Supporting Information for "*SimpleBox4Planet: Environmental Fate Modelling of PFAS and their Alternatives via the Enalos Cloud Platform*"

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S1. Comparison of steady-state mass and concentration calculations using SimpleBox (v4.04) in Excel and the *SimpleBox4Planet* web application

Table S1. Comparison of steady-state mass and concentration calculations for Perfluorobutanoic acid (PFBA), using SimpleBox (v4.04) and the *SimpleBox4Planet* under default scenarios within the regional scale.

Perfluorobutanoic acid (PFBA)					
	SimpleBox (v4.04) in Excel		*SimpleBox4Planet*		
Receiving Compartment	Masses (kg)	Concentrations	Masses (kg)	Concentrations	Concentration Units
Air	6.9E+04	3.0E-07	6.9E+04	3.0E-07	$g.m^{-3}$
Fresh water lake	1.1E+05	2.0E-06	1.1E+05	2.0E-06	$g.L^{-1}$
Fresh water	2.7E+05	1.4E-05	2.7E+05	1.4E-05	$g.L^{-1}$
Fresh water sediment	4.8E+03	2.0E-05	4.8E+03	2.0E-05	$g.kg(w)^{-1}$
Surface sea/ocean water	1.0E+04	1.0E-06	1.0E+04	1.0E-06	$g.L^{-1}$
Deep sea/ocean water	/	/	/	/	$g.L^{-1}$
Marine sediment	5.6E+01	1.4E-06	5.6E+01	1.4E-06	$g.kg(w)^{-1}$
Natural soil	3.2E+01	6.1E-09	3.2E+01	6.1E-09	$g.kg(w)^{-1}$
Agricultural soil	3.1E+06	6.6E-05	3.1E+06	6.6E-05	$g.kg(w)^{-1}$
Other soil	1.2E+01	6.1E-09	1.2E+01	6.1E-09	$g.kg(w)^{-1}$
Total	3.5E+06	/	3.5E+06	/	/

Table S2. Comparison of steady-state mass and concentration calculations for Perfluorobutanoic acid (PFBA), using SimpleBox (v4.04) and the *SimpleBox4Planet* under default scenarios within the continental scale.

Perfluorobutanoic acid (PFBA)					
	SimpleBox (v4.04) in Excel		*SimpleBox4Planet*		
Receiving Compartment	Masses (kg)	Concentrations	Masses (kg)	Concentrations	Concentration Units
Air	1.4E+05	1.8E-08	1.4E+05	1.8E-08	$g.m^{-3}$
Fresh water lake	1.1E+02	1.2E-10	1.1E+02	1.2E-10	$g.L^{-1}$
Fresh water	7.3E+01	2.4E-10	7.3E+01	2.4E-10	$g.L^{-1}$
Fresh water sediment	1.3E+00	3.3E-10	1.3E+00	3.3E-10	$g.kg(w)^{-1}$
Surface sea/ocean water	1.7E+05	2.3E-10	1.7E+05	2.3E-10	$g.L^{-1}$
Deep sea/ocean water	/	/	/	/	$g.L^{-1}$
Marine sediment	4.6E+01	3.2E-10	4.6E+01	3.2E-10	$g.kg(w)^{-1}$
Natural soil	3.2E+01	3.7E-10	3.2E+01	3.7E-10	$g.kg(w)^{-1}$
Agricultural soil	1.3E+02	1.7E-10	1.3E+02	1.7E-10	$g.kg(w)^{-1}$
Other soil	1.2E+01	3.7E-10	1.2E+01	3.7E-10	$g.kg(w)^{-1}$
Total	3.1E+05	/	3.1E+05	/	/

Table S3. Comparison of steady-state mass and concentration calculations for Perfluorobutanoic acid (PFBA), using SimpleBox (v4.04) and the *SimpleBox4Planet* under default scenarios across the global scale within the moderate zone.

Perfluorobutanoic acid (PFBA)					
	SimpleBox (v4.04) in Excel		***SimpleBox4Planet***		
Receiving Compartment	Masses (kg)	Concentrations	Masses (kg)	Concentrations	Concentration Units
Air	4.5E+04	5.8E-10	4.5E+04	5.8E-10	$g.m^{-3}$
Fresh water lake	/	/	/	/	$g.L^{-1}$
Fresh water	/	/	/	/	$g.L^{-1}$
Fresh water sediment	/	/	/	/	$g.kg(w)^{-1}$
Surface sea/ocean water	1.8E+04	4.8E-12	1.8E+04	4.8E-12	$g.L^{-1}$
Deep sea/ocean water	7.5E+04	6.5E-13	7.5E+04	6.5E-13	$g.L^{-1}$
Marine sediment	1.4E+00	9.1E-13	1.4E+00	9.1E-13	$g.kg(w)^{-1}$
Natural soil	/	/	/	/	$g.kg(w)^{-1}$
Agricultural soil	/	/	/	/	$g.kg(w)^{-1}$
Other soil	3.8E+01	1.2E-11	3.8E+01	1.2E-11	$g.kg(w)^{-1}$
Total	1.4E+05	/	1.4E+05	/	/

Table S4. Comparison of steady-state mass and concentration calculations for Perfluorobutanoic acid (PFBA), using SimpleBox (v4.04) and the *SimpleBox4Planet* under default scenarios across the global scale within the arctic zone.

Perfluorobutanoic acid (PFBA)					
	SimpleBox (v4.04) in Excel		***SimpleBox4Planet***		
Receiving Compartment	Masses (kg)	Concentrations	Masses (kg)	Concentrations	Concentration Units
Air	5.0E+03	1.2E-10	5.0E+03	1.2E-10	$g.m^{-3}$
Fresh water lake	/	/	/	/	$g.L^{-1}$
Fresh water	/	/	/	/	$g.L^{-1}$
Fresh water sediment	/	/	/	/	$g.kg(w)^{-1}$
Surface sea/ocean water	5.8E+03	2.3E-12	5.8E+03	2.3E-12	$g.L^{-1}$
Deep sea/ocean water	6.9E+04	9.0E-13	6.9E+04	9.0E-13	$g.L^{-1}$
Marine sediment	1.3E+00	1.3E-12	1.3E+00	1.3E-12	$g.kg(w)^{-1}$
Natural soil	/	/	/	/	$g.kg(w)^{-1}$
Agricultural soil	/	/	/	/	$g.kg(w)^{-1}$
Other soil	1.2E+01	8.6E-12	1.2E+01	8.6E-12	$g.kg(w)^{-1}$
Total	8.0E+04	/	8.0E+04	/	/

Table S5. Comparison of steady-state mass and concentration calculations for Perfluorobutanoic acid (PFBA), using SimpleBox (v4.04) and the *SimpleBox4Planet* under default scenarios across the global scale within the tropic zone.

Perfluorobutanoic acid (PFBA)					
	SimpleBox (v4.04) in Excel		***SimpleBox4Planet***		
Receiving Compartment	Masses (kg)	Concentrations	Masses (kg)	Concentrations	Concentration Units
Air	7.5E+03	5.9E-11	7.5E+03	5.9E-11	$g.m^{-3}$
Fresh water lake	/	/	/	/	$g.L^{-1}$
Fresh water	/	/	/	/	$g.L^{-1}$
Fresh water sediment	/	/	/	/	$g.kg(w)^{-1}$
Surface sea/ocean water	4.4E+02	4.9E-14	4.4E+02	4.9E-14	$g.L^{-1}$
Deep sea/ocean water	1.4E+03	5.3E-15	1.4E+03	5.3E-15	$g.L^{-1}$
Marine sediment	2.6E-02	7.3E-15	2.6E-02	7.3E-15	$g.kg(w)^{-1}$
Natural soil	/	/	/	/	$g.kg(w)^{-1}$
Agricultural soil	/	/	/	/	$g.kg(w)^{-1}$
Other soil	1.9E+00	5.9E-13	1.9E+00	5.9E-13	$g.kg(w)^{-1}$
Total	9.3E+03	/	9.3E+03	/	/

S2. Comparison of steady-state mass flow (kg s^{-1}) calculations using SimpleBox (v4.04) in Excel and the *SimpleBox4Planet* web application

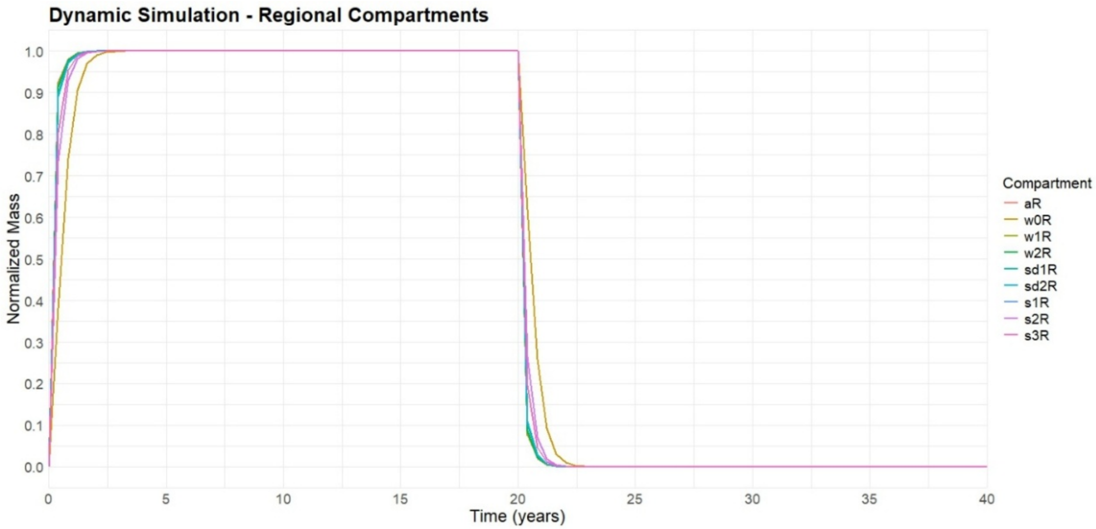
Table S6. Steady-state mass flows (kg s^{-1}) calculations for Perfluorobutanoic acid (PFBA), using SimpleBox (v4.04) under default scenarios.

