Description of 1-D soil biogeochemistry model in ISAM

A scheme explicitly calculating soil organic carbon (SOC) profile has been implemented to Integrated Science and Assessment Model (ISAM). All Parameters in this document are summarized in Table 1.

**Part 1: Updated Model Framework for biogeochemistry component**

Original ISAM biogeochemistry component follows Yang et al., 2009.

**1. SOC pools cascade and structure.**

 In the original ISAM bulk soil model, soil pools have been categorized into aboveground and belowground categories based upon both the impact of litter quality and soil depth on residence time. However, in the vertically-resolved soil model the soil depth information has been explicitly represented so we revised the original model structure. Fine root litter and leaf litter have been put into one category, the fast pool, following the same model structure of aboveground pools in old ISAM version, while stem and coarse root litter are classified into another category, the recalcitrant pools, following belowground pools. This modification is based on their different composition and the recalcitrance to decomposition from litter bag studies including in the arctic ecosystem (Sloan et al., 2013).

 Each soil pool has been separated into 10 layers identical to the soil thermal layers. Each layer has separated soil degradation processes and the exchange of soil organic carbon between two layers can only happen through vertical transport.

**2. Vertical transport of SOC**

 The transport of soil organic matter into deep soil is achieved through two processes: advection and diffusion. Diffusion is used here to describe bioturbation and movement due to gravity, however the gravitational effect on vertical SOC transport is much weaker compared to the bio-turbation effect so the diffusion process is mostly dominated by bioturbation. Advection describes the transportation of the liquid phase SOC into deeper mineral soil. Here we follow equations from Elzein and Balesdent (1995) and apply it to each litter and soil pool:

$$\frac{∂C}{∂t}=D\frac{∂^{2}C}{∂z^{2}}-ν\frac{∂C}{∂z}+S$$

 Where C is the volumetric concentration of soil organic carbon (kgC/m3) in each pool. D is the diffusion coefficient (m2s-1) describing the strength of bioturbation and cryoturbation which specifically occurs in permafrost region. Gravity has been omitted due to its relatively smaller contribution to total transportation), V is the coefficient of advection (m s-1) representing transportation through water. S is the source/sink term describing any reaction happening together with organic carbon transportation simultaneously, including SOC decomposition, litter input into litter pool and the degradation of SOC (transferring between different soil pools). Considering the source/sink term, the equation changes to:

$$\frac{∂C}{∂t}=D\frac{∂^{2}C}{∂z^{2}}-ν\frac{∂C}{∂z}-kC+f\_{d}+\sum\_{i=1}^{N\_{c}}α\_{ij}k\_{i}C\_{i}$$

 Here k is the decomposition rate after considering litter/soil material quality, nitrogen availability and environmental constraints on decomposition. $f\_{d}$ is the litter input into each layer. $α\_{ij}$ is the fraction of the byproducts produced from decomposition of SOC in another pool i that transferring to current pool j.

 The whole convection-diffusion equation is solved by applying boundary condition below:

$$\left\{\begin{array}{c}D\frac{∂C}{∂z}-νC=f\_{s}\left(top,fluxboundary\right)\\\frac{∂C}{∂z}=0\left(bottom,zeroboundary\right)\end{array}\right.$$

 The transport of SOC is solved with the finite difference method, and the power law discretization scheme (Patankar 1980) is applied to prevent numerical instability. The upper boundary condition is discretized through the central difference scheme while lower boundary condition can be directly interpreted as constant SOC densities below the deepest layer. The transport component is simulated weekly.

**3. Discretized litter input, soil decomposition and corresponding environmental modifiers.**

Previously, the litter input was a single flux into corresponding litter pools (Yang et al., 2009). In 1-D soil model we put leaf and stem litters directly into the surface soil layer, and root litter input is distributed into each soil layers depending on the plant root fraction calculated based on root biome mass and biome type (El Masri et al., 2015).

We keep using the same residence time and decomposition formula for organic carbon as described in Yang et al., 2009 but discretize the calculation into each layer. In original ISAM, soil pool cascade had been partitioned into “aboveground” and “belowground.” After modifying the structure fast pools follow the calculation of aboveground pools while recalcitrant pools are derived from the calculation of belowground pools.

 Temperature modifier has been changed to a variant Q10 function in order to differentiate temperature impact on decomposition at different soil depth:

$$\left\{\begin{array}{c}f\_{i,fast}\left(T\right)=a\_{fast}Q\_{10,fast}^{\frac{T\_{i,soil}-T\_{ref,fast}}{10}}\\f\_{i,recal}\left(T\right)=a\_{recal}Q\_{10,recal}^{\frac{T\_{i,soil}-T\_{ref,recal}}{10}}-t\end{array}\right.$$

Here Ti,soil is the soil temperature at soil layer i. Tref,fast is the reference temperature (25 °C) for fast pools and Tref,recal is a lower reference temperature (10°C) for recalcitrant pools to represent higher temperature sensitivity of recalcitrant soil organic matter (Davidson et al., 2006). Q10 values and the correction factors, $a$, have been calibrated to maintain a similar gross temperature impact for first meter soil as the old ISAM version. $t$ (Table 1.) is the intercept term following Gu et al., 2004.

