Sensitivity analysis of a mechanistic model of the rumen *in-vitro* fermentation: Computation of dynamic Shapley effects and Sobol indices

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Rencontres du réseau Mexico 2022, 24-25 Novembre, 2022, Cestas

1. Introduction

Context

Enteric CH_4 emissions produced from the **rumen fermentation** contribute the most to the greenhouse gases (GHG) emitted from ruminants

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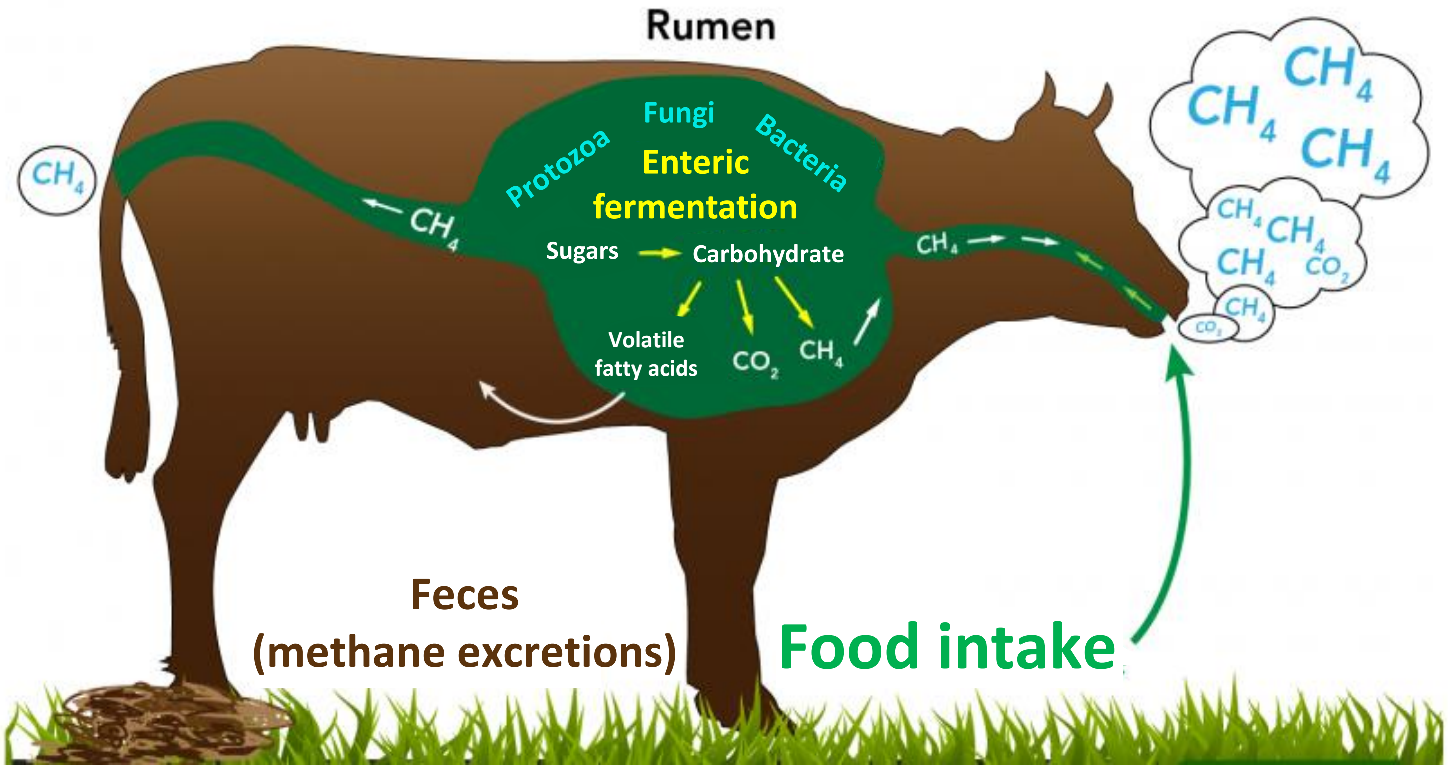

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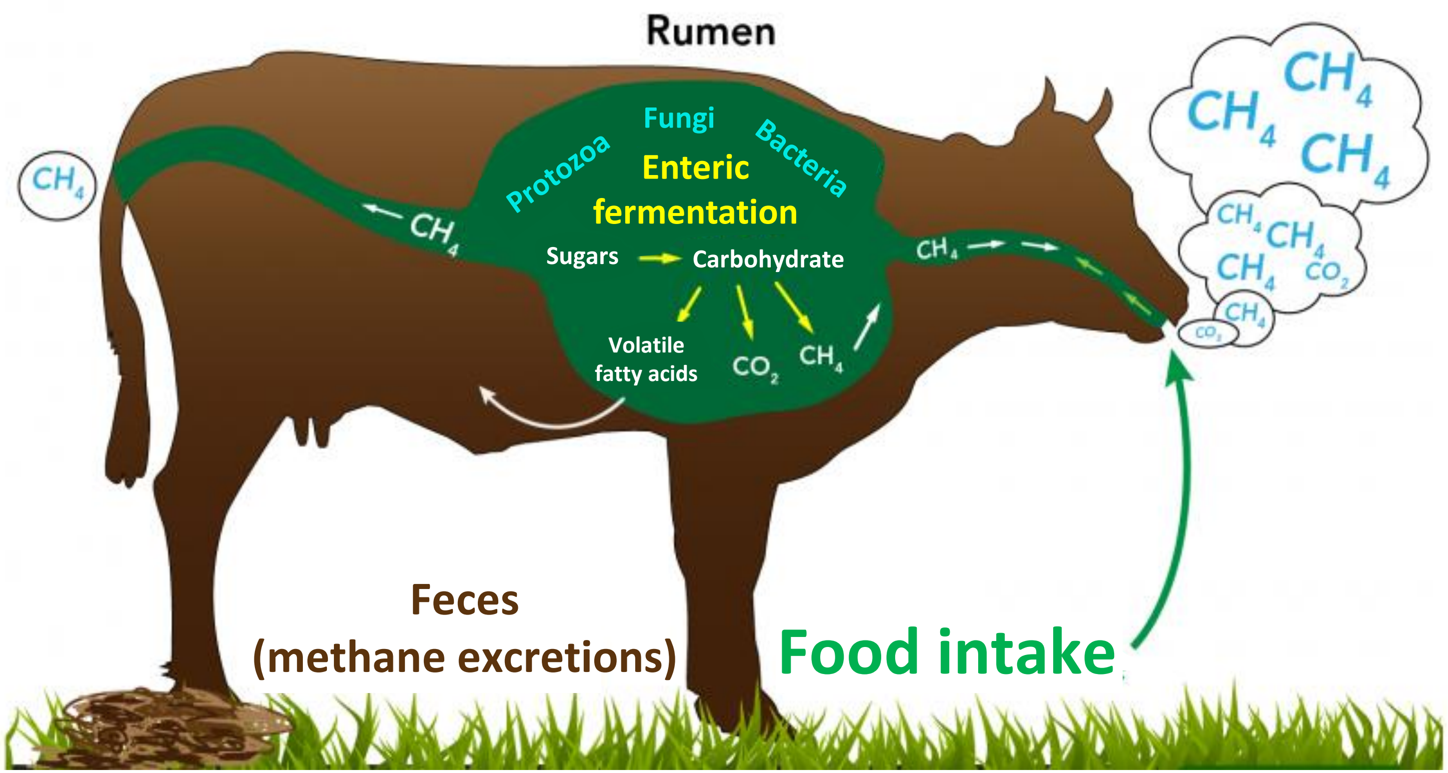

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Mechanistic models are used to:

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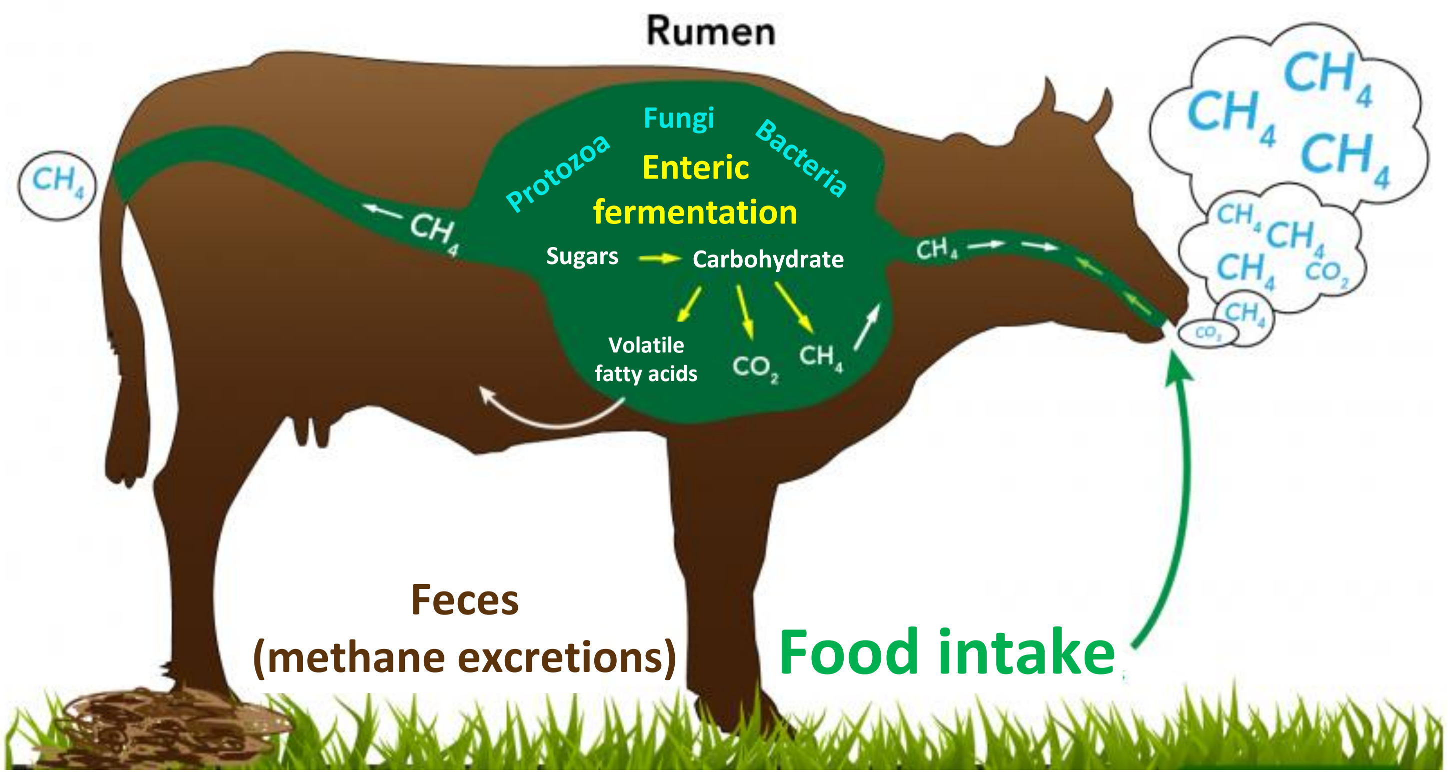

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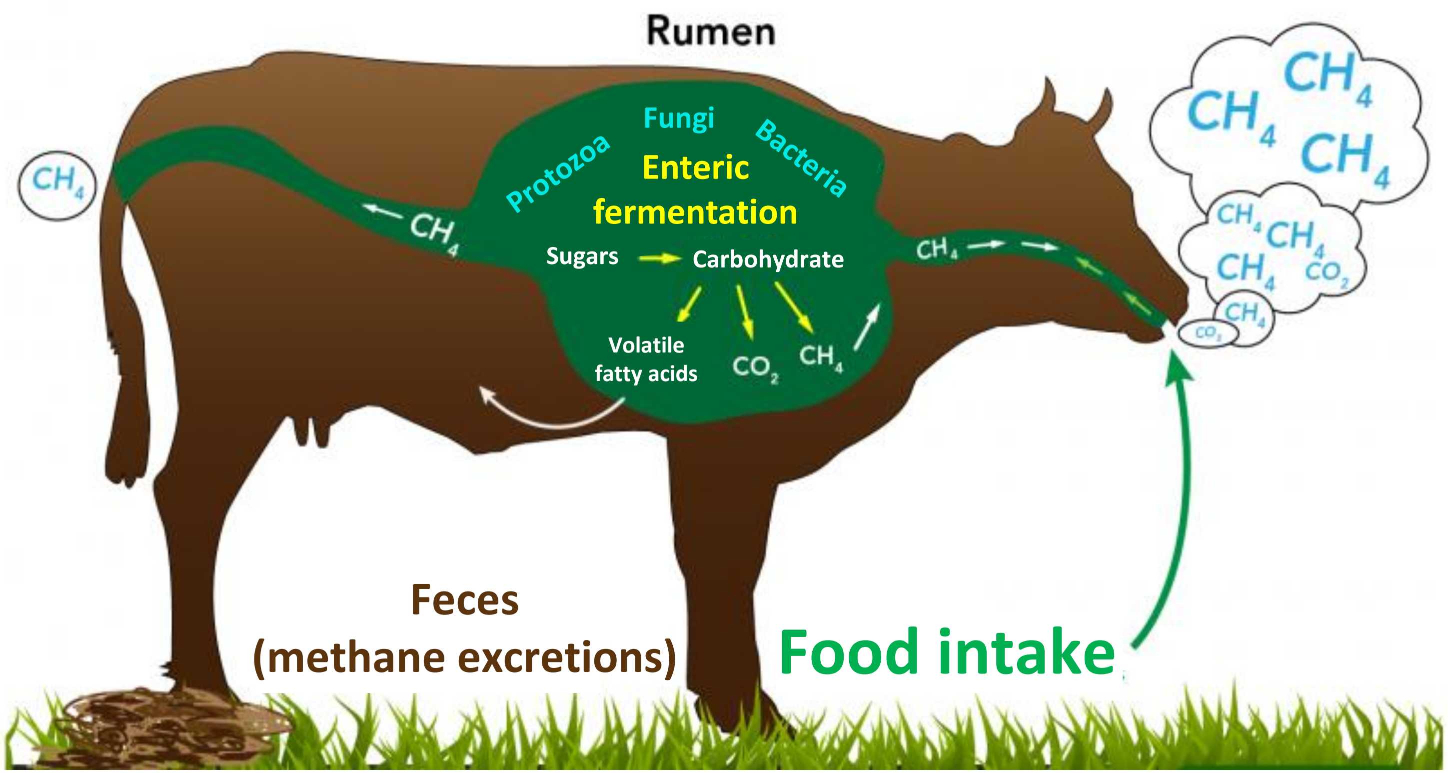

