

Evaluating Brazil's Tiered Approach for Estimating Pesticide Exposure to Soil-dwelling Organisms

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The source of information to perform the modelling is described either in the main manuscript and in the Supplemental Material section (see Supplemental Material _Tables). The sources of information are already mentioned in the References section.

Disclaimer

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1 **Evaluating Brazil's Tiered Approach for Estimating Pesticide Exposure to Soil-** 2 **dwelling Organisms**

3 **Abstract**

4 Brazil's 2023 implementation of mandated ERA frameworks for pesticide registration
5 requires the development of exposure assessment methodologies for soil organisms
6 relevant to local conditions. This Brief Communication evaluates exposure assessment
7 approaches within Brazil's ERA framework, comparing an ESCAPE Climate specific
8 standard local worst-case scenario with locally developed crop-specific scenarios for
9 high-tier exposure tools. Local scenarios were developed by the Brazilian authority for
10 pesticide registration agency (i.e., IBAMA). We analyzed ten pesticides using a tiered
11 approach, beginning with ESCAPE Climate screening and progressing to the USEPA
12 PWC model for higher-tier refinement. Soil exposure was assessed at different depths
13 (i.e., 5 and 10 cm) for earthworms, collembola, and soil microorganisms, incorporating
14 both constant and variable temperature conditions. Initial screening using IBAMA's tier
15 1A standard scenario showed that temperature variability significantly influenced
16 PEC_{SOIL} values, with differences up to 17% between constant and variable
17 conditions. Most of the pesticides failed the risk assessment at this stage. Local scenario
18 development using crop-specific parameters in both ESCAPE Climate and PWC
19 demonstrated refined exposure estimates, with PWC generally producing lower PEC_{SOIL}
20 values due to more comprehensive environmental fate mechanisms being considered..
21 This study highlights the importance of incorporating local scenarios and appropriate
22 refinement tools in regulatory risk assessment schemes for soil organisms, particularly
23 for tropical agricultural conditions. The findings support a tiered exposure assessment
24 framework that balances conservative screening with realistic refinement options for
25 Brazilian agricultural conditions.

26 **Keywords:** Soil organisms, Pesticide Soil Concentration, Soil Exposure Tools, Pesticide
27 Environmental Risk Assessment, Tiered ERA approach

28 **Introduction**

29 The publication of a new regulation for pesticide registration in Brazil in 2023 rendered
30 it mandatory to perform an Environmental Risk Assessment (ERA) as a component of
31 the dossier evaluation (Brasil, 2023). This regulatory amendment highlighted the need to
32 identify knowledge gaps and develop comprehensive ERA processes for non-target

33 organisms (Brasil, 2023; Cione et al., 2024a). The Brazilian Institute of Environment and
34 Renewable Natural Resources (Instituto Brasileiro do Meio Ambiente e dos Recursos
35 Naturais Renováveis, IBAMA), as the responsible environmental agency, has been
36 developing these ERA schemes, with significant progress made through recent research
37 initiatives aimed at establishing frameworks for non-target organism assessment.
38 Regarding soil organisms, the Brazilian environmental agency (henceforth referred to as
39 the agency) started discussing the knowledge gaps in a workshop in 2023 (IBAMA,
40 2023), a prerequisite step before issuing guidelines on ERA schemes for soil organisms.
41 One of the discussions was centered on the most appropriate soil exposure tool to estimate
42 Predicted Environmental Concentrations in the soil (PEC_{SOIL}). During international
43 conferences in Portugal and Germany (see supplemental material), the agency announced
44 its decision to adopt ESCAPE, developed by Klein (2008), as the initial screening tool.
45 ESCAPE is a soil exposure tool, which estimates pesticide concentrations in the soil and
46 in the pore water. The agency subsequently released a worst-case scenario (IBAMA, n.d.)
47 for initial screening, indicating that crop-specific scenarios would be necessary for
48 advancing the ERA scheme for in-soil organisms. For cases where ERA requirements are
49 not met, the agency recommended adopting numerical models for exposure refinement,
50 though this high-tier exposure tool remains undefined.

