

1 **Using Mathcad to facilitate the design of chemical**
2 **reactors involving multiple reactions**

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17 **ABSTRACT**

18 The pedagogy of teaching chemical reaction engineering is continually advancing
19 through the use of new computational tools and, therefore, the integration of these new
20 tools into the Chemical Engineering degree is challenging. This paper reports an
21 educational experience dealing with the use of Mathcad software to complement and to
22 facilitate the design of chemical reactors involving multiple reaction. A continuous stirred
23 tank reactor taking place series reactions and two reactors (continuous stirred tank reactor
24 or plug flow reactor) arranged in series involving parallel reactions were presented as case
25 studies. This experience, which was carried out with the third-year chemical engineering
26 students enrolled in the Chemical Reactors course, revealed that Mathcad facilitates the
27 understanding of the theoretical concepts related to multiple reactions and also reduces
28 the complexity of mathematical calculation to a minimum. Thus, the use of this computer
29 tool allows the teacher: (1) to delve deeper into more issues related to the design of
30 chemical reactors, and (2) to consider this tool perfectly useful for other courses
31 corresponding to the Chemical Engineering degree.

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38 **Keywords:** chemical reactors, multiple reactions, Mathcad, educational experience

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40 1. INTRODUCTION

41 Chemical reaction engineering is recognized as one of the most important courses in any
42 chemical engineering program, dealing with many fundamental concepts that can be
43 applied in a wide variety of fields related to chemical engineering¹. In this sense, while
44 the design of chemical reactors taking place a single reaction is based on optimizing its
45 conversion, this issue becomes more complex when it comes to multiple reactions. In this
46 case, the optimization requires the evaluation of two important concepts like selectivity
47 and yield, as the purification of the reactor output current due to the presence of unwanted
48 products can involve a high economic cost.

49 The traditional way of consolidation or putting into practice the theoretical concepts
50 related to chemical reaction engineering has been accomplished through short-term
51 laboratory experiences²⁻⁵. However, the pedagogy of teaching chemical reaction
52 engineering is continually advancing through the use of new computational tools and,
53 therefore, there is an ongoing effort at many universities to integrate these new tools into
54 the chemical reaction engineering course². In addition to that, higher university education
55 in the 21st requires engineers to master a broad set of competences being the management
56 of new information and communication technologies (ICTs) one of the most relevant^{6,7}.

57 In this context, the use of process simulators with educational purpose has been reported
58 in the literature⁸⁻¹². Moreover, a significant number of computer-aided educational
59 experiences by using mathematical software packages or programs, which were
60 developed both commercially and individually by instructors, can be also found in the
61 chemical engineering pedagogical field. Some illustrative examples are described below:

62 a) IPython software was applied for teaching kinetics of complex heterogeneously-
63 catalyzed reactions¹³; b) DHXA software was used to teach transient analyses of shell-
64 and-tube heat exchangers¹⁴; c) a Submerged Membrane Bioreactor simulator was built

65 with a friendly interface¹⁵; d) Chemical-Workbench system was used for the simulation
66 of a wide spectrum of physical and chemical phenomena¹⁶; e) CHEMSIMUL simulator
67 was applied for chemical kinetics¹⁷; f) heterogeneous chemical kinetics at a gas-surface
68 interface was analyzed by CHEMKIN¹⁸; g) XSEOS is an Excel add-in for computer
69 properties with thermodynamic model often used for teaching chemical engineering
70 thermodynamics¹⁹; h) Matlab is used for educating students in chemical process control²⁰,
71 for the design of continuous contacting countercurrent unit operations²¹ and for solving
72 chemical engineering problems using the arc-length continuation method²²; i) Polymath
73 can be employed for both chemical equilibrium calculations²³ and chemical reaction
74 engineering (e.g., modelling isomerization of unsaturated fatty acid with catalyst
75 deactivation)¹; j) MATHEMATICA was used to illustrate important aspects of nonlinear
76 dynamics drawn from the chemical and biochemical engineering field²⁴ and to estimate
77 the parameters of several models that describe transient chemical engineering processes²⁵.
78 With regards to the software here proposed, Mathcad combines some of the best features
79 of spreadsheets (like MS Excel) and symbolic math programs. Thus, Mathcad provides a
80 good graphical user interface and can be used to manipulate large data arrays, to easily
81 make graphs, and to perform symbolic calculations. In addition to that, one of the main
82 advantages of Mathcad that is not found in other Symbolic Algebraic Systems (e.g.,
83 Maple, MATHEMATICA or Matlab) is its ability to perform calculations with units; this
84 fact makes Mathcad of great interest to be used for engineering students²⁶. As for its main
85 disadvantage, this software requires using a Mathcad program to repeat the analysis steps
86 with different parameters.

87 Some experiences using Mathcad are found in the literature. It has been implemented to
88 supplement and enhance traditional and learning methods for reinforced concrete design²⁷
89 or for the stiffness structural analysis theory of two-dimensional framed structured²⁸, as

90 well as solving piping systems problems²⁹. Interestingly, there are no papers in the
91 literature reporting the use of Mathcad to facilitate the design of reactors involving
92 multiple reactions. Thus, the main objective of this paper lies not only in the fact of using
93 Mathcad to design these reactors, but also in proposing this together with a teaching
94 methodology that favours students' problem-solving skills. Considering our previous
95 educational experience using Mathcad for the calculation of pumping power³⁰, the
96 teaching methodology followed here was similar to that, which consisted of two steps: i)
97 training courses on initiation to Mathcad to learn the basic about Mathcad, and ii) the
98 optimization of chemical reactors design involving multiple reactions. In addition to that,
99 students answered specific questions in order to know their satisfaction degree with the
100 usage of Mathcad for solving chemical reaction engineering problems.

101 **2. USING MATHCAD IN CHEMICAL REACTION ENGINEERING**

102 This section describes the procedure that has been followed to implement Mathcad
103 software in a chemical reactors course to design reactors involving multiple reactions.

104 **2.1. Students**

105 The educational experience was carried out by the third-year chemical engineering
106 students (22 in total) enrolled in the course named Chemical Reactors I (reference:
107 606210212) and tutored by the corresponding author of this contribution. One of the main
108 objectives of this course is the optimization of chemical reactor design taking place
109 multiple reactors, therefore, the prerequisites of this course, among others, includes the
110 adequate application of mass/mole balances and the knowledge on chemical kinetics.