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Mechanistic models are used to:

- estimate CH_4 emissions from ruminants
- better understand the complex mechanism of the rumen fermentation

Mechanistic model of the rumen *in-vitro* fermentation

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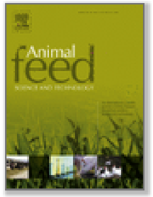
Animal Feed Science and Technology

Volume 220, October 2016, Pages 1-21



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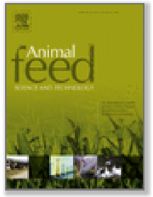

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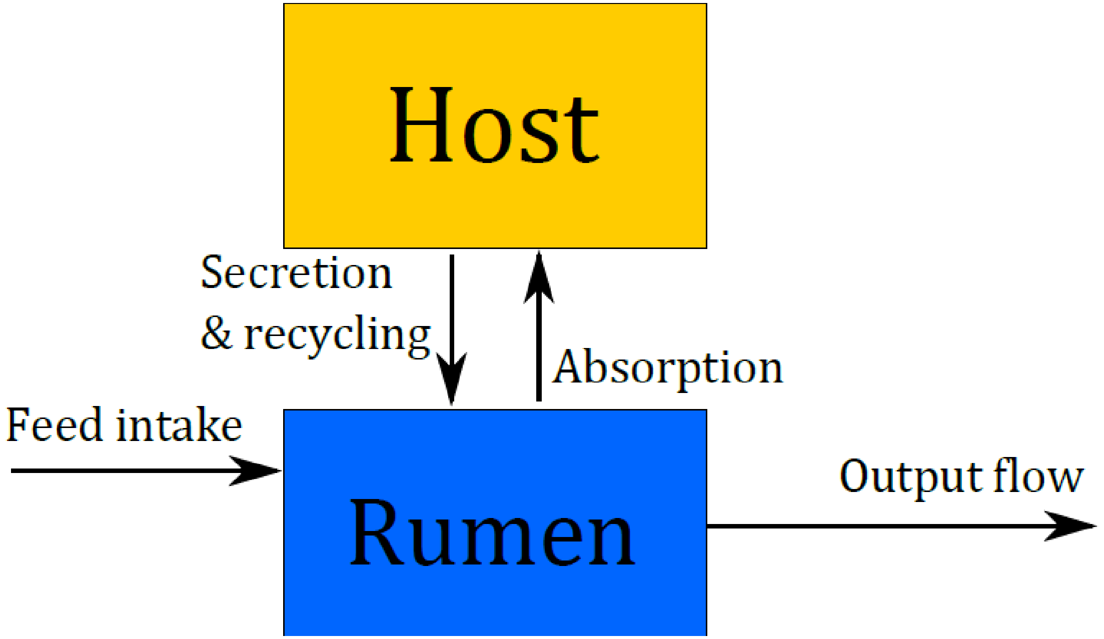

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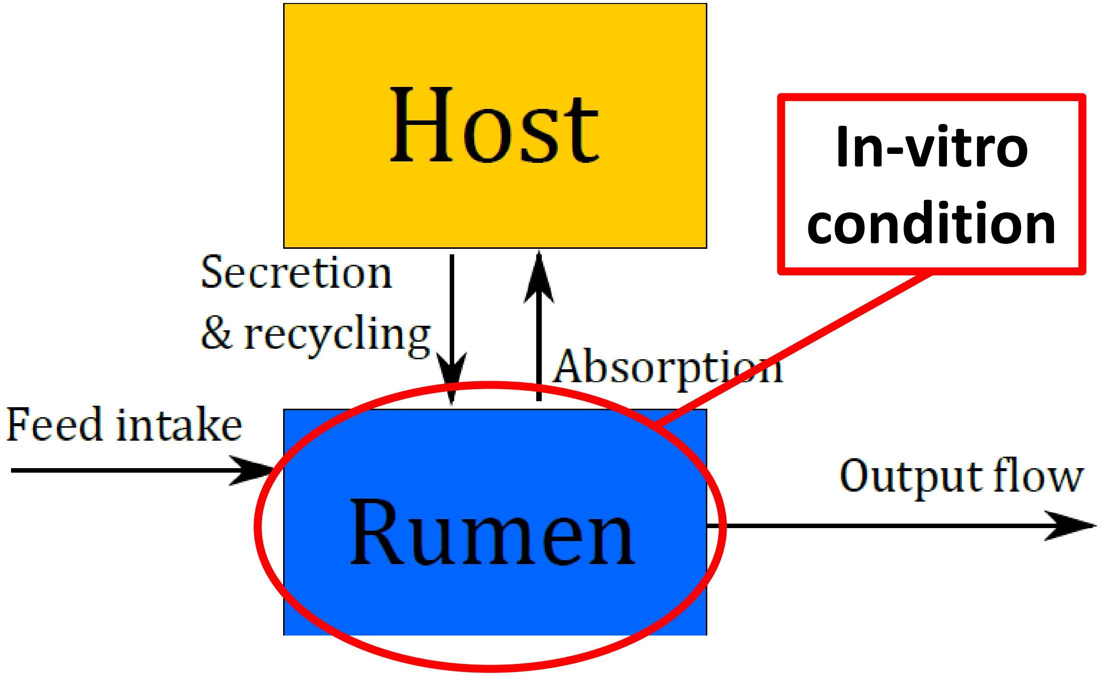

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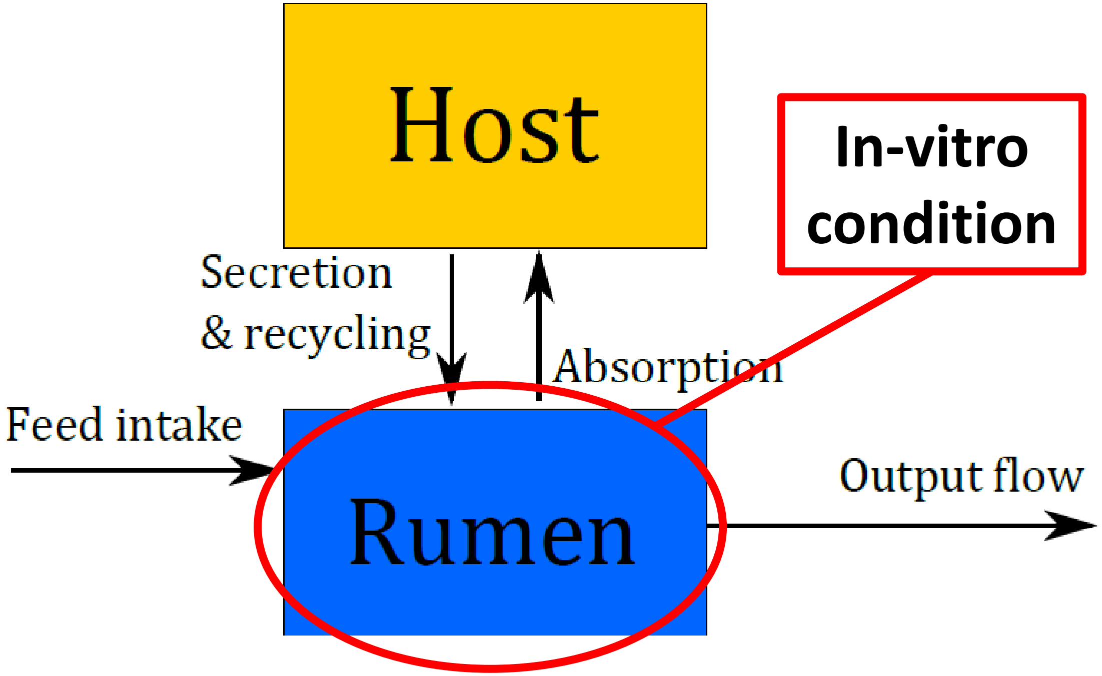

Inputs

biochemical and physicochemical parameters involved in the rumen fermentation → **Model** →

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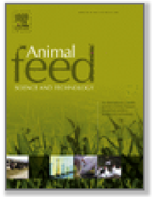

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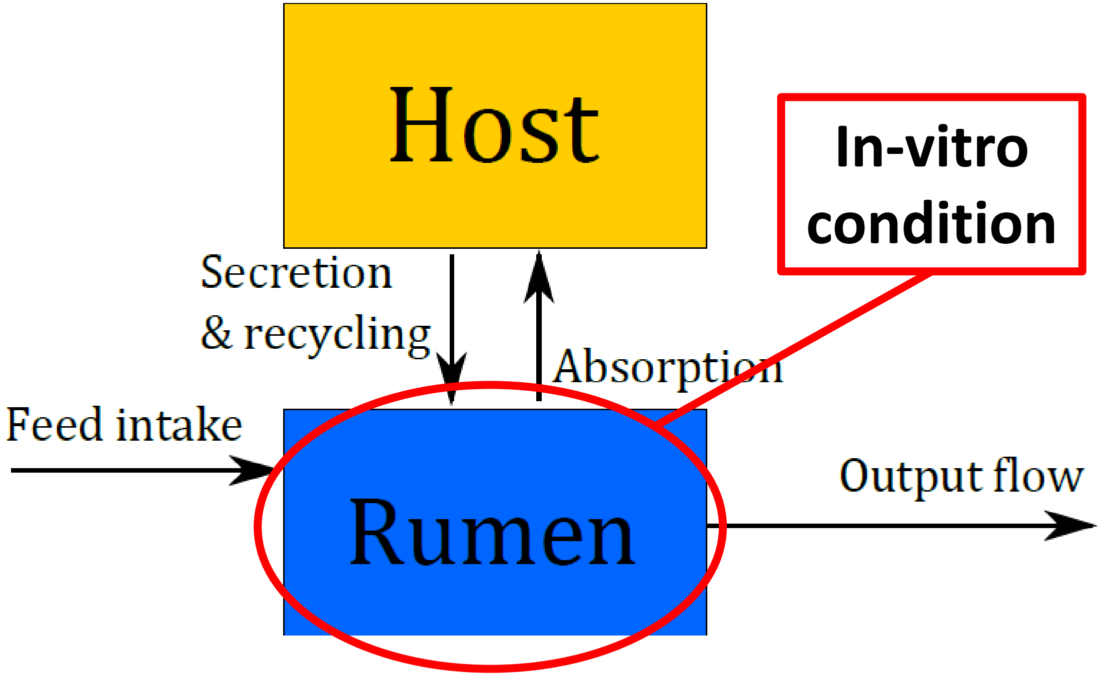

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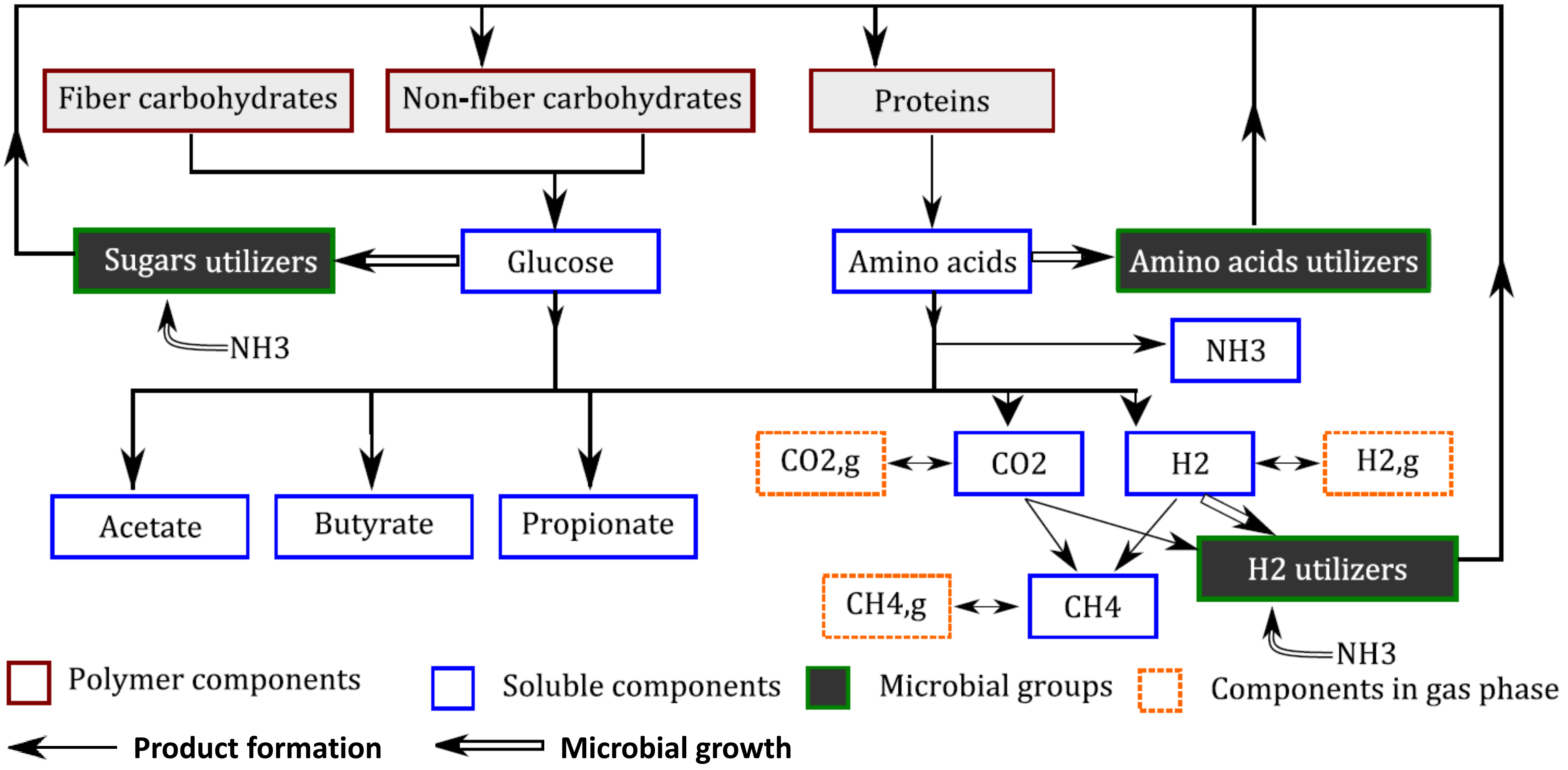
→ **Model** →