For the moisture modifier, we keep using the belowground modifier based on soil water deficit (see Table 1. in Yang et al., 2009) for all soil layers except the first two. Soil content at -33kPa, -100kPa and -1500kPa tension at each soil layer are estimated based on Saxton et al., 2006 rather than read in from an estimated dataset. For the first two layers, we keep using the PET-based water modifier that was used as the aboveground modifier (see eq.8c in Yang et al., 2009). The purpose is to enhance the strong response of heterotrophic respiration (Rh) on precipitation as suggested by Cisneros‐Dozal et al., 2007.

The 1-D soil model also includes a variant sigmoid decay of decomposition rate in order to represent the recalcitrance of SOC in deep soil due to unknown processes (Jenkinson et al., 2008).

$$f\_{i}\left(z\right)=\frac{(-\frac{1}{1+exp⁡(-s\*\left(\left(z\_{i}-z\_{1}\right)-z\_{1}\right))})}{(-\frac{1}{1+exp⁡(-s\*\left(z\_{1}\right))})}+b$$

Where $z\_{i}$ is the node depth of the ith soil layer, $z\_{1}$ is the node depth of first layer. The parameter s = -6.5 is an average value of the estimation in Jenkinson et al., 2008. We added an addition intercept term b = 0.2 in order to match the gross (i.e., SOC mass weighted averaged) depth modifier for the first meter to 1, so we can keep the same residence time consistent for the top first meter of soil as the original bulk soil model.

**4. Nitrogen Cycle**

Currently, soil organic nitrogen has not been explicitly calculated following the advection-diffusion equation. Instead, we calculate C-N ratio at each layer after the soil degradation and SOC transport processes and then implicitly update soil organic nitrogen profile through using this C-N ratio.

We keep using the same scheme as Yang et al., 2009 for mineral nitrogen cycle and the calculation of nitrogen limitation factors.

**Part 2: Modification on model biogeophysics**

ISAM biogeophysics originates from the CoLM (Common Land Model; Barman et al., 2014). Recent updates include plant physiology (Song et al., 2013; El Masri et al., 2013; El Masri et al., 2015), hydrology (Song et al., 2014) and snow/cold region processes (Barman et al., 2015 under review). The modification here mainly focuses on processes related to soil energy and hydrology.

**1. Active Layer Thickness**

 In order to determine the effects of cryoturbation in the top soil layer, active layer thickness (ALT) needs to be treated in detail. Here ALT is determined by interpolating the layer depth through the fraction of unfrozen water to the total water at the layer located above the completely frozen layers, which follows equation (5) in Chadburn et al., 2015.

**2. Soil thermal and hydraulic conductivity**

The thermal conductivity calculation in ISAM is described in Barman et al., 2015. To alleviate the bias of soil thermal storage caused by shallow soil depth (Alexeev et al., 2007), a 42 m deep active thermal soil layer was introduced. Additionally, new snow physics was implemented in the permafrost region (insulation, compaction and depthhoar formation in snow layers), and SOC thermal insulation is included.

 Hydraulic conductivity is also described in Barman et al., 2015.

Here we applied calculated soil organic carbon profile to update soil thermal and hydraulic conductivity in the beginning of every year.

**Part 3: Cryoturbation**

For the permafrost region, we use the cryoturbation diffusive rate instead of the normal bioturbation rate in SOC vertical transport.

The parameterization of cryoturbation diffusive rate follows Koven et al., 2009 and Koven et al., 2013 with slight modification on the layers above active layer depth:

$$D=\left\{\begin{array}{c}D\_{0}(1-(\frac{z\_{ALT}-z}{maxz\_{ALT}})), z<z\_{ALT}\\D\_{0}\left(1-\left(\frac{z-z\_{ALT}}{maxz\_{ALT}-z\_{ALT}}\right)\right), z\_{ALT}<z<maxz\_{ALT}\\0, z>maxz\_{ALT}\end{array}\right.$$

Where, D is the cryoturbation diffusive rate, $D\_{0}$ is a base cryoturbation diffusive constant (see Table1), z is the soil node depth, $z\_{ALT}$ is the active layer thickness, $maxz\_{ALT }=1.53m$ is the lower limit of soil depth for cryoturbation to happen, this number is calculated as 3 times the mean active layer depth from the soil samples we currently have (U. Mishra, unpublished).

**Table 1. Parameters used in ISAM 1-D soil model**

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter Symbol | Parameter name | Value (with unit) | Reference |
| D | Bioturbation diffusive rate constant | 1 cm2yr-1 | Koven et al., 2013 |
| v | Advective rate constant | 0.01\*D cm.yr-1 | This study |
| $$a\_{fast}$$ | Correction factor of Q10 function for fast pools | 1 | This study |
| $$a\_{recal}$$ | Correction factor of Q10 function for recalcitrant pools | 1.3 | Gu et al., 2004, recalibrated in this study |
| $$Q\_{10,fast}^{}$$ | Q10 value for fast pools | 1.6 | This study |
| $$Q\_{10,recal}^{}$$ | Q10 value for recalcitrant pools | 2 | This study |
| T | Intercept term of Q10 function for recalcitrant pools | -0.325 | This study |
| $$s$$ | Coefficient of depth modifier | -6.5 | Jenkinson et al., 2008 |
| b | Intercept term of depth modifier | 0.2 | This study |
| $$D\_{0}$$ | Cryoturbation diffusive rate constant | 5 cm2yr-1 | Koven et al., 2013 |
| $$maxz\_{ALT}$$ | Maximal cryoturbation depth | 1.53 m | Koven et al., 2009 and Mishra, unpublished |

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