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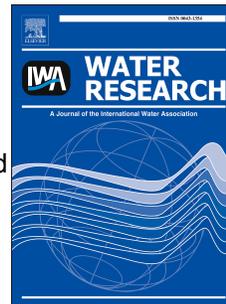
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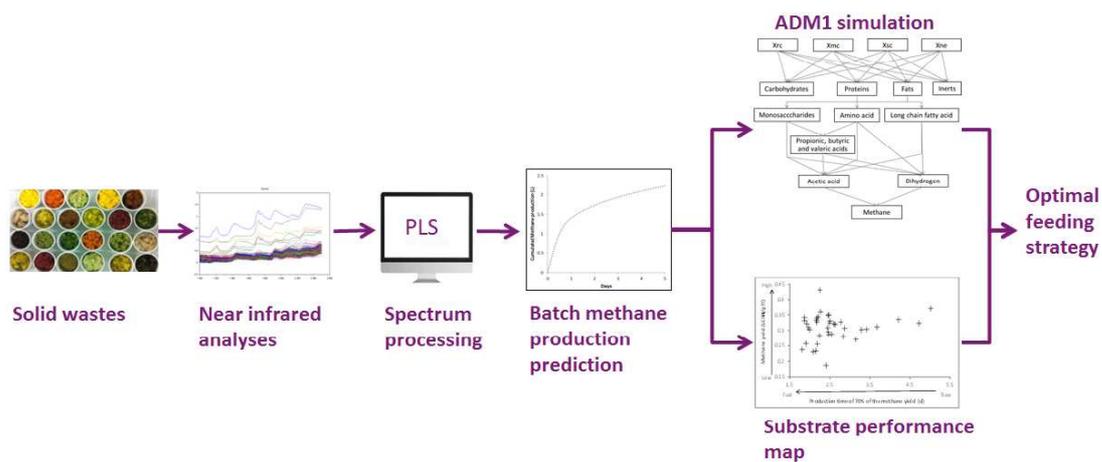
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Fast ADM1 implementation for the optimization of feeding strategy using near infrared spectroscopy

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Abstract

Optimization of feeding strategy is an essential issue of anaerobic co-digestion that can be greatly assisted with simulation tools such as the Anaerobic Digestion Model 1. Using this model, a set of parameters, such as the biochemical composition of the waste to be digested, its methane production yield and kinetics, has to be defined for each new substrate. In the recent years, near infrared analyses have been reported as a fast and accurate solution for the estimation of methane production yield and biochemical composition. However, the estimation of methane production kinetics requires time-consuming analysis. Here, a partial least square regression model was developed for a fast and efficient estimation of methane production kinetics using near infrared spectroscopy on 275 bio-waste samples. The development of this characterization reduces the time of analysis from 30 days to a matter of minutes. Then, biochemical composition

21 and methane production yield and kinetics predicted by near infrared spectroscopy were
22 implemented in a modified Anaerobic Digestion Model n°1 in order to simulate the performance
23 of anaerobic digestion processes. This approach was validated using different data sets and was
24 demonstrated to provide a powerful predictive tool for advanced control of anaerobic digestion
25 plants and feeding strategy optimization.

26 **Keywords**

27 Spectroscopy; Kinetics; Methane potential; Modeling; Anaerobic digestion; ADM1.

28

29 ***1 INTRODUCTION***

30

31 Anaerobic digestion (AD) is probably the major biological process involved in waste valorization. It
32 has a low energy requirement, low sludge production and large potentialities to produce both valuable
33 intermediates and energy. Nonetheless, diversification of substrates and development of Anaerobic co-
34 Digestion (AcoD) are needed in order to keep AD as a highly efficient process. Since feeding strategy is
35 the major factor governing the overall process, the development of AcoD involves optimal feeding
36 strategy definition (Karthikeyan and Visvanathan, 2013). The variability of the available inputs and the
37 diversity of technological processes has made the forecasting of the process performances and the
38 definition of an optimal feeding strategy difficult. In particular, precise substrates characterization and
39 advanced dynamic models are required to predict the performances of the process depending on its
40 feeding strategy (García-Gen et al., 2013). In that aim, the Anaerobic Digestion Model #1 (ADM1) has
41 been developed (Batstone et al., 2002). ADM1 is a detailed model taking into account the main reactions
42 of AD processes. ADM1 has been extensively used and analyzed in both academic and practical
43 applications (Batstone et al., 2006).

44 The first limit is that hydrolysis is recognized as the rate-limiting step in the complex digestion
45 process (Appels et al., 2008) but is represented as a single-order reaction in ADM1. Contois-type
46 equation represents more accurately the hydrolysis of solid substrates (Yasui et al., 2006). Moreover,
47 García-Gen et al., (2015) and Jimenez et al., (2016) recommended to split the organic matter into three
48 to four compartments with different kinetics of hydrolysis to fit the experimental biogas production. The
49 second limit encountered while using such a complex model is that many parameters have to be

50 determined and depend either on the substrate or on the process (Batstone et al., 2015). To set these
51 parameters, a precise characterization of the substrate composition as input variables is needed. Input
52 variables of the model describe the substrate in terms of protein, lipid, carbohydrate content and
53 Chemical Oxygen Demand (COD), biodegradability and kinetics of hydrolysis. Thus, several methods have
54 been proposed to simplify the implementation. Basically, Folin reagent or Kjeldahl procedure are used to
55 estimate the protein content (Souza et al., 2013), hexane extraction for lipid content (Girault et al.,
56 2012) and colorimetric assay using a complexation between phenol and glucose for the carbohydrate
57 content estimation (Ugwuanyi et al., 2005). Kleerebezem and Van Loosdrecht, (2006) proposed to use
58 the elemental composition of the substrate and to transform it into proteins, lipids, carbohydrates, and
59 COD. Zaher et al., (2009) generalized this approach creating a transformer that converts the elemental
60 composition and COD into an input ADM1 vector. The limit of the approaches based on elemental
61 composition is the estimation of the biodegradability and kinetics of hydrolysis. Biodegradability
62 estimation is usually calculated as a rate between COD and Biochemical Methane Potential (BMP). BMP
63 is experimentally obtained by batch digestion experiments which are time-consuming (Angelidaki et al.,
64 2009). However, the laboratory analyses reported above are time consuming and labor intensive, which
65 is an important drawback for industrial application. These characterizations of the substrate are rarely
66 available at industrial scale and must be determined for each new substrate (Appels et al., 2011). The
67 difficulty to estimate the parameters describing the substrate reduces the applicability of the model for
68 the predictions of the digestion performances at industrial scale.