111 **2.2. Teaching methodology**

112 The teaching methodology of this educational experience consisted of two stages: the
113 realization of initiation courses on Mathcad and the optimization of the chemical reactors
114 design taking place multiple reactions. A total of four work sessions using Mathcad were

115 carried out, the first three of which corresponded to the training courses and the last one
116 dealt with the design of chemical reactors. These seminars took place in the computers
117 rooms at the University of Huelva itself, where a version of Mathcad Prime 4.0 is
118 available. It is worth noting that the teaching methodology here implemented were not
119 intended to replace the traditional theoretical lectures, which are absolutely necessary to
120 introduce the fundamentals behind the design of chemical reactors, but to complement
121 theoretical contents and to facilitate the mathematical complexity involved in the design
122 of chemical reactors. Thus, the theoretical concepts related to the design of chemical
123 reactors involving multiple reactions are taught in the traditional theoretical lectures, and
124 leaving its practical application for this educational experience.

125 **2.2.1. Training courses on Mathcad**

126 One of the main shortfalls found in the previous experience using Mathcad³⁰ was the short
127 duration of training courses. In the current experience, the training courses has been
128 expanded to three 5 hour seminars dealing with the basis notions necessary to use
129 Mathcad. The content of each seminar was:

- 130 • Session 1: a) Description of the software-user interface, b) definition of simple
131 functions and c) 2D graphical representation.
- 132 • Session 2: a) Resolution of system of linear equations (“given” and “find” functions),
133 b) use of “root” function and c) numerical resolution of integrals.
- 134 • Session 3: Resolution of simple exercises applying the Mathcad functions studied in
135 the two previous sessions and b) doubts and questions.

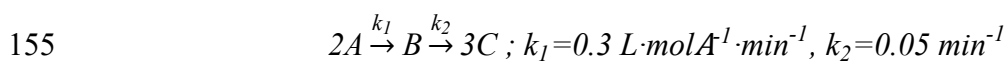
136 All information regarding these training courses to Mathcad were available to students in
137 the Moodle virtual platform of the University of Huelva (<http://moodle.uhu.es/>). Thus,
138 within this platform, a meeting space between the teacher and the students was created.
139 The date and place of each seminar, support material, tutorial videos, as well as the

140 resolution of the different cases studies made during these seminars could be found in this
141 platform.

142 **2.2.2. Addressing the design of chemical reactors involving multiple reactions with** 143 **Mathcad**

144 After completing the sessions corresponding to the initiation to Mathcad, the fourth 5h-
145 seminar was devoted to solving two exercises about the optimization of chemical reactors
146 design applying the knowledge acquired on Mathcad. Before this, the students had
147 available in the Moodle platform a report including the theoretical considerations needed
148 to solve the problems (i.e., all the definitions and design equations that are useful for the
149 chemical reactors design which were previously introduced in the theoretical lectures) as
150 well as the problem statements. During this session, the teacher proposed to the students
151 the main guidelines to solve the exercises with Mathcad and was in permanent support to
152 solve the doubts.

153 The statement of the first exercise was: *In an isothermal continuous stirred tank reactor*
154 *(CSTR) takes place the following series reactions in liquid phase:*



156 *The feed current to the reactor consists of pure A with a concentration of 10 mol·L⁻¹.*

157 *Calculate:*

158 a) *The concentration of species in the output current if the reactor volume is 200 L*
159 *and the volumetric flow rate is 10 L·min⁻¹.*

160 b) *The reactor volume to achieve the maximum production of B and its*
161 *concentration.*

162 c) *The overall yield for the items a) and b).*

163 To solve the item a), it is necessary to make molar balances for species j (i.e., A, B or C)
164 in the CSTR,

165
$$F_{j,i} = F_{j,f} + (-r_r)V \quad (1)$$

166 where V is the reactor volume, r_r are the reaction rate of reaction r th reaction, and $F_{j,i}$ and
 167 $F_{j,f}$ are the molar flow rate in the feed current and in the output of species j , respectively.

168 In addition, the molar flow rate of species j and the reactor volume can be expressed as

169
$$F_j = vC_j \quad (2)$$

170
$$V = \tau v \quad (3)$$

171 where v is the volumetric flow rate, C_j the concentration of species j and τ the space time.

172 From the units of the reaction rate constants (k_1 and k_2) it is possible to state that these
 173 reactions are elementary (i.e., the stoichiometric coefficients are coincident with the
 174 partial orders), and the reaction rates can be expressed as:

175
$$(-r_A) = k_1 C_{A,f}^2 \quad (4)$$

176
$$(-r_B) = -\frac{k_1 C_{A,f}^2}{2} + k_2 C_{B,f} \quad (5)$$

177
$$(-r_C) = -3k_2 C_{B,f} \quad (6)$$

178 Thus, if the equations (2), (3) and (4) are substituted in the molar flow balance for A, the
 179 concentration of species A in the output current results to be

180
$$C_{A,f} = \frac{-1 + \sqrt{1 + 4k_1 \tau C_{A,o}}}{2k_1 \tau} \quad (7)$$

181 For the item a) the space time is a known value (20 min) and the initial concentration of
 182 A is $10 \text{ mol} \cdot \text{L}^{-1}$, therefore according to equation (7) the concentration of A in the output
 183 current ($C_{A,f}$) is $1.210 \text{ mol} \cdot \text{L}^{-1}$. As for the species B, following the same procedure, the
 184 $C_{B,f}$ is dependent on the $C_{A,f}$ by the equation (8)

185
$$C_{B,f} = \frac{\frac{k_1 C_{A,f}^2 \tau}{2}}{1 + k_2 \tau} \quad (8)$$

186 giving a result of $C_{B,f} = 2.197 \text{ mol}\cdot\text{L}^{-1}$. Similarly, the concentration of C in the output
187 current is calculated from

188
$$C_{C,f} = 3k_2 C_{B,f} \tau \quad (9)$$

189 with a value of $6.592 \text{ mol}\cdot\text{L}^{-1}$.

190 The initial objective of the students was to incorporate all these equations in a Mathcad
191 spreadsheet in order to calculate the concentration of the species in the output current. To
192 that end, bearing in mind that the resolution carried out by Mathcad is sequential, the first
193 was to include the known parameters (i.e., reaction rate constants, reactor volume,
194 volumetric flow rate and concentrations of the species in the feed current), as can be
195 observed in Figure 1 (explanatory comments appear in bold type). After that, the space
196 time (referred to as τ_f in the Mathcad spreadsheet) was calculated and the corresponding
197 values of $C_{A,f}$, $C_{B,f}$ and $C_{C,f}$ were obtained by the equations (7), (8) and (9). In addition
198 to that, these concentrations can be also written as a function of the space time and plotted
199 in the Mathcad spreadsheet (Figure 2). As can be seen, the vertical line at 1200 s, which
200 is the actual value for the space time, provides the calculated values of concentrations in
201 the output current.