51 Mackay et al. (2023) analyzed the advantages and limitations of available soil exposure
52 tools and their applicability in Brazil. While agreeing with the agency's recommendation
53 of ESCAPE as a low-tier exposure tool, the authors expressed their concerns about high-
54 tier exposure tools like the Persistence in Soil Analytical Model (PERSAM) - currently
55 used in the European Union's ERA framework (VITO NOV, 2021). They pointed out that
56 such tools are unsuitable for Brazilian conditions due to their rigid parameterization
57 specific to European conditions. These models rely on European-specific databases and
58 fixed scenarios based on European Union soil maps and climate data (Tiktak et.al, 2013,
59 VITO, 2019 and European Food Safety Authority [EFSA], 2015). Unlike the Pesticide
60 Root Zone Model (PRZM) and ESCAPE, which allow for more flexible scenario creation,
61 adapting PERSAM to Brazilian conditions would require extensive soil mapping and
62 parameter adjustments, making it impractical for Brazilian regulatory purposes.

63 In this Brief Communication, we evaluate the benefits of using local scenarios in soil
64 exposure tools (ESCAPE) and demonstrate the applicability of Pesticide in Water
65 Calculator (PWC) tool as a higher-tier exposure tool in Brazilian soil organism ERA. .

66 The PWC is a shell of two modelling tools, Pesticide Root Zone Model (PRZM) and
67 Variable Volume Water Model (VVWM) (U.S. Environmental Protection Agency [EPA],
68 2023). The former estimates pesticide fate and transport in the soil and vadose zone, while
69 VVWM simulates pesticide concentrations in surface water bodies. Through a modeling
70 exercise with 10 plant protection products (PPP), we assess risks according to the soil
71 organism risk scheme discussed by Ibama (IBAMA 2023 and Cione et al. 2024b),
72 exploring exposure refinement options as conveyed by the agency in 2024 (see
73 supplemental material). Our study aims to: (1) demonstrate how developing local
74 scenarios enhances the performance of ESCAPE as a lower-tier tool, making initial
75 screenings more representative of Brazilian conditions, (2) advocate for PWC as a viable
76 higher-tier soil exposure tool for more realistic risk assessments, and (3) highlight the
77 necessity of expanding local scenarios to additional crops for both tools. The findings are
78 expected to contribute significantly to the ongoing development of Brazil's soil organism
79 risk assessment scheme for both lower-tier screening and higher-tier refinement
80 strategies.

81 **Materials and Methods**

82 *Pesticide exposure scheme*

83 Figure 1 shows the pesticide exposure scheme evaluated in this article. The scheme is
84 based on previous public considerations by IBAMA in a workshop held in 2023 (IBAMA,
85 2023; Cione et al., 2024b) and in a presentation at the Akademie Fresenius in June 2025
86 (*see Supplemental Material*). The exposure side of the ERA scheme comprises 3 tiers:
87 1A, 1B, and 1C. The assessment performed in this Brief Communication at each tier is
88 described below. Table 1 presents the soil exposure tools used in each tier and their key
89 parameters. The pesticide application rates are shown in Table S1 (*see Supplemental*
90 *Material*). Additional parameters including application dates, pesticide laboratory and
91 field half-life values (DegT₅₀), and soil characteristics are provided in Tables S2, S3, and
92 S4, respectively.

93 For Tier 1B we developed local ESCAPE Climate crop-specific scenarios for citrus,
94 coffee, cotton and soybeans by adapting soil and weather file inputs from available
95 Brazilian PWC scenarios (*see Exposure calculation in this section*). These scenarios were
96 originally developed for aquatic ERA, and we adapted them to ESCAPE by using soil
97 and weather data from the original scenarios (*see Supplemental Material*).

98 These local scenarios constitute an exercise in the absence of official regulatory scenarios
99 for ESCAPE and that no vulnerability analysis was performed. For potato and tomato, we
100 continued to use IBAMA's worst-case scenario, but, when applicable we incorporated
101 refinements such as crop interception and field DegT₅₀. Crop interception values were set
102 based on Table S1, however because ESCAPE Climate does not allow the user to input
103 crop interception values for each application, we resorted to using the average value. Input
104 crop interception values and field DegT₅₀ are displayed in Table S5, while specific soil
105 input parameters for each scenario are displayed in Table S6

106 **-Soil depth:**

107 (a) Earthworms: 10 cm (b) Collembola and Soil Microorganisms: 5 cm.

108 We used the soil column depth for earthworms and collembola according to the IBAMA's
109 presentation (*see Supplemental Material*). Regarding soil microorganisms, as there was
110 no indication of the soil depth, we considered a soil depth of 5 cm which represents the
111 worst-case scenario..