69 Thus, different methods have been proposed to shorten the time of analysis. Jimenez et al., (2014)
70 used a Partial Least Square (PLS) regression model to predict biodegradability by 3D fluorescence
71 coupled with chemical sequential extractions. It allows reducing the time of analysis from one month to
72 one week. Another method has been proposed by Lesteur et al., (2011) and Jacobi et al., (2012) which
73 reduces the time of BMP analysis to a matter of minute using Near InfraRed (NIR) spectra. NIR spectra

74 are mathematically treated using Standard Normal Variate normalization (SNV), detrending or Savitsky-
75 Golay filtering and used to predict the BMP thanks to a PLS model (see also Ward, 2016). Recently,
76 Charnier et al., (2016) extended the use of the NIR analyses to the prediction of the carbohydrate,
77 protein and lipid content and chemical oxygen demand. Combining the literature on the prediction of
78 the BMP and the biochemical composition, NIR appears to be an efficient method for a fast
79 implementation of the ADM1 model.

80 Kinetic estimation remains a challenge; few methods are available and are all based on biological
81 digestion of the substrates (Jensen et al., 2011). From these digestion experiments, the methane
82 production rate (MPR) is obtained and the kinetic is estimated so that the model fits the MPR (Yasui et
83 al., 2008). Batstone et al., (2009) suggested that this approach underestimates the kinetics of methane
84 production because kinetics depends on the micro-organisms adaptation to the substrate. In order to
85 adapt the micro-organisms to the substrate, García-Gen et al. (2015) estimated the kinetics on eight
86 successive batches using the same substrate to feed the reactor. Thus, methane production kinetics
87 estimation requires batch or continuous digestion experiments which make the kinetics of methane
88 production one of the longest parameter to obtain. To shorten the estimation of methane production
89 kinetics is a hindrance to overcome in order to use ADM1 for industrial purposes (Batstone et al., 2015).

90 Hence, this study aims at reducing the difficulties of ADM1 parameters estimation. It first focuses on
91 the possibility to predict the methane production kinetics of solid substrates using NIR spectroscopy. In a
92 second time, combining the models existing on the literature (Charnier et al., 2016; Jacobi et al., 2012;
93 Lesteur et al., 2011) and the model developed in this study, NIR is used to predict biochemical
94 composition and MPR to implement ADM1. The hydrolysis kinetics of ADM1 is optimized to fit the MPR
95 predicted by NIR. This approach reduces the ADM1 parameters estimation such as BMP or hydrolysis

96 kinetic from 30 days to a matter of hours, making it suitable for industrial application. Eventually, the
97 accuracy of this approach has been estimated based on two case studies.

98 **2 MATERIAL AND METHODS**

99 **2.1 Batch experiments**

100 MPR was estimated from biological degradation of the substrate. Experiments were carried out in
101 8.5 L batch reactors with 6 L of sludge under mesophilic conditions as described in García-Gen et al.,
102 (2015). The substrates were grinded to approximately 1cm. In order to adapt the micro-organisms to the
103 substrate, The reactor was fed at 1 gVS.l^{-1} with the same substrate in eight successive batches, each one
104 lasting for only few days, due to the low amount of substrate added. The biogas produced passed
105 through a moisture trap and through a milligas counter fitted with a digital output (MGC-1 gas flow
106 meters, DR.-ING.RITTER APPARTEBAU GMBH & CO.KG, Bochum, Germany); the data were recorded on-
107 line. The methane production of the last batch (i.e., after adaptation of the microbial ecosystem to the
108 substrate) was used to obtain the MPR. Methane yield was estimated as the maximal methane produced
109 from 1 gTS on the eighth batch. Methane production times were selected on the MPR as values
110 corresponding to the durations required to reach a certain ratio of the methane yield from 5 to 95 %
111 with a regular increment of 5 %.

112 **2.2 NIR analyses**

113 According to Lesteur et al., (2011), freeze-dried and grinded samples were scanned in reflectance
114 over 1000-2500 nm, with a resolution of $2.5 \cdot 10^6 \text{ nm}$, using a spectrophotometer BUCHI NIR-Flex N-500
115 solids fitted with vial accessory (Buchi®, Flawil, Switzerland). For the first chemometric treatment,
116 absorbance (A) was calculated from reflectance (R) as $A = \log(1/R)$ and SNV was applied. For the second

117 treatment, Savitzky–Golay filter with a second derivative was added to previous treatment of the
118 spectra. Eventually, a third treatment was added, based on the first treatment but with a detrending as
119 an additional chemometric treatment.

120 **2.3 Samples analyzed**

121 275 samples representing a wide diversity of substrates were analyzed to build the PLS model for the
122 prediction of the methane production times and BMP. In details, the analyses were conducted on 3 fat or
123 oleaginous samples, 24 fruits, 18 vegetables, 12 farm wastes such as straw, manure or grass, 15 cereals,
124 6 meat or fish extracts, 3 micro-algae and 194 mixed organic wastes. Based on the recommendation of
125 Dardenne (2010), the dataset was split in an independent validation set and a calibration set before
126 establishing any correlation with NIR spectroscopy. A validation set of 42 samples was separated for the
127 model validation composed of 6 vegetables and 36 mixed organic wastes. The remaining 237 samples
128 were used to calibrate the PLS regression model. All the samples were freeze-dried and grinded below 1
129 mm before any analysis. The mean methane yield was about 0.316 L.gTS^{-1} and 0.270 L.gTS^{-1} with a
130 standard deviation of 0.093 L.gTS^{-1} and 0.041 L.gTS^{-1} , a minimal value of 0.129 L.gTS^{-1} and 0.167 L.gTS^{-1} , a
131 maximal value of 0.717 L.gTS^{-1} and 0.351 L.gTS^{-1} for the calibration and validation sets respectively.
132 Figure 1 represents the times required to reach a certain ratio of the methane yield, from 5 to 95%, of
133 both calibration and validation sets. The same samples as described in (Charnier et al., 2016) were used
134 to build the PLS model for the prediction of the biochemical composition.

135 **2.4 Partial least square regression for kinetics prediction.**

136 Methane yield was predicted using the toolbox FACT on Scilab 5.5.0. Methane production times
137 were firstly considered as independent values when running the PLS regression with the tool box FACT,
138 Scilab® 5.5.0. Each of the discrete times (from 5% to 95%) was used to build a specific PLS model leading
139 to 19 independent models with no dependencies between the latent variables for the 19 models.

140 In a second approach, the discrete times (from 5% to 95%) were considered as a vector using the
141 package MixOmics, R[®]3.2.2 leading to one PLS model with a single set of latent variables. In this case the
142 PLS model was built using MixOmics.
143 In both approach, the PLS models for the prediction of the methane production times and the PLS model
144 for the prediction of the methane yield were calibrated using the data from the calibration set. Cross-
145 validations were performed on the calibration set using the Jackknife method (Karaman et al., 2013)
146 which splits randomly the dataset into 15 independent blocks. For each PLS model, the performances of
147 the cross-validation were used to determine the number of latent variables and to choose the best
148 chemometric treatment. The final model was then applied to the independent validation set. The
149 accuracy and robustness of the model were assessed with the indicators recommended in Dardenne
150 (2010). Cross-validation performances were analyzed based on the model Standard Error of Calibration
151 (SEC), the Standard Error of Cross Validation (SECV) and the coefficient of determination between
152 predicted and reference values (R^2). The SEC was unfortunately not accessible using MixOmics but the Q^2
153 and SECV were used to assess the performance of the PLS. The accuracy of the PLS on the validation set
154 was assessed by the Standard error of Prediction (SEP) and bias.

