Description of Peatland DOS-TEM

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2   There are five main modules of peatland DOS-TEM that affect SOC dynamics in the

3   model: 1) the environmental module that simulates the soil temperature, moisture, and water

4   table using the input climate datasets (e.g., air temperature, precipitation); 2) the ecological

5   module that simulates carbon (C) and nitrogen (N) dynamics of both vegetation and soil; 3) the

6   dynamic organic soil module that simulates the structure of SOC above the mineral soil based on

7   relationships between SOC thickness and C mass in soil organic horizons; 4) the disturbance

8   module that simulates the impact of wildfire on vegetation and soil C stocks; and 5) the peatland

9   module, which simulates anaerobic CH_4 and CO_2 production and the dynamics of transport

10   pathways in the soil. The dynamics of the peatland module are affected by information received

11   from the environmental, ecological, and dynamic organic soil modules, and the dynamics of the

12   peatland module influence the ecological and dynamic organic soil modules. The environmental

13   module is described in detail in Yi et al. (2009b), and the ecological and dynamic organic soil

14   modules are described in detail by Yi et al. (2010). Here we brief descriptions of these modules

15   prior to describing the peatland module in detail. Because we did not implement the effect of fire

16   on peatland dynamics in this study, we do not describe the disturbance module; information on

17   the disturbance module can be found in Yi et al. (2010) and Yuan et al. (2012).

18   **The Environmental Module (EnvM)**

19   The EnvM operates at a daily time step using daily air temperature, vapor pressure,

20   surface solar radiation and precipitation, which are downscaled from monthly input data. The

21   EnvM considers the radiation and water fluxes among the atmosphere, canopy, snow pack and

22   soil. Live moss, fibrous, and amorphous organic horizons are considered in the soil column in

23   addition to a mineral soil horizon. Soil moisture and temperature are updated at daily time step.

24   A two-directional Stefan algorithm is used to predict the positions of freezing/thawing fronts in

25   the soil. The temperature of soil layers above first freezing/thawing front and below the last

26   freezing/thawing front is updated separately by solving finite difference equations. Temperatures

27   of the soil layers between the first and last freezing/thawing fronts are assumed to be at the

28   freezing point. Soil moistures are only updated for unfrozen layers by solving Richard equation.

29   Both the thermal and hydraulic properties of soil layers are affected by its water content. The

30   simulated estimates of daily evapotranspiration, soil temperature and moisture are integrated to

31   monthly values, and provided to EcoM. See Yi et al. (2009a) for more details on the EnvM and

32   an evaluation of the performance of the soil temperature and moisture simulations by the module.

33   Other changes to EnvM are described in Yi et al. (2010).

34   **The Ecological Module of Peatland DOS-TEM (EcoM)**

35   The detailed description of most of the ecological processes that calculate the monthly

36   pools and fluxes of carbon and nitrogen in peatland DOS-TEM have largely been documented in

37   previous studies (Euskirchen *et al.*, 2006, McGuire *et al.*, 1992, Raich *et al.*, 1991, Tian *et al.*,

38   1999, Yi *et al.*, 2010, Zhuang *et al.*, 2003). The EcoM operates at monthly time step driven by

39   monthly atmospheric climate input data and simulated environmental data. Monthly leaf area

40   index (LAI) is estimated in EcoM, and provided to EnvM at end of each month. The fibrous and

41   amorphous organic horizon thicknesses are updated at the end of each year, based on the

42   simulated soil C in each horizon. The thicknesses of organic horizons are provided to the

43   dynamic organic soil module. Here, we provide descriptions of the calculations of gross and net

44   primary production, and of the fate of detrital inputs and the calculation of heterotrophic

45   respiration.