Outputs:

Dynamic (time varying from 0 to 24h) of 18 biochemical components concentration produced from the rumen fermentation (acetate, butyrate, propionate, **CH_4**, ammoniac…)

Mechanistic model of the rumen *in-vitro* fermentation



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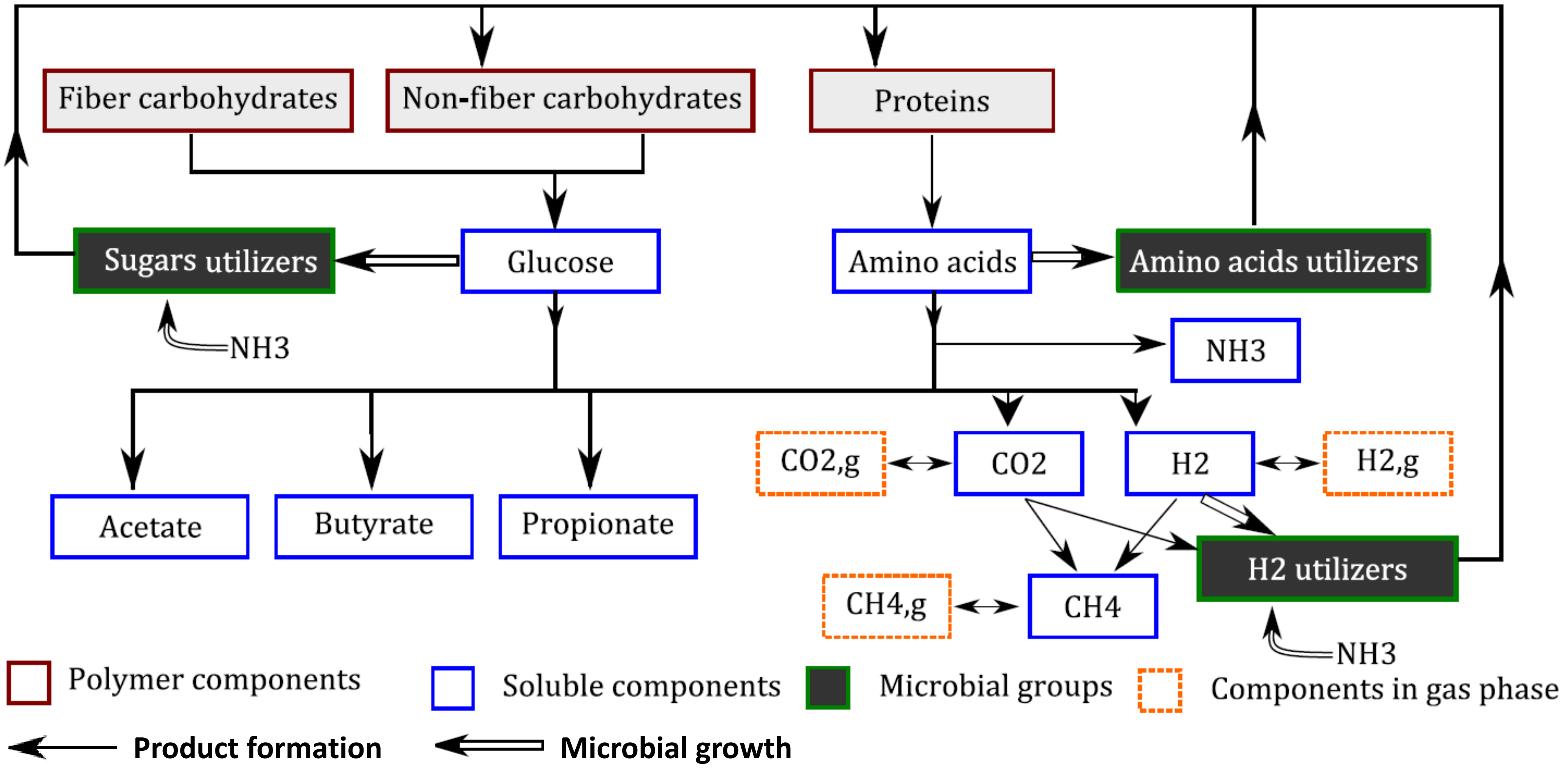

Model complexity: 18 output variables, 32 input parameters

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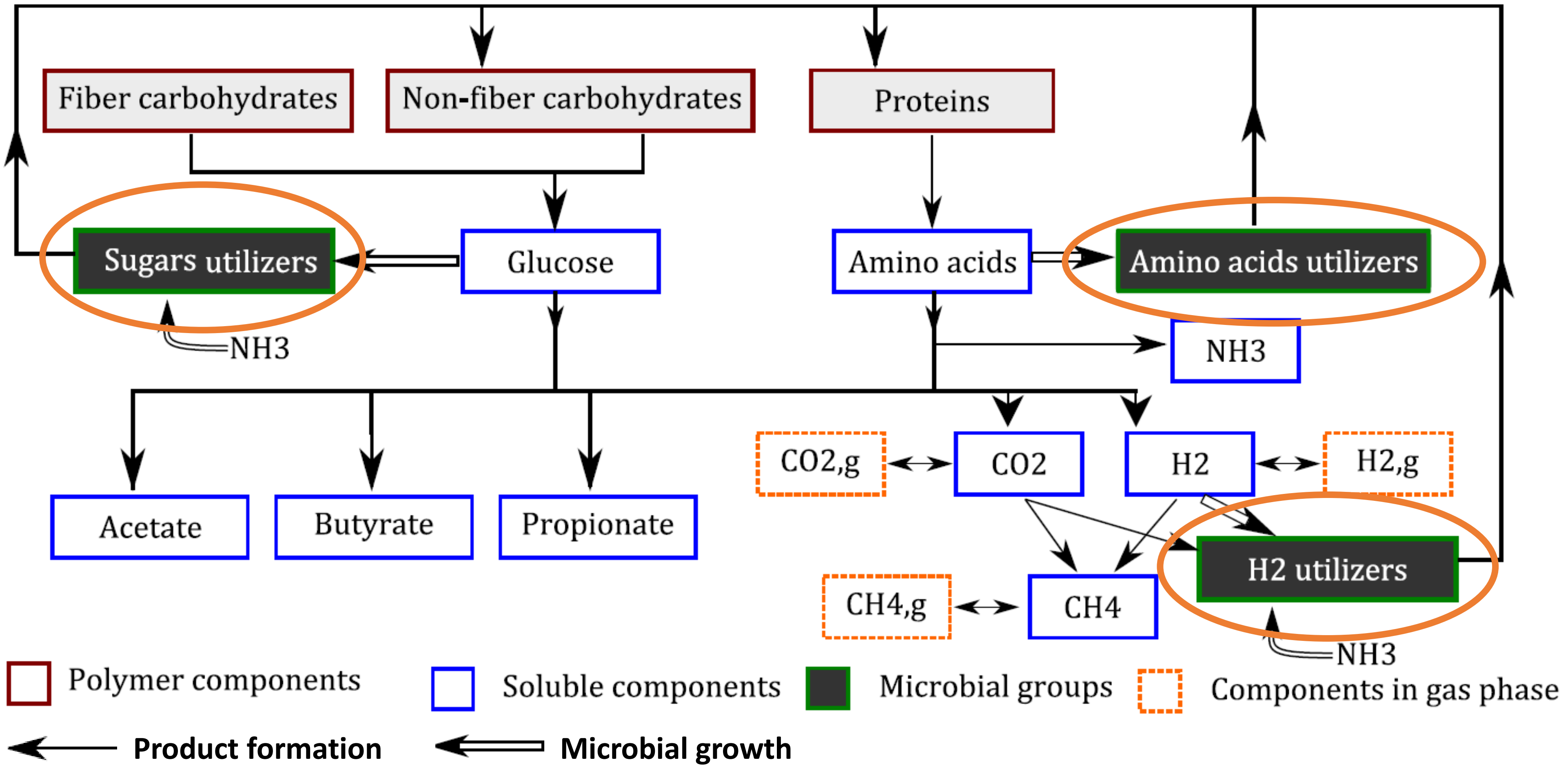

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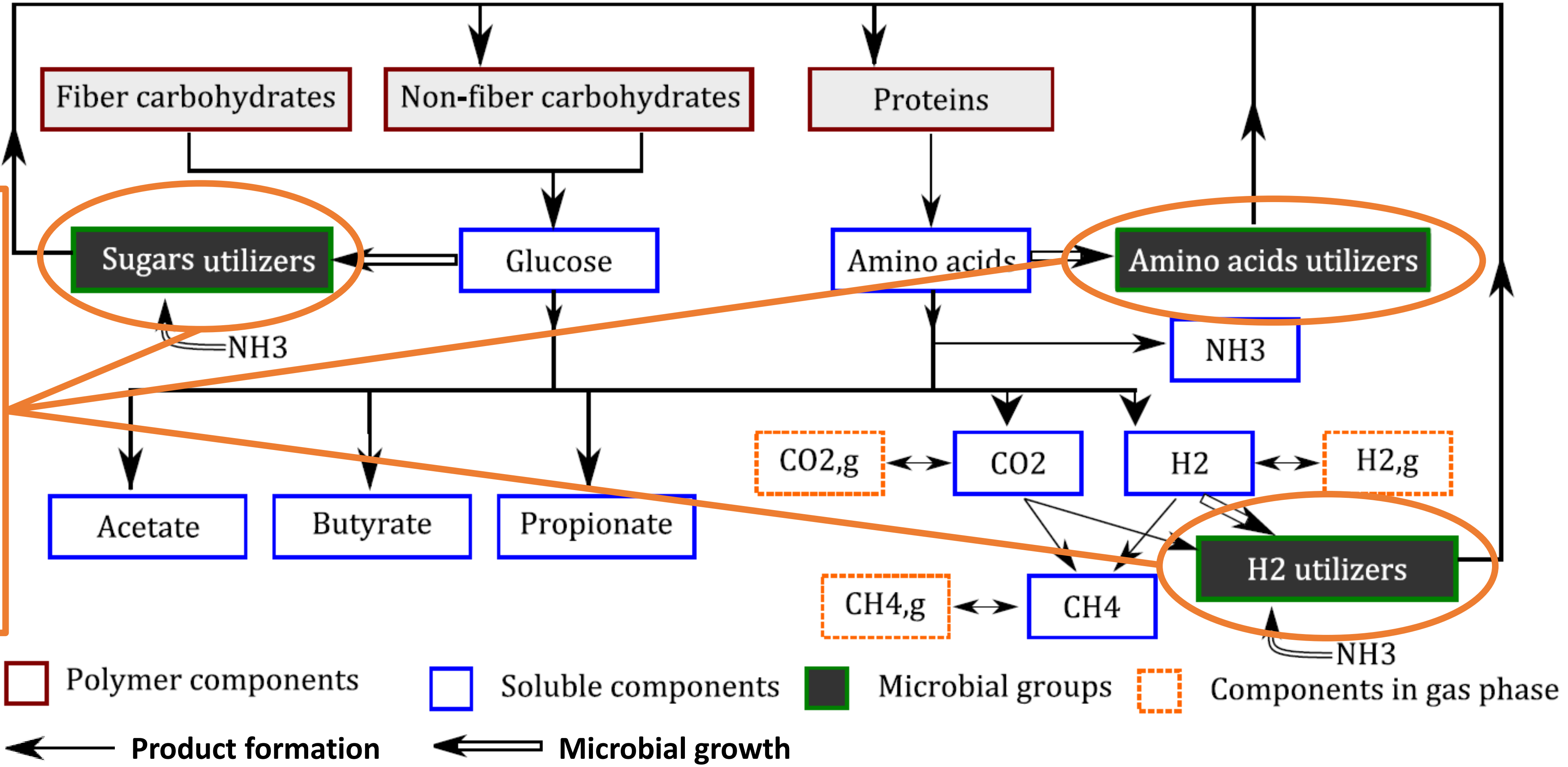
maximum specific utilization rate (k_m, mol substrate/(mol biomass h)) and the Monod constant (K_S, mol/L)