156 **2.5 Modified ADM1**

157 ADM1 benchmarked on the BSM2 report (Rosén and Jeppsson, 2008) was implemented in Scilab
158 5.5.0. ADM1 model was then modified based on the work of (Ramirez et al., 2009). The degradation of
159 the particulate organic matter has been implemented with Contois kinetics to describe both
160 disintegration and hydrolysis. Hydrolysis was supposed to be non-limiting. Three micro-organism groups
161 were considered for the hydrolysis of carbohydrates, proteins and lipids. A consortium regrouping all the
162 hydrolytic micro-organism was considered for the disintegration. An additional modification of this

163 model was tested, as recommended in (Jimenez et al., 2016), four different particulate inputs were
164 implemented, Xrc, Xmc, Xsc and Xne according to their bioaccessibility (Figure 2). Xrc, Xmc, Xsc and Xne
165 stand respectively for the readily accessible, moderately accessible, slowly accessible and not extractible
166 organic matter. These four particulate inputs are considered to have the same composition and to be
167 degraded by the same biomass but with different μ_{\max} in this modified ADM1.

168 **2.6 MPR prediction**

169 The prediction of the MPR curve is made using the predicted methane yield and the 19 methane
170 production times (5-95 %) predicted. At each of the methane production time predicted is associated a
171 methane production using the methane yield multiplied by the percentage reached. Thus 19 points of
172 the MPR curve are estimated based on the NIR prediction. The initial point was added as zero methane
173 produced at time zero. The MPR was then interpolated. A smooth spline with the function *smooth.spline*
174 was done using R[®] 3.2.2 to remove noise. For the prediction of the confidence range, ± 1 SEP was added
175 to the 19 methane production times and the methane production yield before to produce the MPR using
176 this approach, in order to transfer the potential errors of the NIR prediction on the predicted MPR.

177 **2.7 Biochemical composition prediction**

178 The same methods, datasets and models as reported in (Charnier et al., 2016) were used for an
179 accurate prediction of the carbohydrates, nitrogen and lipids content and COD. Thus, the same
180 performances of prediction as described in (Charnier et al., 2016) were obtained. The total
181 carbohydrates content was predicted in $\text{mgO}_2 \cdot \text{gTS}^{-1}$, the total nitrogen content was predicted in $\text{g} \cdot \text{gTS}^{-1}$,
182 the total lipids content was predicted in $\text{g} \cdot \text{gTS}^{-1}$ and the total COD was predicted in $\text{mgO}_2 \cdot \text{gTS}^{-1}$.

183 **2.8 ADM1 modelling approach**

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184 Conversion of the NIR predicted values into ADM1 parameters are presented in Figure 3. Total
 185 nitrogen is converted into protein COD equivalent multiplying the total nitrogen in gram by 6.25*1.54
 186 (Girault et al., 2012). $\frac{1}{6.25}$ is the nitrogen content in protein and 1.54 the mean COD values of proteins
 187 in $\text{gO}_2\cdot\text{g}^{-1}$. Carbohydrates content was directly estimated in COD equivalent. Lipids content was
 188 estimated in gram per gram, thus a conversion rate of 2.8 between gram and COD was applied (Batstone
 189 et al., 2002). 2.8 represents the averaged COD of 1 gram of oil in $\text{gO}_2\cdot\text{g}^{-1}$. COD and methane yield
 190 predictions were used to assess the non-biodegradable content of the substrate using the equation 1
 191 described by Jimenez et al., (2014):

$$192 \quad \text{Biodegradability} = \frac{\text{BMP}}{(\text{COD} * 350)}$$

193 (1)

194 Biodegradability is expressed as a ratio from 0 to 1, BMP in $\text{NmlCH}_4\cdot\text{g}^{-1}$ and COD in $\text{gO}_2\cdot\text{g}^{-1}$. If Xrc, Xmc,
 195 Xsc and Xne inputs were implemented, the repartition of the initial COD in Xrc, Xmc, Xsc and Xne was
 196 determined by analyzing the changes in the methane production slope of the predicted MPR. For the
 197 determination of the initial state of the model variables, a maximal specific growth rate (μ_{\max}) of 3 d^{-1}
 198 was set, representing the mean μ_{\max} found in the 275 samples. The initial state of the ADM1 variables
 199 was simulated in accordance with the experimental protocol (see Material and Methods section 2.1).
 200 Seven batches were successively simulated with an input of $1 \text{ gTS}\cdot\text{l}^{-1}$ in a 6 liter reactor under mesophilic
 201 conditions. The values of the initial state of ADM1 variables were taken as the final values reached on
 202 the seventh batch. Then, on the eighth simulated batch, the kinetics parameters of ADM1 were assessed
 203 based on the MPR predicted by NIR. The estimation of the kinetics was considered as a non-linear
 204 problem based on the root mean square optimization between the MPR predicted by NIR and the MPR
 205 simulated by ADM1. Using the modified ADM1 (see Material and Methods 2.5), the μ_{\max} of the Contois
 206 kinetic terms were optimized by the operator in order to minimize the square value of the difference

207 between the predicted methane production and the simulated methane production. In order to assess
208 the improvements brought by the modifications of the model, the μ_{\max} of the first order disintegration
209 kinetic of the standard ADM1 implementation obtained from (Rosén and Jeppsson, 2008) was also
210 optimized. This was done minimizing the square value of the difference between the predicted methane
211 production and the simulated methane production using the function *leastsq* from Scilab®.5.5.0.

212 **3 RESULTS AND DISCUSSION**

213 **3.1 Prediction of the methane production rate in batch conditions using** 214 **NIR spectroscopy**

215 **3.1.1 Prediction of the methane yield**

216 The methane yield was predicted according to (Lesteur et al., 2011) using the same chemometric
217 treatment, presented in Material and Methods section **Error! Reference source not found.** (absorbance,
218 SNV and Savitzky–Golay filter with a second derivative). Using the data set of the present study and
219 based on the cross-validation performances, the PLS regression model was calibrated using 13 latent
220 variables. The number of latent variables was selected to minimize the SECV. On the calibration set, the
221 SEC was about 0.019 L.gTS⁻¹, SECV about 0.026 L.gTS⁻¹ and R² about 0.92. The model was validated on the
222 independent validation set with SEP of 0.025 L.gTS⁻¹. The SEP found for the methane yield prediction is
223 comparable with the SEP of 0.028 L.gVS⁻¹ reported in (Lesteur et al., 2011). It validates the use of NIR
224 infrared to predict methane yield in this study. If previous models give predictions per gram of volatile
225 solids, predictions per gram of total solid have been preferred since the total solid is faster to estimate
226 than volatile solid and prediction performances were similar.