112 *Evaluated pesticides -agricultural use patterns*

113 We used the same database as Tincani et al. (2023), who initially screened 45 different
114 pesticides. After several refinements, 15 pesticides failed the risk assessment. Of these,
115 five pesticides are registered in other Latin American countries but not in Brazil.
116 Considering our study focuses specifically on Brazil and the development of local
117 scenarios, we excluded these five pesticides and analyzed the remaining ten active
118 ingredients. The list of these pesticides and their critical agricultural practices (cGAP) is
119 provided in the Supplementary Materials. Pesticide names were anonymized.

120 *Exposure calculation*

121 (i) Equations

122 The equations that describe the estimation of the PEC_{SOIL} values in ESCAPE Climate and
123 in the PWC tool are provided in the supplemental material.

124 (ii) Screening with ESCAPE Climate: scenario and input parameters

125 We used a standard worst-case ESCAPE Climate scenario released by IBAMA (IBAMA,
126 n.d.), with input parameters shown in Table S4. The study area is located near the
127 municipality of Itapeva, São Paulo, a region with crops such as soybeans, corn, and wheat

128 (Instituto Brasileiro de Geografia e Estatística, 2023). The GPS coordinates and soil
129 physicochemical parameters were provided by the agency during a workshop in
130 November 2023 and are also described in Cione et al. (2024b). The scenario files are
131 available on the agency's website (IBAMA, n.d.). As this is the only scenario publicly
132 released by the agency, we used it to estimate the PEC_{SOIL} .

133 To compare the effect of the weather file on the modeling output, we have used ESCAPE
134 in (a) constant conditions and (b) variable conditions, which uses the weather file made
135 available by the agency. This weather file contains only the daily average air temperature
136 for the region of Itapeva (*see Figure S1*).

137 (iii) ESCAPE - Development of local scenarios

138 Local scenarios were developed for citrus, coffee, cotton, and soybeans, for which there
139 are Brazilian PWC scenarios available. In this case, we used local weather and soil input
140 parameters from PWC scenarios developed by the agency for aquatic ERA and adapted
141 to ESCAPE Climate (*see Soil exposure tools, item a*). For potato and tomato, although
142 local PWC scenarios are under discussion by IBAMA, they are not available yet;
143 therefore, no exposure assessment was performed in steps 1B and 1C (Figure 1). We used
144 as a template IBAMA's worst case scenario, which contains only average daily
145 temperatures for 2023. Additional details are provided in the Supplemental Material.

146 (iv) PWC scenarios

147 As indicated in the previous item, we have used local PWC scenarios already developed
148 and released by the agency for aquatic ERA (IBAMA, n.d.). A description of how to
149 estimate PEC_{SOIL} values in the PWC tool is provided by Casallanovo et al. (2025). Input
150 parameters can be found in Supplemental Material.

151 (v) PEC_{SOIL} values used in the risk assessment

152 To estimate the risks for soil organisms, we have considered the following conditions:

153 (a) Earthworms and Collembola: time-weighted average (TWA) PEC_{SOIL} values at 28
154 days as indicated by the agency (*see IBAMA's Coimbra presentation 2024 in*
155 *Supplemental Material*)

156 (b) Soil microorganisms: as there was no indication by the agency, we considered the
157 PEC_{SOIL} on the day of the last application (day 0), which represents the worst-case
158 scenario.

159 Regarding ESCAPE Climate, we used the feature “Accumulated PEC”, which estimated
160 the PEC_{SOIL} values after a 10-year period of multiple applications. As for the PWC, as the
161 weather file spans a period of 35 years (1980 to 2015), we used the PEC_{SOIL} values in the
162 last year of application (2015), which typically represents the highest value. For all
163 exposure tools, we used estimated time-weighted average (TWA) PEC_{SOIL} values, as
164 indicated by the agency. (see Supplemental Material).

165 *Pesticide endpoint values*

166 Endpoints for all evaluated soil organisms were retrieved from the Pesticide Properties
167 DataBase (PPDB) (Lewis et al., 2016 and Pesticide Properties DataBase, 2025). They are
168 the same as those used by Tincani et al. (2023).

