INAUGURAL LECTURE
DECEMBER 1, 2022

PROCESS SYSTEMS ENGINEERING IN A CHANGING WORLD

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COLOPHON
Prof. dr. ir. Edwin Zondervan

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During this lecture, klezmer band di Gojim played three tunes:

1. Der Yid in Yerushalayim
2. Vi bistu geweyn far prohibition
3. Firn di mekhetunim aheym

Geachte rector, dear family, friends, colleagues: Welcome to my inaugural lecture! I am really happy to see you all today – in person as well as online!
I would like to kick-off with some music.

Figure 1: Klezmer band di Gojim!

So, that was a great way to kick off an inaugural lecture, right? You were listening to *di Gojim*. And their music is called *klezmer music*. Klezmer is traditional Jewish, eastern European music. I kind of grew up with this music and this band. When I first heard it, it grabbed me, like a virus. The music suits different moods; nostalgic, sad, happy; they say it goes directly into your soul because the instruments (especially the clarinet and violin) sound like human voices expressing emotions. Klezmer music developed in eastern Europe, in the Jewish communities and it absorbed to large extend local, folk influences. The music changed all the time, as Jewish people where moving over the globe – especially in the beginning of the 20th century: from the folk music of the Balkans to jazz- and vaudeville music of the Americas. The klezmorim play different tunes, styles, in different keys, with different rhythms and measures; the measureless doina's, the lively bulgars and freylechs and the strolling hora's. From 4 quarters and 3 quarters to 7/8 measures! Muzikale duizenpoten! (Musical caterpillars)

When I defended my PhD thesis in 2007 in Groningen, I asked if *di Gojim* could come to play at my party. But unfortunately their calendar was busy. Years later, in 2019, when I organized the European Symposium on Computer Aided Process Engineering at the Evoluon in Eindhoven, I asked again, but time fell short and they couldn't come. A couple of months ago I tried again, now for my inauguration and a definite YES came! You cannot imagine my happiness. And I was determined to have them here today, no matter how well they might fit within the topic of my inauguration! I really think that by having di Gojim play music here today we create a unique, festive atmosphere, while I am telling my story.

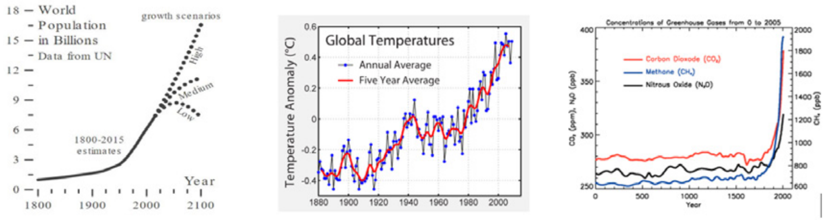


Figure 2: the metrics that describe our progress seem to move exponentially

We live in a changed world. Actually we live in a *changing world*. No matter which metric we take, whether it is population, GDP or greenhouse gas emissions, we can clearly see that things change; all the time. The only constant is change! Of course many of these indicators have only become measurable since the last - say - 200 years, when the industrial revolution started. However, these trends never show steady change. Actually in many cases the change seems to be exponential. You could also argue that this continuous change is countering natural- or biological phenomena, which tend to move towards equilibrium. Maybe that could be a reason that we can never be completely happy, as we are in the middle of a continuous change, while we need stationary conditions for happiness. But let us not get *that* philosophical. On the other hand, it could be very well that our time horizon is just too short to see when we reach an equilibrium. We have very fancy models that help us to study the change over time - the *system dynamics* - and to predict when we might reach a ceiling, a decline or a drama! Think for example of the climate change models.

The climate models tell us that we should act! And there is not a lot of time left! We all know this. Especially our greenhouse gas emissions affect the climate. And these emissions stem from all of our achievements in civilization: how we produce our energy, how we grow our food crops, how we operate our industry, how we deal with our water requirements.