46   Gross primary production (GPP) is calculated at a monthly time step and is affected by

47   several factors (Zhuang *et al.*, 2003):

$$GPP = C_{max}f(PAR)f(PHENOLOGY)f(FOLIAGE)f(T)f(C_a,G_v)f(NA)f(FT) \quad [1]$$

48   where C_{max} is the maximum rate of C assimilation, *PAR* is photosynthetically active radiation,

49   *f(PHENOLOGY)* is monthly leaf area relative to leaf area during the month of maximum leaf

50   area, *f(FOLIAGE)* represents the ratio of canopy leaf biomass relative to maximum leaf biomass,

51   *f(T)* represents the effect of air temperature (ºC), C_a and G_v are atmospheric CO_2 concentration

52   and relative canopy conductance, respectively, *f(C_a, G_v)* represents the effect of stomatal

53   regulation on atmospheric CO_2 uptake, *f(NA)* represents the limiting effect of available inorganic

54   N on GPP, and *f(FT)* represents the effect of freeze and thaw on photosynthetic activity. Except

55   for C_{max}, other factors in the GPP equation range from 0 to 1. The function *f(NA)* is dynamically

56   calculated each month based on the ability of vegetation to mobilize nitrogen from uptake and

57   storage to meet the demands of building new tissue, i.e., net primary production. In other words,

58   at the monthly scale GPP is downscaled so that nitrogen requirement of new production is equal

59   to the amount of nitrogen that vegetation can provide to new production.

60   Net primary production (NPP) is calculated as the different between GPP and autotrophic

61   respiration (R_A). The flux R_A is the sum of maintenance respiration (R_m) and growth respiration

62   (R_g), which is prescribed to be 20% of the difference between GPP and R_m. The flux R_m is a

63   direct function of plant biomass as follows:

$$R_m = K_r C_V e^{rT} \qquad [2]$$

64

65   where K_r is the per-gram-biomass respiration rate of the vegetation at 0 ℃, C_v is the vegetation

66   carbon pool, T is the mean monthly air temperature (℃), and r is the instantaneous rate of change

67   in respiration with the change in temperature.

68   Detrital inputs of C into the soil are divided into aboveground litterfall and belowground

69   detrital inputs. Aboveground litterfall is assigned only to the first soil layer, while belowground

70   detrital inputs are assigned to different soil layers based on fractional distribution of fine roots

71   with depth. We assume that the ratio of aboveground litterfall to total litter input is similar to the

72   ratio of root NPP to total NPP. Soil C is tracked in the fibrous, amorphous, and mineral horizons

73   in peatland DOS-TEM, and heterotrophic respiration for each layer within a soil horizon is

74   calculated based on the soil environmental conditions of that layer:

$$R_{H,i} = K_{co2,i} C_{s,i} f(M_{v,i}) f(T_{c,i}) \qquad\qquad [3]$$

75   where i is soil layer index, $R_{H,i}$ is heterotrophic respiration from layer i (g C m^{-2} h^{-1}), $K_{co2,i}$ is

76   heterotrophic respiration rate at 0℃ of layer i (h^{-1}), $C_{s,i}$ is soil C storage in layer i (g C m^{-2}), and

77    $f(M_{v,i})$ and $f(T_{c,i})$ are moisture and temperature factors affecting decomposition of layer i. $f(M_{v,i})$

78   is parabolic relationship using the pre-defined parameters for the maximum, minimum, and

79   optimal volumetric soil moisture for decomposition, which are 1, 0, and 0.5, respectively. When

80   simulated volumetric soil moisture equals 0.5, $f(M_{v,i})$ equals 1. $f(T_{c,i})$ is calculated based on a Q_{10}

81   (2.0 in this study) and soil temperature of layer i. There is a unique rate limiting parameter for

82   decomposition K_{co2} for the fibrous, amorphous, and mineral soil horizons, that is used to estimate

83   decomposition for each layer within the horizon. The rate limiting parameter is determined by

84   calibrating the model to target values for the C content of the three organic horizons.

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86   **Dynamic organic soil Module (DOSM)**

87   DOSM updates the organic soil structure at the time of fire and at the end of each year,

88   based soil C content of the fibrous and amorphous horizons. DOSM is important in defining the

89   structure of soil organic horizons for the purpose of maintaining the stability and efficiency of

90   soil temperature and moisture calculations when thickness of organic soil C is altered by either

91   wildfire disturbance or ecological processes. The soil organic structure consists of a maximum of

92   1 moss layer, 3 fibrous organic layers, and 10 amorphous organic layers. It is assumed that the

93   minimum soil layer thickness for each horizon is 2 cm. If the thickness of a layer is less than 2