169 *Risk quotient calculation*

170 (i) Earthworms and collembola

171 Based on IBAMA’s recommendation (see IBAMA’s Coimbra presentation in
172 Supplemental Material), we have used the Toxicity Exposure Ratio approach (TER),
173 adopted by the European Union (EFSA, 2017), and calculated as follows:

$$174 \quad (1) \text{ TER} = \frac{\text{Effect}}{\text{Exposure}};$$

175 This approach considers a level of concern (LOC) of 5.0 for chronic risks. Therefore,
176 TER values above the LOC ($TER > 5$) indicate an acceptable risk for both earthworms and
177 collembola. The only difference regarding IBAMA’s proposition and the exercise
178 performed in this Communication is that we did not divide TER by a factor of 2 when the
179 $\log K_{OW}$ is higher than 2 – a procedure adopted for lipophilic PPPs by other regulatory
180 agencies in Europe (Santé et Consommateurs, 2002), Australia (Australian Pesticides and
181 Veterinary Medicines Authority [APVMA], 2019) and the Andean Countries
182 (Comunidad Andina, 2019). According to van Hall et al. (2024), this correction may not
183 be appropriate and is therefore questionable.

184 As for soil microorganisms, the estimated PEC_{SOIL} values were compared directly with
185 the endpoint. If the exposure is below the effect level, the risk is considered acceptable.

186 **Results and Discussion**

187 *Tier 1 A - Screening exposure calculation with ESCAPE Climate and risk calculation*

188 Table 2 displays the TWA PEC_{SOIL} values for both constant (20°C, no weather file) and
189 variable conditions (Tier I IBAMA scenario) for different soil depths and at 0 and 28
190 days. PEC_{SOIL} values were estimated according to the cGAP displayed in Tables S1 (*see*
191 *Supplemental Material*). Soil input data (soil density, field capacity, wilting point and
192 organic carbon content) were the same for both conditions and are based on IBAMA's
193 worst-case scenario; at this stage (Tier 1A), no crop interception values were considered.

194 For half of the pesticides, estimating the exposure under variable temperature conditions
195 resulted in a decrease in the PEC_{SOIL} values when compared to a constant, fixed
196 temperature; in some cases, the decrease was around -17% (Table 2). However, this result
197 was not uniform; for the other half of the pesticides, the modeling output yielded higher
198 PEC_{SOIL} values. The highest increase at 28 days (11 to 17 %) (Table 2) was observed for
199 three potato crop scenarios where the date of the 1st application occurred between July 1st
200 and July 28th (Table S1), corresponding respectively to the cGAP of Fungicide 4 and
201 Insecticides 4 and 11. Conversely, the highest decrease in the PEC_{SOIL} was observed for
202 the cotton scenario (Fungicide 10), for which the date of the first application occurs in
203 December (Table S1). The difference between constant and variable scenarios is higher
204 at 28 days than at 0-day (day of the last application). The only climatic parameter in the
205 Itapeva weather file is the daily average air temperature. To understand its effect on the
206 PEC_{SOIL} , we plotted the air temperature variation throughout the year and compared it
207 with the application date (Figure S1). The month of July corresponds to the winter season
208 in the Itapeva region, while December is already within the summer. Therefore, in July,
209 the average air temperature is below the standard 20°C used in ESCAPE under constant
210 conditions, while the opposite behavior is observed in December – temperatures are above
211 20°C. Because air temperature directly influences soil temperature, soil temperature is
212 expected to follow similar seasonal patterns. According to the ESCAPE manual (Klein,
213 2008), the equation that is used to estimate the PEC_{SOIL} is influenced by the soil
214 temperature, where the estimated residues are corrected/normalized against daily soil
215 temperatures. Consequently, this normalization process can explain the different trends
216 according to time of application.

217 The PEC_{SOIL} values estimated with the agency's standard scenario was then used to
218 estimate risks to soil organisms for each PPP (Table 3). As indicated, only Fungicide 4

219 passed the risk assessment. This result was expected because Fungicide 4 is not persistent
220 in soil and only moderately toxic to soil organisms (Tincani et al., 2023). For the
221 remaining 9 pesticides, the assessment then escalated to Tier 1B.

222 *Tier 1B - Exposure refinement with local Brazilian scenarios in ESCAPE Climate*

223 According to the flowchart in Figure 1, the next step at Tier 1B is to develop specific crop
224 scenarios in ESCAPE Climate for those cases where the risk assessment fails and include
225 refinement options such as crop interception values and field DegT₅₀. As discussed by
226 Tincani et al. (2023), accounting for crop interception values will depend on the label
227 GAP, for instance, if the label indicates a soil application, there is no crop interception.
228 Likewise, as indicated in Tables S3 and S6, for some pesticides the field DegT₅₀ does not
229 differ much from the ones estimated under laboratory conditions. Regarding local
230 scenarios for aquatic organisms, IBAMA has already developed and released Brazilian
231 crop-specific exposure scenarios for the PWC, including coffee, cotton, citrus and
232 soybeans, while scenarios for crops such as potatoes and tomatoes are under discussion,
233 but are not available yet. Therefore, in the latter case we have resorted to using the current
234 worst-case IBAMA scenario (Itapeva) and consider, where applicable, refinements such
235 as crop interception and/or field DegT₅₀, which are displayed on Table S6), while the
236 refined TER calculation is in Table 4.