		Emission	Inflow	Outflow	Removal	Degra dation	air-water transport	water-air transport	air-soil transport	soil-air transport	soil-water transport	water-sed transport	sed-water transport	mass balance
Regional Scale														
air	aR	3.2E-01	4.0E-02	6.5E-01	2.5E-05	2.2E-01	1.4E-04	4.2E-01	2.2E-05	9.5E-02				*0.0E+00*
fresh water lakes	w0R	0.0E+00	0.0E+00	2.7E-04		6.0E-03	1.0E-05	5.3E-03			1.2E-02			*0.0E+00*
fresh water	w1R	3.2E-01	2.7E-04	1.9E-02		1.4E-02	1.1E-04	4.1E-01			1.3E-01	2.6E-03	2.6E-03	*0.0E+00*
coastal sea water	w2R	0.0E+00	1.9E-02	1.4E-02		5.5E-04	1.8E-05	4.8E-03				2.9E-05	2.9E-05	*0.0E+00*
fresh water sediment	sd1R				1.4E-05	1.3E-05						2.6E-03	2.6E-03	*0.0E+00*
coastal marine sediment	sd2R				5.1E-08	1.5E-07						2.9E-05	2.9E-05	*0.0E+00*
natural soil	s1R	0.0E+00			2.1E-08	8.5E-07			6.2E-06	2.2E-06	3.2E-06			*0.0E+00*
agricultural soil	s2R	3.2E-01			9.4E-04	8.2E-02			1.4E-05	9.5E-02	1.4E-01			*0.0E+00*
other soil	s3R	0.0E+00			7.9E-09	3.2E-07			2.3E-06	8.0E-07	1.2E-06			*0.0E+00*
Continental Scale														
air	aC	0.0E+00	6.6E-01	2.3E-01	5.0E-05	4.3E-01	4.2E-03	4.0E-03	2.2E-05	7.0E-06				*0.0E+00*
fresh water lakes	w0C	0.0E+00	0.0E+00	2.6E-07		5.8E-06	1.0E-05	5.0E-06			8.6E-07			*0.0E+00*
fresh water	w1C	0.0E+00	2.6E-07	5.3E-06		3.9E-06	1.1E-04	1.1E-04			9.4E-06	7.2E-07	7.1E-07	*0.0E+00*
coastal sea water	w2C	0.0E+00	1.4E-02	5.3E-03		9.0E-03	4.1E-03	3.9E-03				2.4E-05	2.4E-05	*0.0E+00*
fresh water sediment	sd1C				3.8E-09	3.6E-09						7.2E-07	7.1E-07	*0.0E+00*
coastal marine sediment	sd2C				0.0E+00	1.2E-07						2.4E-05	2.4E-05	*0.0E+00*
natural soil	s1C	0.0E+00			2.1E-08	8.5E-07			6.2E-06	2.1E-06	3.1E-06			*0.0E+00*
agricultural soil	s2C	0.0E+00			4.0E-08	3.5E-06			1.4E-05	4.1E-06	6.0E-06			*0.0E+00*
other soil	s3C	0.0E+00			7.8E-09	3.1E-07			2.3E-06	8.0E-07	1.2E-06			*0.0E+00*
Global Scale - Moderate climate zone														
air	aM	0.0E+00	1.9E-01	5.2E-02	1.6E-05	1.4E-01	1.3E-03	8.6E-04	7.4E-06	2.6E-06				*0.0E+00*
upper ocean water	w2M	0.0E+00	5.9E-03	5.4E-03		9.9E-04	1.3E-03	8.6E-04			3.8E-06			*0.0E+00*
deep sea	w3M		4.7E-03	7.2E-04		4.0E-03						7.1E-07	7.1E-07	*0.0E+00*
ocean sediment	sdM				4.1E-12	3.7E-09						7.1E-07	7.1E-07	*0.0E+00*
soil	sM	0.0E+00			2.5E-08	1.0E-06			7.4E-06	2.6E-06	3.8E-06			*0.0E+00*
Global Scale - Arctic climate zone														
air	aA	0.0E+00	1.7E-02	3.5E-03	1.8E-06	1.3E-02	5.5E-04	2.6E-04	7.1E-07	1.8E-07				*0.0E+00*
upper ocean water	w2A	0.0E+00	1.3E-03	1.6E-03		6.7E-05	5.5E-04	2.6E-04			4.5E-07			*0.0E+00*
deep sea	w3A		1.6E-03	7.5E-04		8.0E-04						6.5E-07	6.5E-07	*0.0E+00*
ocean sediment	sdA				2.7E-12	7.3E-10						6.5E-07	6.5E-07	*0.0E+00*
soil	sA	0.0E+00			3.0E-09	7.3E-08			7.1E-07	1.8E-07	4.5E-07			*0.0E+00*
Global Scale - Tropical climate zone														
air	aT	0.0E+00	2.9E-02	3.0E-03	2.7E-06	2.6E-02	1.7E-04	2.1E-05	8.0E-07	3.2E-07				*0.0E+00*
upper ocean water	w2T	0.0E+00	1.1E-05	1.1E-04		5.8E-05	1.7E-04	2.1E-05			3.5E-07			*0.0E+00*
deep sea	w3T		2.0E-04	1.1E-05		1.9E-04						1.3E-08	1.3E-08	*0.0E+00*
ocean sediment	sdT				5.4E-14	1.7E-10						1.3E-08	1.3E-08	*0.0E+00*
soil	sT	0.0E+00			2.4E-09	1.3E-07			8.0E-07	3.2E-07	3.5E-07			*0.0E+00*
		9.5E-01			*1.0E-03*	*9.5E-01*								*0.0E+00*

Table S7. Steady-state mass flows (kg s-1) calculations for Perfluorobutanoic acid (PFBA), using *SimpleBox4Planet* under default scenarios.

Compartments	Emission	Inflow	Outflow	Removal	Degrad.	air-water transport	water-air transport	air-soil transport	soil-air transport	soil-water transport	water-sed transport	sed-water transport	mass balance
Regional Scale													
air	3.2E-01	4.0E-02	6.5E-01	2.5E-05	2.2E-01	1.4E-04	4.2E-01	2.2E-05	9.5E-02				0.0E+00
fresh water lakes	0.0E+00	######	2.7E-04		6.1E-03	1.0E-05	5.3E-03			1.2E-02			0.0E+00
fresh water	3.2E-01	2.7E-04	1.9E-02		1.4E-02	1.1E-04	4.1E-01			1.3E-01	2.6E-03	2.6E-03	0.0E+00
coastal sea water	0.0E+00	1.9E-02	1.4E-02		5.5E-04	1.8E-05	4.8E-03				2.9E-05	2.9E-05	0.0E+00
fresh water sediment				1.4E-05	1.3E-05						2.6E-03	2.6E-03	0.0E+00
coastal marine sediment				5.1E-08	1.5E-07						2.9E-05	2.9E-05	0.0E+00
natural soil	0.0E+00			2.1E-08	8.5E-07			6.2E-06	2.2E-06	3.2E-06			0.0E+00
agricultural soil	3.2E-01			9.4E-04	8.2E-02			1.4E-05	9.5E-02	1.4E-01			0.0E+00
other soil	0.0E+00			7.9E-09	3.2E-07			2.3E-06	8.0E-07	1.2E-06			0.0E+00
Continental Scale													
air	0.0E+00	6.6E-01	2.3E-01	5.0E-05	4.3E-01	4.2E-03	4.0E-03	2.2E-05	7.0E-06				0.0E+00
fresh water lakes	0.0E+00	######	2.6E-07		5.8E-06	1.0E-05	5.0E-06			8.6E-07			0.0E+00
fresh water	0.0E+00	2.6E-07	5.3E-06		3.9E-06	1.1E-04	1.1E-04			9.4E-06	7.2E-07	7.1E-07	0.0E+00
coastal sea water	0.0E+00	1.4E-02	5.3E-03		9.0E-03	4.1E-03	3.9E-03				2.4E-05	2.4E-05	0.0E+00
fresh water sediment				3.8E-09	3.6E-09						7.2E-07	7.1E-07	0.0E+00
coastal marine sediment				0.0E+00	1.2E-07						2.4E-05	2.4E-05	0.0E+00
natural soil	0.0E+00			2.1E-08	8.4E-07			6.1E-06	2.2E-06	3.1E-06			0.0E+00
agricultural soil	0.0E+00			4.0E-08	3.5E-06			1.4E-05	4.1E-06	6.0E-06			0.0E+00
other soil	0.0E+00			7.8E-09	3.1E-07			2.3E-06	7.9E-07	1.2E-06			0.0E+00
Global Scale - Moderate climate zone													
air	0.0E+00	1.9E-01	5.2E-02	1.6E-05	1.4E-01	1.3E-03	8.6E-04	7.4E-06	2.6E-06				0.0E+00
upper ocean water	0.0E+00	5.9E-03	5.4E-03		9.9E-04	1.3E-03	8.6E-04			3.8E-06			0.0E+00
deep sea		4.7E-03	7.2E-04		4.0E-03						7.1E-07	7.1E-07	0.0E+00
ocean sediment				4.1E-12	3.6E-09						7.1E-07	7.1E-07	0.0E+00
soil	0.0E+00			2.5E-08	1.0E-06			7.4E-06	2.6E-06	3.8E-06			0.0E+00
Global Scale - Arctic climate zone													
air	0.0E+00	1.7E-02	3.5E-03	1.8E-06	1.3E-02	5.5E-04	2.6E-04	7.1E-07	1.8E-07				0.0E+00
upper ocean water	0.0E+00	1.3E-03	1.6E-03		6.7E-05	5.5E-04	2.6E-04			4.5E-07			0.0E+00
deep sea		1.6E-03	7.5E-04		8.0E-04						6.5E-07	6.5E-07	0.0E+00
ocean sediment				2.7E-12	7.3E-10						6.5E-07	6.5E-07	0.0E+00
soil	0.0E+00			3.0E-09	7.3E-08			7.1E-07	1.8E-07	4.5E-07			0.0E+00
Global Scale - Tropical climate zone													
air	0.0E+00	2.9E-02	3.0E-03	2.7E-06	2.6E-02	1.7E-04	2.1E-05	8.0E-07	3.2E-07				0.0E+00
upper ocean water	0.0E+00	1.1E-05	1.1E-04		5.8E-05	1.7E-04	2.1E-05			3.5E-07			0.0E+00
deep sea		2.0E-04	1.1E-05		1.9E-04						1.3E-08	1.3E-08	0.0E+00
ocean sediment				5.4E-14	1.7E-10						1.3E-08	1.3E-08	0.0E+00
soil	0.0E+00			2.4E-09	1.3E-07			8.0E-07	3.2E-07	3.5E-07			0.0E+00
	9.5E-01			1.1E-03	9.5E-01								0.0E+00

S3. Comparison of dynamic output



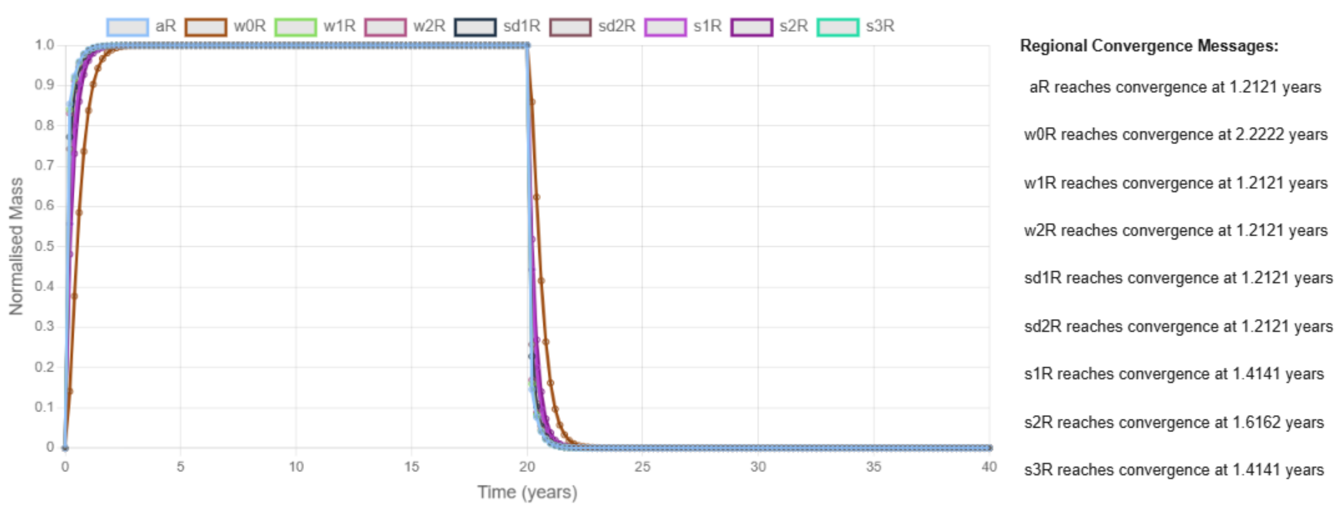


Figure S1. Comparison of dynamic calculations of normalized mass (defined as the ratio of dynamic mass divided by the steady-state mass) over time for Perfluorobutanoic acid (PFBA), determined using the Dynamic Rshell for SimpleBox (v4.04) (top panel) and the SimpleBox4Planet (bottom panel), under default scenarios within the regional scale. aR: Arctic Region; w0R: freshwater lakes; w1R: freshwater; w2R: coastal sea water; s1R: natural soil; s2R: agriculture soil, s3R: other soil, sd1R: fresh water sediment, sd2R: coastal marine sediment.