202 The results obtained so far are those corresponding to the reaction under consideration;
203 however, one of the main advantage of using Mathcad software is that it is possible to
204 configure a template valid for any series reactions. Thus, after resolving the item a), the
205 next objective proposed to the students, with the assistance of the teacher, was to create
206 this template. Figure 3 displays a Mathcad template to calculate the concentration of
207 species in the output current of a CSTR for a general series reactions as



209 where na , nb and nc are the stoichiometric coefficients. Thus, the procedure for using this
210 template is very simple: a) firstly, the known parameters (i.e., stoichiometric coefficients,

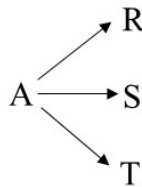
211 reaction rate constants, concentrations of the species in the feed current, reactor volume
212 and volumetric flow rate) are introduced and, b) secondly, the system of 6 equations with
213 6 unknowns (i.e., concentrations of the species in the output current and the reaction rates)
214 is solved by using the “given” and “find” Mathcad functions. The success of this template
215 lies in the fact that the first three equations gather the reaction rates as a function of any
216 stoichiometric coefficients. The template displayed in the Figure 3 was applied to the
217 series reactions proposed in the item a) and, as can be seen, the concentrations of the
218 species in the output current ($C_{A,f}$, $C_{B,f}$ and $C_{C,f}$) are coincident with those obtained by
219 equations (7), (8) and (9), thereby validating the usage of this Mathcad template. It is
220 worth noting that this template is of special interest to study the effect that the
221 concentration of the species in the feed current exert on the final result, since equations
222 (8) and (9) result from a feed current containing only the specie A (i.e., $C_{B_0} = C_{C_0} = 0$).

223 Returning to the exercise 1, item b) asked students to calculate the reactor volume to
224 achieve the maximum concentration of specie B as well as this concentration. As the
225 concentration of B in the output current depends on the space time and this in turn on the
226 reactor volume, the optimum reactor volume requires deriving the $C_{B,f}(\tau)$ function with
227 respect to the space time and then to determine its roots. It is clear that the “manual”
228 derivation of $C_{B,f}(\tau)$ function can become a rather complex task; however, it is extremely
229 simple with Mathcad (see Figure 4). The derivative function of $C_{B,f}(\tau)$ is defined (named
230 as $DerCb(\tau)$ in the Mathcad spreadsheet) and the “root” Mathcad function calculates the
231 roots of this function (τ_{opt}), and then the optimum reactor volume (V_{opt}), as well as the
232 maximum concentration of B, are directly obtained. As can be seen in the graph of Figure
233 4, the calculated optimum space time corresponds to the maximum of $C_{B,f}(\tau)$ function.

234 Finally, the overall yield (ψ) is defined as the concentration of the desired specie (B) at
235 the end of the reaction (i.e., in the output current) divided by the concentration of specie

236 A converted (i.e, the difference of concentrations in the feed and output current).
 237 Therefore, the calculation of this parameter (Figure 5) needs the concentrations of species
 238 A and B for the space time achieved in each item (τ_f and τ_{opt}), which is calculated taking
 239 into account the reaction stoichiometry and equations (7) and (8). As expected, the overall
 240 yield in the optimized conditions (ψ_{opt}) is higher than that observed for the item a)
 241 conditions (ψ_a).

242 The statement of the second exercise was: *Two reactors are arranged in series taking*
 243 *place the following parallel reactions in liquid phase,*



244
 245 *where S is the desired product. 15 L·s⁻¹ of a current containing 2000 mol·m⁻³ of A is*
 246 *introduced in the first reactor and its concentration is reduced to 50 mol·m⁻³ in the output*
 247 *of the second one. Knowing that the concentration of A in the output of the first reactor*
 248 *corresponds to that for the maximum instantaneous yield, what is the total amount of S*
 249 *produced if the configuration is i) CSTR+PFR or ii) PFR+CSTR?*

250 *Data: $k_R=2000 \text{ molA}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$; $k_S=1 \text{ s}^{-1}$; $k_T=1\cdot 10^{-3} \text{ m}^3\cdot\text{molA}^{-1}\cdot\text{s}^{-1}$*

251 This exercise addresses the association of two reactors involving parallel reactions.
 252 Before solving it, some theoretical concepts must be clarified. In a continuous stirred tank
 253 reactor (CSTR), the amount of the desired species produced (ΔC_S) is calculated from the
 254 instantaneous yield (φ) and the amount of A converted ($-\Delta C_A$) as

255
$$\Delta C_S = \varphi(-\Delta C_A) \quad (11)$$

256 and for a plug flow reactor (PFR) its corresponding equation is

257
$$\Delta C_S = \int_{C_{Af}}^{C_{Ao}} \varphi dC_A \quad (12)$$

258 where C_{A0} and C_{Af} are the concentrations of A in the feed and output currents,
259 respectively. The instantaneous yield (ϕ) is defined as the rate of production of the desired
260 product (S) divided by the rate of consumption of A, at the current time:

$$261 \quad \phi = \frac{(r_s)}{(-r_A)} \quad (13)$$

262 Before using Mathcad the teacher explained to the students these theoretical concepts,
263 and the nomenclature to be used for each possible configuration (CSTR+PFR or
264 PFR+CSTR, referred to as Option A or B, respectively) with the help of the graph
265 included in Figure 6. Next, similar to exercise 1, the known parameters (i.e., reaction rate
266 constants, volumetric flow rate and the concentrations C_{A0} , C_{S0} and C_{A2}) are included in
267 the Mathcad spreadsheet. After that, it was proposed to the students that they introduce
268 the reaction rates from the units of the reaction rate constants supplied, being the correct
269 expressions those displayed in Figure 7. The C_{A1} value should be calculated from the
270 maximum of the instantaneous yield (ϕ), therefore the next step was to define this
271 parameter as a function of the concentration of A, and then calculate its maximum value
272 with the “root” Mathcad function. As deduced from graph in Figure 7, the concentration
273 of specie A at the output of the first reactor, C_{A1} , is $1414 \text{ mol}\cdot\text{m}^{-3}$, and it is the same for
274 the two possible configurations. The optimum association will be one that provides the
275 maximum production of the desired specie (S), i.e., the maximum concentration of S in
276 the output current of the second reactor (C_{S2}), which corresponds to the sum of the
277 concentrations produced in both reactors. Figure 8 shows the procedure followed to
278 calculate the final concentration of S according to the Option A (CSTR+PFR), referred
279 to as “Cs2_optA” in the Mathcad spreadsheet. The amount of S produced in the CSTR is
280 a direct calculation, but that corresponding to the PFR requires the resolution of an
281 integral, which depending on the complexity of reaction rates can become difficult;
282 however, this question is easily solved by the powerful symbolic calculation of Mathcad.