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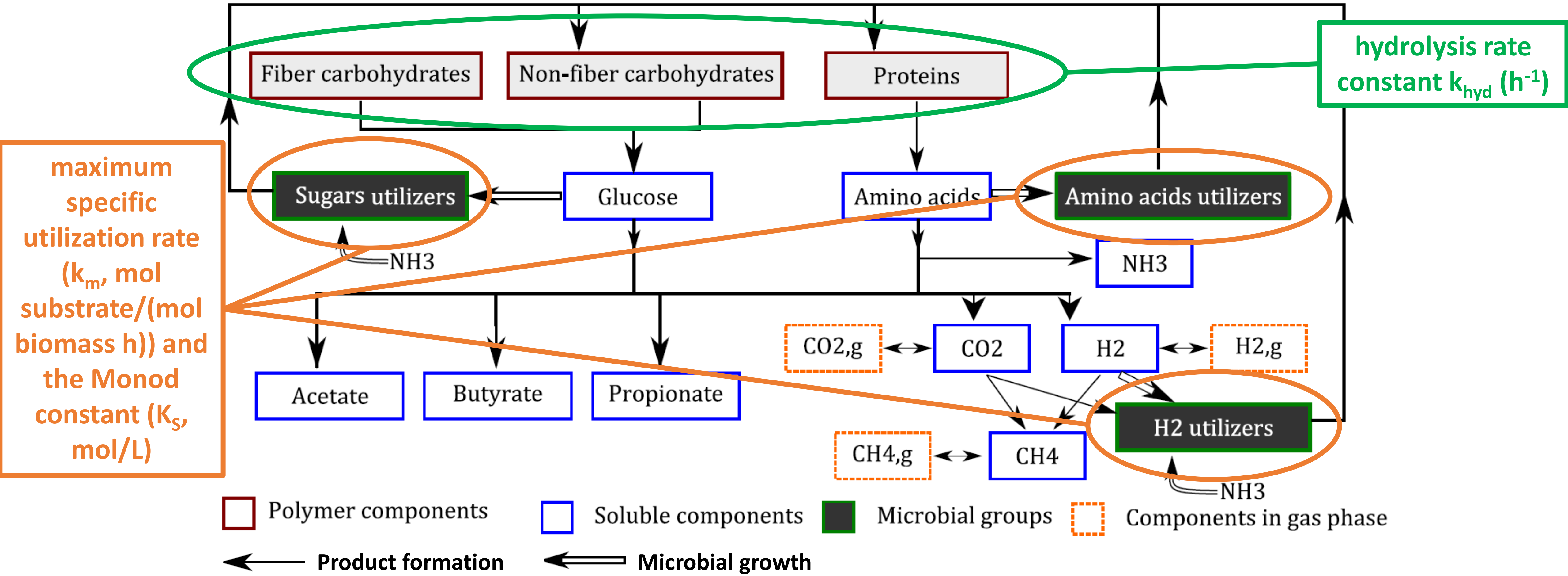

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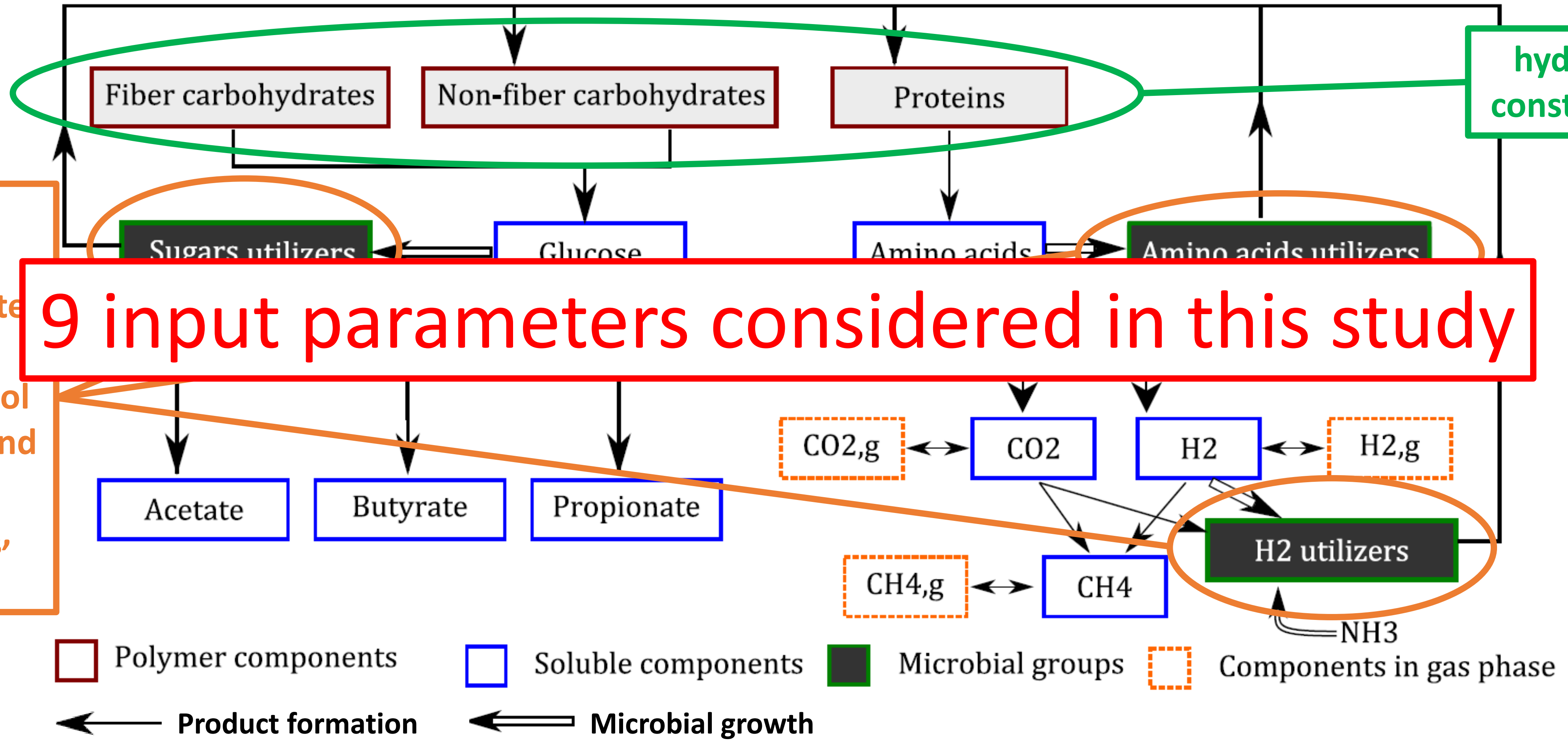

hydrolysis rate constant k_{hyd} (h^{-1})

maximum specific utilization rate (k_m, mol substrate/(mol biomass h)) and the Monod constant (K_S, mol/L)

9 input parameters considered in this study

Model complexity: 18 output variables, 32 input parameters

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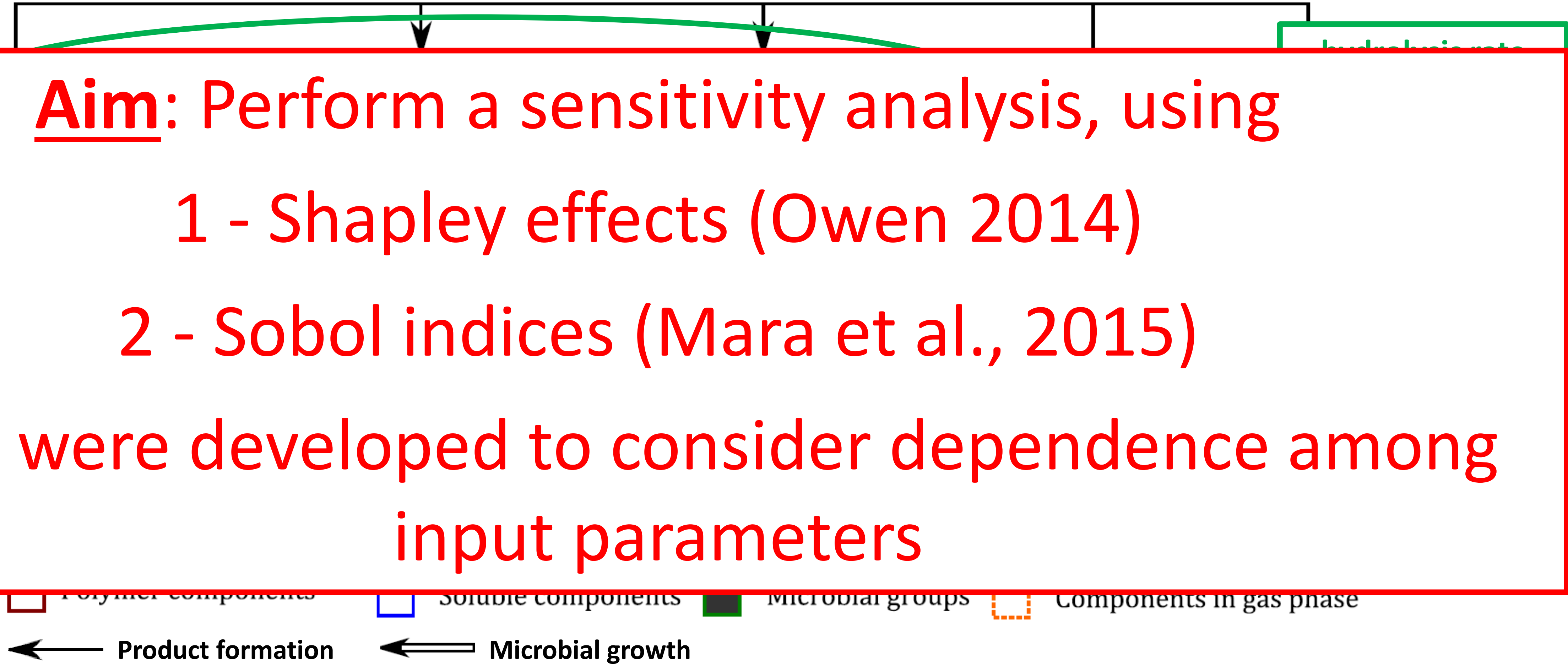


Aim: Perform a sensitivity analysis, using

1 - Shapley effects (Owen 2014)

2 - Sobol indices (Mara et al., 2015)

which were developed to consider dependence among input parameters

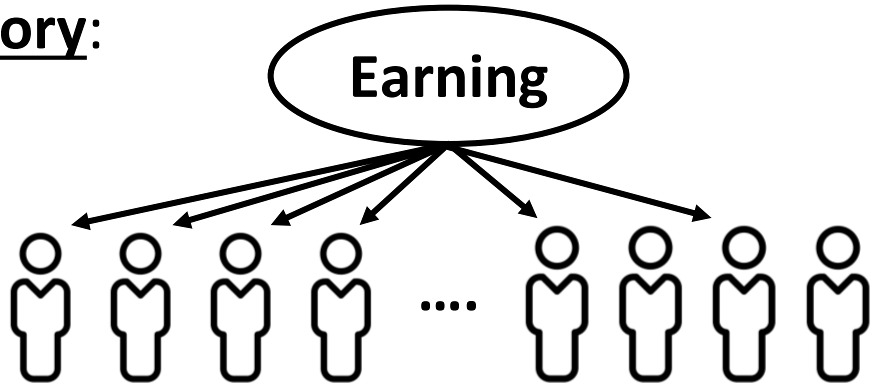
Model complexity: 18 output variables, 32 input parameters

2. Method 1: Shapley effects

Method

Game theory:

n players



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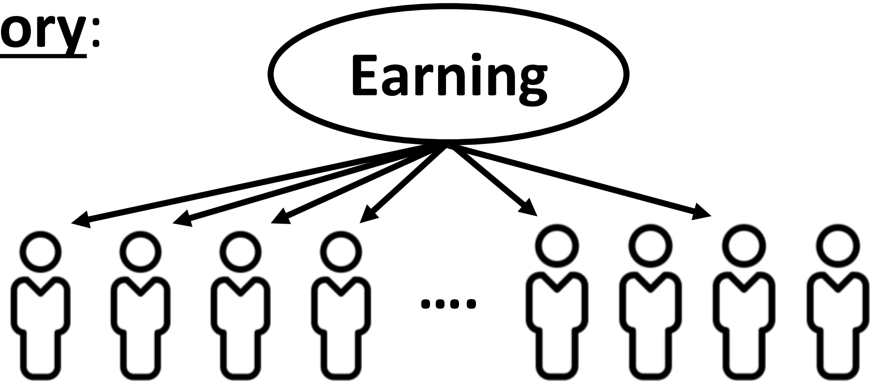

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define a relevant way to allocate the earnings between players

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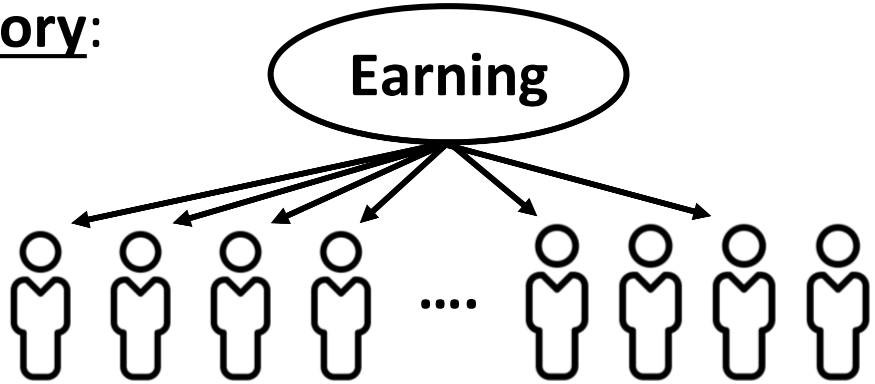

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Shapley, 1953 proposed a fair share of earnings of a n players coalition