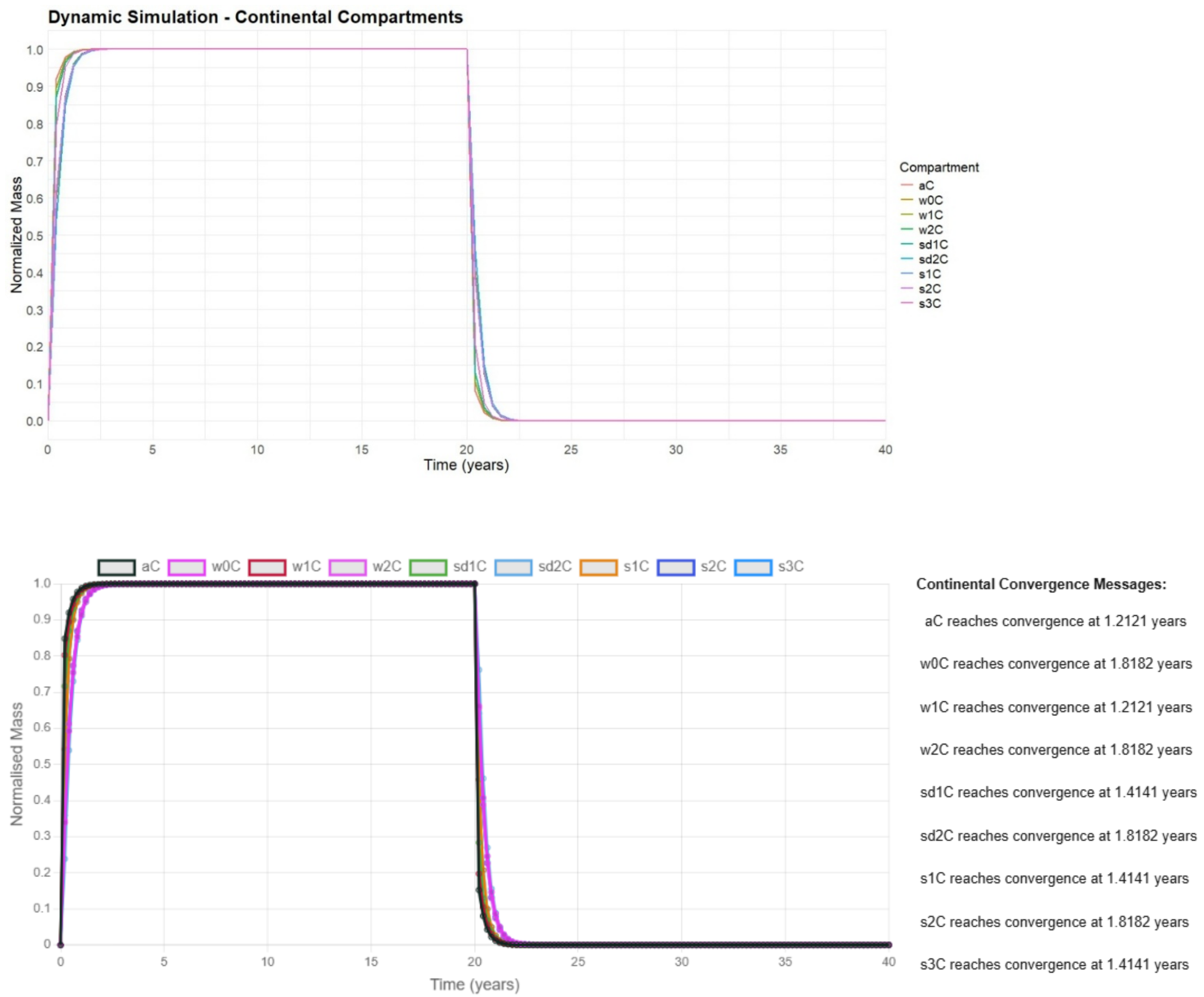


Figure S2. Comparison of dynamic calculations of normalized mass (defined as the ratio of dynamic mass divided by the steady-state mass) over time for PFBA, using the Dynamic Rshell for SimpleBox (v4.04) (top panel) and the SimpleBox4Planet (bottom panel), under default scenarios within the continental scale.

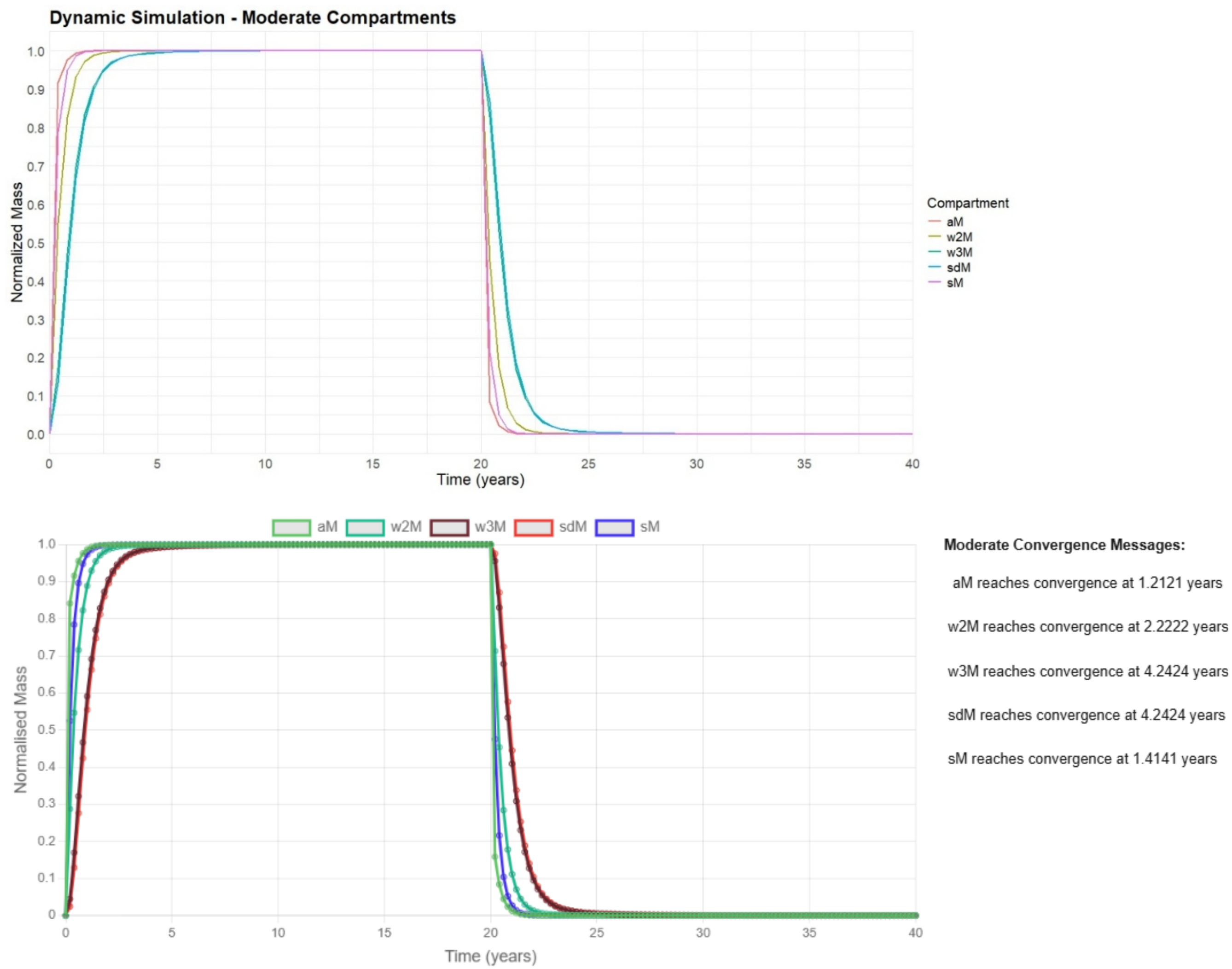


Figure S3. Comparison of dynamic calculations of normalized mass (defined as the ratio of dynamic mass divided by the steady-state mass) over time for PFBA, using the Dynamic Rshell for SimpleBox (v4.04) (top panel) and the SimpleBox4Planet (bottom panel), under default scenarios across the global scale within the moderate zone.

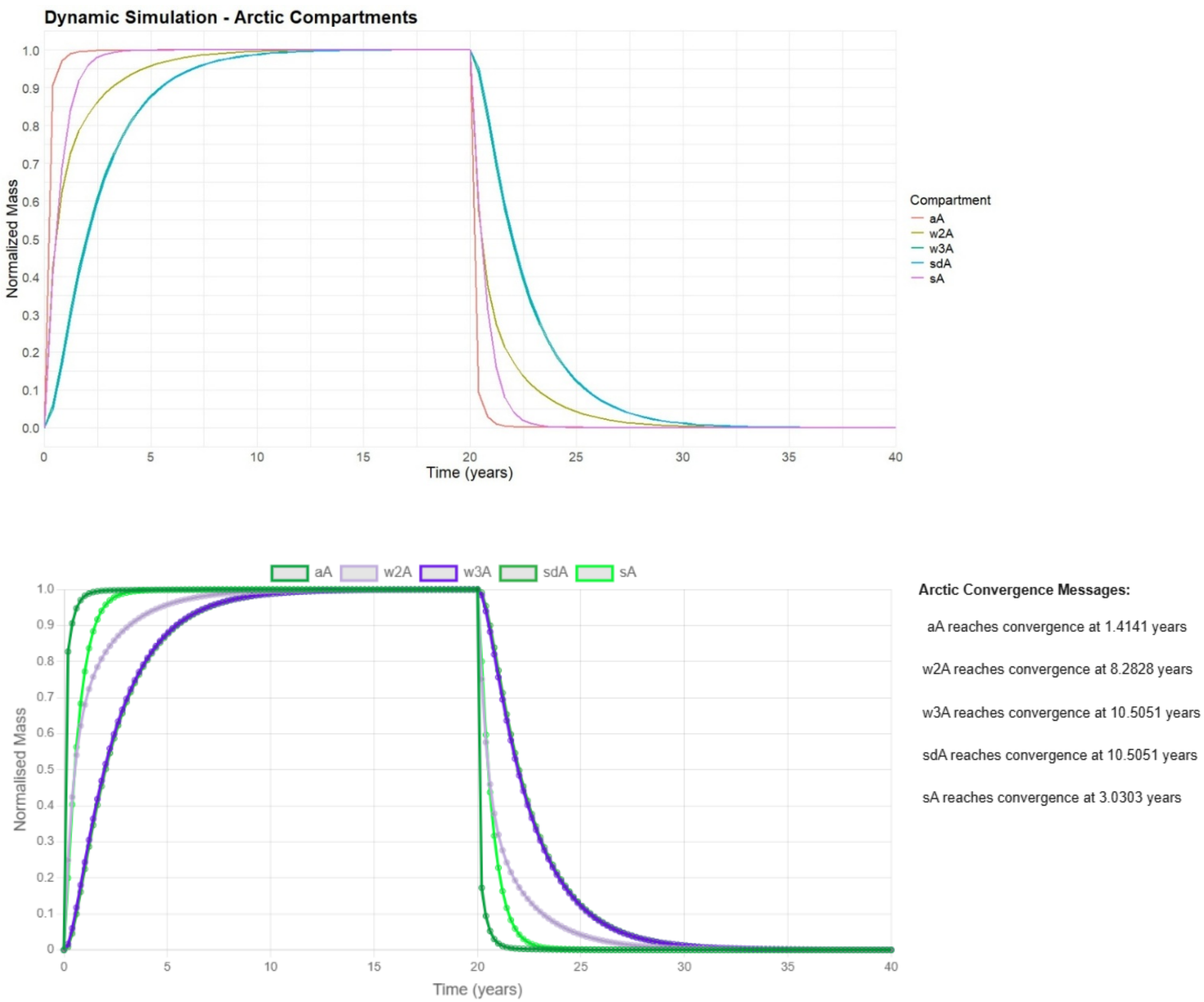


Figure S4. Comparison of dynamic calculations of normalized mass (defined as the ratio of dynamic mass divided by the steady-state mass) over time for PFBA, using the Dynamic Rshell for SimpleBox (v4.04) (top panel) and the SimpleBox4Planet (bottom panel), under default scenarios across the global scale within the arctic zone.