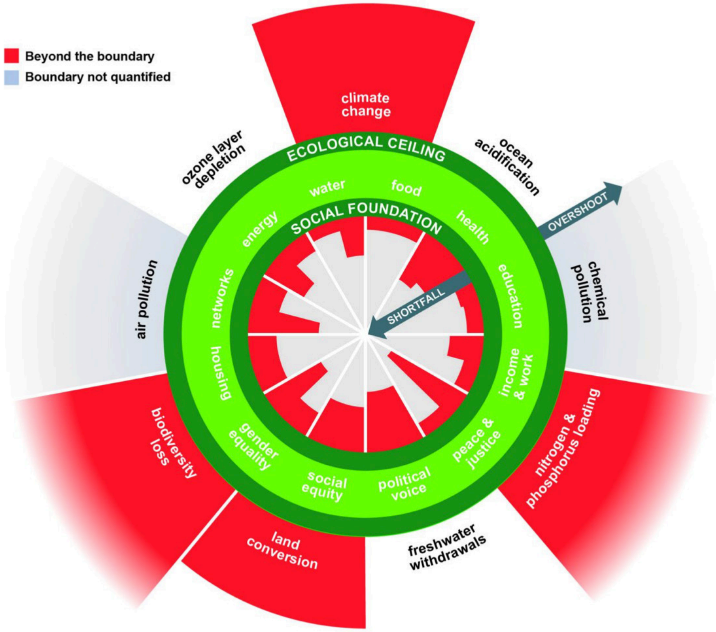


Figure 3: The doughnut model by Kate Raworth

In our development the priority has been on establishing and improving our social foundations; but we realize that in getting to our social foundation we are overshooting and hit the ecological ceiling! Of course there has to be a balance between the two, as is shown in the famous doughnut model, introduced by Kate Raworth in her Oxfam paper *A Safe and Just Space for Humanity* of 2011. This balance is required to battle climate change, but it is also needed to prevent the depletion of our resources.

The big question is; what is the best way of achieving such balance with such a complex, interconnected system of energy, water, food and industry (often called the nexus)? Maybe there are two ways of achieving balance: the first way is to go through a *transition*, which is by itself a gradual change towards a balance. The alternative is by what I call *shock therapy*, or a step change.

In this step change we have to make abrupt changes to achieve balance. Maybe at first glance this seems a very unrealistic way of achieving balance. And I agree! Although I want to point to you an earlier transition that we went through in the Netherlands, in the 1960s.

Figure 5: The Dutch gas transition in the 1960's

Yes, this was also an energy transition! The Dutch government managed to completely change its energy infrastructure in the 1960s and moved to a gas powered energy system. Within a period of 5-10 years this new energy system was in place and in full use! There has been a very nice documentary in 2020 produced by *Andere tijden - De slag om het gas* (the battle for the gas) that describes this transition. This was a step change! And what made it possible to set out such a step change?

Maybe I am thinking too simplistic, but I think there were three factors that made this abrupt change possible: 1) Opportunity – in the north of the Netherlands huge gas reserves were discovered; 2) Green field development – no serious pipeline grid was in place yet, in other words the grid could be developed from scratch; 3) Not too many alternatives; basically gas was the only alternative to coal. There was not yet a serious prospect of generating energy in a renewable fashion.

Of course the circumstances are very different today, although there are many opportunities to valorise renewable- and still fossil sources, we are facing limitations in the current hardware (e.g. grid) and it turns out that we have many alternatives to choose from when we want to renovate our technological world. It should be clear that I am not only thinking about energy, but also about our food-, water- and industrial chains, that are highly interconnected. In our mobility chains and our information networks we have similar issues, but as I am a chemical engineer I would not consider them here in scope.

