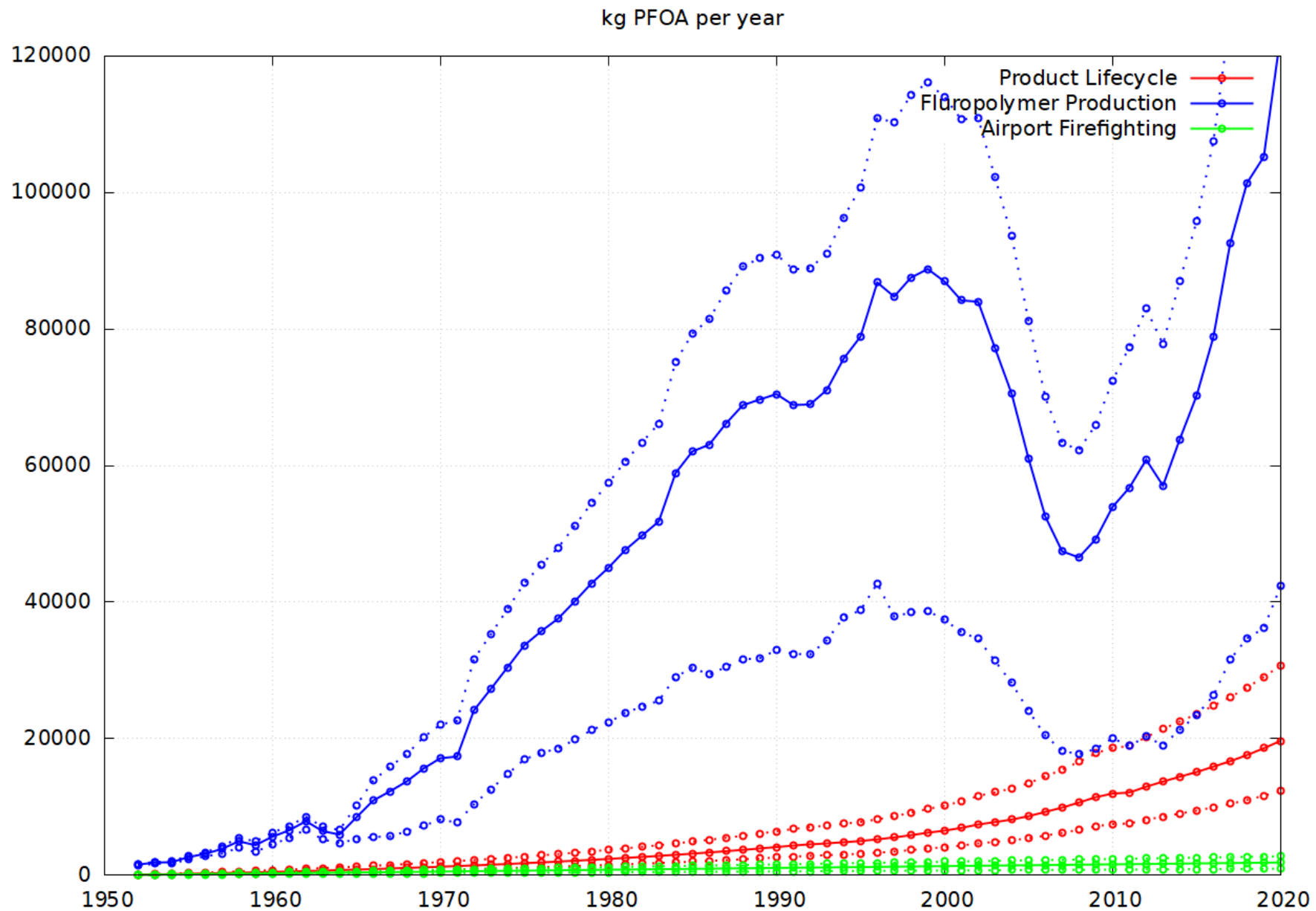
# Exploring some results



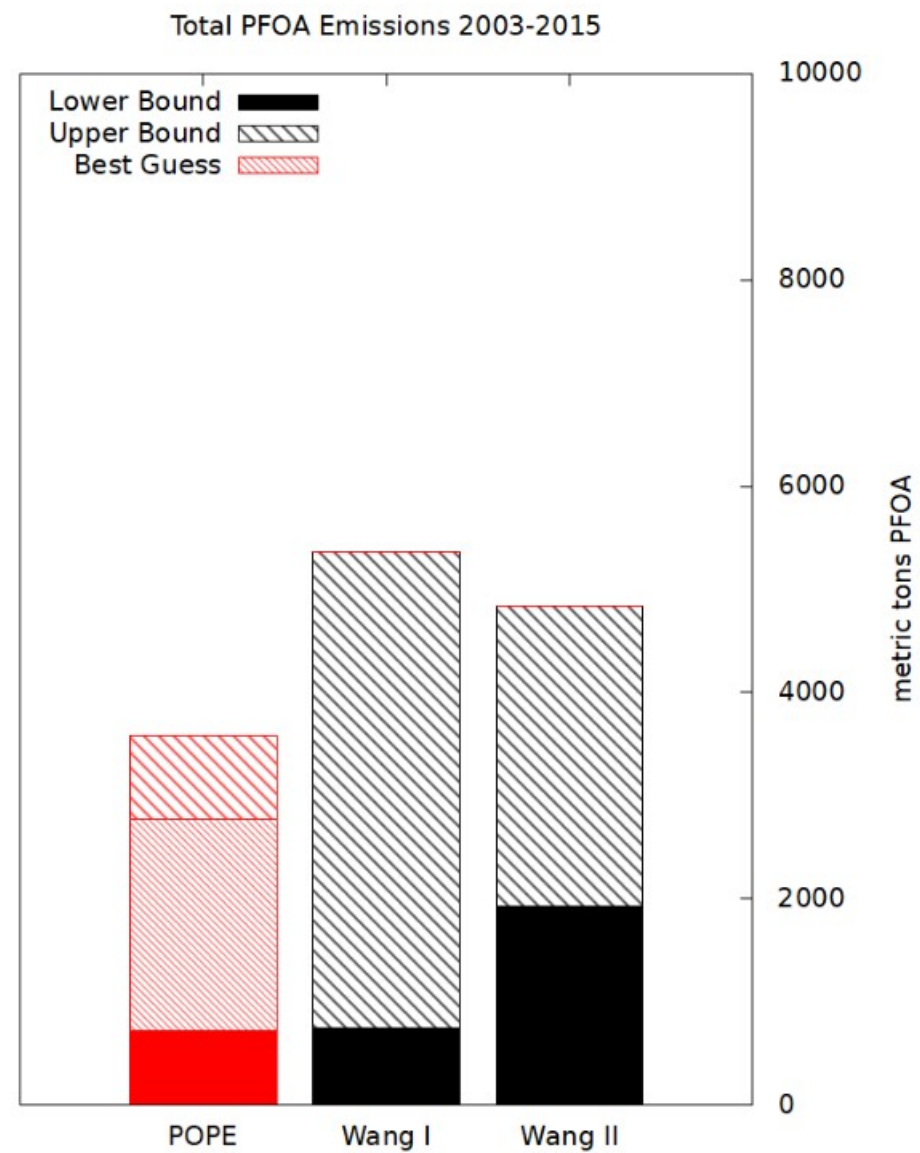
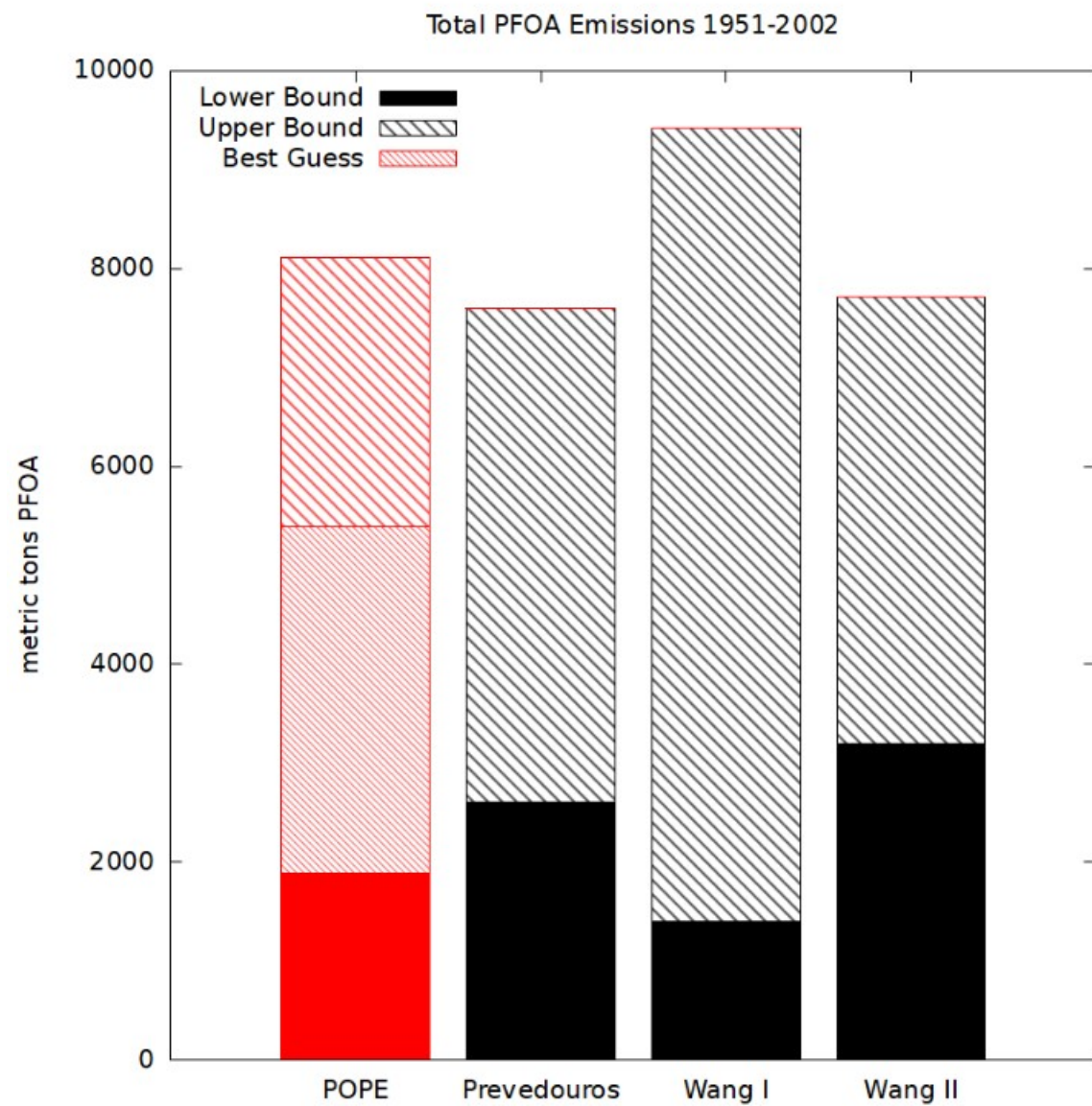
# The parameter space

## 4 basic degrees of freedom

- **Scaling of Riverinput**
  - Upper bounds and lower bounds from emission model
  - Is validated on its own with measurements
- **Scaling of Air Sea exchange**
  - High uncertainty due to unreliable Henry`s Law constants
  - Requires data on atmospheric concentrations
- **Scaling of partitioning coefficients**
  - May be able to be analysed independantly with the right dataset
- **Scaling of degradation coefficients**
  - Photolytic degradation fixed, but plays a small part
  - Other degradation is a educated guess









# Vapor pressure

From Hanna Joerss (KBT)