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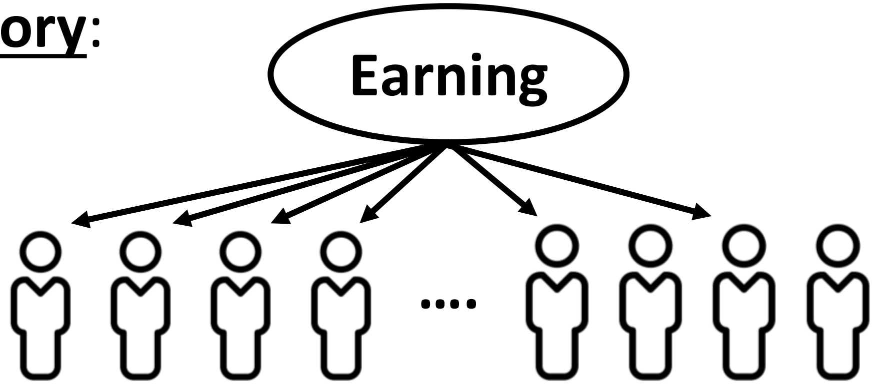

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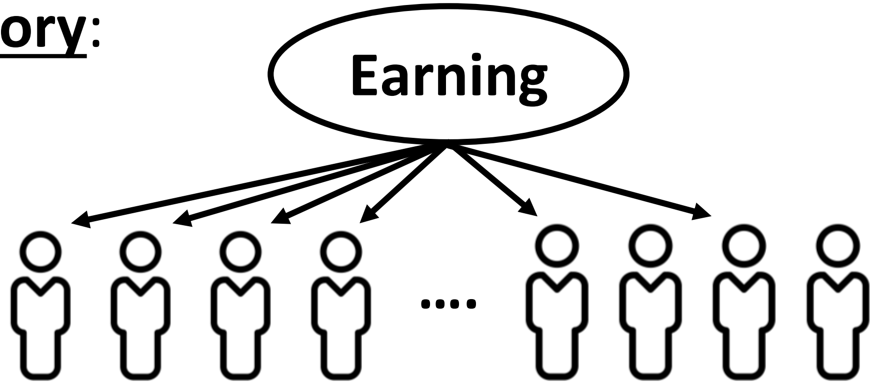

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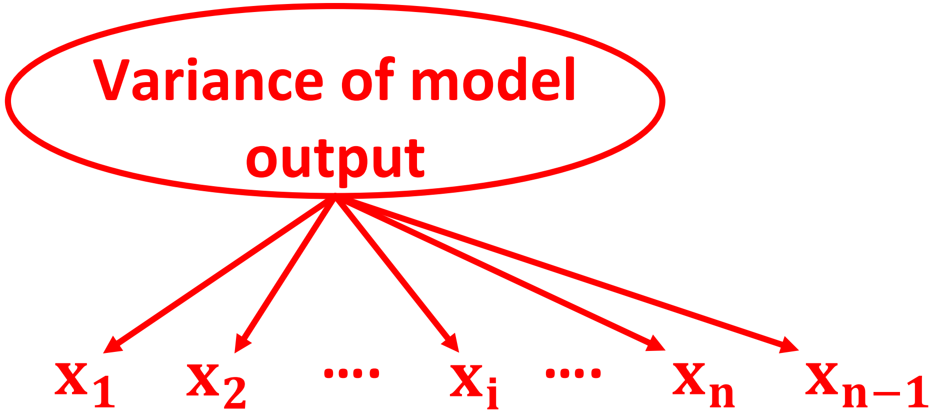

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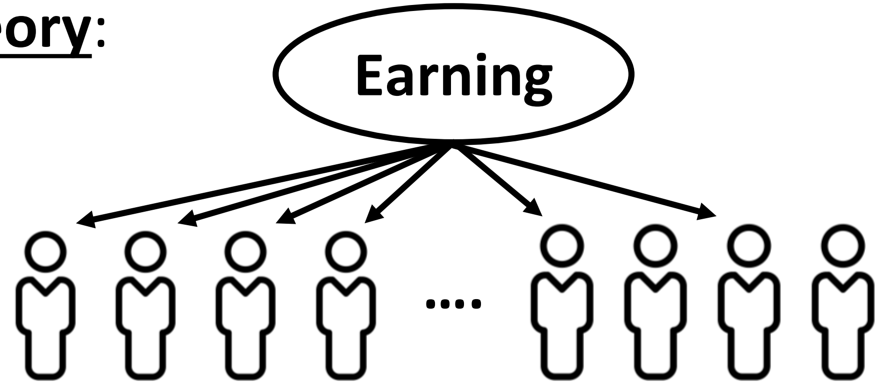

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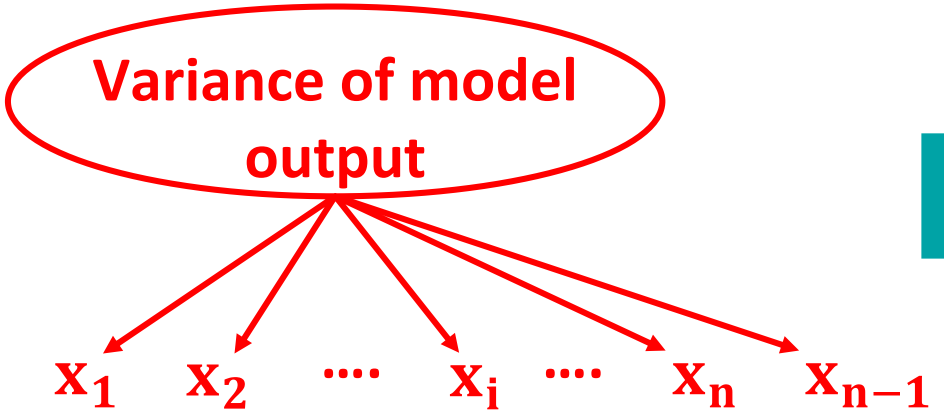

n inputs

Shapley effects measure the part of variance of model output caused by the uncertainty of the inputs and allow an allocation of the interaction and dependence contributions between the inputs

Sensitivity indices computed

Shapley effects

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➡ Advantage: condensed and easy-to-interpret (sum equal to 1)

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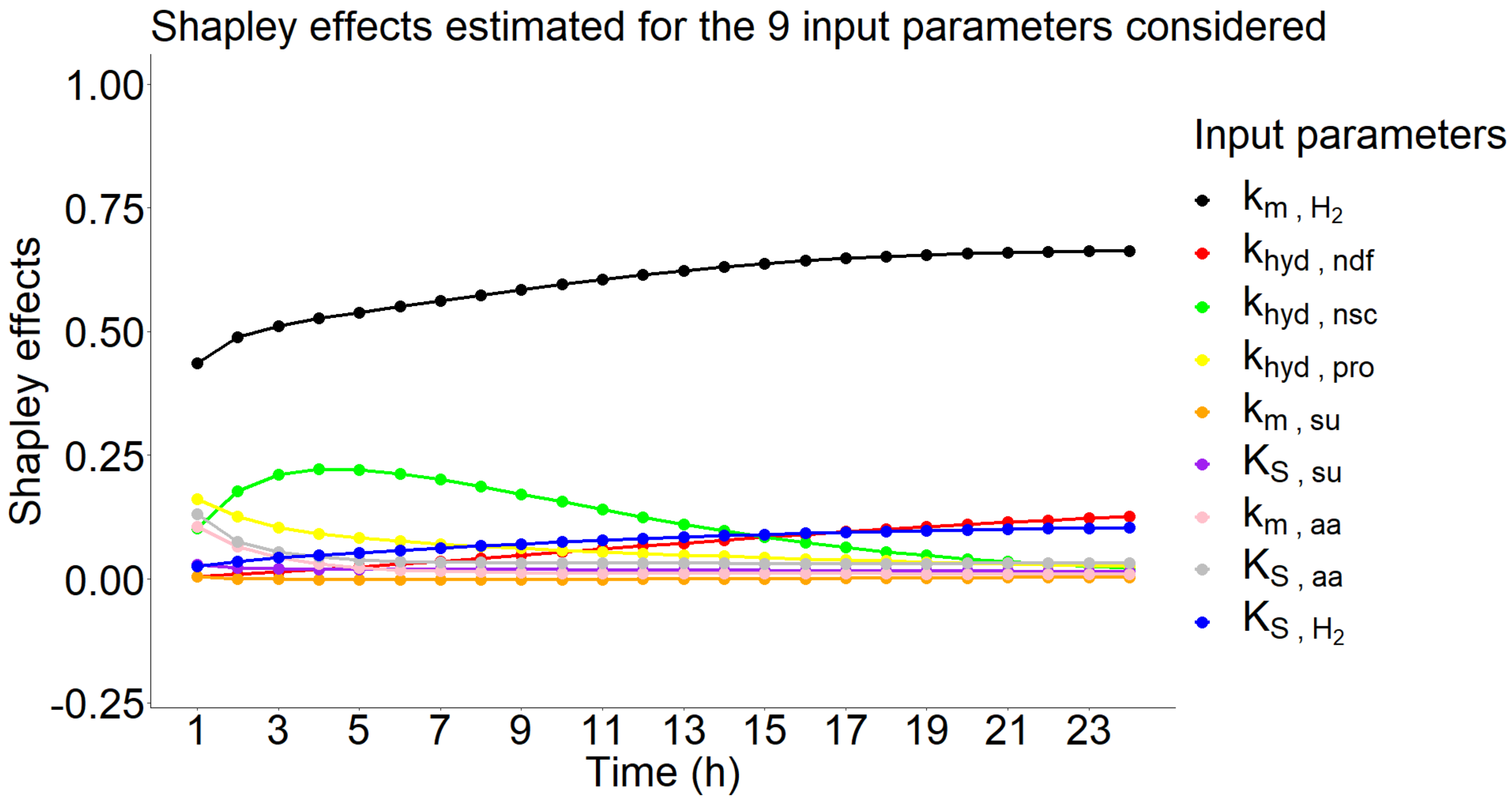
- $m = 10{,}000$ permutations were performed

Application on CH_4 concentration dynamic



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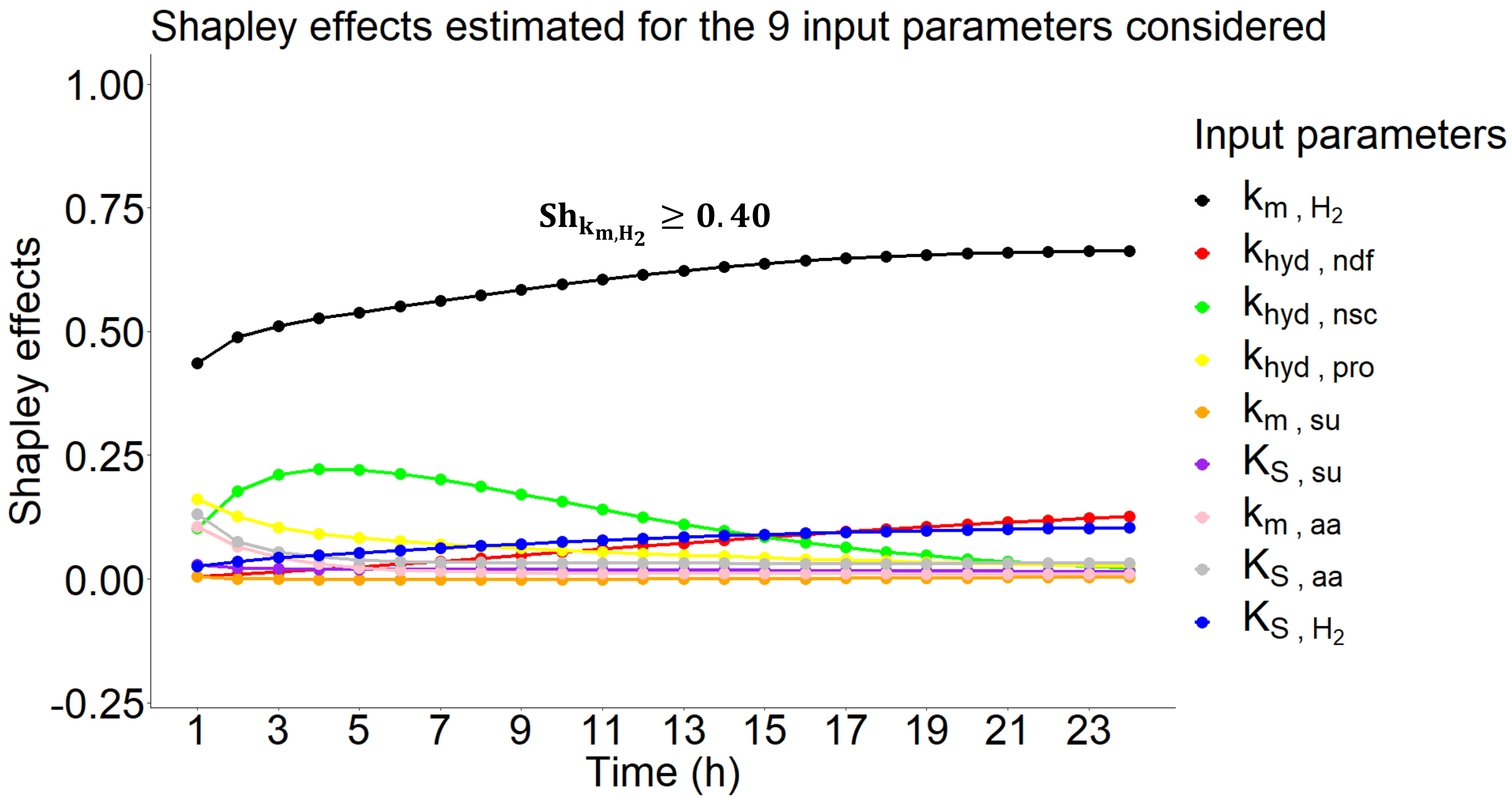
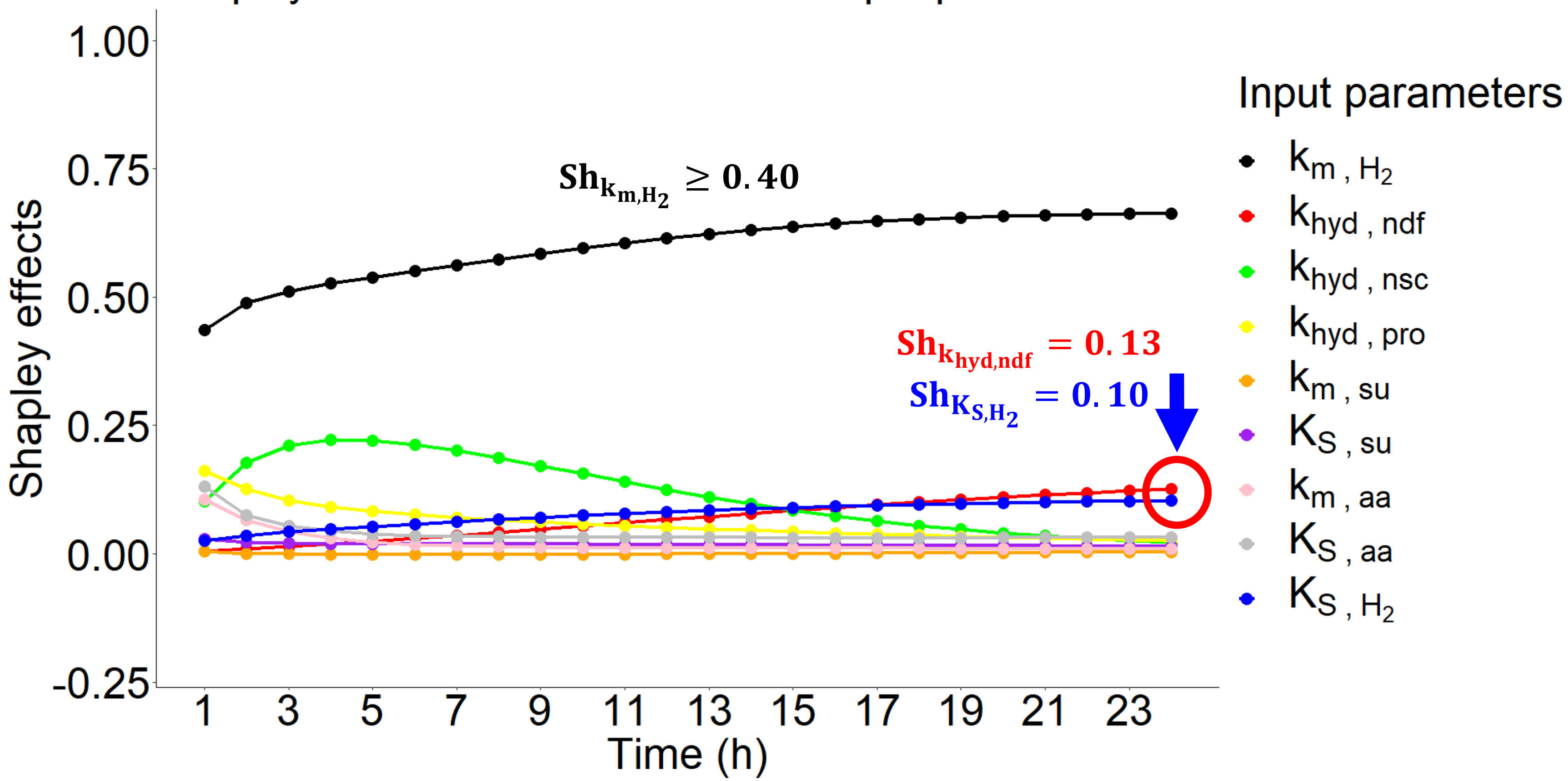