237 The refined TER calculation indicates that Fungicide 10 and Insecticide 15 pass the
238 refined risk assessment. Regarding the pesticides, the exposure can be further refined with
239 a high-tier exposure tool (Tier 1C). However, as potatoes and tomatoes do not have local
240 crop scenarios available, we did not continue with refinements for Fungicide 2,
241 Insecticides 4, 5, 10 and 11. This is a data gap that can be addressed either by the agency
242 or the scientific community, but it is not within the scope of this manuscript.

243 *Tier 1C - Exposure estimation with PWC and with local Brazilian scenarios*

244 As a higher-tier option (1C) for the soil exposure tool, we use the USEPA PWC to
245 estimate the PEC_{SOIL}. The feasibility of using this exposure tool has already been
246 discussed by Casallanovo et al. (2025). As previously described in Materials and
247 Methods, we used local crop-specific exposure scenarios for coffee and soybeans released
248 by the agency for aquatic ERA and recalculated the TER only for the soil organism for
249 which concerns have been observed in the previous steps, namely collembola for
250 Fungicide 3 and earthworms for Fungicide 6. The refined risk assessment is displayed in

251 Table 5. The outcome indicates that Fungicide 3 passes the risk assessment for all
252 scenarios, while Fungicide 6 fails the risk assessment for all scenarios. In the latter case,
253 as no additional exposure refinements are available, to continue the ERA scheme, risk
254 assessors may resort to refining the the effect endpoint by considering the geomean,
255 SSDs, Toxicokinetic-Toxicodynamic (TKTD) approaches, or higher-tier field studies.
256 This approach has already been discussed by the agency in previous workshops (IBAMA,
257 2023; Cione et al, 2024b) and might be a viable option to continue the ERA for highly
258 toxic PPPs to soil organisms.

259 **Conclusion**

260 We have evaluated the exposure side of the ERA scheme for soil organisms according to
261 Brazilian environmental authority proposition, aiming both to evaluate its feasibility and
262 to contribute to discussions regarding the adoption of a soil organism risk assessment
263 scheme in Brazil. The results indicated that developing local scenarios can help refine the
264 exposure estimates further. While ESCAPE scenarios generally produce results close to
265 worst-case estimates (Table 2), using PWC as a high-tier exposure tool (step 1C in
266 IBAMA's proposition) showed further reductions in PEC_{SOIL} values. However, these
267 reductions were not always sufficient to eliminate risk concerns, as demonstrated with
268 Fungicide 6 (Table 5). Nonetheless, it still demonstrates the potential of using this tool,
269 as it considers mechanisms that are not accounted for in ESCAPE (Casallanovo et al.,
270 2025). To add further realism to the evaluation, an additional step that could be addressed
271 either by the Brazilian environmental agency and/or by the academic community is to
272 develop crop- specific exposure scenarios for an ERA scheme for soil organisms.

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360

Table Caption

361

Table 1. Soil exposure assessment tools and parameters by tier level

362

Table 2. PEC_{SOIL} values for pesticides at different soil depths under constant (20°C) and

363

variable temperature conditions and their percent difference (%).

364

Table 3. Tier 1A risk estimation based on ESCAPE Climate and IBAMA worst-case

365

scenario output. In bold, PPPs which failed the risk assessment

366

Table 4. Tier 1B risk estimation based on ESCAPE Climate, refined IBAMA worst-case

367

scenario and local crop scenarios. In bold, PPPs which failed the risk assessment

368

Table 5. Tier 1C risk estimation based on PWC and local crop scenarios. In bold, PPPs

369

which failed the risk assessment

370

371 **Figure Caption**

372 **Figure 1.** Overview of soil organism ERA exposure assessment. (A) IBAMA-specified
373 soil column depths by organism type, and (B) tools for PEC_{SOIL} estimation. Panel A
374 illustration created using Microsoft Copilot Artificial Intelligence (AI); Panel B content
375 based on IBAMA (2023) and Supplemental material.