283 Thus, the production of S in the CSTR and PFR was of 153 and 268 mol·m⁻³, respectively,
284 whose area has been represented in the “instantaneous yield” vs. “concentration of A”
285 graph in Figure 8, giving rise a final concentration of 421 mol·m⁻³ (“Cs2_optA” value).
286 As for the Option B (PFR+CSTR), the production of S in the PFR was similar to that
287 obtained in the CSTR for the Option A (as may be deduced from their corresponding
288 areas), but the production of S in the CSTR is much lower than that noticed on the PFR
289 for the Option A. Therefore, the optimum configuration to achieve the maximum
290 production of S is the Option A.

291 Finally, the Mathcad spreadsheets followed to solve these exercises, as well as the
292 template for the series reactions, can be downloaded in Cuadri et al.³¹

293 **3. EVALUATION OF THE EDUCATIONAL EXPERIENCE**

294 **3.1. Student feedback and evaluation**

295 The degree of satisfaction of the students with the usage of Mathcad software for the
296 design of chemical reactors involving multiple reactions was carried out through students’
297 survey made in the last work session. It consisted of 10 questions, which were answered
298 by all the students (22 in total), the first three of which referred to the training courses on
299 initiation to Mathcad; the questions and their corresponding scores and standard
300 deviations are displayed in Figure 10. The main conclusions derived from the students’
301 survey are:

- 302 • As mentioned before, one of the faults detected in the previous educational
303 experience with Mathcad³⁰ was the little time devoted to the training courses. In
304 the current experience, it was increased in one more session which resulted in an
305 acceptable score in the question Q1 (3.8). Therefore, it can be assume that three
306 training seminars are suitable for future experiences.

307 • Moodle platform is considered a useful way of student-teacher communication
308 (Q2) and the exercises proposed in the three training workshops are adequate
309 (Q3). However, as regards to the latter question, some responses in the opening-
310 ended question (see Student 3 below) provide valuable information about future
311 actions.

312 • Regarding the use of Mathcad for the design of chemical reactors involving
313 multiple reactions, students consider this educational experience positively (Q10),
314 since it reduces the mathematical problems (Q4) and helps students to better
315 understand the theoretical concepts (Q5).

316 • Interestingly, students feel empowered to address other problems related to the
317 design of chemical reactors autonomously (Q6). Therefore, the educational
318 experience here proposed enables the achievement of efficient learning, which
319 favours students' problem-solving skills.

320 Beyond the scores obtained in each question, which in the end are only numbers, the
321 responses in the opening-ended question should be considered as matter of discussion.

322 Some of them are shown below:

323 • Student 1: *"It was easy to see how the mathematical problems are solved quickly
324 and I can rest assured that I will not fail in that"*.

325 • Student 2: *"After using Mathcad I don't see any sense to keep solving problems
326 of chemical reactors by hand"*.

327 • Student 3: *"More exercises solving system of equations should be done before
328 starting with the exercise of reactors"*.

329 • Student 4: *"What I liked the most was the template for series reactions, it's great.
330 The worst, the difficulty in making graphs"*.

331 **3.2. Authors' reflections**

332 After completing the education experience, in order to improve future actions related to
333 the use of Mathcad software for solving engineering problems related to Chemical
334 Engineering, some authors' reflections are presented:

- 335 • It is absolutely necessary in today's knowledge society that future chemical
336 engineers acquire in their own university the skills for the management of
337 mathematical software packages or programs.
- 338 • The use of Mathcad creates a classroom atmosphere in which students can
339 exchange impressions about the different resolution methodologies, which
340 enriches learning.
- 341 • In the last working session, it would be very interesting to solve the two proposed
342 exercises about the design of chemical reactors following the "traditional"
343 procedure, in order to highlight the enormous advantages of calculation (e.g.,
344 resolution of system of equations or integrals) that Mathcad offers.
- 345 • With the goal to ensure the concepts acquired during the training courses on
346 initiation to Mathcad, some exercises are proposed by the teacher to do outside
347 school hours.
- 348 • The easy mathematical resolution using Mathcad means removing the focus on
349 the mathematical problem, which allow the teacher to spend more time addressing
350 other engineering issues.

351 **4. REMARKS CONCLUSIONS**

352 This paper shows the great potential of math software Mathcad to address the design of
353 chemical reactors taking place multiple reactions. To that end, the educational experience,
354 which was carried out with third-year chemical engineering students enrolled in the
355 Chemical Reactors course, included (1) training courses on initiation to Mathcad, (2) the
356 resolution of two examples related to the design of chemical reactors, and (3) a meeting

357 space supported by the Moodle virtual platform of the University of Huelva. As
358 illustrative examples, a continuous stirred tank reactor taking place series reactions and
359 two reactors (continuous stirred tank reactor or plug flow reactor) arranged in series
360 involving parallel reactions were solved by Mathcad software. After this task, a student
361 survey gave a very positive assessment of this educational experience. Their main reasons
362 were two: Mathcad allows them to better understand the theoretical concepts related to
363 the design of chemical reactors involving multiple reactions and the mathematical
364 difficulties are negligible. Because of this, students feel the need to extend the use of
365 Mathcad to solve other engineering problems related to Chemical Engineering by the
366 creation of their own Mathcad spreadsheets. Finally, the educational experience here
367 proposed enables the achievement of efficient learning, which favours students' problem-
368 solving skills.

