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Sensibility testing of a NH_3 volatilisation model for APSIM

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Abstract: The majority of atmospheric NH_3 is estimated to stem from agriculture. The currently released version of APSIM does not include volatilisation and this is a major omission in the model. Reliable data quantifying volatilisation is too sparse to use as the sole source of testing for the model. Here we describe a sensibility-based process for elucidating knowledge as narrative statements and then using those statements to more rigorously test the model with the aim of avoiding serendipitous equifinality in the parameterisation.

Keywords: *APSIM, Cropping Systems Model, Model Testing, Model Development*

1. INTRODUCTION

Globally, over 75% of atmospheric NH_3 is estimated to stem from agriculture (Lan et al., 2024). Studies have found that volatilisation is highly influenced by environment (soil moisture, temperature, pH, wind speed), the location (primarily depth in the soil), and concentration of N pools (Sommer, 2004). Volatilisation is difficult to measure so field studies are limited in number and scope. In addition, volatilisation is a highly sporadic process – providing further challenges to conducting robust field measurements and obtaining reliable data.

Process-based models are a valuable tool to expand the scope of the available studies, simulating NH_3 volatilisation beyond the bounds of controlled experiments. In 2010, Cichota et al. developed a prototype of the volatilisation process for APSIM (Holzworth et al., 2014) v7 using methods based largely on Génermont and Cellier (1997). The model has been applied in several studies including Vogeler et al. (2013) and Snow et al. (2025) but, until recently, was not adopted into the updated version of APSIM (Holzworth et al., 2018), partly for lack of testing.

Given the complexity inherent to any field experiment and the scarcity of field experiments available for testing the model, we decided to rely on a combination of traditional data-based testing with sensibility analysis to verify the robustness of the model. Sensibility tests reduce the risk of serendipitous equifinality, i.e. modelling the correct outcome *via* incorrect mechanisms or parameters, and enhance the scope of soils and environments in which the model can be used with some confidence. Testing the major processes independently in controlled simulations first builds confidence that the model is working as expected such that subsequent tests of the model against field experiments (wherein those processes will interact with each other and site-specific conditions) yield meaningful conclusions about the model's performance. This paper concentrates on the sensibility analysis and describes our approach to this methodology.

2. OUR SENSIBILITY TESTING APPROACH

Drawing from a combination of established theory and a literature review, we first devised eight sensibility tests directed at the range of mechanisms in the volatilisation process. These were to evaluate the model's response to: (1) applying urea fertiliser to soils of varying moisture; (2) a range of initial soil pHs and soil buffering capacities; (3) wind speed; (4) the concentration of urea in the soil at application; (5) the depth of urea application; (6) a reduction in the nitrification rate; (7) the effect of varying ambient temperature; (8) the time course of emissions after a fertiliser application. These are mapped against a volatilisation process diagram (Figure 1). Each of these tests are backed by published literature to support narrative assertions that reflect what we expect the model to produce. For example, taking the first test, we make the statement:

> Application of urea onto a dry (vs. moist) soil surface with no subsequent rain will result in low volatilisation losses due to slow hydrolysis which then allows the nitrification process to moderate the soil pH necessary for high volatilisation losses.

Stating the tests and our expectations in this narrative style (followed by supporting literature) allowed us to devise simulation tests that reflect the major process interactions without needing detailed ancillary experimental data. While alignment of the model's predictions with these evidence-based expectations provides confidence in the model, any combinations of environmental and chemical drivers that defy the expectations are particularly valuable as that leads to further, detailed examinations.

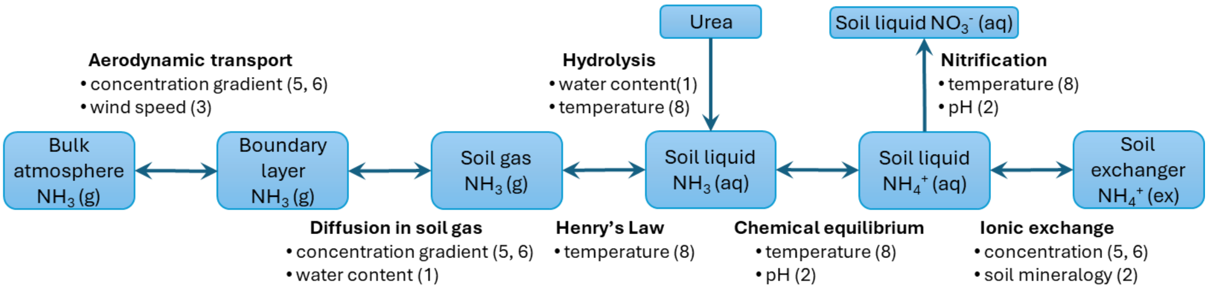

Figure 1. Diagram of APSIM model for NH_3 volatilisation (adapted from Cichota and Snow, 2012). The numbers in parenthesis correspond to the list of sensibility tests. Most of the processes are non-linear so the effect of source strength (test number 4) is tested throughout.

3. CONCLUSIONS

Before its release for general use, the prototype ammonia volatilisation model needs to undergo various tests, including a sensibility test. Sensibility tests evaluate whether the model outputs are logical, the code is working as expected, and the model is responding reasonably to changes in the system's environment and management (Holzworth et al., 2011). Such tests increase confidence and transparency in the model's performance, providing a foundation for future model users in their interpretation of the simulation results.

These initial tests focus on volatilisation from the application of urea fertiliser. Future work will look at how well the model simulates more complex additives and conditions (e.g., urine patches, manure slurry). Following the sensibility tests, the model will be further tested in model-data comparisons using datasets collected in Australia, New Zealand, and Europe.

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