✓ $\mathbf{k_{m,H_2}}$ contributed the most to the variability of CH_4 concentration dynamic over all the time considered

Application on CH_4 concentration dynamic

Shapley effects estimated for the 9 input parameters considered



- ✓ $\mathbf{k_{m,H_2}}$ contributed the most to the variability of CH_4 concentration dynamic over all the time considered
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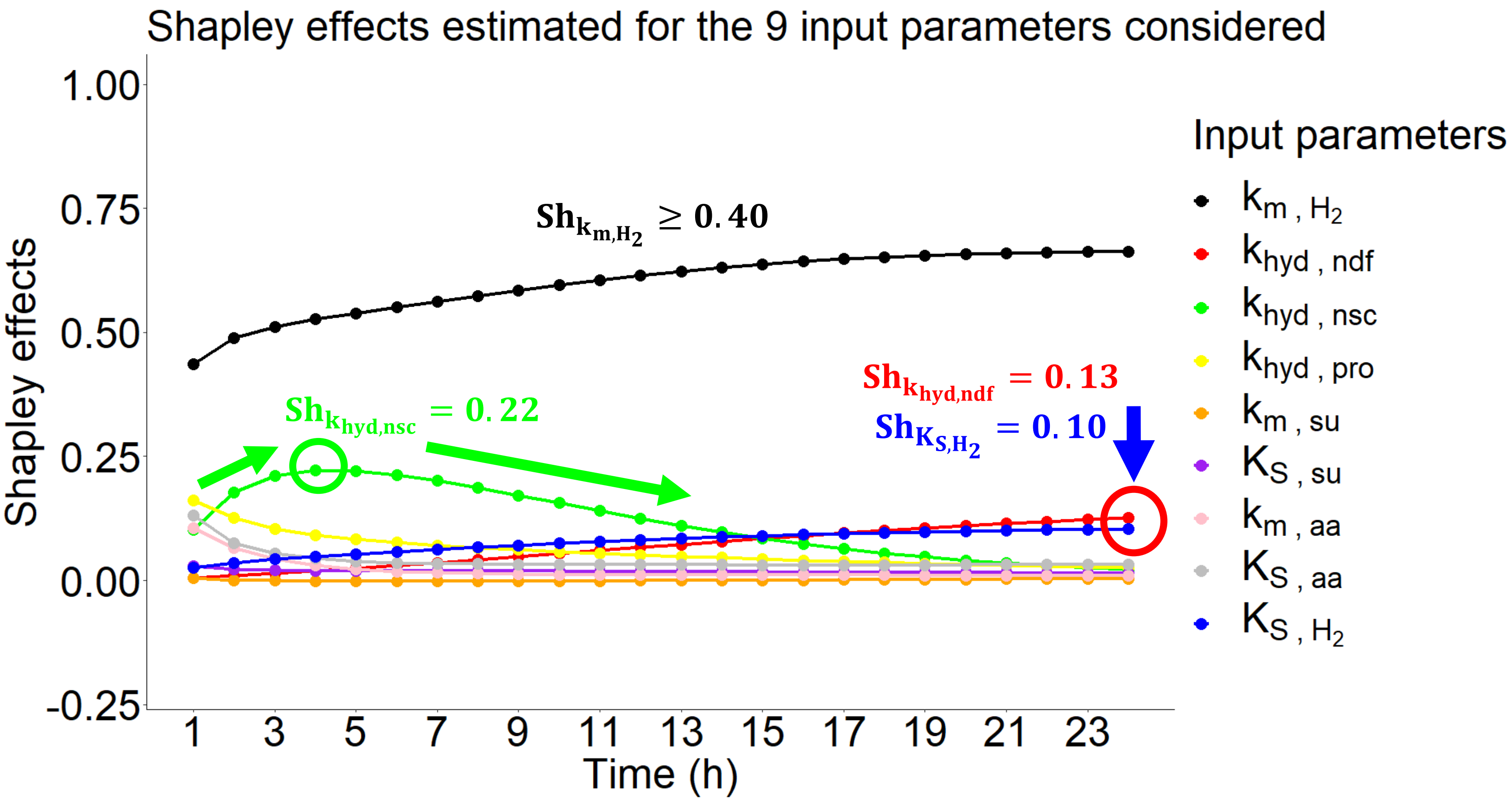

- ✓ $\mathbf{k_{m,H_2}}$ contributed the most to the variability of CH_4 concentration dynamic over all the time considered
- ✓ $\mathbf{k_{hyd,ndf}}$ and $\mathbf{K_{S,H_2}}$ were the other influential input parameters at t = 24h
- ✓ $\mathbf{k_{hyd,nsc}}$ had a rather important contribution at the beginning of the fermentation before to slowly decreased to 0

3. Method 2: Full and independent Sobol indices

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Dependent inputs **Rosenblatt transformation** → **Independent inputs**

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n circular reordering of $x = (x_1, x_2, \ldots, x_{n-1}, x_n)$:

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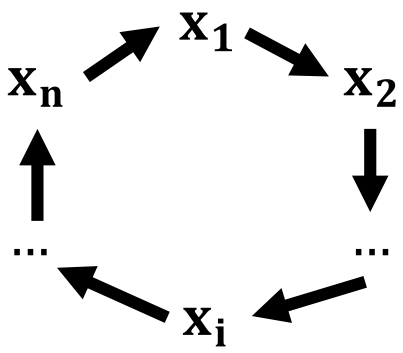

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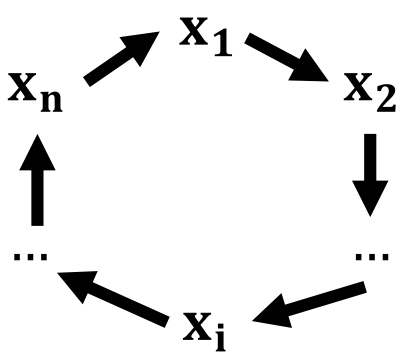

1st reordering : $(x_1, x_2, \dots, x_i, \dots, x_n)$

⋮

ith reordering : $(x_i, x_{i+1}, \dots, x_1, \dots, x_{i-1})$

⋮

nth reordering : $(x_n, x_1, \dots, x_i, \dots, x_{n-1})$

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

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$$\left[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, \left(x_{i-1}\middle|x_{\sim(i-1)}\right)\right] \xrightarrow{RT} \left(u_1^i, u_2^i, \dots, u_n^i\right)$$

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$\mathbf{u_1^i}$ include the effects of the dependence of $\mathbf{x_i}$ with the other inputs

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Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

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Full Sobol indices of x_i (S_i^{full}, T_i^{full})

Sensitivity indices computed

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Full Sobol indices of x_i $\left(S_i^{full}, T_i^{full}\right)$

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

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Full Sobol indices of x_i $\left(S_i^{full}, T_i^{full}\right)$

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

Independent Sobol indices of x_{i-1} $\left(S_{i-1}^{ind}, T_{i-1}^{ind}\right)$

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

$$[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, (x_{i-1}|x_{\sim(i-1)})] \xrightarrow{RT} (u_1^i, u_2^i, \dots, u_n^i)$$

u_1^i include the effects of the dependence of x_i with the other inputs

⬇

Full Sobol indices of x_i (S_i^{full}, T_i^{full})

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

⬇

Independent Sobol indices of x_{i-1} $(S_{i-1}^{ind}, T_{i-1}^{ind})$

Interpretation:

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

$$\left[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, (x_{i-1}|x_{\sim(i-1)})\right] \xrightarrow{RT} (u_1^i, u_2^i, \dots, u_n^i)$$

u_1^i include the effects of the dependence of x_i with the other inputs

⇩

Full Sobol indices of x_i (S_i^{full}, T_i^{full})

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

⇩

Independent Sobol indices of x_{i-1} $(S_{i-1}^{ind}, T_{i-1}^{ind})$

Interpretation:

1. Comparison of the total indices T_i^{full} and T_i^{ind}

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

$$[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, (x_{i-1}|x_{\sim(i-1)})] \xrightarrow{RT} (u_1^i, u_2^i, \dots, u_n^i)$$

u_1^i include the effects of the dependence of x_i with the other inputs

Full Sobol indices of x_i (S_i^{full}, T_i^{full})

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

Independent Sobol indices of x_{i-1} $(S_{i-1}^{ind}, T_{i-1}^{ind})$

<u>Interpretation</u>:

1. Comparison of the total indices T_i^{full} and T_i^{ind}
   - ✓ If $T_i^{ind} \approx 0$ and $T_i^{full} \gg 0$ → contribution of x_i is only due to its dependence with other inputs

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

$$[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, (x_{i-1}|x_{\sim(i-1)})] \xrightarrow{RT} (u_1^i, u_2^i, \dots, u_n^i)$$

u_1^i include the effects of the dependence of x_i with the other inputs

⬇

Full Sobol indices of x_i (S_i^{full}, T_i^{full})

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

⬇

Independent Sobol indices of x_{i-1} $(S_{i-1}^{ind}, T_{i-1}^{ind})$

Interpretation:

1. Comparison of the total indices T_i^{full} and T_i^{ind}
   - ✓ If $T_i^{ind} \approx 0$ and $T_i^{full} \gg 0$ ➡ contribution of x_i is only due to its dependence with other inputs
   - ✓ If $T_i^{ind} \gg 0$ ➡ contribution of x_i is due to x_i alone and /or its interactions with other inputs

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

$$[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, (x_{i-1}|x_{\sim(i-1)})] \xrightarrow{RT} (u_1^i, u_2^i, \dots, u_n^i)$$

u_1^i include the effects of the dependence of x_i with the other inputs

Full Sobol indices of x_i (S_i^{full}, T_i^{full})

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

Independent Sobol indices of x_{i-1} $(S_{i-1}^{ind}, T_{i-1}^{ind})$

<u>Interpretation</u>:

1. Comparison of the total indices T_i^{full} and T_i^{ind}

- ✓ If $T_i^{ind} \approx 0$ and $T_i^{full} \gg 0$ ➡ contribution of x_i is only due to its dependence with other inputs
- ✓ If $T_i^{ind} \gg 0$ ➡ contribution of x_i is due to x_i alone and /or its interactions with other inputs
- ✓ If $T_i^{ind} \approx 0$ and $T_i^{full} \approx 0$ ➡ x_i has no contribution on output variance