369 **5. LIST OF SYMBOLS**

| | | |
|-----|-----------|---|
| 370 | k_r | reaction rate constant of the rth reaction [variable] |
| 371 | r_r | reaction rate of the reaction r [$\text{mol}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$] |
| 372 | V | reactor volume [m^3] |
| 373 | $F_{j,i}$ | molar flow rate in the feed current of species j [$\text{mol}\cdot\text{s}^{-1}$] |
| 374 | $F_{j,o}$ | molar flow rate in the output current of species j [$\text{mol}\cdot\text{s}^{-1}$] |
| 375 | C_j | concentration of species j |
| 376 | τ | space time [s] |
| 377 | v | volumetric flow rate [$\text{m}^3\cdot\text{s}^{-1}$] |
| 378 | φ | instantaneous yield [-] |
| 379 | ψ | overall yield [-] |

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387 **CONFLICT OF INTERESTS**

388 The authors declare that there are no conflict of interests.

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- 468

FIRST EXERCISE

Item a)

reaction rate constants

$$k_1 := 0.3 \frac{\text{L}}{\text{min} \cdot \text{mol}} \quad k_2 := 0.05 \cdot \frac{1}{\text{min}}$$

reactor volume

$$V := 200 \text{L}$$

volumetric flow rate

$$v_0 := 10 \frac{\text{L}}{\text{min}}$$

concentration of the species in the feed current

$$C_{a0} := 10 \frac{\text{mol}}{\text{L}} \quad C_{b0} := 0 \frac{\text{mol}}{\text{L}} \quad C_{c0} := 0 \frac{\text{mol}}{\text{L}}$$

469

470 **Figure1.** A portion of the Mathcad spreadsheet including all known variables values for

471

example 1, item a).

472

space time

$$\tau_f := \frac{V}{v_o} = 20 \text{ min}$$

concentration of the species in the output current

$$C_{af} := \frac{-1 + \sqrt{1 + 4 \cdot k_1 \cdot \tau_f \cdot C_{ao}}}{2 \cdot k_1 \cdot \tau_f} = 1.21 \cdot \frac{\text{mol}}{\text{L}}$$

$$C_{bf} := \frac{\frac{k_1 \cdot C_{af}^2 \cdot \tau_f}{2}}{1 + k_2 \cdot \tau_f} = 2.197 \cdot \frac{\text{mol}}{\text{L}}$$

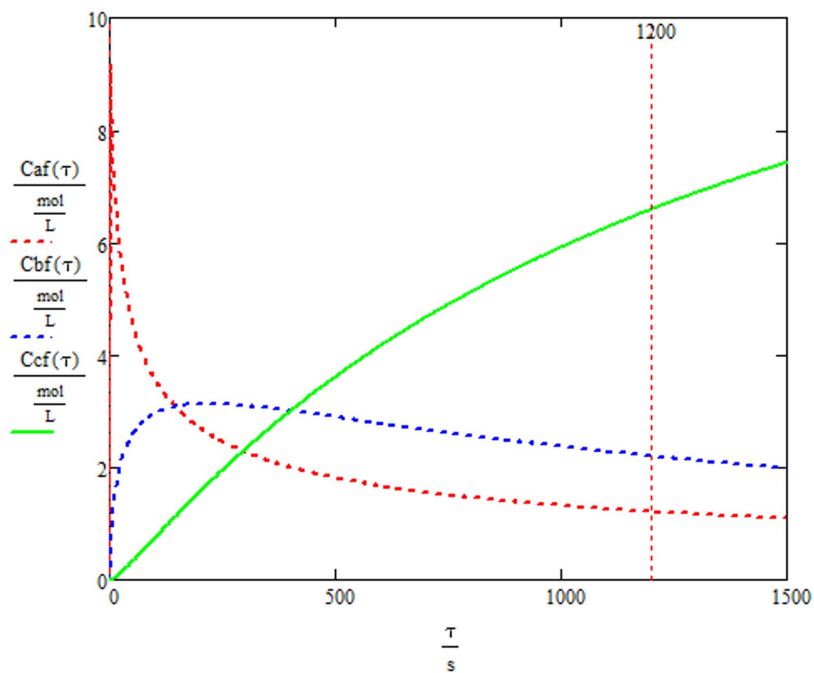
$$C_{cf} := 3 \cdot k_2 \cdot C_{bf} \cdot \tau_f = 6.592 \cdot \frac{\text{mol}}{\text{L}}$$

concentration of the species as a function of space time

$$C_{af}(\tau) := \frac{-1 + \sqrt{1 + 4 \cdot k_1 \cdot \tau \cdot C_{ao}}}{2 \cdot k_1 \cdot \tau}$$

$$C_{bf}(\tau) := \frac{\frac{k_1 \cdot C_{af}(\tau)^2 \cdot \tau}{2}}{1 + k_2 \cdot \tau}$$

$$C_{cf}(\tau) := 3 \cdot k_2 \cdot C_{bf}(\tau) \cdot \tau$$



473

474

Figure 2. A portion of the Mathcad spreadsheet with the procedure to calculate the

475

concentration of the species in the output current, and its graphic representation,

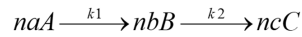
476

corresponding to the example 1, item a).

477

SERIES REACTIONS (TEMPLATE)

general expression series-reactions



stoichiometric coefficients

$$na := 2 \quad nb := 1 \quad nc := 3$$

reaction rate constants

$$k_1 := 0.3 \quad k_2 := 0.05$$

concentration of the species in the feed current

$$C_{a0} := 10 \quad C_{b0} := 0 \quad C_{c0} := 0$$

volume reactor and volumetric flow rate

$$V := 200 \quad v_0 := 10$$

space time

$$\tau := \frac{V}{v_0} = 20$$

guess values

$$C_a := 1 \quad C_b := 1 \quad C_c := 1 \quad r_a := 1 \quad r_b := 1 \quad r_c := 1$$

system of equations

Given

$$r_a = -k_1 \cdot C_a^{na}$$

$$r_b = \frac{nb \cdot k_1 \cdot C_a^{na}}{na} - k_2 \cdot C_b^{nb}$$

$$r_c = \frac{nc}{nb} \cdot k_2 \cdot C_b^{nb}$$

$$C_a = C_{a0} + r_a \cdot \tau$$

$$C_b = C_{b0} + r_b \cdot \tau$$

$$C_c = C_{c0} + r_c \cdot \tau$$

$$\begin{pmatrix} r_{af} \\ r_{bf} \\ r_{cf} \\ C_{af} \\ C_{bf} \\ C_{cf} \end{pmatrix} := \text{Find}(r_a, r_b, r_c, C_a, C_b, C_c) = \begin{pmatrix} -0.439 \\ 0.11 \\ 0.33 \\ 1.21 \\ 2.197 \\ 6.592 \end{pmatrix}$$

concentration of the species in the output current

$$C_{af} = 1.21 \quad C_{bf} = 2.197 \quad C_{cf} = 6.592$$

478

479 **Figure 3.** Mathcad template to calculate the concentration of species in the output

480

current of a CSTR for a general series reactions.