227 **3.1.2 Prediction of the methane production times**

228 First of all, the times required to reach a certain percentage of the methane yield ranging from 5
229 to 95 % of the final value has been considered as independent values at each ratio of the methane yield.
230 The choice of the chemometric treatment was based on the PLS performance during cross-validation and
231 calibration. SEC, SECV and R^2 between predicted and reference values in cross-validation are represented
232 in Figure 4. For all the treatments, SEC and SECV increase from 5 to 70% of the methane yield, this
233 corresponds to an approximate 6-fold change. SEC and SECV then decrease with the methane yield
234 ratio from 70 % to 95 %. The variation of SEC and SECV is correlated with the variance within the dataset
235 which increases with the ratio of the methane yield to reach a maximal variance between 65 % and 70 %
236 of the methane yield as suggested in Figure 1. The experimental standard deviation and the standard
237 deviation of the predicted values in cross-validation are plotted in Figure 4. The standard deviation
238 reaches a maximum of 1.24 day at 65 % of the methane yield. Thus, the most important difference of
239 production time between the samples is reached at 65 % of the methane yield. It explains the increase of
240 both SEC and SECV up to this point. Then, the variance decreases indicating a homogenization of the
241 samples. It can be concluded that 65 % of the methane yield is the most discriminant production time. It
242 can be observed in figure 4 that, regardless of the chemometric treatment, using independent PLS
243 model, R^2 increases with the methane yield ratio. It means that model predictions are less accurate on
244 early methane production. It can be mainly explained by two factors. First, to restore anaerobic
245 conditions after having fed the digester, the head space is flushed using nitrogen. As a consequence, the
246 very first biogas production is due to both liquid gas equilibrium and substrate biodegradation, which
247 disturbs the estimation of the methane produced from the substrate biodegradation. Secondly, the early
248 methane production is due to 5 to 15 % of the organic matter. Thus the information related to this early
249 production can be diluted in the NIR spectrum which is made on the overall substrate.

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250 About the chemometric treatments, both SEC and SECV were minimized using treatment
251 absorbance, SNV and Savitzky–Golay filter with a second derivative at any ratio of the methane yield
252 with respectively values from 0.05 to 0.37 days and 0.07 to 0.55 days. R^2 was maximal using treatment
253 absorbance, SNV and Savitzky–Golay filter with a second derivative until 70% of the methane yield
254 whereas treatment absorbance, SNV and detrending slightly improved R^2 after 70% of the methane yield
255 compared to treatment absorbance, SNV and Savitzky–Golay filter with a second derivative. Treatment
256 absorbance, SNV and Savitzky–Golay filter with a second derivative maximized the PLS regression
257 performances for the prediction of production time and was chosen as the reference chemometric
258 treatment for this purpose.

259 PLS regression was also built to treat the production time as a vector of correlated values. In this
260 case, a global set of latent variables is used. The advantage of this approach is to acknowledge the
261 correlation between the production times at any ratio of the methane yield. The disadvantage is the
262 necessity to set a unique number of latent variables for every ratio of the methane yield. Using
263 treatment absorbance, SNV and Savitzky–Golay filter with a second derivative, both approaches were
264 compared considering either the time of production as a correlated vector or as independent values. SEC
265 was not accessible using MixOmics and is thus absent of the Figure 4. Q^2 was used to set the number of
266 latent variables to 5 which corresponds to the first Q^2 value below 0.0975 with a local minimum. The
267 number of latent variables considering production time as independent values varies from 6 to 12. A
268 reduction of the number of latent variables is usually acknowledged as a gain in robustness.
269 Nonetheless, SECV was higher considering production time as a vector with values from 0.07 to 0.60 days
270 than considering the methane production times as independent values. Moreover, the R^2 was lower with
271 values from 0.47 to 0.79. On average, considering the methane production time as a vector increased
272 the SECV by 8.5% and decreased R^2 by 6.1%. From these results, it can be concluded that the

273 performances are maximized considering the time of production as independent values with treatment
274 absorbance, SNV and Savitzky–Golay filter with a second derivative.

275 The resulting PLS regression model was then tested on the validation set. SEP values are
276 presented in Figure 5. The same patterns as for SECV and SEC estimation were observed for SEP and
277 RMSEP which reached maximal values at 0.65 point of the methane yield with respectively 0.47 and 0.46
278 day. The standard deviation of the validation set confirmed an increase of the dispersion until 65 % of
279 the methane yield (Figure 5). SEP and RMSEP are approximately 2 times lower than the standard
280 deviation of the validation set which proves that PLS was able to discriminate the production time of the
281 samples. It also shows that the errors of prediction are low, for instance at 65 % of the methane yield
282 the SEP was 0.47 day to predict values in a range from 1.15 to 4.75 day with a mean value of 2.32 day.
283 The model previously built on the calibration set can thus be considered as suitable to predict the times
284 of degradation at any methane yield ratio.

285 The cross-validation and validation results using treatment absorbance, SNV and Savitzky–Golay
286 filter with a second derivative and considering the times required to reach a certain percentage of the
287 methane yield as independent values are detailed in the bottom of Figure 5. In these two figures, the
288 methane production times are represented without any distinction on the methane yield ratio. Figure 5
289 confirms the accuracy of the PLS model but also shows that the error of prediction decreases with the
290 predicted time. The methane production times above 6 days mostly represent a methane production
291 above 65 % of the final methane yield. It has been previously observed that the variance decreased after
292 65 % of the methane yield and that this goes with a decrease of SECV, SEP and RMSEP, which explains
293 the decrease in the error of prediction. From the cross-validation results, it can be seen that one sample
294 is strongly under-predicted at several methane yield ratios. It is actually the only sample represented by
295 oil. It shows that oil is under-estimated on the current dataset of calibration. This error is not found

296 during the validation step because no oil was contained in the validation set. Nonetheless, from these
297 results, it can be concluded that the prediction of production time is feasible using NIR spectroscopy and
298 PLS model, even if an improvement of the dataset could be made including more oil samples.

299 **3.1.3 Prediction of the methane production rates**

300 A case study was carried out on two samples from the validation set to assess the feasibility of the
301 MPR prediction. As explained in the section 2.6, the MPR was predicted using both methane production
302 times and methane yield predicted by NIR analyses. Then MPR was interpolated from these 19 points.
303 These curves are represented as “NIR predictions” in Figure 6 and compared to the experimental
304 cumulated methane production. It shows that NIR prediction represents properly the production of
305 methane. Both methane yield and production time were correctly predicted. The errors of prediction on
306 the methane yield were about 6.7 % on salad and 3.5 % on cauliflower. On the experimental data, the
307 methane flow decreased after 0.4 and 1 day and increased again after 1 and 1.5 day for respectively
308 salad and cauliflower (Figure 6.A-B). These behaviors were not accurately predicted by NIR. One possible
309 explanation is an inhibition of the readily degradable substrate on the slowly degradable substrate that
310 was not predicted by NIR. Another hypothesis leading to similar results can be found in Yasui et al.,
311 (2008): the readily accessible organic matter is degraded first followed by the slowly accessible organic
312 matter, keeping in mind that kinetics of disintegration and accessibility are independent.