376 **Note:** IBAMA – Instituto Brasileiro do Meio Ambiente e Recursos Renováveis [*Brazilian Institute of*
377 *Environment and Renewable Natural Resources*], PEC_{SOIL} -Predicted Environmental Concentration in the
378 soil

379 **Alt text:** A two-part diagram illustrating a tiered environmental risk assessment (ERA) framework for soil
380 organisms. Panel A is a cross-section of a soil profile showing the required assessment depths: 5 cm for
381 collembola, soil mites, and microorganisms, and 10 cm for earthworms. Panel B is a flowchart detailing
382 the three-tiered assessment process: Tier 1A involves initial screening using the ESCAPE analytical model
383 with a worst-case scenario; Tier 1B involves refined assessment using ESCAPE with crop-specific
384 scenarios if Tier 1A fails; and Tier 1C involves higher-tier assessment using the USEPA PWC model to
385 consider additional environmental transformation mechanisms if Tier 1B fails

Figure 1.

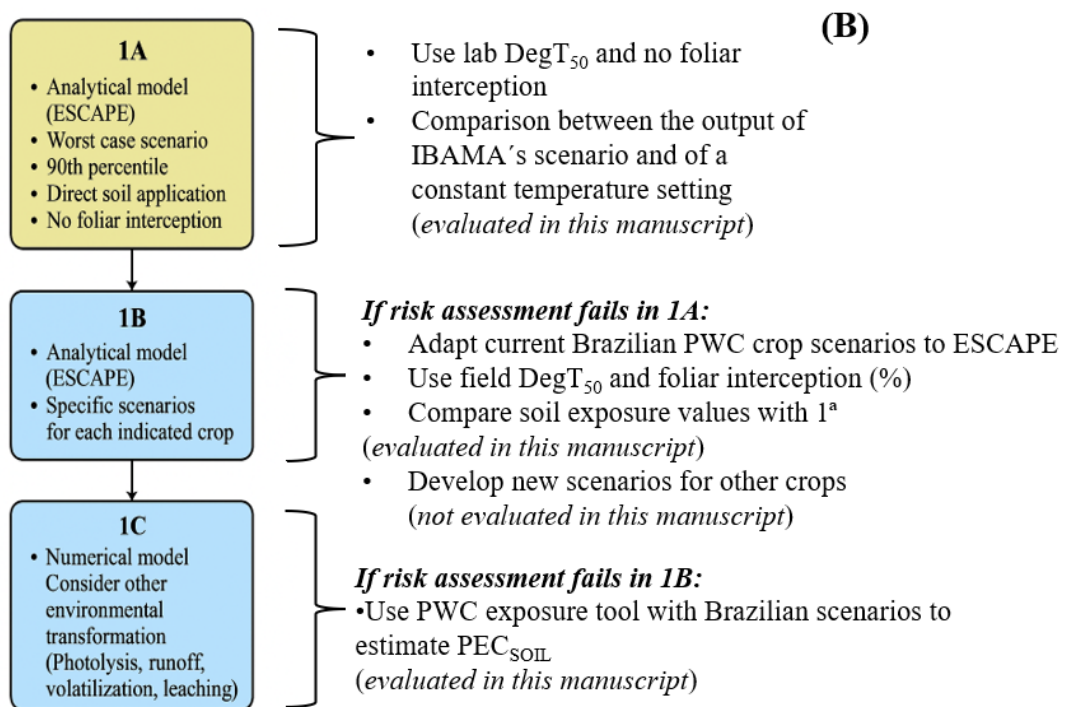
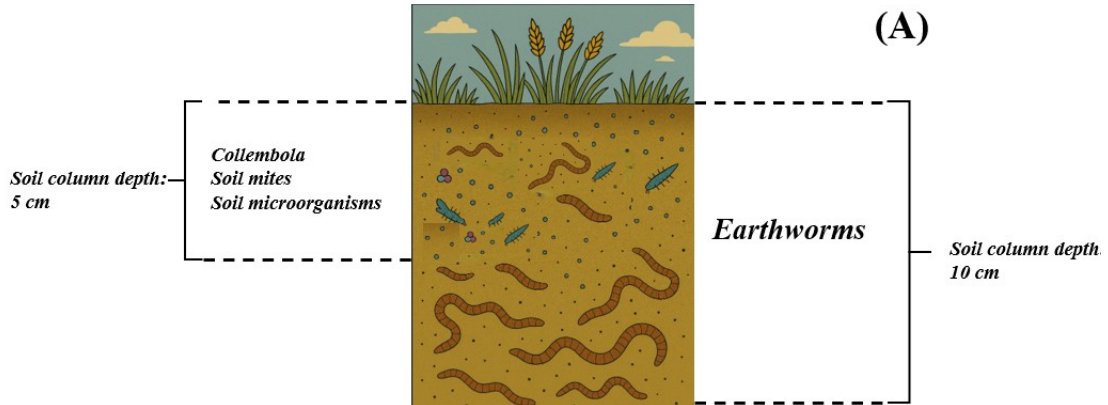