481

482

FIRST EXERCISE

Item b)

Derivative of $C_b(\tau)$

$$\text{Der}C_b(\tau) := \frac{d}{d\tau} C_b(\tau)$$

Optimum space time

$$\tau_{\text{opt}} := 200\text{s} \text{ (guess value)}$$

$$\tau_{\text{opt}} := \text{root}(\text{Der}C_b(\tau_{\text{opt}}), \tau_{\text{opt}}) = 213.742\text{ s}$$

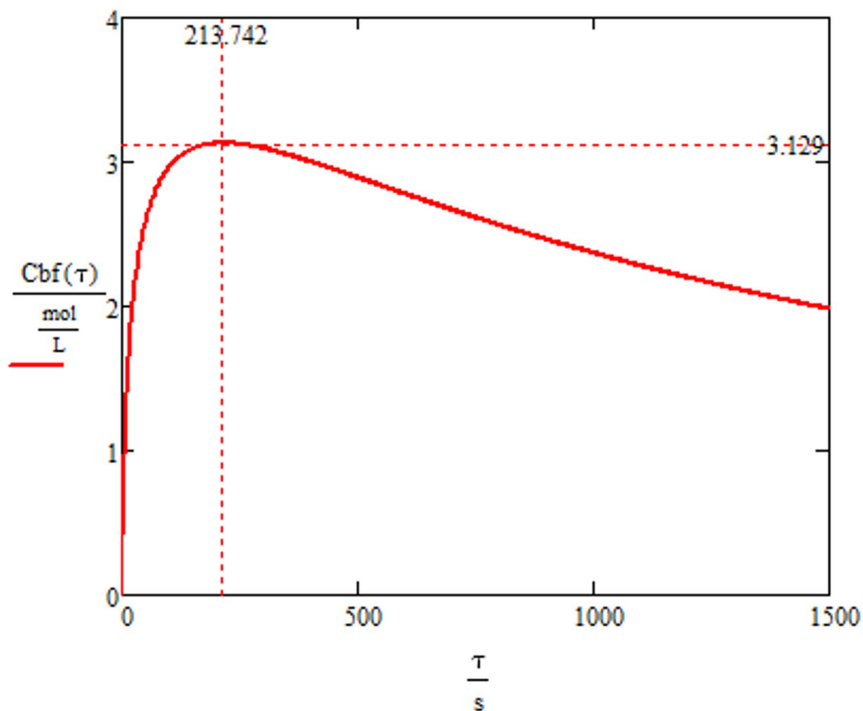
$$\tau_{\text{opt}} = 213.742\text{ s}$$

Optimum volume reactor

$$V_{\text{opt}} := v_0 \cdot \tau_{\text{opt}} = 35.624\text{ L}$$

Maximum concentration of B

$$C_b(\tau_{\text{opt}}) = 3.129 \cdot \frac{\text{mol}}{\text{L}}$$



483

484 **Figure 4.** A portion of the Mathcad spreadsheet with the procedure to calculate the

485 maximum concentration of B corresponding to example 1, item b).

FIRST EXERCISE

Item c)

Concentration of species in the output current for item a) conditions

$$C_{af}(\tau_f) = 1.21 \cdot \frac{\text{mol}}{\text{L}} \quad C_{bf}(\tau_f) = 2.197 \cdot \frac{\text{mol}}{\text{L}}$$

Overall yield for item a) conditions

$$\psi_a := \frac{C_{bf}(\tau_f)}{C_{ao} - C_{af}(\tau_f)} \cdot \frac{2}{1} = 0.5$$

Concentration of species in the output current for item b) conditions

$$C_{af}(\tau_{opt}) = 2.627 \cdot \frac{\text{mol}}{\text{L}} \quad C_{bf}(\tau_{opt}) = 3.129 \cdot \frac{\text{mol}}{\text{L}}$$

Overall yield for item b) conditions

$$\psi_{opt} := \frac{C_{bf}(\tau_{opt})}{C_{ao} - C_{af}(\tau_{opt})} \cdot \frac{2}{1} = 0.849$$

486

487 **Figure 5.** A portion of the Mathcad spreadsheet with the procedure to calculate the

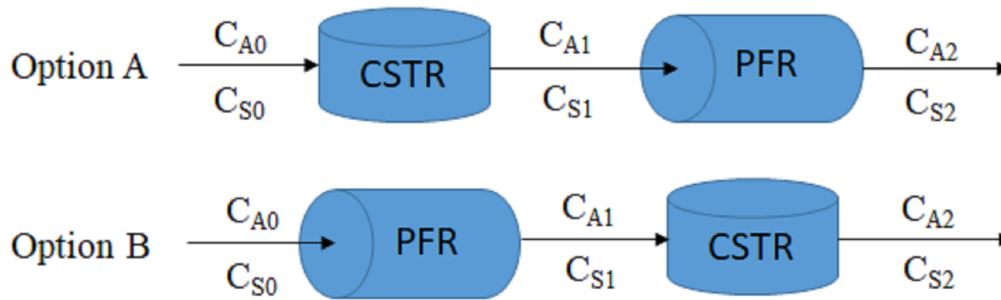
488 overall yields corresponding to example 1, item c).

489

490

491

SECOND EXERCISE



reaction rate constants

$$k_1 := 2000 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \quad k_2 := 1 \cdot \frac{1}{\text{s}} \quad k_3 := 0.001 \frac{\text{m}^3}{\text{mol} \cdot \text{s}}$$

volumetric flow rate

$$v_0 := 0.015 \cdot \frac{\text{m}^3}{\text{s}}$$

known concentrations

$$C_{A0} := 2000 \frac{\text{mol}}{\text{m}^3} \quad C_{S0} := 0 \frac{\text{mol}}{\text{m}^3} \quad C_{A2} := 50 \cdot \frac{\text{mol}}{\text{m}^3}$$

492

493 **Figure 6.** A portion of the Mathcad spreadsheet including all known variables values

494

for example 2.

