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Chemical Engineering Education and the New Paradigm of Open-Source Software

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Free and open-source platform-independent software is now a reality that even Chemical Engineering (ChemE) can no longer ignore but it is also a new way of international co-operation for disseminating and interchanging information. Aspen Plus [1], MatLab [2] and other proprietary software are of major importance, expensive and usually Microsoft Windows platform-dependent but they are in a way or another already integrated in students training. LATEX [3], Python [4], SAGE [5], COPASI [6], OpenFOAM [7], etc. continue to be in some countries, for instance in Portugal, a totally new field to ChemEstudents.

The answer to "Why this happens and continues to happen in our days" could perhaps give a solution to that ambiguity. To answer this question it's important to review some facts and previous cases:

-Aspen Suite in 1992 (firstly the MAX ver. 1.1) was presented to the Chemical Engineering Department of Técnico of the present Lisbon University, and it took 10 or more years of hard work to finally be introduced in the student's curriculum.

-In Law nº 36/2011, the Portuguese parliament [8] establishes the necessity of adoption of open source rules for all the government informatics (The Cabinet Office of the UK government did the same on July 2014 [9]) but in 2014 a PhD thesis in ChemE continues to be written in Microsoft Word (.docx) in more than 95% of the cases.

- In July 1, 2014 CRC Press published "Introduction to Software for Chemical Engineers" [10]. According to the editor, "provide an introduction that serves as a quick reference guide for the use of different computer software in chemical engineering applications so that students become familiar with the capabilities." (p.vii). Open-source software is cited only three or four times to establish its existence or advantages.

-LATEX with R, SAGE (SAGETEX) or Python integration is not even imagined by the students and even less by the teachers and almost not used in manuscript submission in the world of chemistry and chemical engineering.

-Expensive software university/enterprise contracts, like Microsoft, MathWorks or COMSOL are still paid when there is little money for laboratory even for exemplification work.

For instance, COPASI, well used in biochemical networks and their dynamics is easily extensible to chemical reaction kinetics analysis and fast mechanistic discrimination in batch or continuous reactors [11], is almost unknown by ChemE teachers groups or Chemical Reaction Engineering/Catalysis PhD students. Even the SBML standard [12], easily translated to pure chemical reaction mechanism, using common sense, is not standard and almost unused.

Why teach MatLab and not SciPy [13]? Why use Microsoft Word and not LibreOffice/ Open Office (equation insertion in similar LATEX format) or LATEX? Why have bad graphic quality YouTube classroom presentations and not well-written RUBY/HTML pages?

Lets take the synergies of LATEX embedded SAGE/Python environment and compare them with Microsoft Word with Excel tables and statistical treatment. If we compare software price, hardware demand, resulting productivity or quality for large documents like PhD Thesis, Word/Excel is far from being acceptable but is the preferred choice.

The lack of tutorial documentation or examples or hard configurability cannot be an excuse because it is not true. Due to the pure lack of interest in subjects that are not within the central scope of the teachers work these new capabilities are not transmitted to students. Like so, ChemE is waking up late for software/hardware fast development like demonstrated in biology, biochemical and *omics*, etc.

Of course it doesn't make sense to be too dogmatic about the use of open source when proprietary software works better or is of generalized use as a standard. In this case we can't replace for instance Aspen Plus teaching in a ChemE course by ASCEND (or by the new CAPE-OPEN DWSIM[14]) or Aspen Dynamics (or HYSYS) by OpenModelica [15]. There is no enough time in the classroom to build the complete P&I and develop the needed thermodynamic properties correlations and teach OpenModelica or even DWSIM at the same time.

This discussion has been longstanding in other areas and produced some extreme positions and for instance the proprietary software defenders talk about open source defenders as evangelists.

The importance over the subject can be expressed with the number of answers to the questions in Google search engine for "why not open-source" 6.0×10^{8}results (in October 14, 2014, query = why OR not open-source).

Perhaps another Google experience, like the one presented in Table 1 could help to characterize the ChemE position attitude towards open-source.

Table 1: Number of Google search engine answers for queries, which are only one word different.

'word' in Google query*: "open-source 'word' engineering"	**Number of answers (October 2014)**
	16,800
Civil	2,170
Chemical	60,200
Biological	4,020
Biochemical	2,160,000

* The query must include the quotation mark at the beginning and end.

The nearly two orders of magnitude achieved by the experiment shown in Table 1 mean that biochemical related knowledge is connected to Open Source and we know that is in fast development (proteomics and other *omics*, DNA mapping, PCA analysis, etc.). On the other hand, ChemE is not so correlated with Open Source. Is ChemE stagnating? I think not. For instance heterogeneous catalysis won a Nobel prize in 2007, catalysis in 2010, development of multiscale models for complex chemical systems in 2013.There are numerous subjects to develop like exothermic trickle bed catalytic reactors are far from being well described at microscopic, particle and reactor levels, etc., etc. We, ChemE engineers know that we need computers and how to talk with them. Can universities pay software and not laboratory-scale demonstration unit operations and don't care about it? This cannot be understood!

Unfortunately, perhaps the upcoming restricting policies in Research and Development funding coming from national politicians and European leaders [16] will introduce a new driving-force on the subject. Perhaps we are close to a paradigm shift in the discipline, which has been predicted for some time [17].

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