Sensitivity indices computed

Let's consider the i^{th} reordering $(x_i, x_{i+1}, \dots, x_n, x_1, x_2, \dots, x_{i-1})$

$$[(x_i), (x_{i+1}|x_i), \dots, (x_1|(x_i, x_{i+1}, \dots, x_n)), \dots, (x_{i-1}|x_{\sim(i-1)})] \xrightarrow{RT} (u_1^i, u_2^i, \dots, u_n^i)$$

u_1^i include the effects of the dependence of x_i with the other inputs

⇓

Full Sobol indices of x_i (S_i^{full}, T_i^{full})

u_n^i represent the effects of x_{i-1} that are not due to its dependence with the other inputs $x_{\sim(i-1)}$

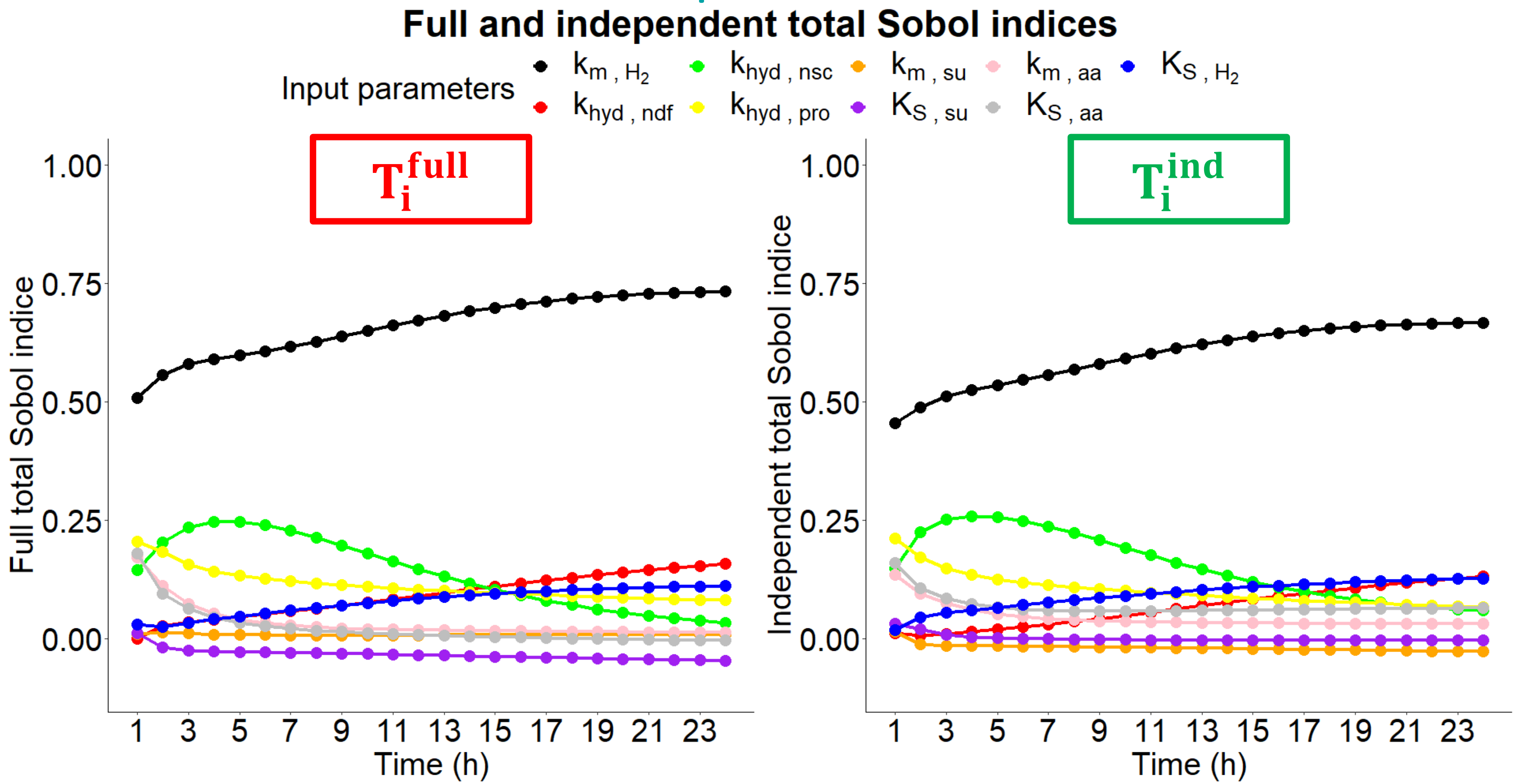
⇓

Independent Sobol indices of x_{i-1} $(S_{i-1}^{ind}, T_{i-1}^{ind})$

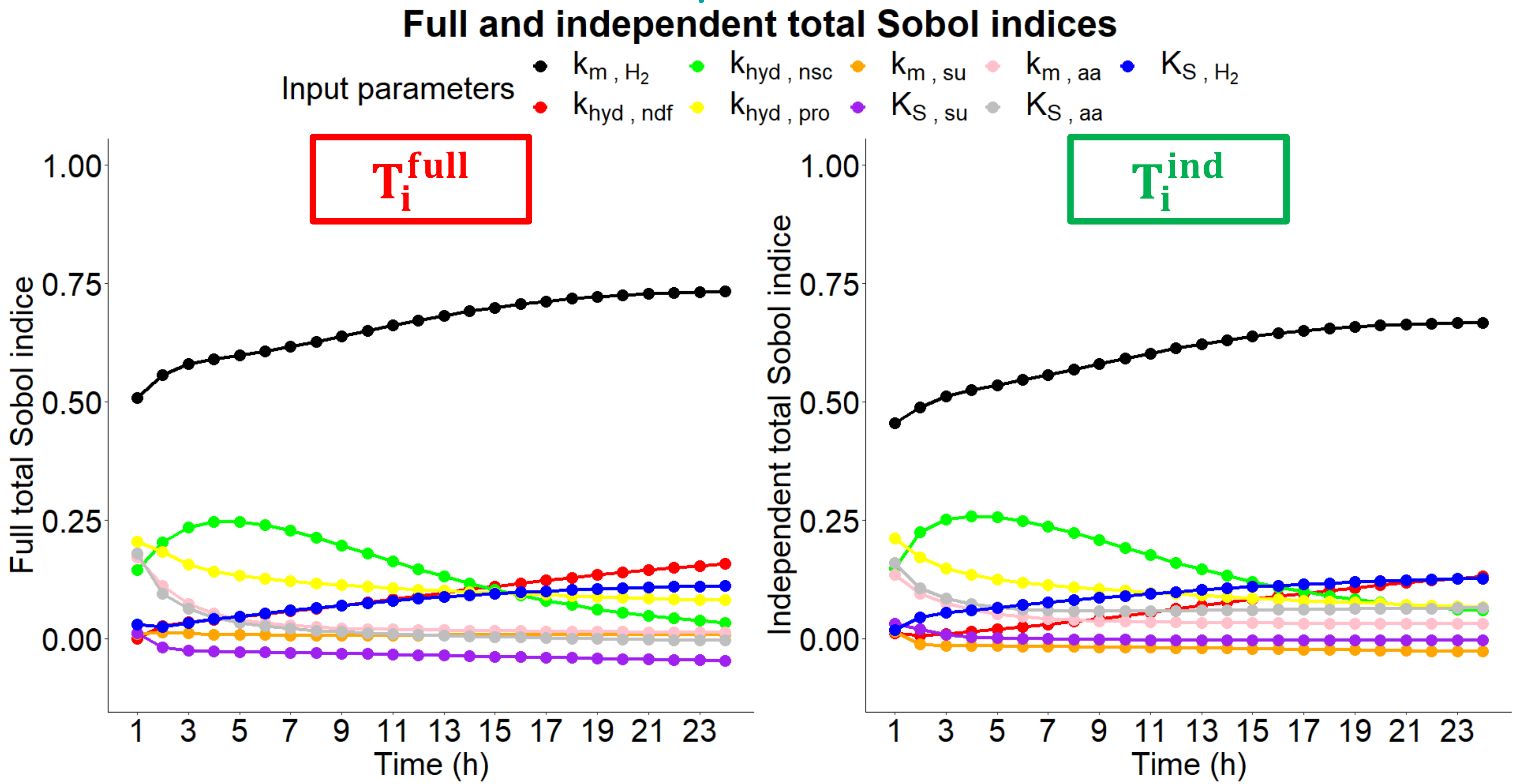
Interpretation:

1. Comparison of the total indices T_i^{full} and T_i^{ind}
   - ✓ If $T_i^{ind} \approx 0$ and $T_i^{full} \gg 0$ ⟹ contribution of x_i is only due to its dependence with other inputs
   - ✓ If $T_i^{ind} \gg 0$ ⟹ contribution of x_i is due to x_i alone and /or its interactions with other inputs
   - ✓ If $T_i^{ind} \approx 0$ and $T_i^{full} \approx 0$ ⟹ x_i has no contribution on output variance
2. Comparison of S_i^{full} and T_i^{full} or S_i^{ind} and T_i^{ind} to analyze the effects of the interactions