495

496

497

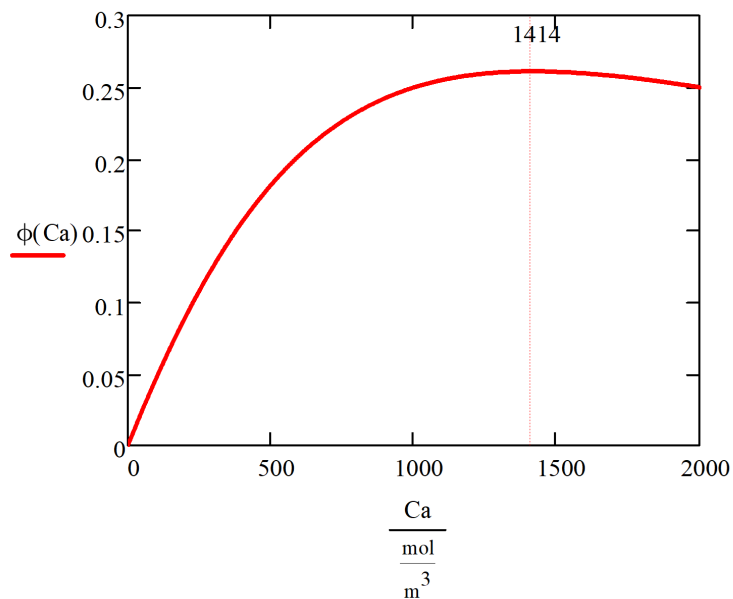
reaction rates

$$r_r(\text{Ca}) := k_1 \cdot \text{Ca}^0 \quad r_s(\text{Ca}) := k_2 \cdot \text{Ca}^1 \quad r_t(\text{Ca}) := k_3 \cdot \text{Ca}^2$$

Definition of the instantaneous yield (ϕ)

$$r_a(\text{Ca}) := r_r(\text{Ca}) + r_s(\text{Ca}) + r_t(\text{Ca})$$

$$\phi(\text{Ca}) := \frac{r_s(\text{Ca})}{r_a(\text{Ca})} \quad \text{instantaneous yield as a function of Ca}$$



$$\text{Ca1} := 500 \frac{\text{mol}}{\text{m}^3} \quad \text{guess value}$$

$$\text{Ca1} := \text{root}\left(\frac{d}{d\text{Ca1}} \phi(\text{Ca1}), \text{Ca1}\right) = 1.414 \times 10^3 \frac{\text{mol}}{\text{m}^3}$$

$$\text{Ca1} = 1414.214 \frac{\text{mol}}{\text{m}^3} \quad \text{Concentration of A at the output of the first reactor}$$

498

499 **Figure 7.** A portion of the Mathcad spreadsheet with the procedure to calculate the

500

optimum concentration of A corresponding to example 2.

501

502

503

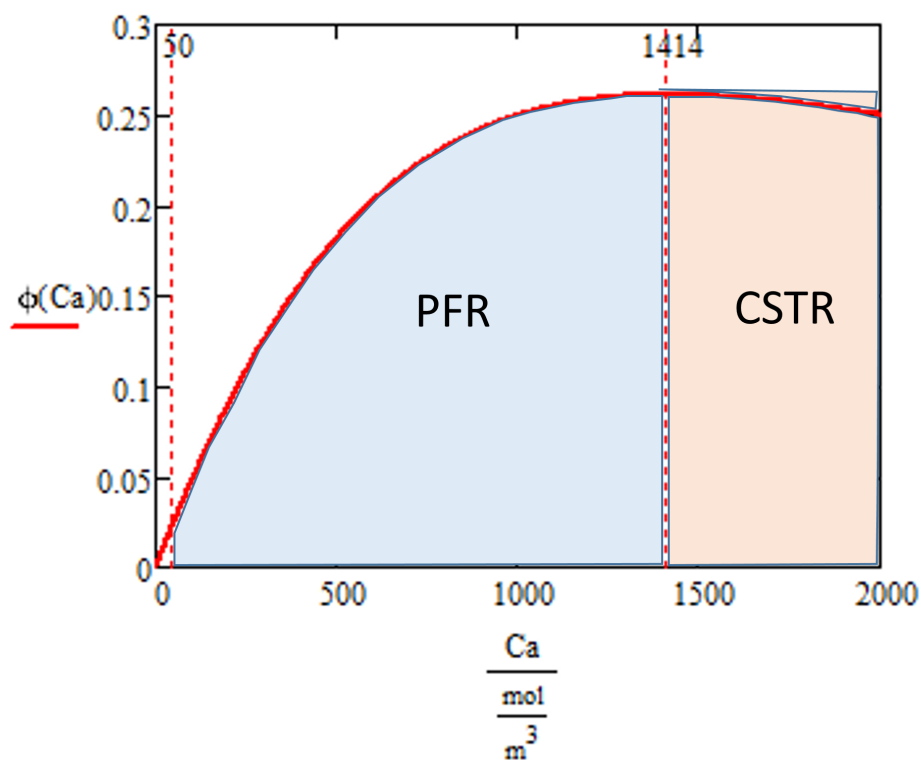


$$\phi(Ca1) \cdot (C_{A0} - Ca1) = 153.01 \frac{\text{mol}}{\text{m}^3} \quad \text{Amount of S produced in the CSTR}$$

$$\int_{Ca2}^{Ca1} \phi(Ca) dCa = 268.765 \frac{\text{mol}}{\text{m}^3} \quad \text{Amount of S produced in the PFR}$$

$$Cs2_{\text{optA}} := \phi(Ca1) \cdot (C_{A0} - Ca1) + \int_{Ca2}^{Ca1} \phi(Ca) dCa$$

$$Cs2_{\text{optA}} = 421.775 \frac{\text{mol}}{\text{m}^3} \quad \text{Total amount of S produced}$$



504

505 **Figure 8.** A portion of the Mathcad spreadsheet with the procedure to solve the