94   cm, a layer will be combined with other layers of the same horizon, or be reset to 2 cm if there is

95   only one layer for a horizon (except for live moss, which will not be included in the soil column

96   if it is less than 2 cm). The rationale behind the assignment of the organic soil layer thickness is

97   that the upper layers in the soil column should be thinner than deeper layers, following the

98   common practice of land surface models and ecosystem models in simulation soil thermal and

99   moisture dynamics. At the same time, the upper layer should not so thin that it leads to instability

100   and inefficiency in calculations of soil thermal and moisture dynamics. The assignment of layer

101   thickness for the fibrous organic horizon is provided in Table D1 of Yi et al. (2010). The

102   thicknesses and number of layers in the amorphous organic horizon (n_{amp}) are based the

103   thickness of deepest fibrous horizon layer ($d_{fib,bot}$) and the total thickness of amorphous organic

104   horizon (d_{amp}):

$$n_{amp} = \begin{cases} 1 & d_{amp} \leq d_{fib,bot} \\ 2 & d_{fib,bot} < d_{amp} \leq 2d_{fib,bot} \\ \vdots & \\ 9 & 8d_{fib,bot} < d_{amp} \leq 9d_{fib,bot} \\ 10 & d_{amp} > 9d_{fib,bot} \end{cases} \qquad [4]$$

105   The thicknesses of layers with the amorphous horizon are calculated as:

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$$d_{amp,n} = \frac{n}{\left(\dfrac{n_{amp}\left(n_{amp}+1\right)}{2}\right)}, \quad n = 1,2,\ldots,n_{amp} \tag{5}$$

106   where $d_{amp,n}$ is the thickness of layer n.

107   At the beginning of each year, the thicknesses of the moss layer, fibrous organic layers,

108   and amorphous organic layers are checked. If any of these layers have thickness less than

109   minimum value, or if the total thickness and total number of fibrous layers are not consistent

110   with those in Table D1 of Yi et al. (2010), then all layers of that horizon (fibrous/amorphous) are

111   combined together, and then split according Table D1 of Yi et al. (2010) and/or equations 4 and

112   5. The temperature of each new layer is determined by linear interpolation of the nearest soil

113   temperatures of old organic soil structure. Soil freezing/thawing fronts are reassigned to new soil

114   structure with the relative distance to the top of a horizon (moss, fibrous, amorphous) unchanged.

115   Soil water content of each new organic soil layer is first retrieved by comparing the boundary of

116   new and old soil layer structure. For example, if a new organic soil layer is completely located in

117   an old organic soil layer, than the new organic soil layer is assigned a fraction of old organic soil

118   layer's water content based on the ratio of thicknesses of both layers; if a new organic soil layer

119   originated from two different old layers, the soil water content of new layer is assigned the sum

120   of soil water contents retrieved from both old layers using the above method. After the

121   determination of soil water content, the soil liquid and ice contents are retrieved with the position

122   of freezing and thawing fronts in a layer.

123   The growth of moss is determined by a number of factors, including moss type, radiation,

124   wind speed, and precipitation (Bisbee *et al.*, 2001). In peatland DOS-TEM, the biomass and NPP

125   of moss are not simulated explicitly, as they are considered as part of overall vegetation biomass

126   and NPP. However, the thickness of moss is explicitly considered for the purposes of soil

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127   temperature and moisture calculations. Moss thickness is simulated as an empirical function of

128   years since last fire based on (Yi *et al.*, 2009a):

$$d_{moss} = d_{moss,\max} \frac{y_{sf}}{y_{sf} + y_{half}} \qquad [6]$$

129   where d_{moss} is the thickness of moss (cm), $d_{moss, max}$ is the maximum thickness of moss (m), y_{sf} is

130   number of years since last fire (year), and y_{half} is number of year which was need for moss to

131   reach half of $d_{moss,max}$. In this study, we assigned 3.5 cm to $d_{moss,max}$ and 5 to y_{half} based on *Yi et al.*

132   (2009a).

133   The thicknesses of fibrous and amorphous layers are calculated using the simulated soil C

134   content of each horizon and the equation:

$$C_{mass} = ad^b \qquad [7]$$

135   where C_{mass} is C content (g C cm^{-2}) of an organic horizon, d is organic horizon thickness (cm),

136   and a and b are fitted coefficients for the fibrous or amorphous horizons [See Yi et al. (2009a)

137   for more detail and estimates of a and b].