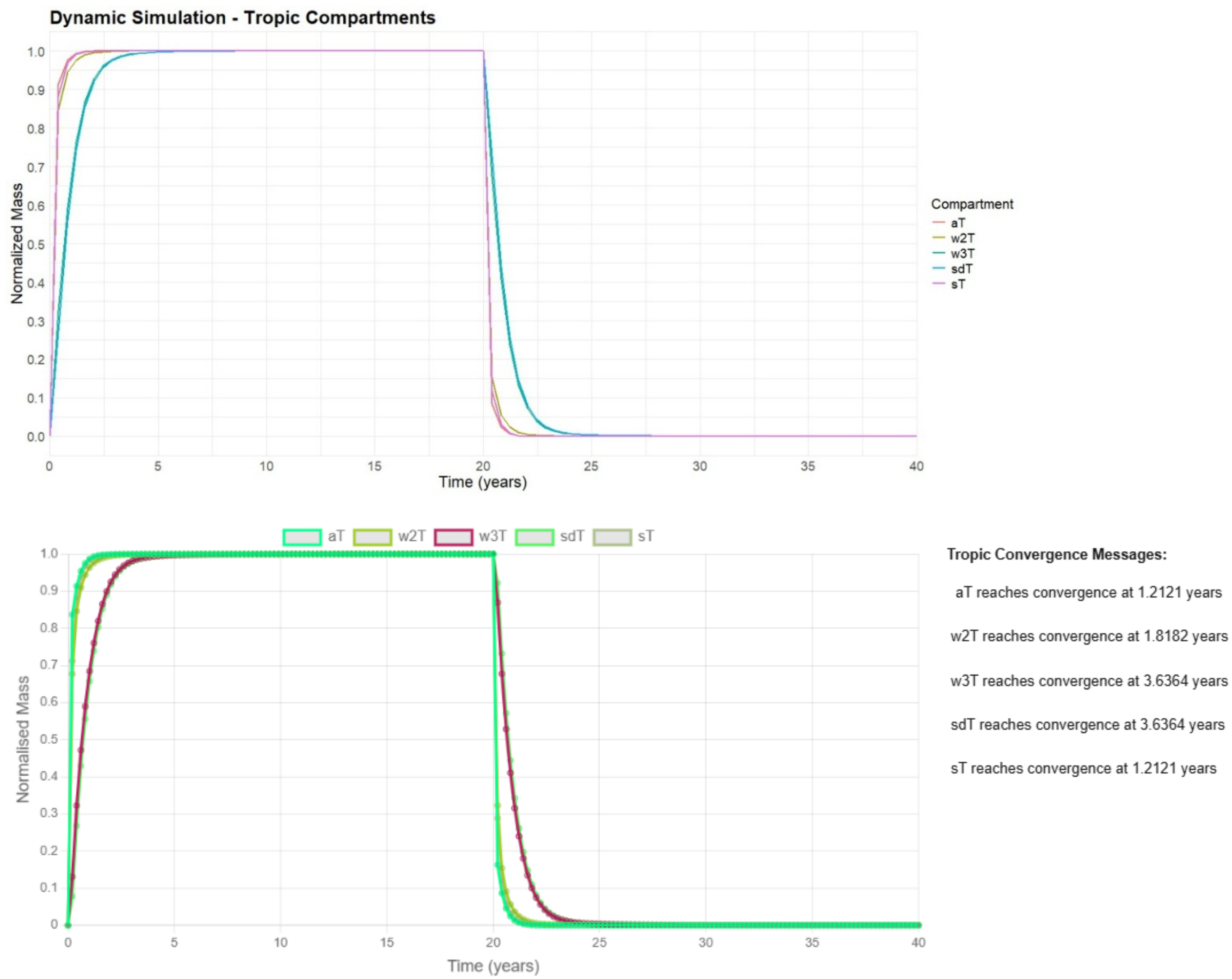


Figure S5. Comparison of dynamic calculations of normalized mass (defined as the ratio of dynamic mass divided by the steady-state mass) over time for PFBA, using the Dynamic Rshell for SimpleBox (v4.04) (top panel) and the SimpleBox4Planet (bottom panel), under default scenarios across the global scale within the tropic zone.

S4. Output window after selecting 'Execute Steady-State Simulation'

Results

Back

Steady-State Simulation

Objective: To determine the equilibrium distribution of a chemical under constant input conditions.

Mathematical Basis: The system assumes that the inputs (emissions) and outputs (degradation, advection, etc.) are constant, and the net change in mass (i.e., dM/dt) is **zero** in each compartment.

Key Equation: The steady-state mass balance equation is solved by setting:

$$\frac{dM}{dt} = 0 \Rightarrow \mathbf{K} \cdot \mathbf{M}_{\infty} + \mathbf{E} = 0$$

where:

K (s^{-1}) is the matrix of transfer rate coefficients between compartments,

$\mathbf{M}_{\infty}$ (kg) is the vector of masses (or fugacities) in compartments at steady-state,

E (kg s^{-1}) is the vector of constant emission rates

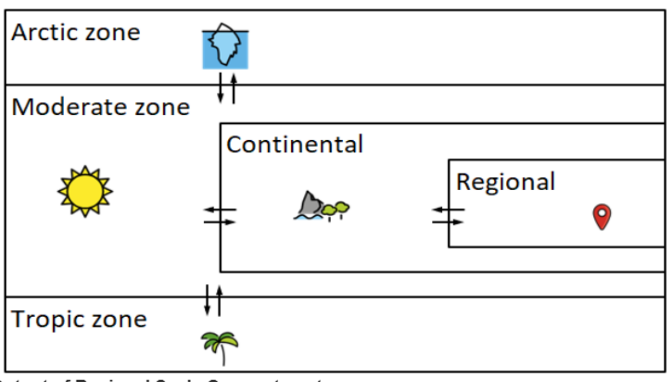
The model computes the **steady-state fugacity or mass** in each compartment using algebraic methods such as matrix inversion (e.g., solving $\mathbf{M} = -\mathbf{K}^{-1} \cdot \mathbf{E}$). The result tells you the **long-term average concentrations** assuming emissions are constant.

Output table 1: Steady-state Masses and Concentrations

Media	Masses (kg)					Concentrations					
	Reg	Cont	Mod	Arct	Trop	Reg	Cont	Mod	Arct	Trop	Units
Air	9.81E4	5.60E5	1.04E6	4.09E5	1.03E6	4.28E-7	7.54E-8	1.34E-8	9.63E-9	8.11E-9	g.m-3
Fresh water lake	5.49E3	2.92E2	0.0	0.0	0.0	9.61E-8	3.15E-10	0.0	0.0	0.0	g.L-1
Fresh water	1.74E5	2.42E2	0.0	0.0	0.0	9.24E-6	7.91E-10	0.0	0.0	0.0	g.L-1
Fresh water sediment	4.63E4	6.43E1	0.0	0.0	0.0	1.89E-4	1.61E-8	0.0	0.0	0.0	g.kg(w)-1
Surface sea/ocean water	6.44E3	1.76E5	8.84E4	1.93E5	4.44E4	6.44E-7	2.37E-10	2.29E-11	7.56E-11	4.97E-12	g.L-1
Deep sea/ocean water	0.0	0.0	2.64E5	1.74E6	4.71E4	0.0	0.0	2.27E-12	2.27E-11	1.76E-13	g.L-1
Marine sediment	4.45E2	6.09E2	6.08E1	4.54E2	8.91E0	1.14E-5	4.21E-9	4.03E-11	4.56E-10	2.56E-12	g.kg(w)-1
Natural soil	2.27E2	6.49E2	0.0	0.0	0.0	4.32E-8	7.62E-9	0.0	0.0	0.0	g.kg(w)-1
Agricultural soil	3.29E6	2.39E3	0.0	0.0	0.0	7.05E-5	3.16E-9	0.0	0.0	0.0	g.kg(w)-1
Other soil	8.39E1	2.40E2	4.45E3	5.18E3	1.37E3	4.32E-8	7.62E-9	1.35E-9	3.58E-9	4.20E-10	g.kg(w)-1
Total	3.62E6	7.41E5	1.39E6	2.35E6	1.13E6	0.0	0.0	0.0	0.0	0.0	0.0

Export Results

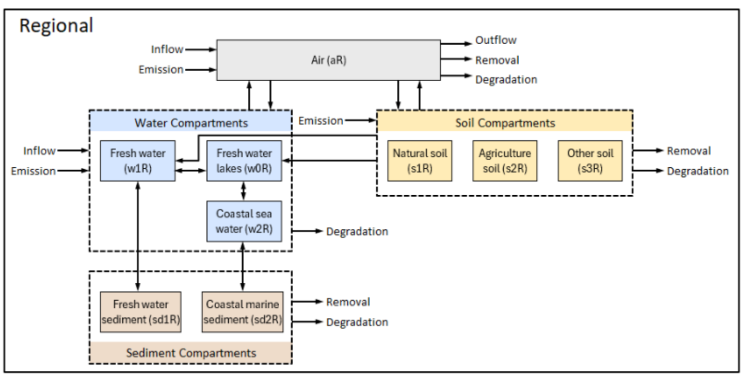
Graphical Output of Scale Zone Compartments



Regional: 3.62E6 kg (39.22%) Show
Continental: 7.41E5 kg (8.03%) Show
Moderate: 1.39E6 kg (15.06%) Show
Arctic: 2.35E6 kg (25.46%) Show
Tropical: 1.13E6 kg (12.24%) Show
Total Mass: 9.23E6 kg

Graphical Output of Regional Scale Compartments

aR: 4.28E-7 g.m⁻³
w0R: 9.61E-8 g.L⁻¹
w1R: 9.24E-6 g.L⁻¹
w2R: 6.44E-7 g.L⁻¹
sd1R: 1.89E-4 g.kg(w)⁻¹
sd2R: 1.14E-5 g.kg(w)⁻¹
s1R: 4.32E-8 g.kg(w)⁻¹
s2R: 7.05E-5 g.kg(w)⁻¹
s3R: 4.32E-8 g.kg(w)⁻¹



aR: 9.81E4 kg (2.71%)
w0R: 5.49E3 kg (0.15%)
w1R: 1.74E5 kg (4.81%)
w2R: 6.44E3 kg (0.18%)
sd1R: 4.63E4 kg (1.28%)
sd2R: 4.45E2 kg (0.01%)
s1R: 2.27E2 kg (0.01%)
s2R: 3.29E6 kg (90.86%)
s3R: 8.39E1 kg (0.00%)

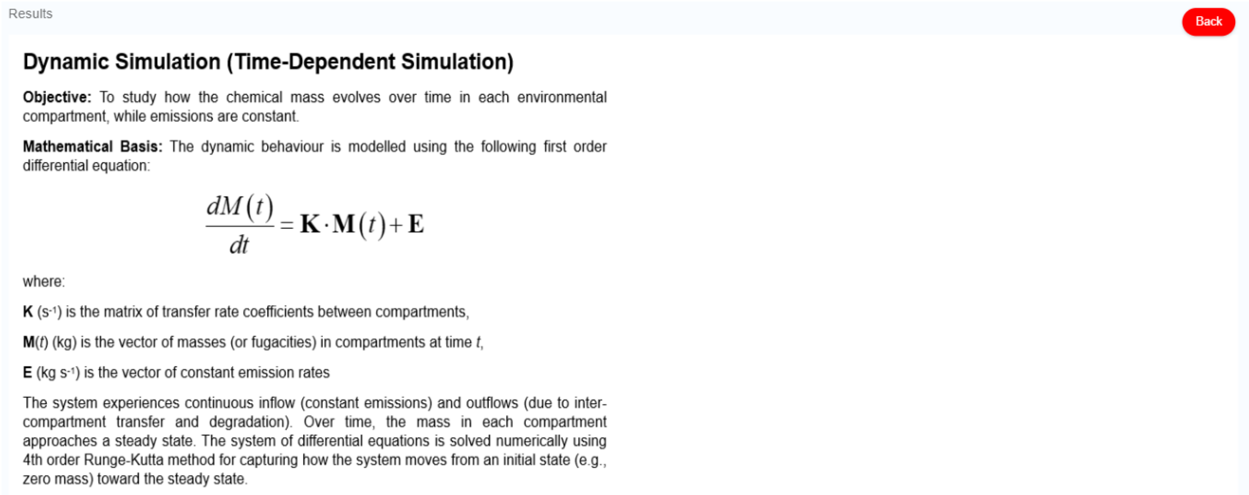
Output table 2: Steady-state mass flows ($kg.s^{-1}$)