Table 1. Soil exposure assessment tools and parameters by tier level

Tier	Tool Used	Description	Key Parameters
1A	ESCAPE Climate	Initial screening	- IBAMA's worst-case scenario (Tier-1_IBAMA) - 0% crop interception - Laboratory DegT ₅₀
1B	ESCAPE Climate	Refined assessment	- Local crop-specific scenarios - Crop interception (if applicable) - Field DegT ₅₀
1C	USEPA PWC	Higher-tier assessment	- Local crop-specific scenarios - Crop interception (if applicable) - Field DegT ₅₀ - Most refined parameters: application method, soil layers*, crop-specific parameters**

*Multiple of soil horizons and its parameters (e.g. soil horizon thick, soil horizon density)

**Emergence, maturity and removal dates, root depth, canopy details (cover, height and hold-up)

Note:

USEPA – United States Environmental Agency, PWC – Pesticide in Water Calculator, IBAMA – Instituto Brasileiro do Meio Ambiente e Recursos Renováveis [*Brazilian Institute of Environment and Renewable Natural Resources*]

DegT₅₀ – pesticide half-life in soil

Table 2

Molecule	Crop	Soil depth (cm)	PEC _{SOIL} (mg a.i./kg soil dw)					
			0-day			28-day, TWA		
			Constant	Variable	Difference (%)	Constant	(b)Variable	Difference (%)
Fungicide 2	Potato	5	5.57	5.41	- 2.88	5.49	5.33	- 2.94
		10	2.79	2.71		2.75	2.67	
Fungicide 3	Soybeans	5	2.10	2.19	+ 4.59	1.56	1.71	+ 10.1
		10	1.05	1.09		0.778	0.857	
Fungicide 4	Potato	5	3.35	3.71	+ 10.8	2.00	2.35	+ 17.3
		10	1.67	1.86		1.00	1.17	
Fungicide 6	Coffee	5	0.525	0.520	- 0.93	0.493	0.485	- 1.46
		10	0.263	0.260		0.246	0.243	
Fungicide 10	Cotton	5	0.265	0.231	- 12.8	0.198	0.164	-17.4
		10	0.133	0.116		0.099	0.0817	
Insecticide 4	Potato	5	10.3	11.0	+ 6.36	7.60	8.58	+ 12.9
		10	5.17	5.50		3.80	4.29	
Insecticide 5	Tomato	5	7.43	7.18	- 3.36	7.29	7.00	- 3.92
		10	3.72	3.59		3.64	3.50	
Insecticide 10	Potato	5	1.49	1.50	+ 0.66	1.39	1.42	+ 1.94
		10	0.743	0.748		0.697	0.710	
Insecticide 11	Potato	5	2.11	2.20	+ 4.73	1.17	1.31	+ 11.6
		10	1.05	1.10		0.587	0.655	
Insecticide 15	Citrus	5	0.513	0.510	- 0.58	0.470	0.456	- 2.83
		10	0.256	0.255		0.235	0.228	

Note 1: values were rounded up

Note 2: PEC_{SOIL} -Predicted Environmental Concentration in the soil, TWA – time-weight average

Table 3.

Molecule	Earthworm, NOEC	28-day PEC _{SOIL} TWA, 10 cm	TER	Collembola, NOEC	28-day PEC _{SOIL} TWA, 5 cm	TER	C&N, effect	0-day PEC _{SOIL} , 5 cm	Risks?	Final Result
Fungicide 2	1.2	2.67	0.45	1000	5.33	187	8	5.41	No	Fail
Fungicide 3	1.0	0.857	1.17	0.36	1.71	0.21	2	2.19	Yes	Fail
Fungicide 4	50	1.17	42	18	2.35	7.66	4.8	3.71	No	Pass
Fungicide 6	0.75	0.243	3.09	55.8	0.485	115	3.33	0.520	No	Fail
Fungicide 10	0.315	0.082	3.86	5	0.164	30.6	1	0.231	No	Fail
Insecticide 4	0.84	4.29	0.19	0.21	8.58	0.02	4.0	11.0	Yes	Fail
Insecticide 5	12.7	3.50	3.6	0.08	7.00	0.01	6.4	7.18	Yes	Fail
Insecticide 10	500	0.710	704	0.08	1.42	0.06	0.893	1.50	Yes	Fail
Insecticide 11	1.8	0.655	2.75	9.26	1.31	7.07	3.33	2.20	No	Fail
Insecticide 15	0.29	0.228	1.27	3.38	0.456	7.41	8	0.51	No	Fail