313 **3.1.4 Simple predicted indicator of methane production performances**

314 MPR is a relevant indication that allows to differentiate the methane production performances
315 of two substrates, but MPR analysis becomes difficult when the number of samples to compare
316 increases. Methane yield and kinetics of methane production are two key parameters to elaborate an
317 optimal feeding strategy. It is indeed in the interest of the plant operator to maximize both methane
318 yield and kinetics. The time needed to reach 70 % of the methane yield has been reported in section

319 3.1.2 to be the most discriminant time. The observation of this time allows differentiating a substrate
320 with a fast kinetic of methane production. In Figure 7, the samples of the validation set have been
321 plotted depending on their predicted methane production time needed to reach 70% of the methane
322 yield and their predicted methane yield. Figure 7 shows that the fast NIR spectroscopy analysis of the
323 substrate provides the opportunity to the plant operator to select the most relevant substrates on a
324 simple graph.

325 **3.2 ADM1 calibration from NIR prediction**

326 It has been proven that NIR spectroscopy can be used to estimate MPR in batch conditions. It turns
327 to be also a powerful method to implement an ADM1 model able to predict the substrate methane
328 production performances. The approach was applied to the case studies of salad and cauliflower. As
329 described in Materials and Methods section **Error! Reference source not found.**, carbohydrates, nitrogen
330 and lipids content, COD and methane production rate were used to implement ADM1. The curve
331 predicted by NIR was then used as a reference for the μ_{\max} optimization of the Contois kinetic
332 parameters. The model using only one particulate input (Batstone et al., 2002) was first tested.
333 Respectively for salad (Figure 6.A) and cauliflower (Figure 6.B), μ_{\max} were estimated at 1.92 and 4.33 d⁻¹.
334 It can be seen that, while optimizing μ_{\max} , the model does not represent accurately the predicted MPR.
335 Indeed, it tends to under-estimate the kinetics at the beginning of the production and to over-estimate it
336 in the second part. More kinetic parameters are thus needed to represent efficiently the curve. Hence, a
337 second optimization was done using the modified ADM1 described in section 2.5 with four fractions and
338 four distinct μ_{\max} kinetic parameters for disintegration. It can be seen that four kinetics of disintegration
339 improved the fit between the simulated cumulated biogas production and the predicted cumulated
340 biogas production. The degradation of X_{rc} is faster than when considering a single input while the
341 degradation of X_{mc}, X_{sc} and X_{ne} are slower, which fits the predicted data. It can be seen in Figure 6.A-B

342 that the NIR predicted data allows calibrating a modified ADM1 that accurately represents the
343 experimental batch data.

344

345 If we consider a normal distribution of errors, 68.2 % of the reference values are contained in a range
346 of ± 1 SEP of the predicted value. Thus, an error of ± 1 SEP was applied to each methane production
347 time, to the methane yield and to the parameters describing the biochemical composition predicted by
348 NIR in order to obtain an envelope where 68 % of the possible MPR curves will be included. μ_{\max} of the
349 Contois kinetic parameters were optimized on the most optimistic MPR, minus one SEP on the methane
350 production time and plus one SEP on the methane yield, and on the most pessimistic MPR, plus one SEP
351 on the methane production time and minus one SEP on the methane yield. The confidence range of the
352 simulations is presented in Figure 6.C-D. It can be seen that the experimental MPR is included in the
353 simulated range of confidence of the MPR. It shows that the predicted confidence range represents
354 accurately the experimental MPR. Since the experiments focus on the methane production under non
355 inhibitory conditions, the impact of the errors of prediction on the biochemical composition cannot be
356 observed. This approach is interesting in order to predict the performance of the plant depending on the
357 feeding strategy. The introduction of potential errors of prediction in the model also provided an
358 estimation of the risk that the plant operator is taking (Južnič-Zonta et al., 2012). Thus, it could provide
359 key information to the human operator to optimize safely the production of a real plant.

360 **3.3 Discussion on the MPR prediction using NIR**

361 Batstone et al., (2009) have demonstrated that hydrolysis kinetic parameters estimated in BMP
362 tests translated to very poor model performance when BMP-estimated values were used to simulate
363 continuous reactors. On the other hand, García-Gen et al., (2015) demonstrated that the calibrated
364 ADM1 kinetic parameters from batch assays that allow micro-organisms to adapt to individual substrates

365 can be used to model semi-continuous co-digestion operation treating simultaneously 5 wastes. In our
366 case, we used the same experimental protocol as García-Gen et al., (2015) and thus the model
367 parameters can be assumed to be valid for continuous operation of the digester. The main drawback of
368 the batch experiments with adapted micro-organisms is the time needed, from 6 to 12 weeks, which
369 reduces its use. This study also shows that NIR spectrometry can be efficiently used to predict
370 experimental batch MPR on adapted micro-organisms. Kinetic parameters of the ADM1 model calibrated
371 on the predicted batch MPR can be used for continuous co-digestion simulation. This approach gives the
372 opportunity to replace time-consuming biological experiments by fast NIR analysis for feeding strategy
373 optimization. Two drawbacks must be highlighted. First, NIR remains an expensive and unusual device
374 and only laboratories and large plants can afford to own a NIR spectrometer. Second, the analysis can be
375 done on dry samples only. Two disadvantages are linked to drying: volatile compounds cannot be
376 analyzed and on-line application cannot be considered. A further interesting development or
377 improvement of this technology would be to work with wet samples and install an online sensor able to
378 characterize in real time any input coming to the plant. The obstacle is the absorption of water using NIR
379 that disturb the analysis. Mayer (2015) provides for example some hints about the estimation of
380 methane yield on wet samples using NIR.

381 **4 Conclusion**

382 The current study shows that:

- 383 • The kinetics of methane production was the main hindrance to overcome for a fast
384 implementation of the ADM1 model using NIR. Thus, a PLS model has been developed to
385 estimate properly the kinetics of methane production from a large set of solid substrates
386 using NIR spectroscopy.

- 387 • Based on the actual and previous studies on biochemical composition, methane production
388 yield and kinetics prediction using NIR, it is demonstrated that NIR is a powerful tool for the
389 prediction the main parameters needed to optimize AD plants with a single analysis of few
390 minutes on dry samples.
- 391 • The predicted parameters using NIR spectroscopy are transformed in ADM1 parameters to
392 implement a modified ADM1. From this virtual plant, it becomes possible to predict the
393 performance of degradation of any input. It gives access to every parameters estimated in
394 the ADM1 model such as the concentration of VFA, nitrogen or the biogas composition.

395 This study demonstrates that the use of NIR spectroscopy coupled with PLS regression and ADM1
396 modeling can help the human operators to monitor the plant. This approach can be used as a powerful
397 tool for plant monitoring and feeding strategy optimization.