Compartm.	Emission	Inflow	Outflow	Removal	Degrad.	air-water transport	water-air transport	air-soil transport	soil-air transport	soil-water transport	water-sed transport	sed-water transport	mass balance
Regional Scale													
air	3.17E-1	1.63E-1	9.25E-1	3.60E-5	2.12E-2	1.92E-4	3.01E-1	1.30E-4	1.65E-1				0.00E0
fresh water lakes	0.00E0	0.00E0	1.32E-5		4.77E-4	1.40E-5	2.81E-4			7.58E-4			0.00E0
fresh water	3.17E-1	1.32E-5	1.27E-2		1.51E-2	1.54E-4	2.97E-1			8.34E-3	3.90E-3	3.32E-3	0.00E0
coastal sea water	0.00E0	1.27E-2	8.82E-3		5.59E-4	2.45E-5	3.30E-3				2.90E-5	2.43E-5	0.00E0
fresh water sediment				1.34E-4	4.47E-4						3.90E-3	3.32E-3	0.00E0
coastal marine sediment				4.07E-7	4.30E-6						2.90E-5	2.43E-5	0.00E0
natural soil	0.00E0			9.24E-9	9.85E-6			3.62E-5	2.50E-5	1.38E-6			0.00E0
agricultural soil	3.17E-1			6.10E-5	1.43E-1			8.05E-5	1.65E-1	9.09E-3			0.00E0
other soil	0.00E0			3.42E-9	3.65E-6			1.34E-5	9.26E-6	5.10E-7			0.00E0
Continental Scale													
air	0.00E0	1.06E0	9.27E-1	2.05E-4	1.21E-1	1.65E-2	4.94E-3	3.73E-4	2.18E-4				0.00E0
fresh water lakes	0.00E0	0.00E0	7.01E-7		2.54E-5	4.01E-5	1.50E-5			1.00E-6			0.00E0
fresh water	0.00E0	7.01E-7	1.76E-5		2.10E-5	4.41E-4	4.13E-4			1.10E-5	5.43E-6	4.62E-6	0.00E0
coastal sea water	0.00E0	9.38E-3	5.59E-3		1.53E-2	1.60E-2	4.51E-3				3.96E-5	3.37E-5	0.00E0
fresh water sediment				1.85E-7	6.22E-7						5.43E-6	4.62E-6	0.00E0
coastal marine sediment				0.00E0	5.89E-6						3.96E-5	3.37E-5	0.00E0
natural soil	0.00E0			2.65E-8	2.82E-5			1.04E-4	7.16E-5	3.94E-6			0.00E0
agricultural soil	0.00E0			4.44E-8	1.04E-4			2.31E-4	1.20E-4	6.61E-6			0.00E0
other soil	0.00E0			9.80E-9	1.04E-5			3.84E-5	2.65E-5	1.46E-6			0.00E0
Global Scale - Moderate climate zone													
air	0.00E0	1.46E0	1.21E0	3.79E-4	2.24E-1	2.97E-2	4.53E-3	7.11E-4	4.90E-4				0.00E0
upper ocean water	0.00E0	8.52E-3	2.60E-2		7.68E-3	2.97E-2	4.53E-3			2.70E-5			0.00E0
deep sea		2.54E-2	2.53E-3		2.29E-2						3.95E-6	3.37E-6	0.00E0
ocean sediment				1.81E-10	5.87E-7						3.95E-6	3.37E-6	0.00E0
soil	0.00E0			1.81E-7	1.93E-4			7.11E-4	4.90E-4	2.70E-5			0.00E0
Global Scale - Arctic climate zone													
air	0.00E0	3.94E-1	2.83E-1	1.50E-4	7.39E-2	4.61E-2	9.58E-3	1.85E-4	1.24E-4				0.00E0
upper ocean water	0.00E0	1.90E-2	5.19E-2		3.65E-3	4.61E-2	9.58E-3			1.13E-5			0.00E0
deep sea		5.19E-2	1.90E-2		3.29E-2						2.61E-5	2.51E-5	0.00E0
ocean sediment				9.59E-10	9.54E-7						2.61E-5	2.51E-5	0.00E0
soil	0.00E0			7.54E-8	4.90E-5			1.85E-4	1.24E-4	1.13E-5			0.00E0
Global Scale - Tropical climate zone													
air	0.00E0	6.82E-1	4.13E-1	3.79E-4	2.48E-1	2.22E-2	2.29E-3	5.32E-4	3.71E-4				0.00E0
upper ocean water	0.00E0	3.56E-4	1.08E-2		9.49E-3	2.22E-2	2.29E-3			1.54E-5			0.00E0
deep sea		1.04E-2	3.56E-4		1.01E-2						7.06E-7	4.93E-7	0.00E0
ocean sediment				1.88E-11	2.12E-7						7.06E-7	4.93E-7	0.00E0
soil	0.00E0			1.03E-7	1.46E-4			5.32E-4	3.71E-4	1.54E-5			0.00E0
	9.51E-1			1.35E-3	9.50E-1								0.00E0

Export Mass Flows

Figure S6. The output window of the Steady-State Simulation in *SimpleBox4Planet* presenting a summary of the steady-state simulation results, including a table displaying steady-state masses and concentrations for each scale and compartment. Users can visualize the mass distribution across different scales through graphical outputs and interactively explore compartment-specific mass distributions using the 'Show' button. Additionally, a second table provides detailed mass flow information for key transfer processes, ensuring mass balance verification. Users can export both steady-state results and mass flows in Excel format for further analysis and reporting.

S5. Output window after selecting ‘Execute Dynamic Simulation’


Results

Back

Dynamic Simulation (Time-Dependent Simulation)

Objective: To study how the chemical mass evolves over time in each environmental compartment, while emissions are constant.

Mathematical Basis: The dynamic behaviour is modelled using the following first order differential equation:

$$\frac{dM(t)}{dt} = \mathbf{K} \cdot \mathbf{M}(t) + \mathbf{E}$$

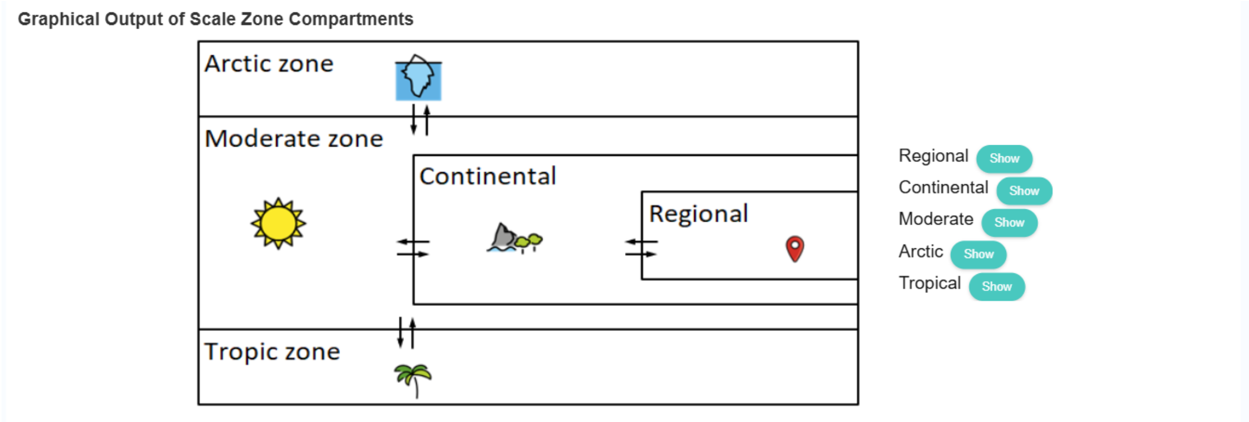
where:

K (s^{-1}) is the matrix of transfer rate coefficients between compartments,

M(*t*) (kg) is the vector of masses (or fugacities) in compartments at time *t*,

E (kg s^{-1}) is the vector of constant emission rates

The system experiences continuous inflow (constant emissions) and outflows (due to inter-compartment transfer and degradation). Over time, the mass in each compartment approaches a steady state. The system of differential equations is solved numerically using 4th order Runge-Kutta method for capturing how the system moves from an initial state (e.g., zero mass) toward the steady state.



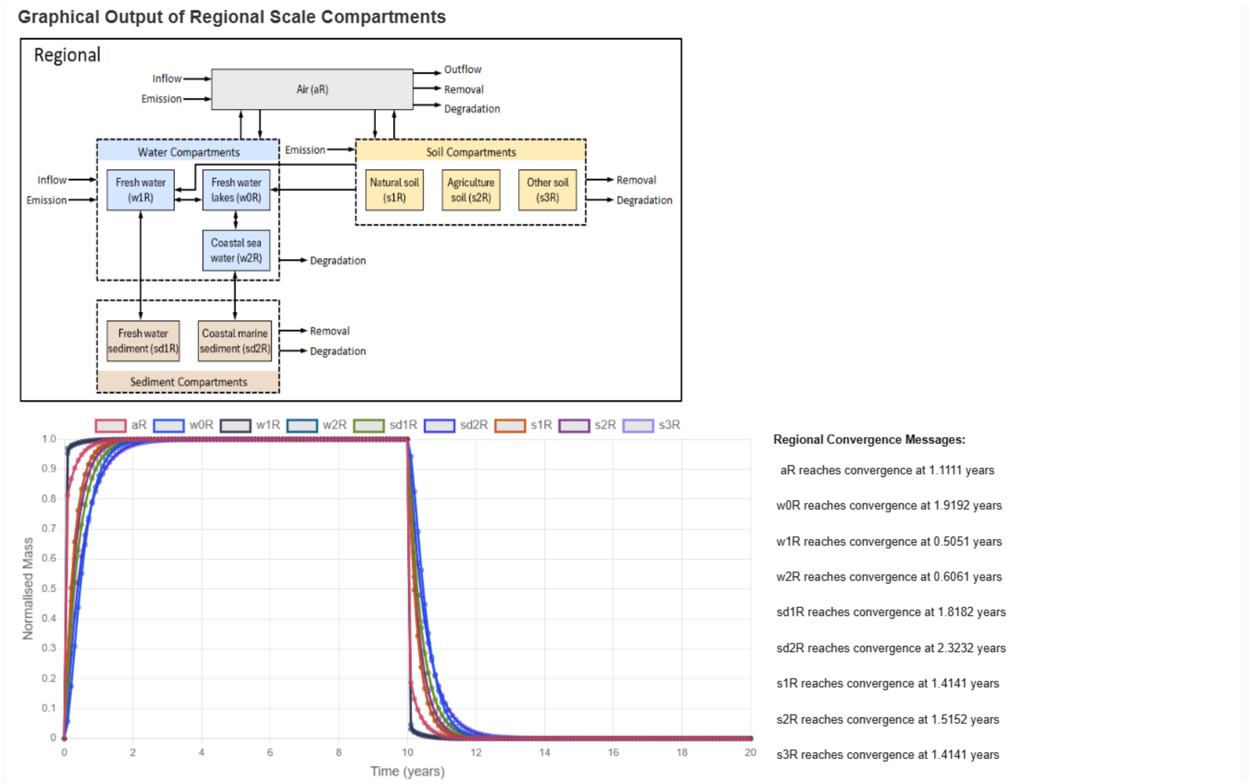


Figure S7. The output window of the Dynamic Simulation in *SimpleBox4Planet*, providing a brief description of the quasi-dynamic simulation and presenting a graphical representation of mass distribution across different scales. Users can select a specific scale using the ‘Show’ button to visualize the dynamic evolution of mass, normalized by the steady-state mass, as a function of time.