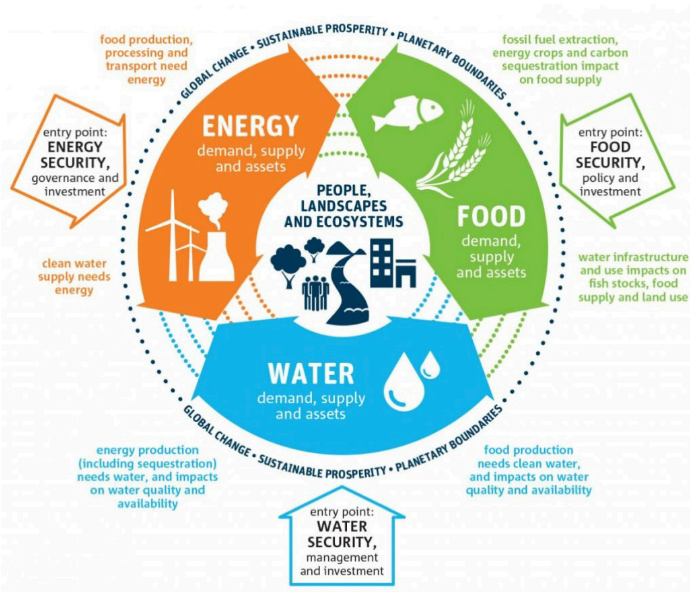


Figure 6: The water-energy-food nexus

Here is an illustrative example: *The bio-economy*. There have been over the last 5 years several European directives that state that the EU should further develop and extend its bio-economy. In short: a bio-economy valorises biomass in to food, energy and chemicals. Economists have mentioned that already 8% of Europe's workforce is active in this bio-economy, and that by 2030 an additional one million jobs can be created. Each euro invested will yield another euro. It is said that a bio-economy will also mitigate greenhouse gas emissions and restore the ecosystems with at least 15% by 2025. Now, what are the considerations when developing a bio-economy.

Well we have to decide which variety of plant species to cultivate, or agricultural waste to collect, in which way we will harvest and handle the feedstock, which intermediate products are of interest, which conversion and separation technologies to select and which final products should be produced. In other words, many decisions to make, and I always say: *decisions multiply*! These decisions hold for individual technologies, for factories and, for supply chains. They hold for the decisions to be made on the short term (how to operate certain equipment) and for the intermediate- to longer term; tactical- and strategic decisions: where to build factories, where to grow crops, and so forth. I have not even mentioned the connections that a bio-economy might carbon capture and utilization, energy transition and water requirements. I believe that in such complex decision-making process PSE can play an important role.
But, what is PSE? *Process systems engineering*?

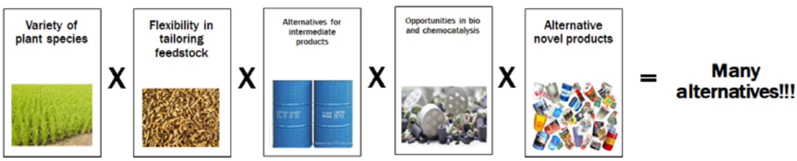


Figure 7: Decisions for the bio-economy

There have been several definitions of what PSE actually is. But when I ask it in a group, nobody can really come up with a clear description. It is of course a discipline within chemical engineering that makes use of mathematics and computers. And many of you will consider process design, process control and simulation as core activities of PSE. PSE was first coined in the 1960's at Imperial college by *Prof. Sargent*. In 1982 the first PSE conference was organized in Japan. And actually this year the PSE conference returned to Kyoto for its jubilee celebration. I prefer to use a description provided by *Ignacio Grossmann* in the beginning of the 2000's. PSE concerns the systematic design, analysis and optimization of decision-making processes for the discovery, design, manufacture and distribution of products. The emphasis is on decision-making, and for me this means optimization. Companies that employ systematic decision-making tools and strategies typically become the industrial leaders of the world. You might browse for a book by *Steve Sashihara* titled "*The optimization edge*" to get impressed by the power of optimization and decision-making.

I like this quote from Dwight Eisenhower. In a way it also resembles process systems engineering: whenever I run in a problem I can't solve, I make it bigger. It is this zoom-in/zoom-out attitude that distinguishes the process systems engineer from others. Alternatively, as a philosophy of life: don't be part of the problem, be the entire problem!

Anyways, the process systems engineer is typically a generalist. Maybe a generalist does not have deep knowledge, but he has overview. A specialist on the other hand has deep knowledge but not always the overview, or maybe not even a vision on the end product. I recognize this sometimes also in discussions with my colleagues. This difference can be shown in the following figure:

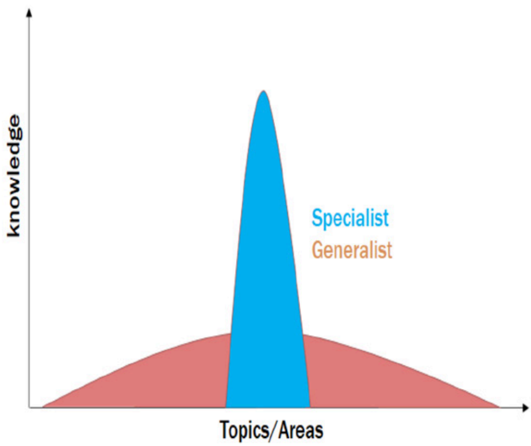


Figure 8: Specialist and generalist

If you would take this to the extreme case: the specialist will know everything about nothing and the generalist knows nothing about everything. For sure I am a generalist.