398

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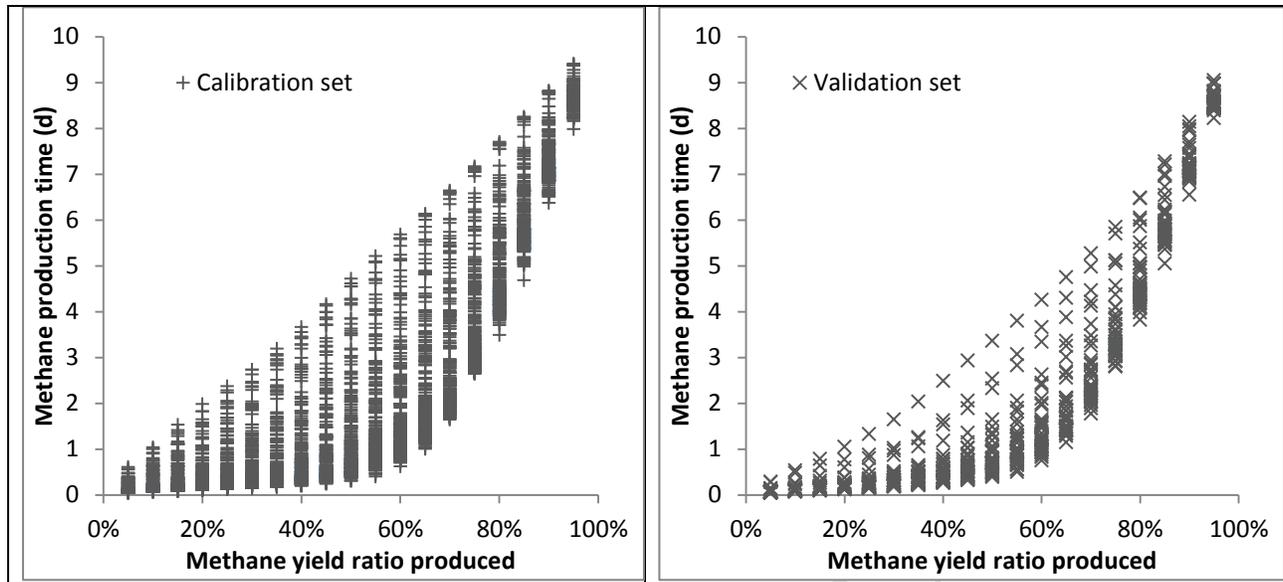


Figure 1: Calibration and validation set features of the experimental data. Description of the methane production time required to reach a certain ratio of the methane yield from 5 to 95 %.

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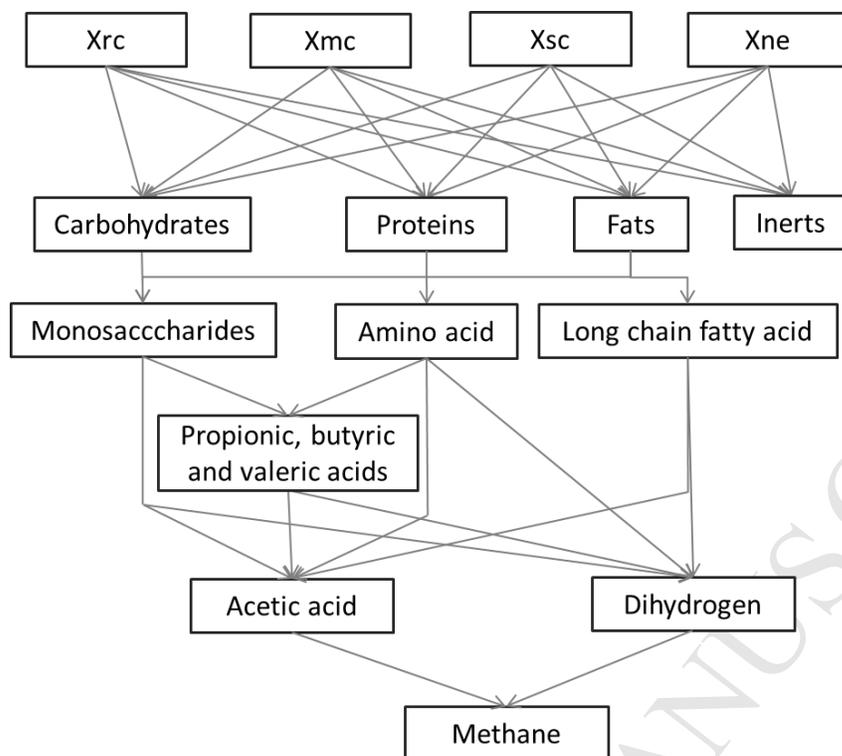


Figure 2: Modified ADM1 with four different particulate inputs Xrc, Xmc, Xsc and Xne.

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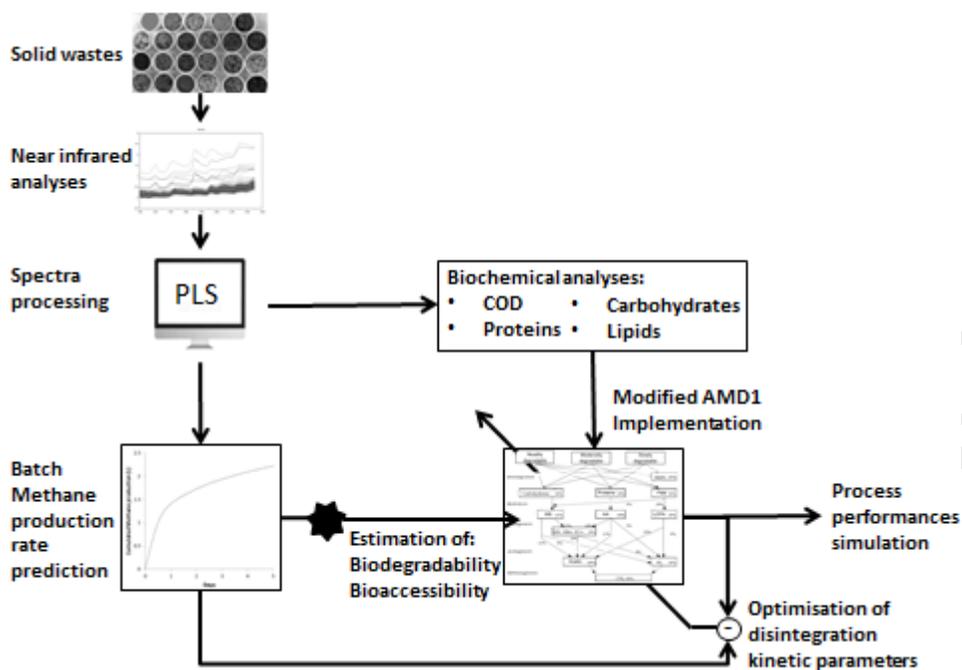