S6. Output window after selecting ‘Calculate Fate Factors’

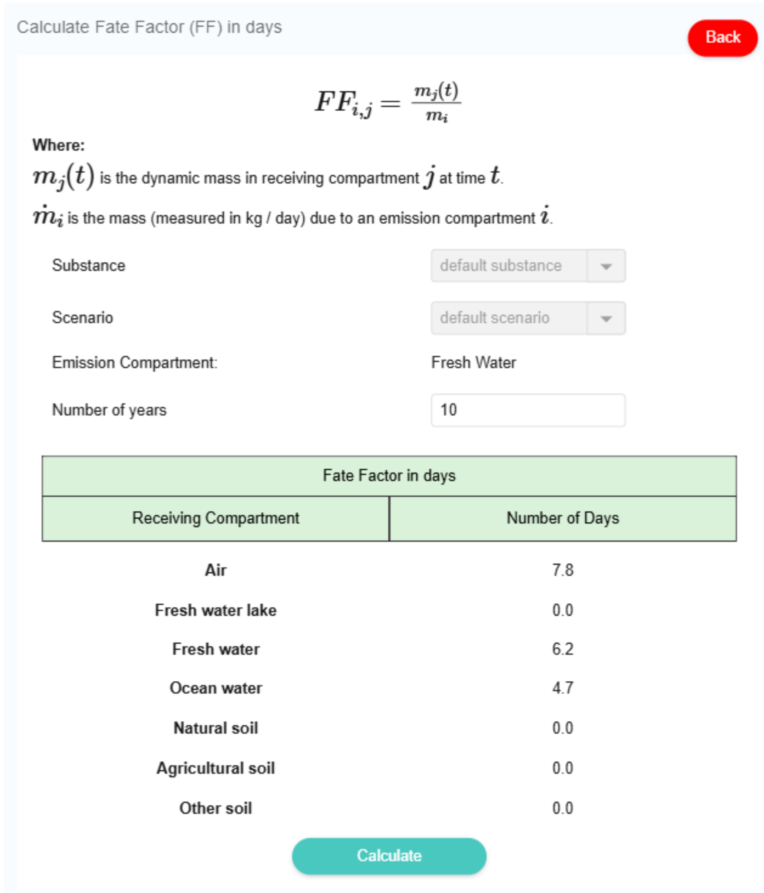


Figure S8. Output of the ‘Calculate Fate Factors’ function in the SimpleBox4Planet web application. Computation is only enabled under continental-scale scenarios with a single specified emission compartment. Users may also define a custom time (in years) to analyze the fate behavior over a relevant temporal scale.

S7. REST APIs

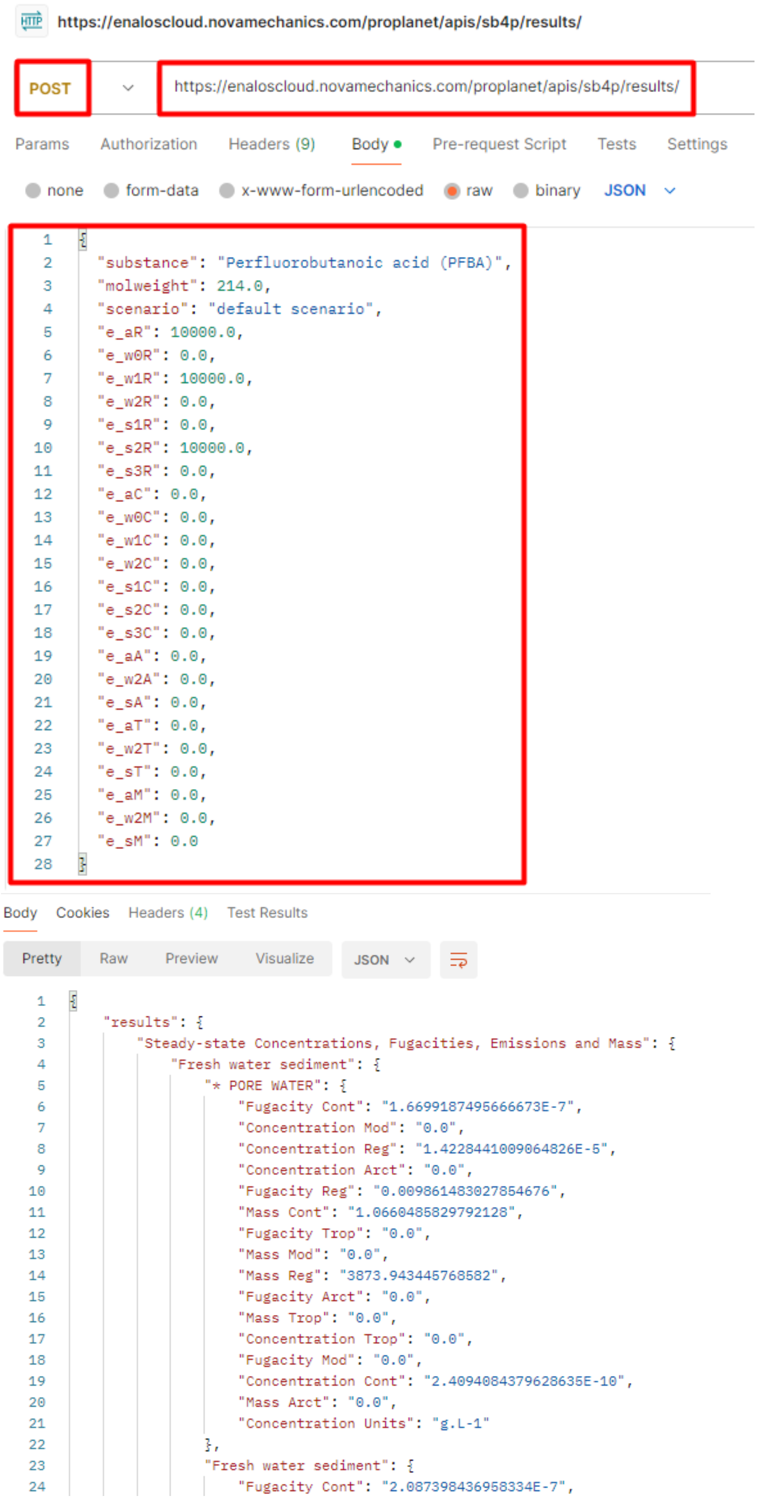


Figure S9. Using Postman to test the functionality of a 'POST' request for the endpoint https://enaloscloud.novamechanics.com/proplanet/apis/sb4p/results/, including input data and response validation.

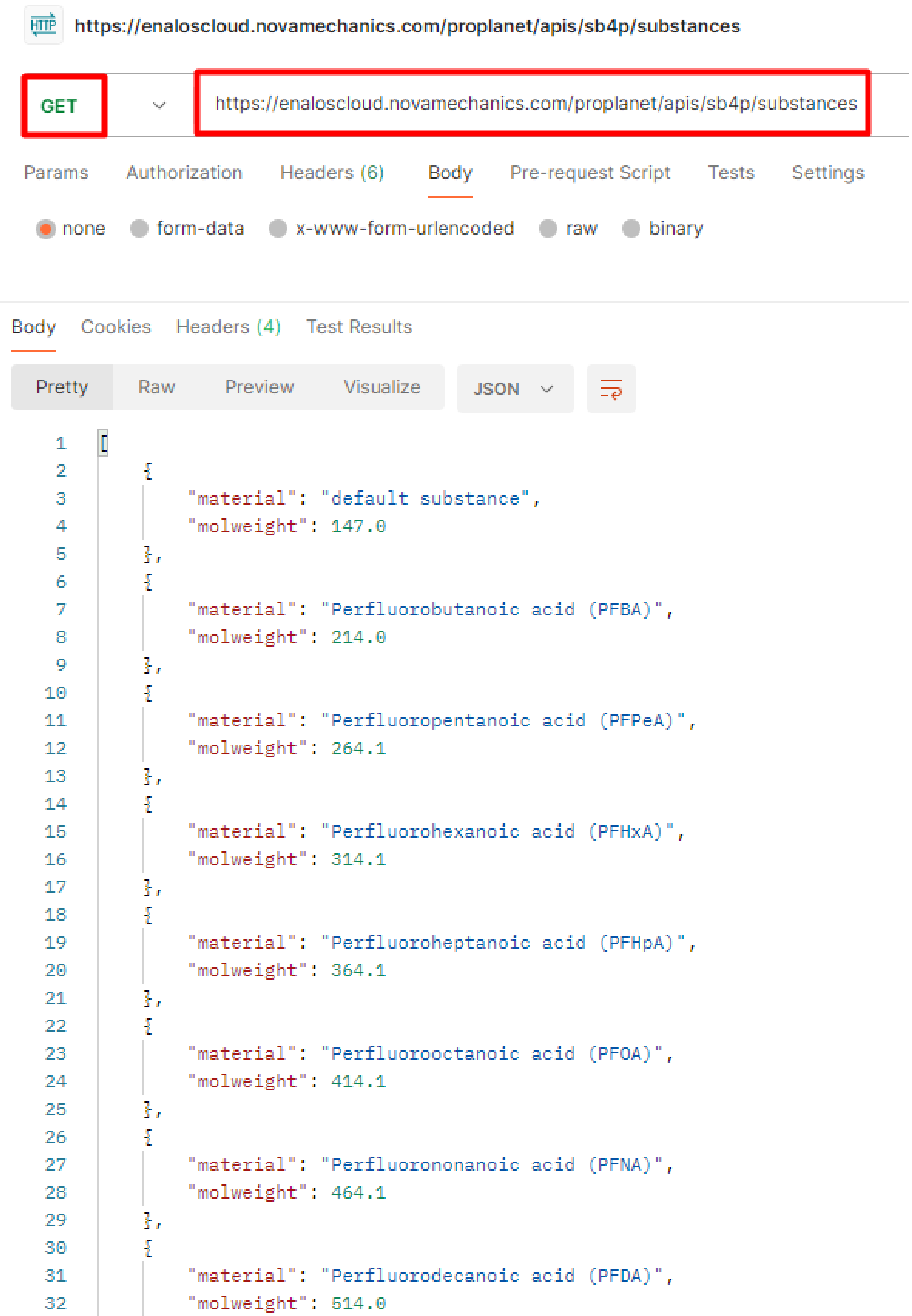


Figure S10. Using Postman to test the functionality of a 'GET' request for the endpoint https://enaloscloud.novamechanics.com/proplanet/apis/sb4p/substances, verifying the request parameters and the expected response.

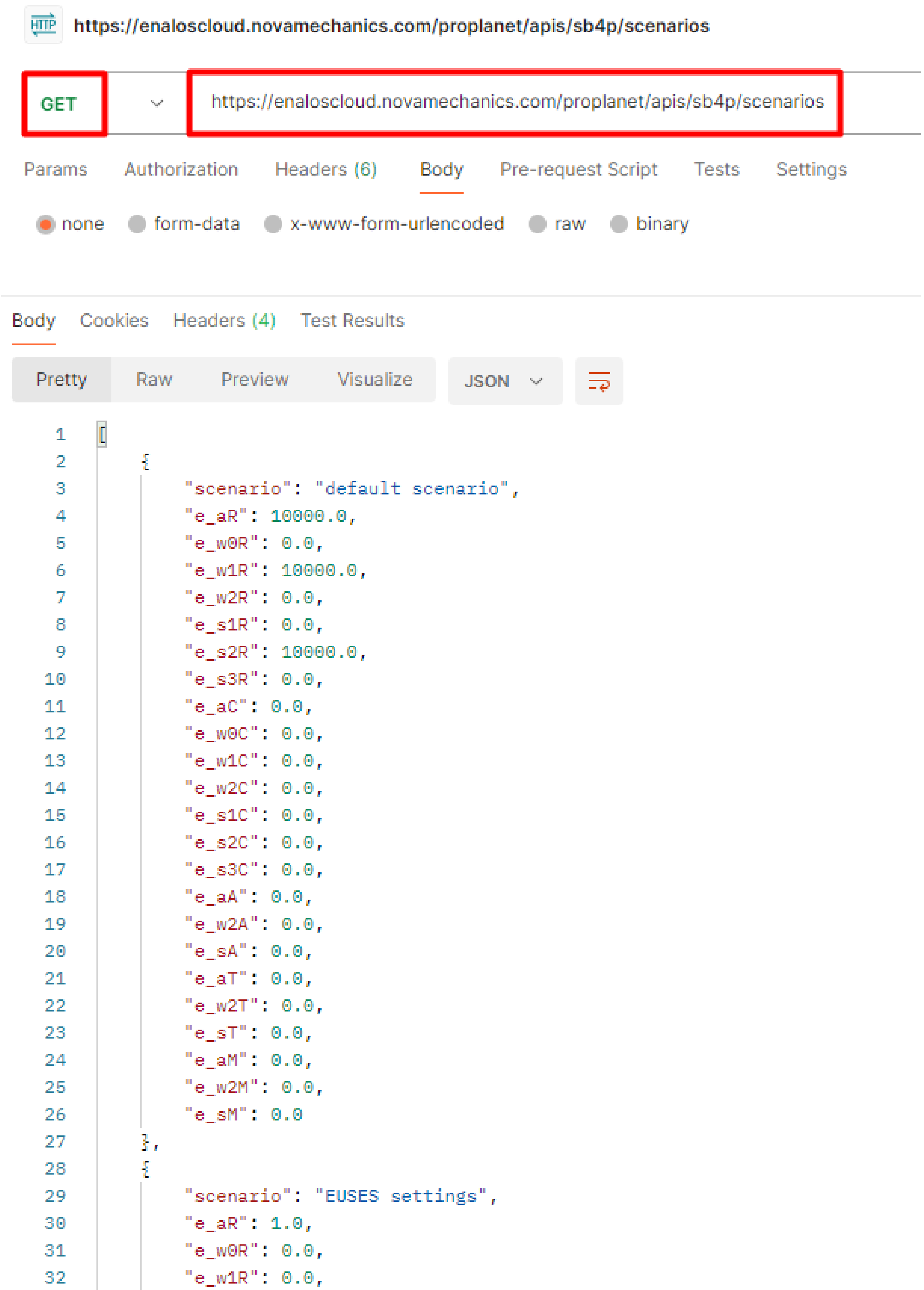


Figure S11. Using Postman to test the functionality of a 'GET' request for the endpoint https://enaloscloud.novamechanics.com/proplanet/apis/sb4p/scenarios, verifying the request parameters and the expected response.