Note 1: values were rounded up

Note 2: NOEC = No Observed Effect Concentration, values in mg a.i./kg soil

PEC_{SOIL} -Predicted Environmental Concentration in the soil, values in mg a.i./kg soil dw

TWA – time-weight average

TER = Toxicity Exposure Ratio

C&N = carbon and nitrogen studies. Units are in mg a.i./kg soil

Table 4.

Molecule	Scenario name	Earthworm, NOEC	28-day PEC _{SOIL} TWA, 10 cm	TER	Collembola, NOEC	28-day PEC _{SOIL} TWA, 5 cm	TER	C&N, effect	0-day PEC _{SOIL} , 5 cm	Risks?	Final Result
Fungicide 2	IBAMA Tier I	1.2	1.41	0.85	1000	2.82	355	8	2.92	No	Fail
Fungicide 3	Alegria	1.0	0.134	7.48	0.36	0.267	1.35	2	0.373	No	Fail
	LEM		0.105	9.51		0.210	1.71		0.312	No	
	Nova Candelaria		0.133	7.51		0.267	1.35		0.373	No	
Fungicide 6	Coqueiral	0.75	0.245	3.06	55.8	0.477	117	3.33	0.530	No	Fail
	Jaguaré		0.178	4.21		0.353	158		0.403	No	
	Santana da Vargem		0.245	3.06		0.477	117		0.530	No	
Fungicide 10	Brasnorte	0.315	0.0268	11.7	5	0.0536	93.3	1	0.0848	No	Pass
	LEM		0.0219	14.4		0.0438	114		0.0709		
	Sapezal		0.0221	14.3		0.0442	113		0.0696		
	Sorriso		0.0262	12.0		0.0525	95.2		0.0838		
Insecticide 4	IBAMA Tier I	0.84	2.74	0.31	0.21	5.47	0.04	4.0	9.17	Yes	Fail
Insecticide 5	IBAMA Tier I	12.7	0.527	24.1	0.08	1.05	0.08	6.4	1.37	No	Fail
Insecticide 10	IBAMA Tier I	500	0.614	814	0.08	1.22	0.06	0.893	1.37	Yes	Fail
Insecticide 11	IBAMA Tier I	1.8	0.479	3.76	9.26	0.958	9.66	3.33	1.69	No	Fail
Insecticide 15	Avai/Duartina*	0.29	0.0386	7.51	3.38	0.0772	43.8	8	0.120	No	Pass
	Ipigua		0.0367	7.90		0.0735	46.0				
	Itajobi		0.0376	7.71		0.0752	44.9				
	José Bonifacio		0.0366	7.92		0.0732	46.2				

*Local soil input data (see Table S5) and weather file are the same

Note 1: values were rounded up

Note 2: NOEC = No Observed Effect Concentration, values in mg a.i./kg soil

PEC_{SOIL} -Predicted Environmental Concentration in the soil, values in mg a.i./kg soil dw

TWA – time-weight average

TER = Toxicity Exposure Ratio

C&N = carbon and nitrogen studies. Units are in mg a.i./kg soil

Table 5.

Molecule	Crop	Scenario name	Collembola, NOEC	28-day TWA PEC_{SOIL} (mg a.i./kg soil dw), 5 cm	TER
Fungicide 3	Soybeans	Alegria	0.36	0.0423	8.51
		LEM		0.0496	7.25
		Nova Candelária		0.0054	66
Molecule	Crop	Scenario name	Earthworm, NOEC	28-day TWA PEC_{SOIL} (mg a.i./kg soil dw), 10 cm	TER
Fungicide 6	Coffee	Coqueiral	0.75	0.172	4.36
		Jaguaré		0.156	4.81
		Santana da Vargem		0.197	3.81

Note: LEM – Luis Eduardo Magalhães, Bahia state

NOEC = No Observed Effect Concentration, values in mg a.i./kg soil

PEC_{SOIL} -Predicted Environmental Concentration in the soil, values in mg a.i./kg soil dw

TWA – time-weight average

TER = Toxicity Exposure Ratio