Figure 3: Modeling approach diagram

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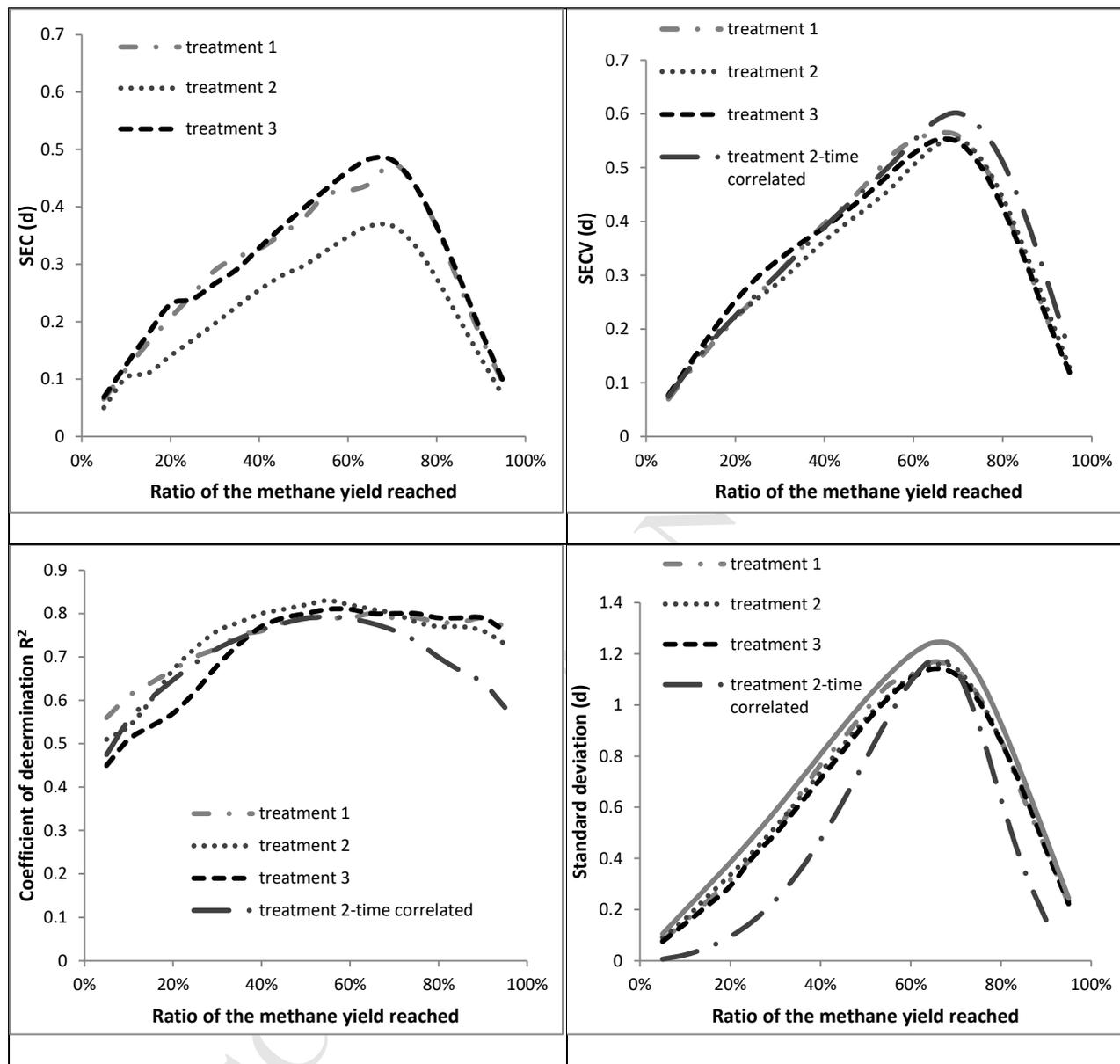


Figure 4: PLS regression performances on cross-validation with 3 different chemometric treatments and considering the methane production times as correlated or independent values. Treatment 1 correspond to absorbance and SNV, treatment 2 to absorbance, SNV and Savitzky-Golay filter and treatment 3 to absorbance, SNV and detrending.

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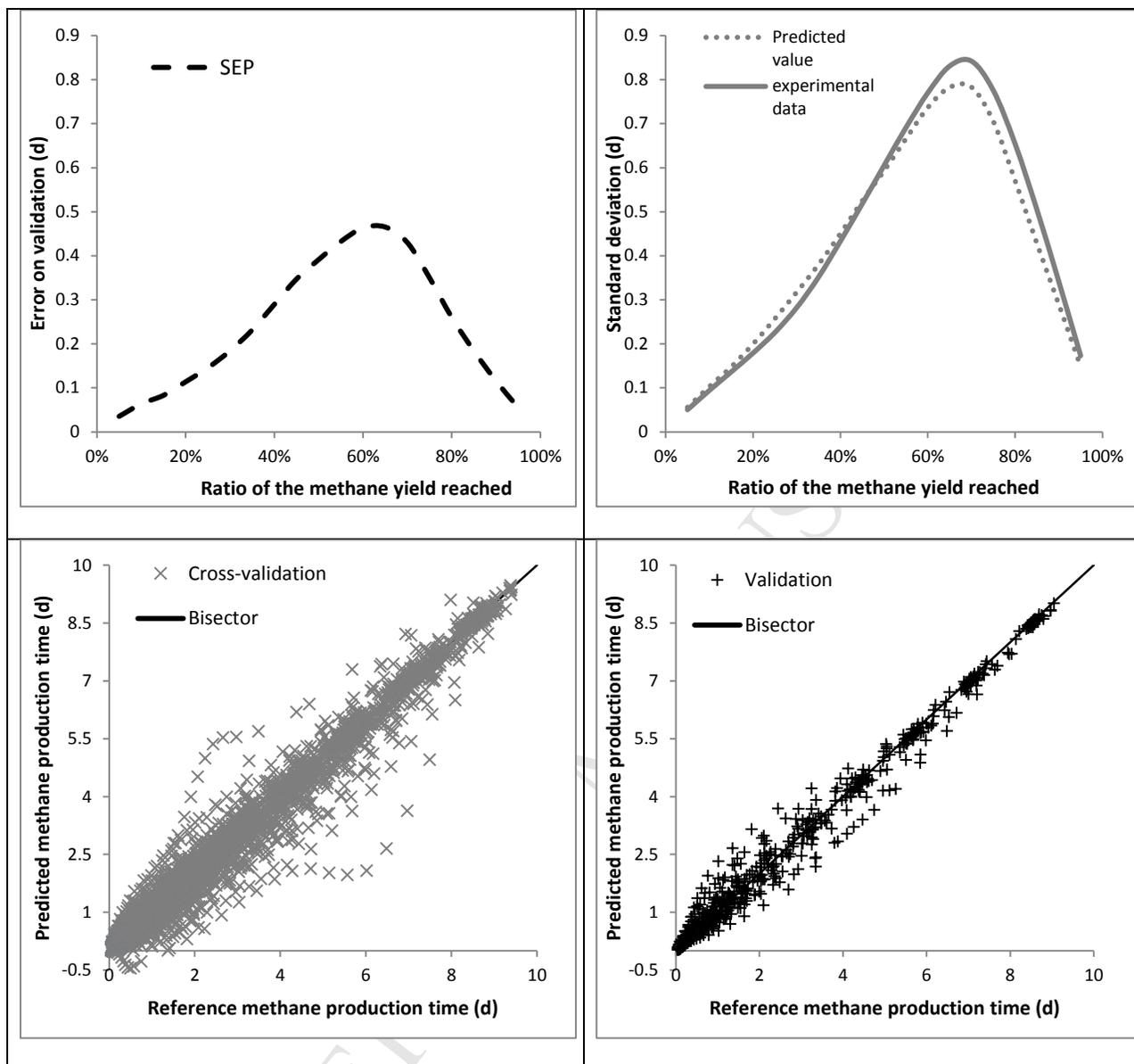


Figure 5: PLS performances on the validation set (up) and representation of the predicted value of both cross-validation and validation (bottom).