138   As the fibrous organic horizon grows thicker, the bottom layer of the fibrous organic

139   horizon is transferred to the amorphous organic horizon. A threshold method is used to mimic

140   the process of humification, i.e. when the fibrous organic horizon becomes thicker than the

141   threshold, the component of the fibrous organic horizon above the threshold is transferred to the

142   amorphous organic horizon.

143   **The Peatland Module**

144   In the peatland module, microbial decomposition of SOC in peatlands/wetlands is divided

145   into aerobic and anaerobic decomposition. Aerobic decomposition, i.e. heterotrophic respiration,

146   is assumed to exclusively occur in the unsaturated zone (above water table) and CO_2 is the only

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147 terminal product of aerobic decomposition. Aerobic decomposition is estimated by the

148 heterotrophic respiration calculations described for the EcoM above. Anaerobic decomposition

149 occurs exclusively in the saturated zone (below the water table) and both CH_4 and CO_2 are the

150 terminal products of anaerobic decomposition.

151   The production of CH_4 in the model (anaerobic decomposition of SOC) is a function of a

152 decomposition rate limiting parameter, SOC mass, and soil temperature (Q_{10} of 2.0) in each SOC

153 layer. The anaerobic decomposition rate limiting parameters of fibric, amorphous, and mineral

154 SOC are unknown and were calibrated with field observations as discussed later. Once CH_4 is

155 produced in the soil, its transport is controlled by various mechanisms. Below we describe the

156 processes that affect the mass balance of CH_4 in the soil of peatland DOS-TEM.

157   The mass balance of CH_4 in a given soil layer is defined as:

$$\frac{\partial C_{CH4}}{\partial t} = P - \frac{\partial diff}{\partial z} - E - O - R_p \qquad [8]$$

158   where C_{CH4} is the CH_4 concentration (μmol L^{-1}), t is the time, P is the CH_4 production

159 rate (μmol L^{-1} h^{-1}), $diff$ is the diffusion transport of CH_4 (μmol cm L^{-1} h^{-1}), z is the soil depth

160 (cm), E and R_p represents the CH_4 emission rates through ebullition and plant-mediated

161 processes (μmol L^{-1} h^{-1}), respectively, and O represents the CH_4 oxidation rate (μmol L^{-1} h^{-1}).

162   The production of CH_4 is strongly related to soil carbon quality as well as soil moisture

163 and temperature conditions, and defined separately for each soil organic layer in our study,

164 following Ise et al. (2010) as:

$$P = \begin{cases} U \dfrac{K_{CH4,i} C_{s,i} f(T_{c,i})}{Z_i \theta_w} & \text{if } Z_i \leq Z_{WT} \\ 0 & \text{if } Z_i > Z_{WT} \end{cases} \qquad [9]$$

165   where P is the CH$_4$ production rate (μmol L^{-1} h^{-1}), U is the unit conversion factor, $K_{CH4,i}$ is the

166   CH$_4$ production rate (h^{-1}) at 0°C of layer i, Z_i is the layer thickness (cm), $f(T_{c,i})$ represents the

167   dependence of decomposition SOC to CH$_4$ on soil temperature, θ_w is the soil moisture content

168   (cm^3 cm^3), Z_i is the depth of given soil layer (positive number with zero at the soil surface), Z_{WT}

169   is the depth of water table (positive number with zero at the soil surface). It was assumed in the

170   model that the anaerobic condition only occurs when soil was totally saturated [i.e., the soil layer

171   is below water table (Z_{WT})]. There is a unique rate limiting parameter for decomposition K_{CH4} for

172   the fibrous, amorphous, and mineral soil horizons, that is used to estimate decomposition for

173   each layer within the horizon. The rate limiting parameter is determined by calibration using the

174   measured CH$_4$ efflux data as presented in the model calibration section.