Application on CH_4 concentration dynamic

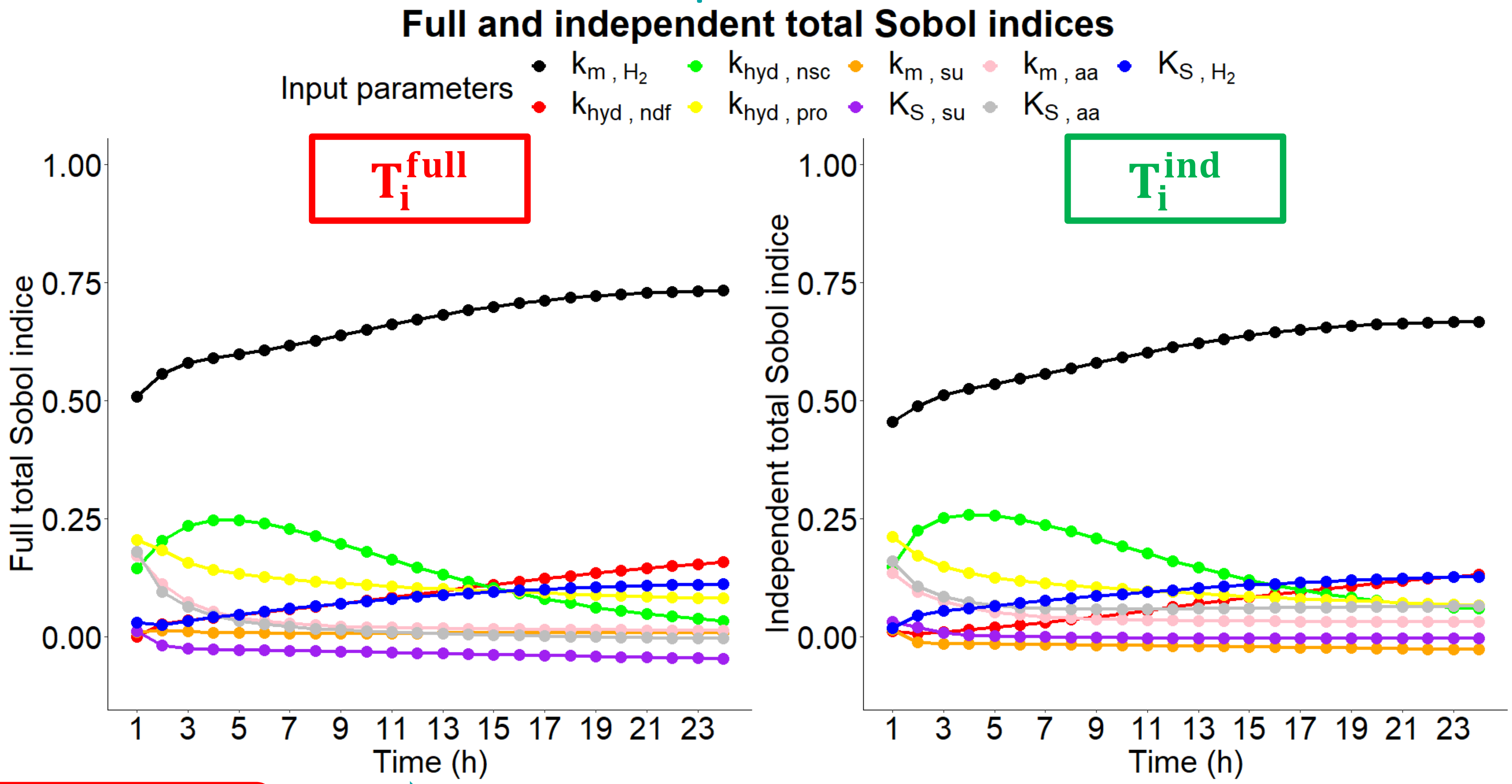


Application on CH_4 concentration dynamic



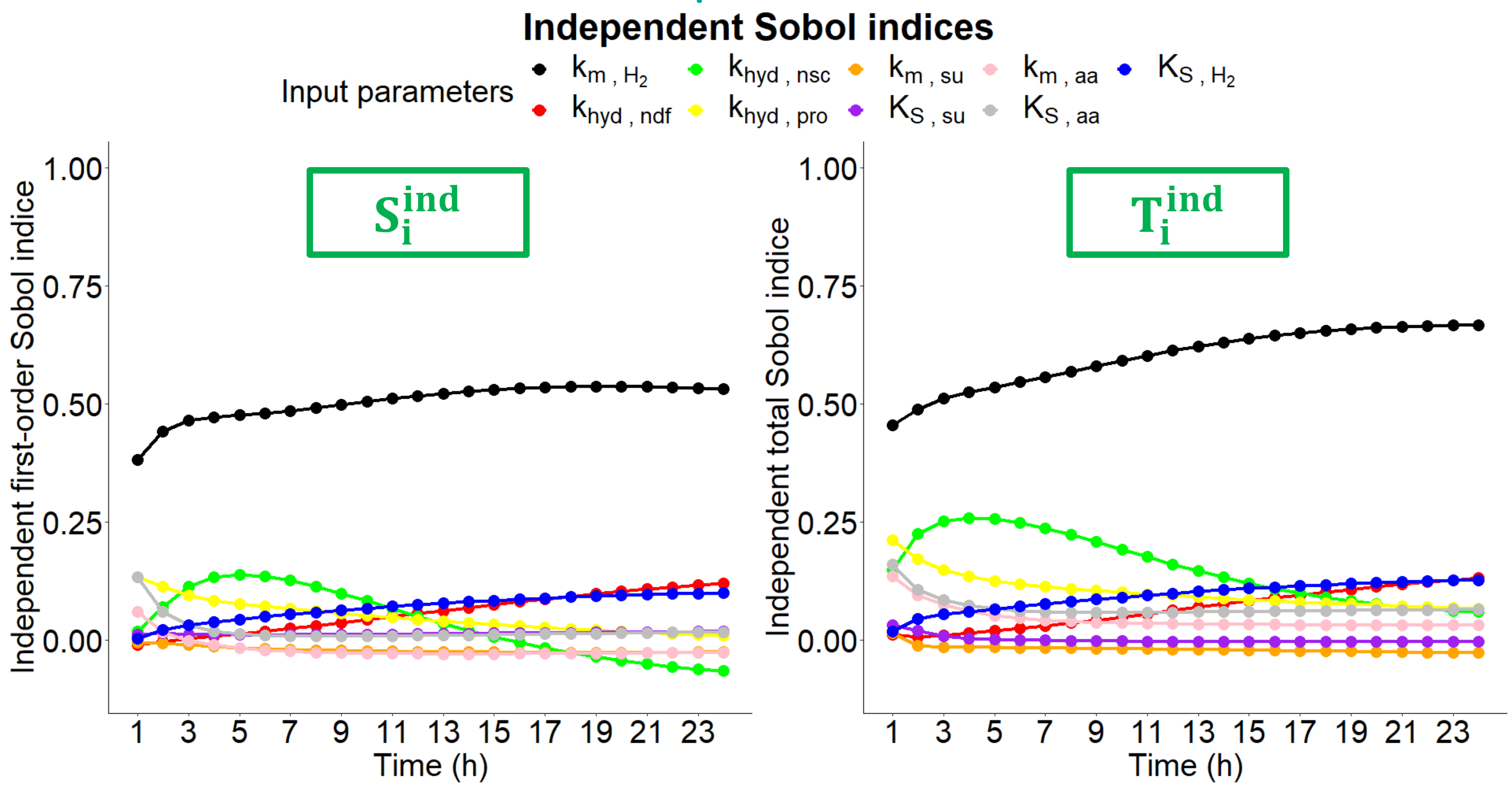
$$T_i^{full} - T_i^{ind} \leq 0.07$$

Application on CH_4 concentration dynamic

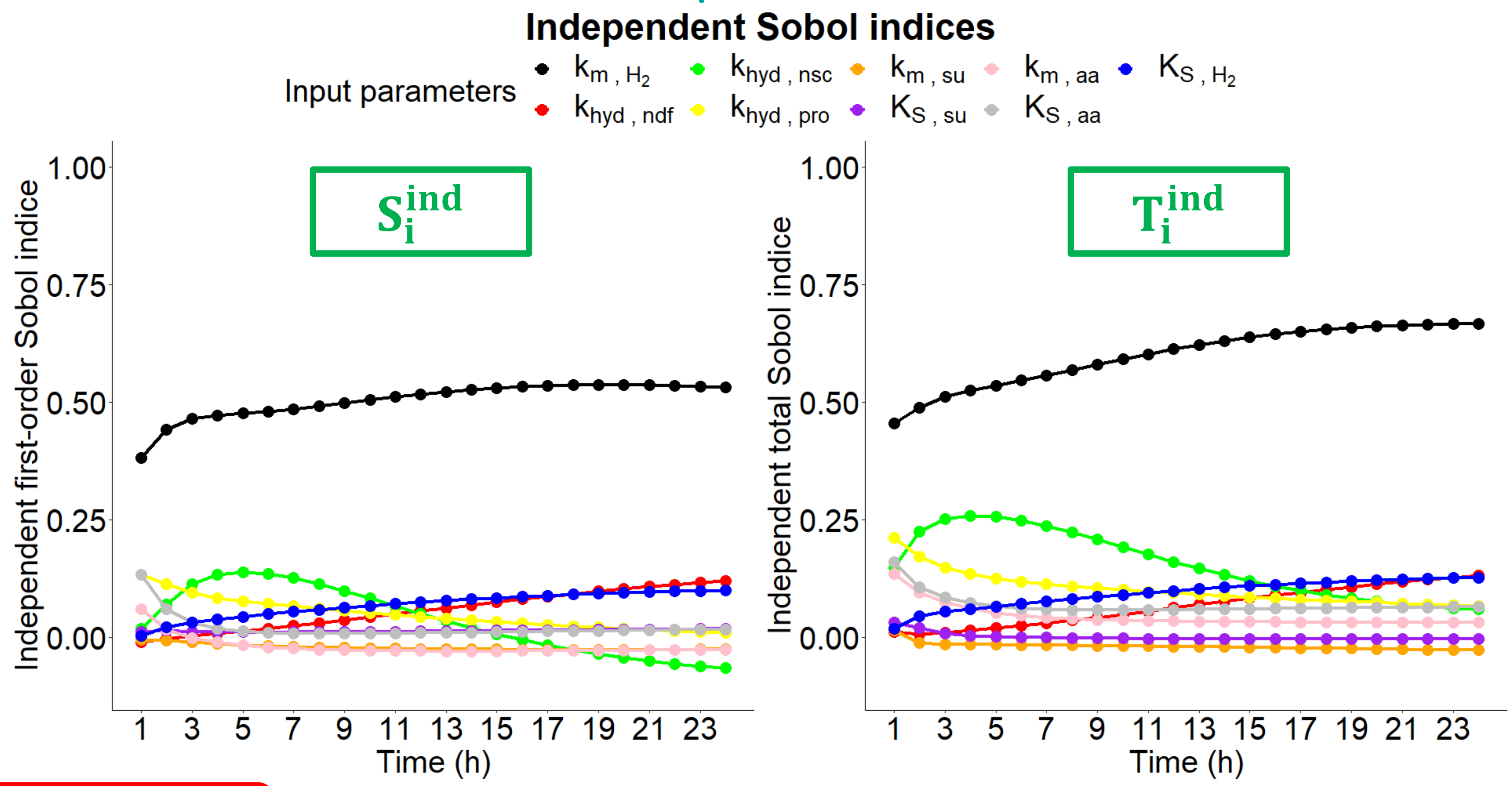


$T_i^{full} - T_i^{ind} \leq 0.07$ → **dependencies among input parameters contributed very few to the variance of the CH_4 concentration dynamic (as expected)**

Application on CH_4 concentration dynamic

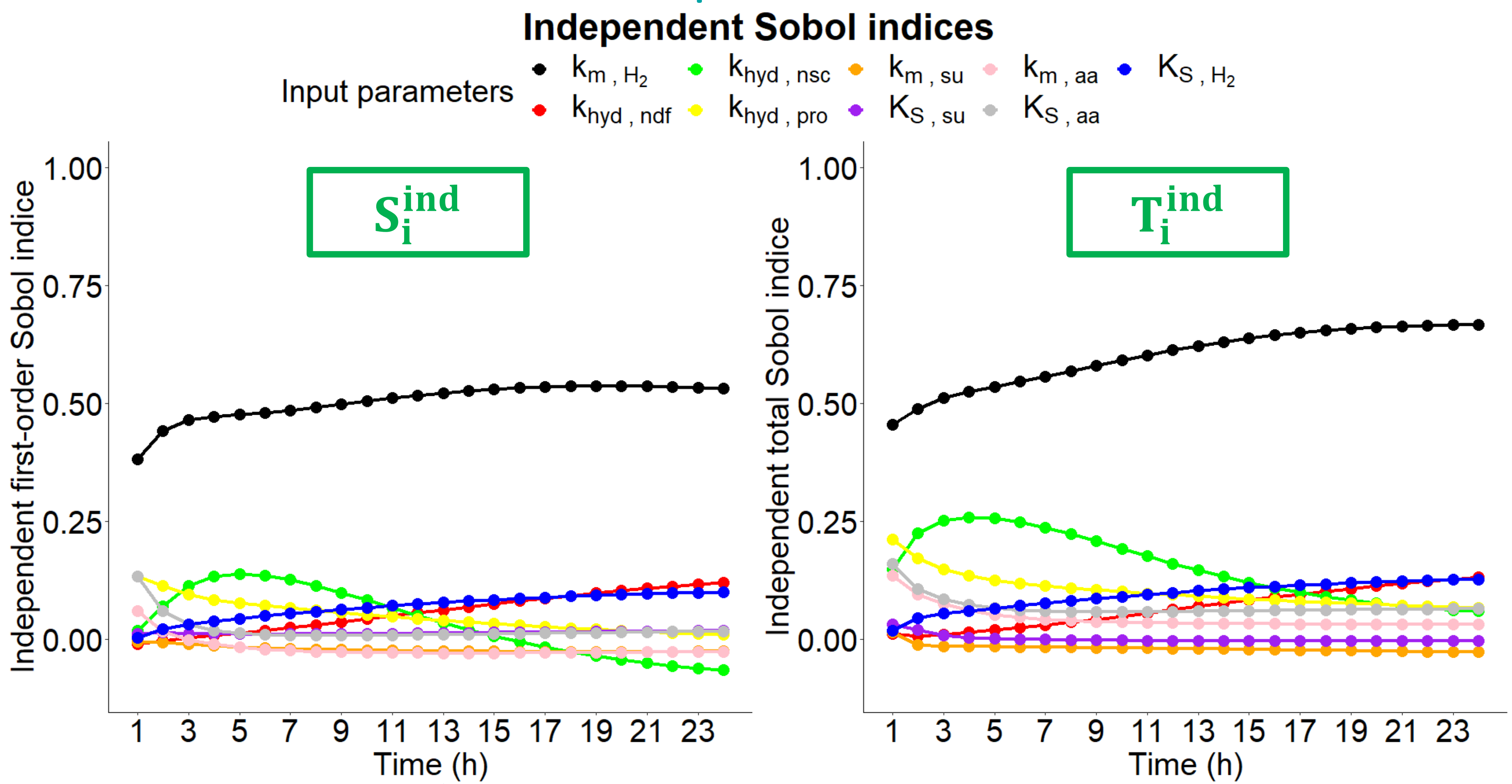


Application on CH_4 concentration dynamic



$$T_i^{ind} - S_i^{ind} \leq 0.15$$

Application on CH_4 concentration dynamic



$$T_i^{ind} - S_i^{ind} \leq 0.15$$

Interactions between input parameters contributed very few to the variance of the CH_4 concentration dynamic

4. Conclusion

Take home messages

Shapley effects

k_{m,H_2} was the most influential input parameter to the variation of the dynamic of CH_4 concentration

Take home messages

Shapley effects

- **k_{m,H_2} was the most influential input parameter to the variation of the dynamic of CH_4 concentration**
- $k_{hyd,nsc}$ showed a non-negligible contribution to CH_4 concentration variability at the beginning of the fermentation

Take home messages

Shapley effects

- **k_{m,H_2} was the most influential input parameter to the variation of the dynamic of CH_4 concentration**
- $k_{hyd,nsc}$ showed a non-negligible contribution to CH_4 concentration variability at the beginning of the fermentation
- $k_{hyd,ndf}$ and K_{S,H_2} showed a low contribution at t = 24h

Take home messages

Shapley effects

- **k_{m,H_2} was the most influential input parameter to the variation of the dynamic of CH_4 concentration**
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Full and independent Sobol indices

- **Dependency (expected) and interaction contributions were low**

Take home messages

Shapley effects

- $\mathbf{k_{m,H_2}}$ **was the most influential input parameter to the variation of the dynamic of CH_4 concentration**
- $k_{hyd,nsc}$ showed a non-negligible contribution to CH_4 concentration variability at the beginning of the fermentation
- $k_{hyd,ndf}$ and K_{S,H_2} showed a low contribution at t = 24h

Full and independent Sobol indices

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Perspectives

Take home messages

Shapley effects

- **k_{m,H_2} was the most influential input parameter to the variation of the dynamic of CH_4 concentration**
- $k_{hyd,nsc}$ showed a non-negligible contribution to CH_4 concentration variability at the beginning of the fermentation
- $k_{hyd,ndf}$ and K_{S,H_2} showed a low contribution at t = 24h

Full and independent Sobol indices

- **Dependency (expected) and interaction contributions were low**

Perspectives

1. **Extend these implementations to a mechanistic model of the rumen *in-vivo* fermentation with dependent input parameters**

Take home messages

Shapley effects

- **k_{m,H_2} was the most influential input parameter to the variation of the dynamic of CH_4 concentration**
- $k_{hyd,nsc}$ showed a non-negligible contribution to CH_4 concentration variability at the beginning of the fermentation
- $k_{hyd,ndf}$ and K_{S,H_2} showed a low contribution at t = 24h

Full and independent Sobol indices

- **Dependency (expected) and interaction contributions were low**

Perspectives

1. **Extend these implementations to a mechanistic model of the rumen *in-vivo* fermentation with dependent input parameters**

2. **PhD: Uncertainty analysis of several outputs of the rumen fermentation computed by the model**

Thank you for your attention!

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Thanks to INRAE research department PHASE and the ABIES doctoral school for funding this PhD