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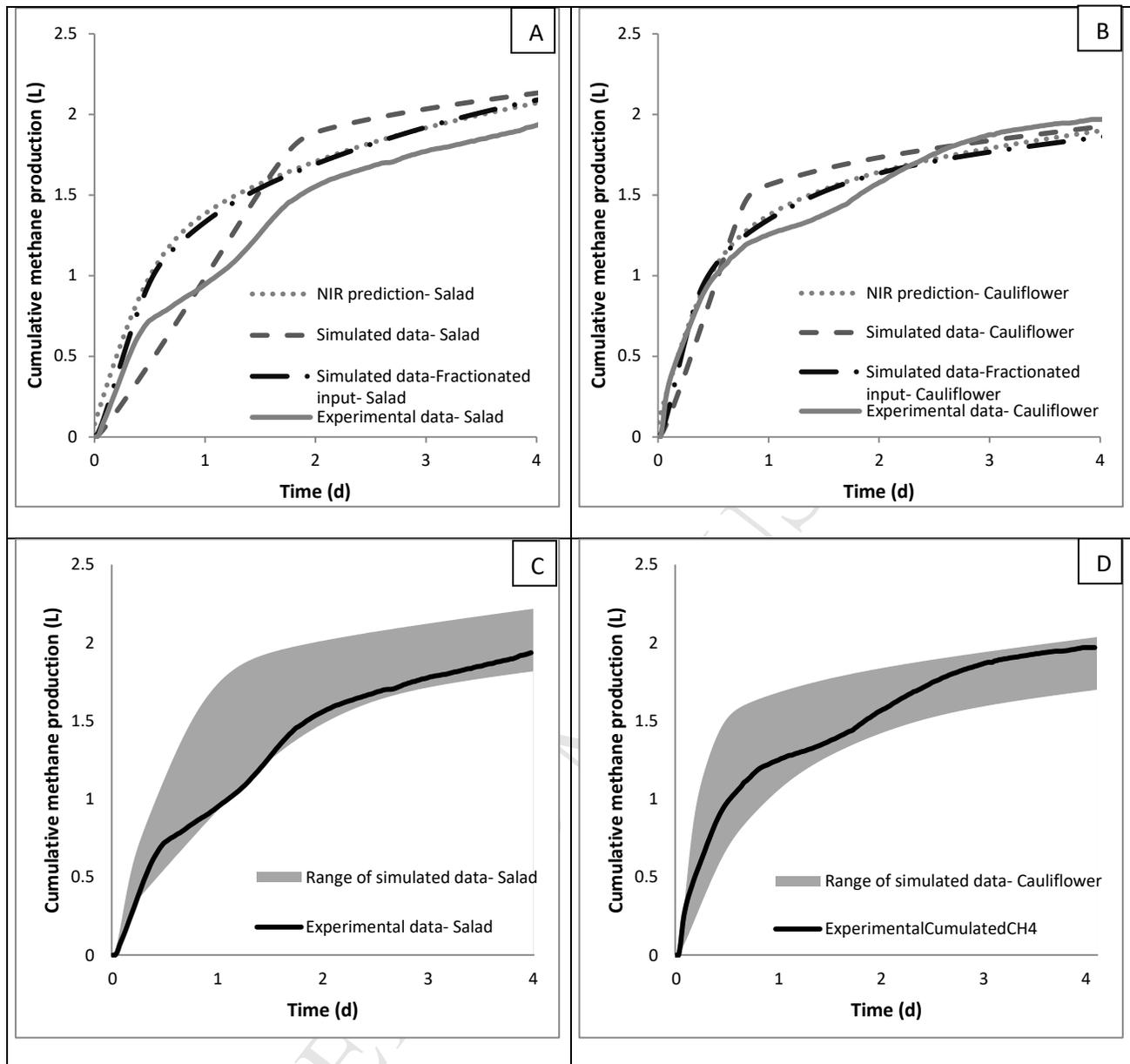


Figure 6: Cumulative methane production curve for anaerobic of salad (left) and cauliflower (right) in batch. A and B, comparison of predicted and simulated data using ADM1 considering the particulate organic matter as a single input or fractioning the particulate organic matter in four inputs with their own kinetics of disintegration for salad and cauliflower respectively. B. C and D, modelling of the methane cumulative production for salad and cauliflower AD taking into account the error of prediction for salad and cauliflower respectively. Methane production times and methane yield were chosen at ± 1 SEP of the predicted value. The grey area represents the range of confidence.

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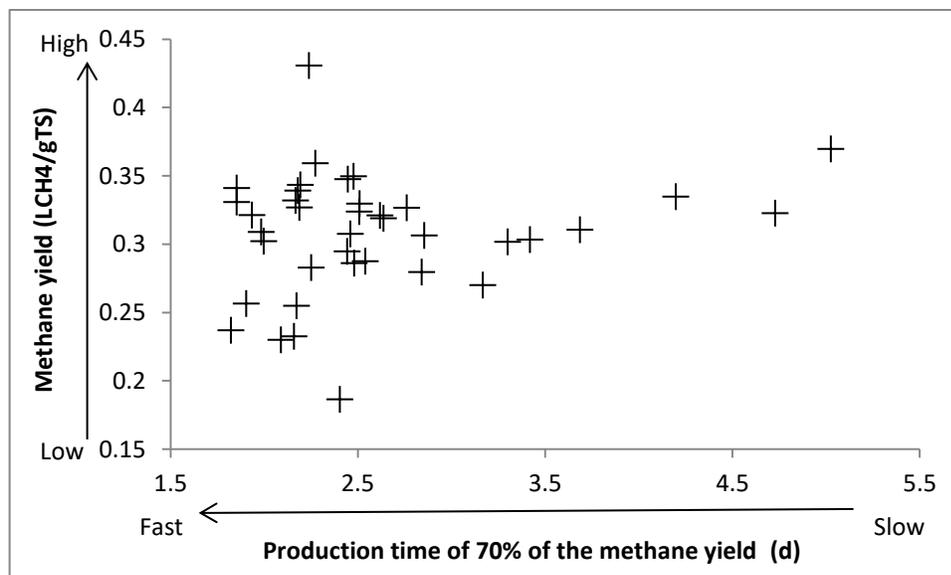


Figure 7: Performances of the substrates from the validation set expressed as a function of the methane yield and the production time of 70% of the methane yield. Abscissa arrow indicates the methane production kinetics and ordinate arrow the methane yield.

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Highlights

- Near infrared prediction of the methane yield and kinetics
- Use of near infrared spectroscopy to implement ADM1
- Prediction of co-digestion performances assisted with ADM1 simulation
- Feeding strategies optimization using the developed predictive methodology

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