175   The diffusion of CH$_4$ in the gaseous and liquid phase is defined, based on Fick's Law, as:

$$diff = -D_g \frac{\partial C_{CH4}}{\partial z} \qquad [10]$$

176   where D_g is the CH$_4$ diffusion coefficient (cm^2 h^{-1}) that is defined as:

$$D_g = D_0 \tau \left(\frac{T_{k,i}}{293.15} \right)^{1.75} \qquad [11]$$

177   where D_0 is the CH$_4$ diffusion coefficient in the atmosphere (cm^2 h^{-1}), τ is the soil tortuosity in

178   gaseous or liquid phase (unitless), and $T_{k,i}$ is the absolute soil temperature (K). D_0 was set to 720

179   cm^2 h^{-1} (Walter & Heimann, 2000). The traditional Penman (1940) and Millington and Quirk

180   (1961) models are known to overestimate and underestimate diffusion coefficient, respectively,

181   at high moisture content (or low air-filled porosity). Pingintha et al. (2010) used six tortuosity

182   models to calculate the soil gas efflux and then compared the results of six most commonly used

183   diffusion models with the laboratory measured gas efflux. The results indicated that the Moldrup

184   et al. (1997) model was the most robust model to calculate soil gas efflux in soils with high

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185   moisture content (e.g., peatlands). Therefore, the tortuosity in gaseous and liquid phases is

186   defined as:

$$\begin{cases} \tau = 0.66(\rho_s - \theta_w)\left(\dfrac{\rho_s - \theta_w}{\rho_s}\right)^{\frac{12-m}{3}} & \text{for gaseous phase} \\ \tau = 0.66\theta_w\left(\dfrac{\theta_w}{\rho_s}\right)^{\frac{12-m}{3}} & \text{for liquid phase} \end{cases} \qquad [12]$$

187   where ρ_s is the soil porosity (cm^3 cm^{-3}), and m is an empirical parameter (unitless) set to 3.0

188   following Pingintha et al. (2010).The upper boundary condition for Eq. [3] is defined as a

189   Dirichlet condition:

$$C_{CH4}(t, z = 0) = 0.076 \ \mu\text{mol L}^{-1} \qquad [13]$$

190   where 0.076 µmol L^{-1} is the CH$_4$ concentration in the atmosphere. The lower boundary condition

191   is defined as a Neumann condition:

$$\frac{\partial C_{CH4}}{\partial z} = 0 \qquad [14]$$

192   It is assumed in the model that bubbles are formed in the saturated zone when the CH$_4$

193   concentration in the soil water is greater than a certain threshold value (i.e., saturation

194   concentration of CH$_4$). The threshold value is a function of soil temperature and determined

195   based on the observed solubility of CH$_4$ in pure water at different temperatures (Wania *et al.*,

196   2010, Yamamoto *et al.*, 1976):

$$S_B = 0.05708 - 0.001545T_{c,i} + 0.00002069T_{c,i}^{2} \qquad [15]$$

197   where S_B is the Bunsen solubility coefficient defined as the volume of CH$_4$ dissolved per unit

198   volume of water at standard atmospheric pressure and a given temperature ($T_{c,i}$). Therefore the

199   mass-based Bunsen solubility coefficient (S_M, µmol L^{-1}) can be calculated with the ideal gas law:

$$S_M = U\frac{pV_{CH4}}{RT_k} = U\frac{(p_{atm} + \rho_w gh)V_{CH4}}{RT_k} \qquad [16]$$

200   where U is the unit conversation factor, p is the partial pressure of CH_4 that is the sum of

201   atmospheric (p_{atm}) and hydrostatic pressure ($\rho_w gh$), h is the water height (m), V_{CH4} is the volume

202   of CH_4 (m^3), R is the gas constant (8.3145 m^3 Pa K^{-1} mol^{-1}), and T is the absolute temperature

203   (K).