The PSE community has been around for quite some time, at least 60 years. We are not a very large community. If I would have to guess I would say that we may have around 2000 members in our community, worldwide. We meet each other typically at two events, the yearly ESCAPE, a European symposium and the PSE a three years event that moves through Europe, Asia and the Americas. Our magazine is the Elsevier journal "Computers & chemical engineering". And over the last decades we have been instrumental in the development of process design, simulation, control and optimization tools. Think of software packages like Aspen or GProms. All of it to improve the decision-making for new processes and products. Traditionally PSE was active within the (petro)chemical industry, but over the years new frontiers were sought towards specialty chemicals and pharmaceuticals and more recent to agri-food-, water- and energy sectors. I believe PSE is also the perfect candidate to develop and advertise new technological development in sustainability and circularity (think of Life cycle assessment) and Artificial intelligence (in understanding and interpreting information and as means to enhance decision-making for new processes and products). PSE has in the last 5 years also made a very successful revival in the Netherlands via new appointments in universities (including myself) but also by establishing the network organization PSE-NL and by hosting European events like the ESCAPE in 2019 and this year here at Twente University the CAPE Forum!

Despite being such a small community, I have the feeling that we are delivering!

I guess the most important thing that we deliver is the skilled engineer by high quality education and training!

Figure 9: Pioneers of the klezmer music, in the middle sits Naftule Brandwein

Time for a musical intermezzo! [Assemble in the mean time the distillation set up]

The tune that you have been listening to is called "*Vi bistu geweyn far prohibition*". Which is Yiddish and means: "Who were you before the prohibition". The prohibition was the result of the recession of the 1920's. People got desperate and took resort to alcohol. So a general prohibition was enforced. Klezmer clarinettist Naftule Brandwein was known for playing this tune in the beginning of the twentieth century. Naftule was an Austrian born Jew that emigrated to the U.S. He also honoured his last name (Brandy) as he was a strong drinker. But he was also a virtuous clarinettist. He was really a show man, dressing up for his performance in a suit full of light bulbs. It was reportedly said that there was this one time an incident where his suit caught fire! He played so virtuously that he was afraid that others might steal his fingering technique; for that reason he played often standing with his back to the audience. Well; one way of making moonshine is by distillation. The setup that I was assembling here. I guess what I tried to say here is that students might learn more by actually doing things.

Here at Twente University we have excellent education to train this next generation chemical engineer in the best possible way. Although I believe further improvements can be made.

In the way we teach for example. The COVID crisis forced us to use online teaching methods, to record classes and pen casts to use contact time with students more efficiently: much less towards classical lecturing and more towards active discussion with students. Maybe a bit less towards communicating technical skills (there are so many resources available to students to master a specific skill) and more towards handling, understanding and solving problems! We should also make sure that inputs, such as problems, cases, projects etc are brought in via real stakeholders (e.g. the industry) and we must not be scared to provide hands-on training to our students. I am for example thinking of having here at Twente a real process control lab; where students can touch valves and tune real PID controllers. I also envision a virtual reality component in teaching process design; where students can walk – with their 3D googles – in an augmented reality of a factory and go through scenario analysis and calamity training. We must also make sure that the new technological developments in sustainability, circularity and artificial intelligence find their way into our courses. These are the tools of the future and we should make sure that the next generation chemical engineer knows how to use them. These ideas are in line with two surveys amongst academia and industry that were conducted over the last years. 2-3 years ago Prof. Grievink and colleagues surveyed the Dutch situation and more recently an international survey was conducted by Daniel Lewin and colleagues for the same purpose. If we do not act, the threat is a potential disconnect between what we teach in academia and what is required by industry. We all understand that industry needs to change. But, to transform the industry, we should equip the next generation of chemical engineers during their training with the tools for developing sustainable processes and products. David Attenborough reportedly said: “Bringing nature into the classroom can kindle a fascination and passion for the diversity of life on earth and can motivate a sense of responsibility to safeguard it”.