S8. Environmental fate modelling of PFOA

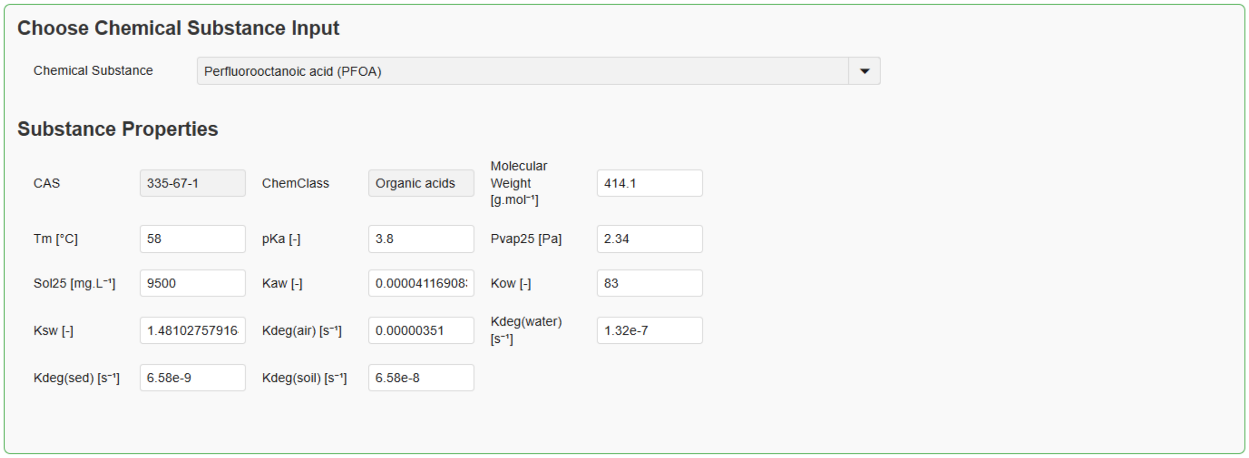


Figure S12. Physicochemical properties of perfluorooctanoic acid (PFOA) used in the SimpleBox4Planet web application to simulate its environmental fate and transport. These include key parameters such as molecular weight, melting temperature (Tm), acid dissociation constant (pKa), vapor pressure at 25 °C (Pvap25), water solubility at 25 °C (Sol25), air-water partition coefficient (Kaw), octanol-water partition coefficient (Kow), soil-water partition coefficient (Ksw), degradation rate in air (Kdeg(air)), degradation rate in water (Kdeg(water)), degradation rate in sediment (Kdeg(sed)) and degradation rate in soil (Kdeg(soil)). The values have been obtained from previous studies.[1-4]

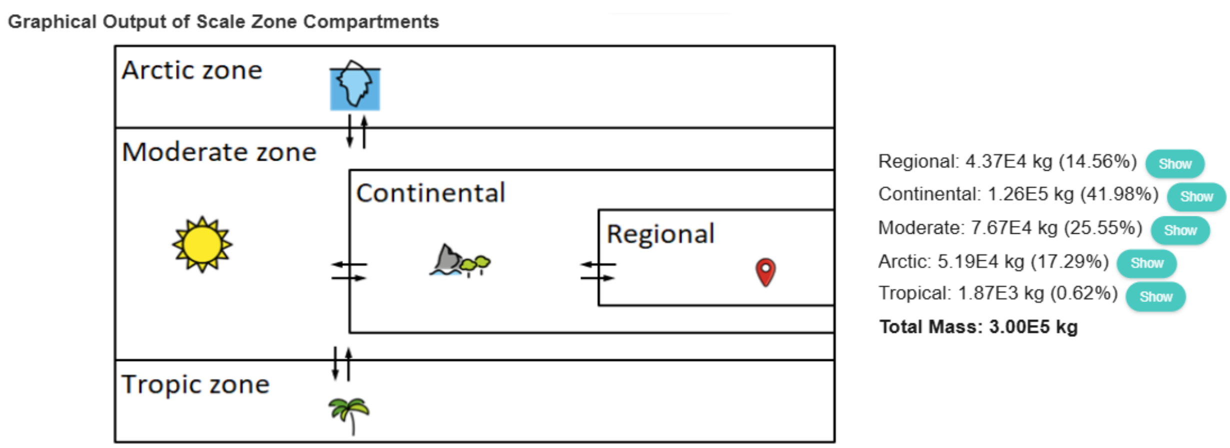


Figure S13. Mass distribution of PFOA across spatial environmental scales following direct emissions of 1,000 tonnes per year to air at the regional scale, as simulated by the *SimpleBox4Planet* web application.

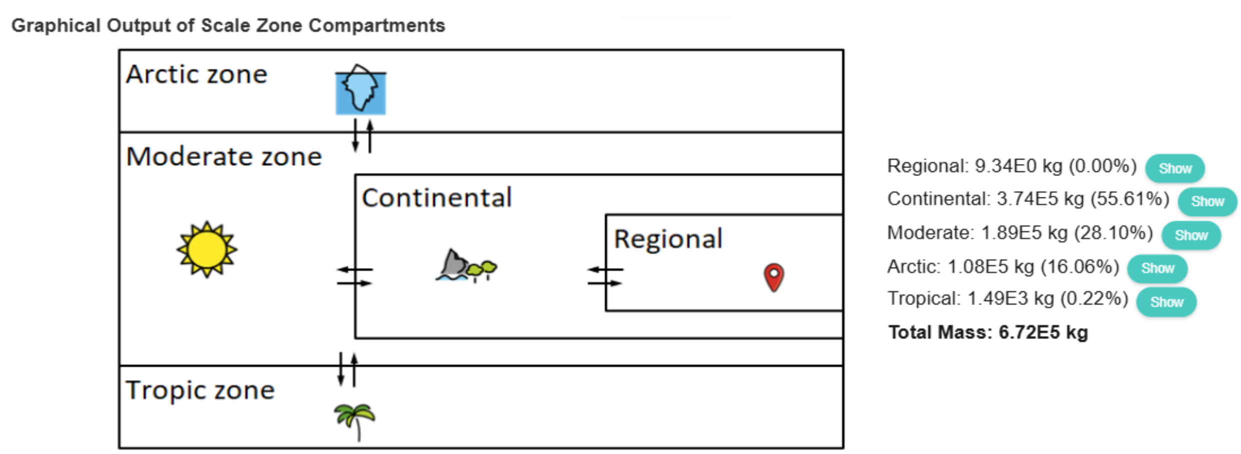


Figure S14. Mass distribution of PFOA across spatial environmental scales following direct emissions of 1,000 tonnes per year to seawater at the continental scale, as simulated by the *SimpleBox4Planet* web application.

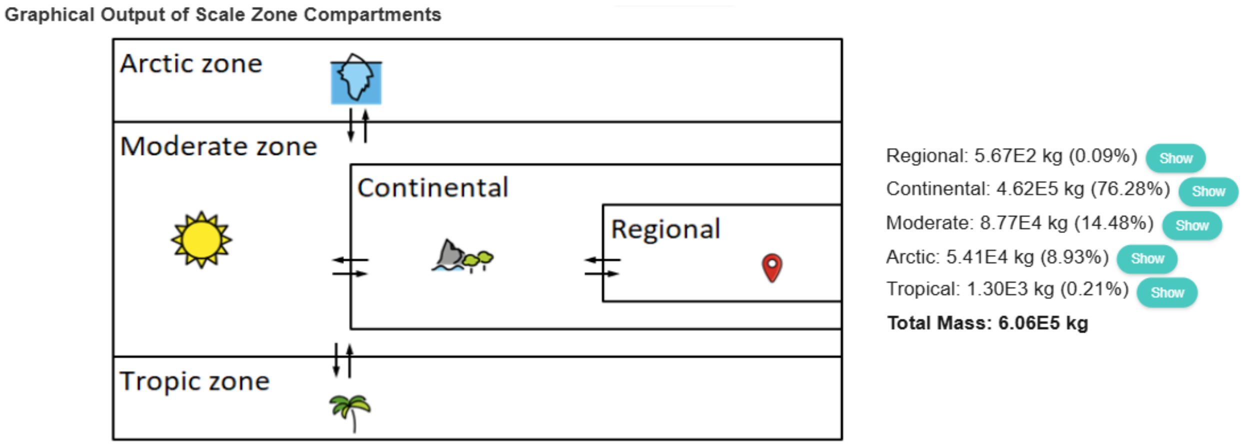
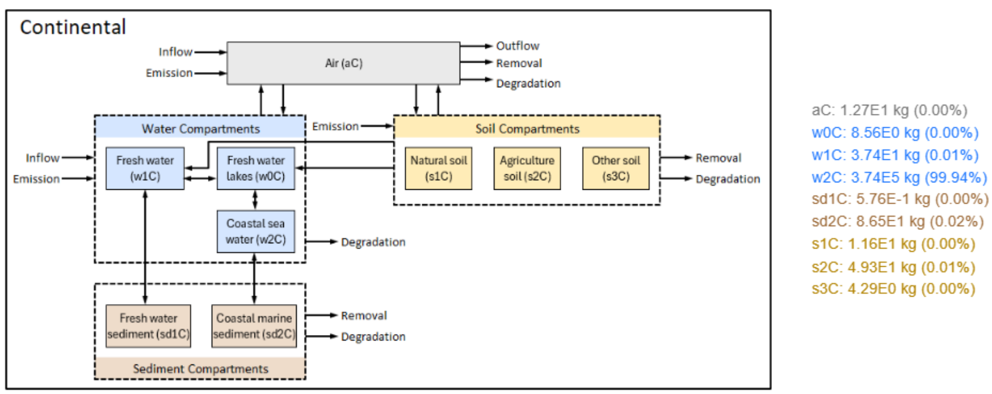
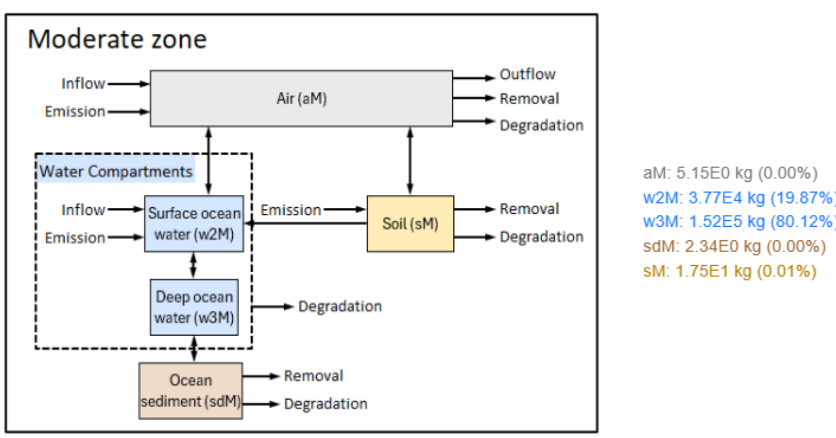


Figure S15. Mass distribution of PFOA across spatial environmental scales following direct emissions of 1,000 tonnes per year to natural soil at the continental scale, as simulated by the *SimpleBox4Planet* web application.