204   Therefore, the ebullition emission rate of CH_4 from the saturated zone to the unsaturated

205   zone is defined as:

$$E = \begin{cases} k_h(C_{CH4} - S_M) & \text{if } C_{CH4} > S_M \text{ and } Z_i \leq Z_{WT} \\ 0 & \text{if } Z_i > Z_{WT} \end{cases} \qquad [17]$$

206   where k_h is a rate constant (1.0 h^{-1}).The oxidation of CH_4 ($CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$) in

207   the unsaturated soil layers is assumed to follow Michaelis-Menten kinetics and strongly

208   controlled by soil temperature (Walter & Heimann, 2000)

$$O = \begin{cases} \dfrac{V_{max}C_{CH4}}{k_m + C_{CH4}} f(T_{c,i}) & \text{for } Z_i \geq Z_{WT} \\ 0 & \text{for } Z_i < Z_{WT} \end{cases} \qquad [18]$$

209   where V_{max} and k_m are the Michaelis-Menten kinetics parameter and set to 5 µmol L^{-1} h^{-1} and 20

210   µmol L^{-1} (Walter & Heimann, 2000), respectively.

211   The CH_4 lost through the vascular plant aided transport is defined as (Walter & Heimann,

212   2000):

$$R_p = k_p f_{root} f_{grow} T_{veg} C_{CH4} \qquad [19]$$

213   where R_p is the CH_4 emission rate through plant at a given soil layer (µmol L^{-1} h^{-1}), k_p is the rate

214   constant (1.0 h^{-1}), f_{root} is the root distribution in soil, T_{veg} is a factor describing how different

215   types of vegetation/plants affect CH_4 transport, f_{grow} is the growing stage of plants/vegetation,

216   and C_{CH4} is the CH$_4$ concentration at a given soil layer. The growing state of plants/vegetation

217   was calculated based on the soil temperature and leaf area index:

$$f_{grow} = \frac{LAI_c}{LAI_{max}}$$ [20]

218   where LAI_c is the stand LAI at the stand age c and LAI_{max} is the maximum LAI when

219   plants/vegetation reach maturity. Equation (20) implies that the seasonal variations on the plant-

220   mediated CH$_4$ transport are negligible based on the results of Shea (2010). Shea (2010) also

221   reported that the vegetation species and functional groups (e.g., *Carex*) are important to plant-

222   mediated CH$_4$ transport, which is reflected as T_{veg} in the model.

223   The total CH$_4$ efflux from the soil to the atmosphere is be calculated as:

$$F = \begin{cases} U\left(Q_p + diff_a(t, z = 0)\right) & \text{if } Z_{WT} \leq 0 \\ U\left(Q_p + E + diff_w(t, z = 0)\right) & \text{if } Z_{WT} > 0 \end{cases}$$ [21]

224   where F is the CH$_4$ emission flux (μmol m^{-2} h^{-1}) from the soil to the atmosphere, U is the unit

225   conversion factor, Q_p is the total plant-aided CH$_4$ transport (μmol m^{-2} h^{-1}), $diff_a$ and $diff_w$ are the

226   diffusion transport of CH$_4$ in the gaseous and liquid phases (μmol m^{-2} h^{-1}), respectively. In the

227   model, it is assumed that 50% of CH$_4$ transported by plant is oxidized by rhizospheric oxidation

228   before being released into the atmosphere (Walter & Heimann, 2000). The total plant mediated

229   CH$_4$ transport (Q_p) is calculated by integrating through the root zone:

$$Q_p = 0.5 \int_{Z_{root}}^{0} R_p dz$$ [22]

230   where z_{root} is the root depth (soil depth at the soil surface is assumed to be zero).

231   The total CO$_2$ release from the soil is calculated as the sum of CO$_2$ produced from

232   decomposition of SOC under aerobic conditions (i.e., heterotrophic respiration), CO$_2$ produced

233   during the microbial oxidation of CH$_4$ in the oxic zone, and the anaerobic production of CO$_2$.

234   The aerobic production of CO_2 in the model is described above in the description of the EcoM.

235   The anaerobic production of CO_2 in the model is calculated based on the aerobic production of

236   CO_2. Many laboratory incubation studies (e.g., Bergman *et al.*, 1999, Glatzel *et al.*, 2004, Kane

237   *et al.*, 2012, Lee *et al.*, 2012, Updegraff *et al.*, 1995) indicate that aerobic:anaerobic CO_2

238   production ratios in high-latitude peatland ecosystems range between 0.28:1 and 5:1. Therefore,

239   we assumed that the ratio of aerobic CO_2 to anaerobic decomposition is 2 for an aerobic CO_2

240   flux calculated for simulated soil temperature and an optimum soil moisture of 50% saturation.

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