Or to repeat myself: our most important product is the skilled engineer!

Of course an important source of knowledge for our students stems from the research that we do. So I would like to use the opportunity to also tell you something about my work.

My academic career started almost 20 years ago when I took up a PhD position here at Twente University. Over the years I moved to different places and I worked with different people. I was always under the impression that my movements were kind of erratic. Different topics, tools and application areas. But while preparing this lecture, I realized that throughout this journey there actually is a vision, a connection between my contributions. Churchill said: to know your future you must know your past. From information to knowledge and from knowledge to wisdom. And maybe from wisdom to conspiracy theory … who knows.

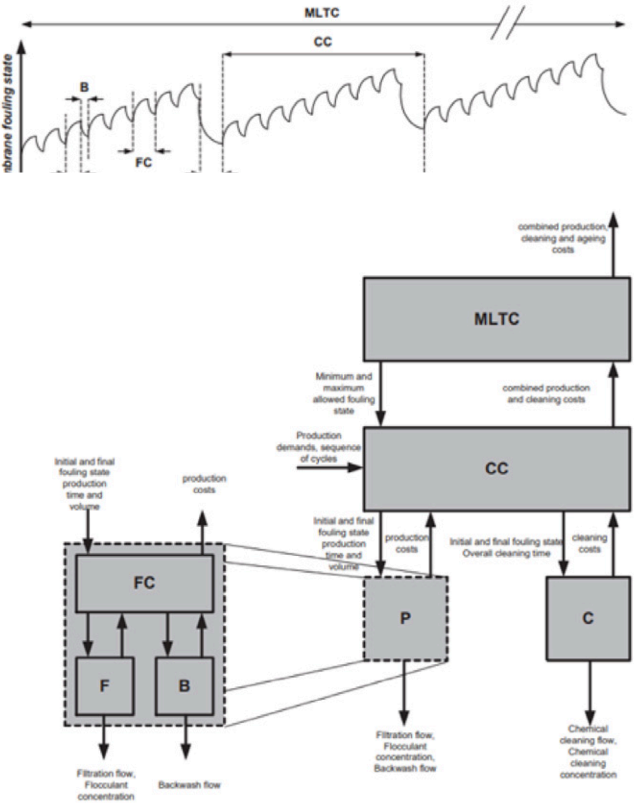


Figure 10: The ultrafiltration control hierarchy

From 2003 to 2007 I was a PhD candidate at Twente University – ultimately defending the thesis at Groningen University. Under the guidance of professor Roffel I developed a modeling framework to optimize the performance of ultrafiltration membranes for the purification of surface water. I described the performance of such a membrane system at different time scales. From short term phenomena such as filtration and backwashing via medium term cleaning cycles up to the level of the membrane life time. From seconds to years. The models were used to define operational strategies that would reduce costs, and chemicals and increase lifetime. The models were organized in a kind of hierarchy.

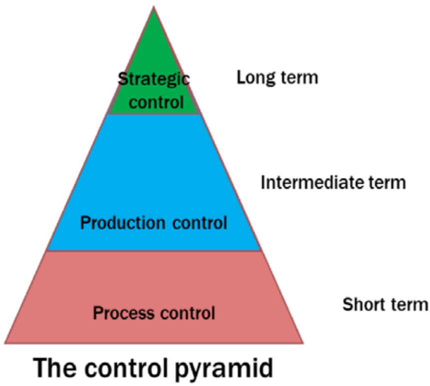


Figure 11: The control pyramid

When I wrote the summary of my thesis I realized that this hierarchy could be represented by a pyramid: the control pyramid! Reflecting control strategies at different time scales.

I finished my PhD and got a job as assistant professor at Eindhoven University of technology with Professor André de Haan; who just started a chair on process systems engineering in 2006. André coupled me to a number of his PhD students that were working on process intensification problems, especially reactive distillation. At the same time I could work on my own research ideas and Andé allowed me to spend time abroad at some of the renowned places for PSE. I went to UPC with Prof. Puigjaner, to CMU with Prof. Grossmann, to DTU with Prof. Gani and then to IC with Prof. Pistikopoulos. I see this travels as a way of filling up my PSE toolbox. I also realized that process design and process control are intertwined.