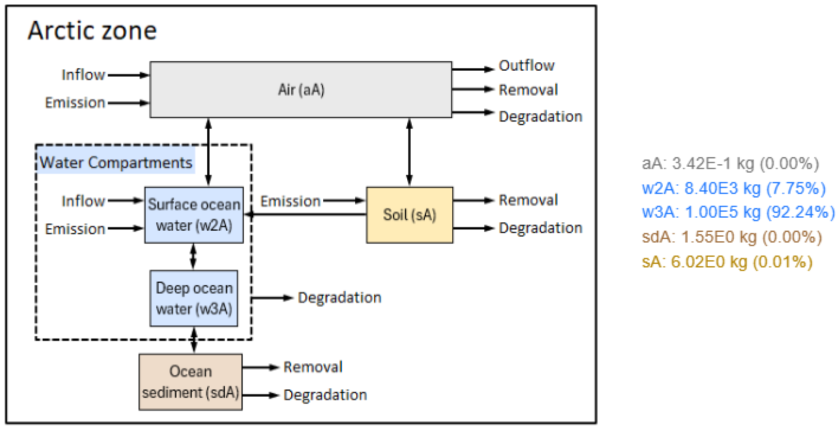
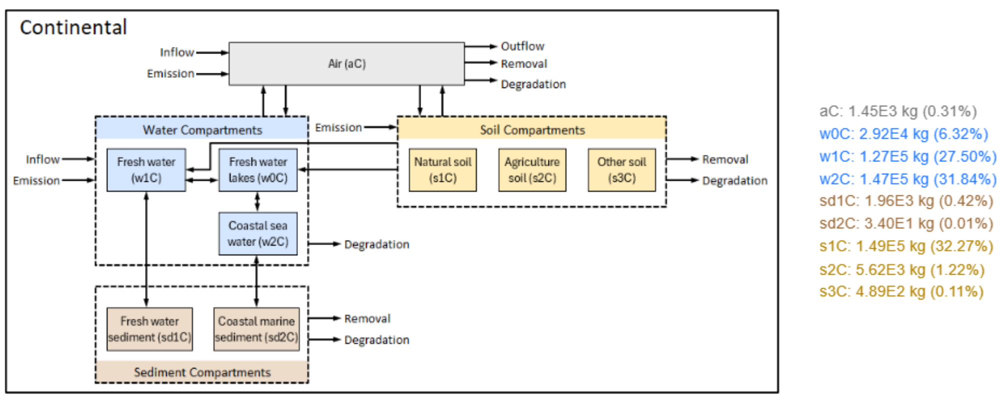
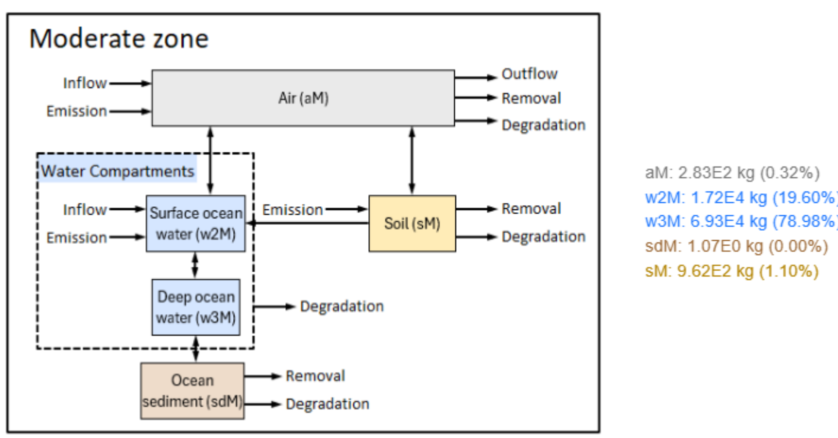


Figure S16. Compartmental-level mass distribution of PFOA simulated using the *SimpleBox4Planet* web application under a direct emission scenario of 1,000 tonnes per year released to seawater at the continental scale. The figure illustrates the percentage of PFOA mass distributed across four environmental compartments—air, water, soil, and sediment—within the continental scale and the moderate and arctic zones of the global scale.





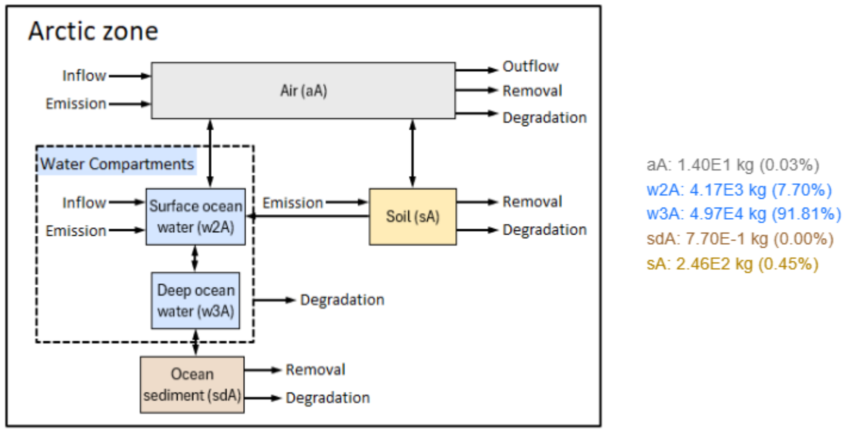


Figure S17. Compartmental-level mass distribution of PFOA simulated using the *SimpleBox4Planet* web application under a direct emission scenario of 1,000 tonnes per year released to natural soil at the continental scale. The figure illustrates the percentage of the PFOA mass distributed across four environmental compartments—air, water, soil, and sediment—within the continental scale and the moderate and arctic zones of the global scale.

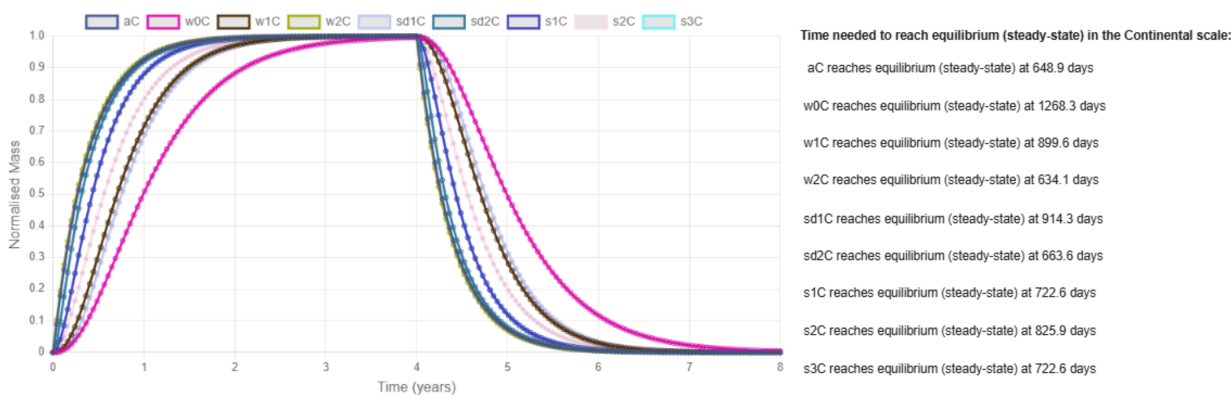


Figure S18. Time-resolved simulation of the normalized mass of PFOA in each environmental compartment at the continental scale, conducted using the SimpleBox4Planet web application under a direct sea water emission scenario of 1,000 tonnes per year. The y-axis represents the normalized mass (i.e., the ratio of dynamic mass to steady-state mass), where a value of 1 indicates that steady-state has been reached. The figure also shows the time to equilibrium for each compartment, annotated in days, and demonstrates that the time required to reach steady-state during the emission phase equals the time required for mass decay following emission cessation, consistent with first-order kinetic behavior.

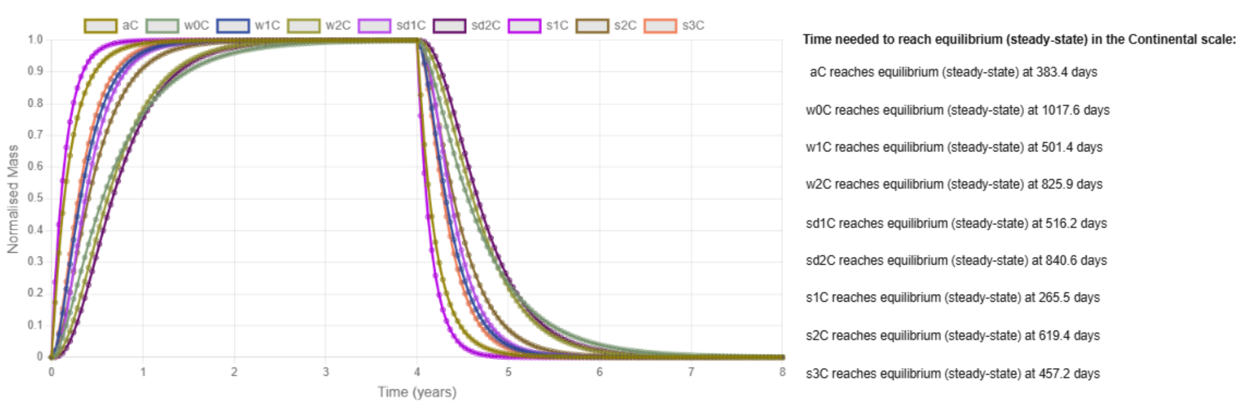


Figure S19. Time-resolved simulation of the normalized mass of PFOA in each environmental compartment at the continental scale, conducted using the SimpleBox4Planet web application under a direct natural soil emission scenario of 1,000 tonnes per year. The y-axis represents the normalized mass (i.e., the ratio of dynamic mass to steady-state mass), where a value of 1 indicates that steady-state has been reached. The figure also shows the time to equilibrium for each compartment, annotated in days, and demonstrates that the time required to reach steady-state during the emission phase equals the time required for mass decay following emission cessation, consistent with first-order kinetic behavior.

Table S8. Experimental matrix of the Plackett–Burman design, consisting of 20 simulation runs, generated using the Isalos Data Analytics Platform. The resulting total mass of PFOA distributed (in kg) was calculated using the *SimpleBox4Planet* web application under a continental-scale direct seawater emission scenario.

T_m	pK_a	*P*vap25	Sol25	K_{aw}	K_{ow}	K_{sw}	Mass distributed (tonnes)
60	0	12	500	0.0000000808	83	1	675.49441
60	3.8	0.1	500	0.0000010000	83	1	675.49459
40	3.8	12	50	0.0000010000	3981	1	675.49468
40	0	12	500	0.0000000808	3981	100	679.49537
60	0	0.1	500	0.0000010000	83	100	678.4957
60	3.8	0.1	50	0.0000010000	3981	1	675.4946
60	3.8	12	50	0.0000000808	3981	100	679.49537
60	3.8	12	500	0.0000000808	83	100	678.49524
40	3.8	12	500	0.0000010000	83	1	675.49467
60	0	12	500	0.0000010000	3981	1	675.49468
40	3.8	0.1	500	0.0000010000	3981	100	679.49581
60	0	12	50	0.0000010000	3981	100	679.49603
40	3.8	0.1	500	0.0000000808	3981	100	679.49535
40	0	12	50	0.0000010000	83	100	678.49588
40	0	0.1	500	0.0000000808	3981	1	675.49441
40	0	0.1	50	0.0000010000	83	100	678.49568
60	0	0.1	50	0.0000000808	3981	1	675.49441
60	3.8	0.1	50	0.0000000808	83	100	678.49522
40	3.8	12	50	0.0000000808	83	1	675.49441
40	0	0.1	50	0.0000000808	83	1	675.4944

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