506 CSTR+PFR configuration corresponding to example 2.

507

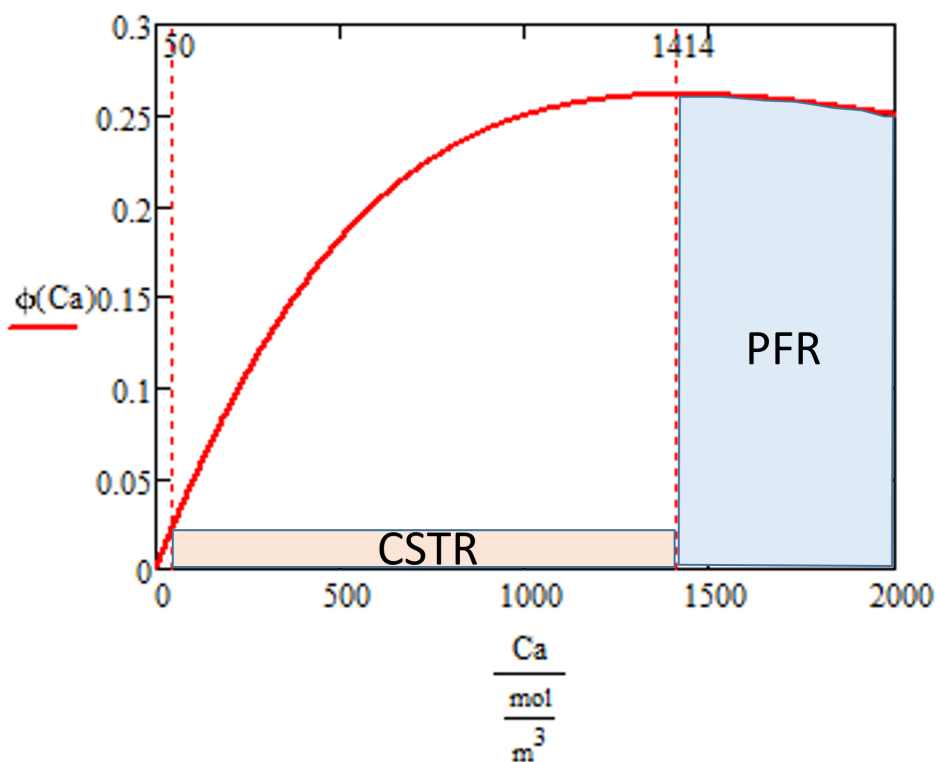


$$\int_{Ca1}^{Cao} \phi(Ca) dCa = 150.6 \frac{\text{mol}}{\text{m}^3} \quad \text{Amount of S produced in the PFR}$$

$$\phi(Ca2) \cdot (Ca1 - Ca2) = 33.233 \frac{\text{mol}}{\text{m}^3} \quad \text{Amount of S produced in the CSTR}$$

$$Cs2_{\text{optB}} := \int_{Ca1}^{Cao} \phi(Ca) dCa + \phi(Ca2) \cdot (Ca1 - Ca2)$$

$$Cs2_{\text{optB}} = 183.833 \frac{\text{mol}}{\text{m}^3} \quad \text{Total amount of S produced}$$



508

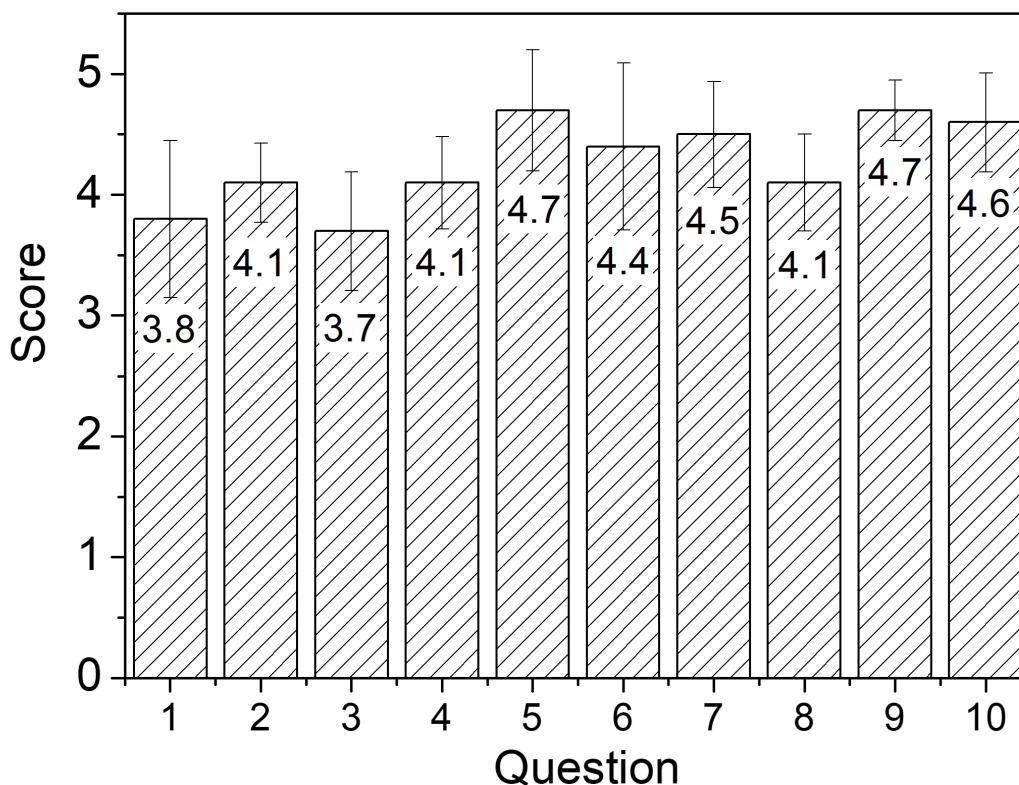
509 **Figure 9.** A portion of the Mathcad spreadsheet with the procedure to solve the

510 PFR+CSTR configuration corresponding to example 2.

511

512

| EVALUATION OF THE EDUCATION EXPERIENCE | | | | | | |
|---|--|---|---|---|---|---|
| 1-Strongly disagree ; 5- Strongly agree | | | | | | |
| | | 1 | 2 | 3 | 4 | 5 |
| Q1 | I consider that the time devoted to training courses is sufficient | | | | | |
| Q2 | The Moodle platform was useful to facilitate the communication with the teacher and to solve doubts | | | | | |
| Q3 | The exercises proposed in the third seminar on initiation to Mathcad were adequate | | | | | |
| Q4 | Through the use of Mathcad the mathematical resolution problems were minimal | | | | | |
| Q5 | The software has helped me to better understand some theoretical concepts involved in the multiple reactions | | | | | |
| Q6 | I consider myself ready to use this software autonomously | | | | | |
| Q7 | The knowledge acquired in this course is perfectly applicable to solve other engineering problems | | | | | |
| Q8 | I would like to further deepen the use of Mathcad | | | | | |
| Q9 | I consider that this tool should be extended for the rest of courses for the Chemical Engineering degree | | | | | |
| Q10 | I value this educational experience very positively | | | | | |
| | Some comments: | | | | | |



513

514

Figure 10. Student survey questions about this educational experience and their

515

corresponding responses.