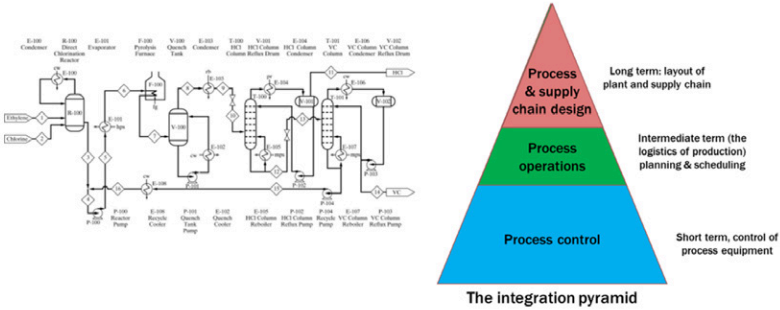


Figure 12: The integration pyramid; integrating control and design

On top of the control pyramid was another level: the process design level. The decisions that you make during the process design stage, affect the decisions that you can make at the process control level. Actually; they were not directly connected. In between there was an "operational" level that considered scheduling/planning decisions. With the projects I was moving around on the different stages of the pyramid and I wondered why we use this preemptive, or sequential way of making decisions. Could you not get rid of the levels and integrate all decision making into one monolithic type of model? Finding a way to integrate the pyramid was the holy grail of PSE! There has been effort to reach integration, but nobody could do this in a really good fashion, and the consequence was that after integration the pyramid was broken up again to smaller parts that were solved sequentially. Integrate to decompose … that is a paradox … that is the integration paradox!

Now, the big hurdle was that at each of these levels different modeling methods were used. Dynamic models, steady state models, models that are linear or nonlinear, with continuous and or discrete variables, and so on. In addition it often was also not clear how the levels should interact. I spend big part of my time with André de Haan in search of a universal modeling language and towards a standard for integrating levels. I got in touch with a systems engineering group at the department of mechanical engineering where a new process algebra was developed to really create universal models; and as part of my stay at UPC I realized that there are international integration standards such as the ISA95. But my attention and interest moved when I got connected to the late professor Peter Bongers.

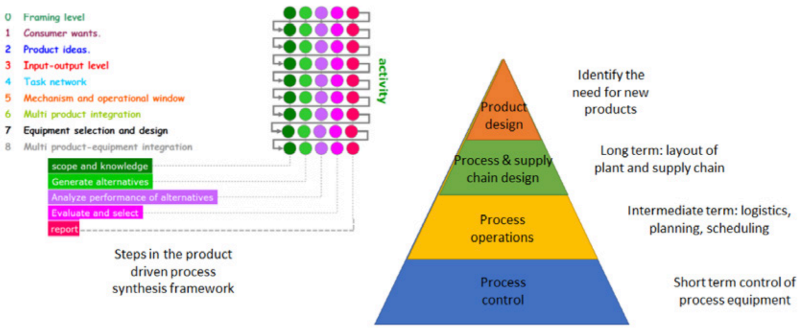


Figure 13: The extended integration pyramid including product design.

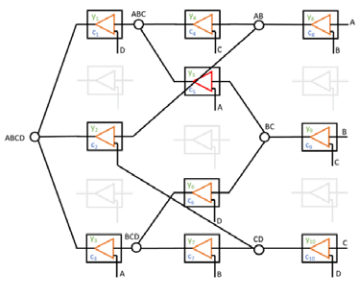
Prof. Bongers obtained the Hoogewerff chair on product design. Bongers was head of R&D at Unilever in Vlaardingen and was one day per week in Eindhoven to develop the methodology on product-driven process synthesis (PDPS) that he developed together with his colleague Crishian Almeida Rivera. We got introduced and together we coached a team of PhD candidates that were all covering a part of the PDPS. Sadly, Bongers got ill and passed away within about 2 years of his appointment. He could not see the result of his PhD candidates! And he could not see that Cristhian and I organized all the work into a great textbook!
For me this period came with a new insight: that the pyramid should be extended again, on top of the process design level there is another level: the product design level. A process can only be designed, after you realize which product you would like to make! The product drives the process! I ran a couple of very exciting projects from making ice cream and mayonnaise up to creating food-health products based on antioxidants.

But we were reaching 2015 and I made a career move.

I moved to Germany and was promoted to professor at the University of Bremen with my own chair on PSE. The move also meant again a change of topic, namely: the energy transition.

I moved a step away from the question how to integrate the pyramid and I realized that there are three challenges that we face at all levels of the pyramid!

The challenge of flexibility, sustainability and complexity. How to design/operate processes when we have uncertainty in feedstock, equipment performance and demand for products? How do we design/operate processes when we have conflicting objectives, for example: environmental targets versus economic targets? And how do we deal with the complexity that originates from making models to design/operate processes? I was answering these questions on the basis of four topics in the energy transition: biobased production, hydrogen economy, carbon capture and utilization and electrochemical storage of energy. In the middle of this very vibrant developments in Bremen an opportunity arose to come back to the Netherlands and establish Process systems engineering as discipline here at Twente university!



Suppose we have a mixture of P=4 components: A,B,C,D (ranked by increasing boiling point)... How many distillation columns do I need to separate all components? (Sharp separations possible, no azeotropes or other complications) Well ... you need (P-1) distillation columns, i.e. 3 columns ... We can design 5 different sequences!

$$N_S = \frac{[2(P-1)]!}{P!\,(P-1)!}$$

If we only consider one separation technique (distillation)

P	Ns
4	5
5	14
6	42
7	132
8	429
9	1430
10	4862

But if we also have the option to choose from different separation techniques (T) ...

$$N_S = T^{P-1}\frac{[2(P-1)]!}{P!\,(P-1)!}$$

	T=1			T=2			T=3
P	Ns		P	Ns		P	Ns
4	5		4	40		4	135
5	14		5	224		5	1134
6	42		6	1344		6	10206
7	132		7	8448		7	96228
8	429		8	54912		8	938223
9	1430		9	366080		9	9382230
10	4862		10	2489344		10	95698746

In classical process design we rule out many alternatives by using heuristics and only focus on evaluating a limited number of alternatives ... we might miss a surprising good alternative!

Figure 14: The superstructure framework

And here at Twente University I am now in full swing in establishing my PSE method! The product is kind of a tom-tom navigator that can be used to find the best route from raw material to final product via the selection of different technologies. We work on the production of added value chemicals from algae biomass, or the production of methanol from renewable hydrogen and carbon dioxide, or the production of green ammonia. My PSE method has 5 ingredients that are inspired by the dilemma that I proposed a minute ago: 1) Convert the problem to a network (superstructure), 2) Setup the mathematical model, 3) Reduce the complexity (make linear what is nonlinear, make convex what is not convex), 4) Incorporate the uncertainty (via scenario's, probability distributions and stochastic tools) and 5) Assess multiple conflicting objectives (via creating pareto frontiers).

The superstructure is the cherry on the pie!

It is the keyword to which I would like to be associated. The superstructure is a visual representation from feedstock to product and shows all possible routes. Each node in the superstructure represent a technology. You can imagine that by evaluating multiple feedstock, technologies and end products the combinatorial complexity goes up, factorial. Superstructure optimization is done by several people/groups, but there has not been a standardization. This is what I see as my core activity in Twente for the coming period, to establish a pitstop for superstructure optimization. I call it pitstop because of the Formula 1. In the 1980's a pitstop took about 2 minutes, nowadays it takes just a few seconds. This major improvement comes from standardization! The same holds for the superstructure, if we standardize the superstructure approach we can generate and solve them much more efficiently. With my current team we are developing this standardization; a convention for drawing the superstructure, in the way how we formulate the mathematics (mass balance, energy balance, recycles, conversion, separation, etc.) and how we code and document the superstructure.

The superstructure can be seen as a web.
And PSE is the spider in the web of a changing world.

Thank you all for listening and for coming to my inaugural lecture.

When the rector closes the meeting and the cortege moves, *di Gojim* will accompany us with more klezmer!

Ik heb gezegd!

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