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SPIRE 8 – 2015 – Solids handling for intensified process technology

Title: Intensified by Design© for the intensification of processes involving solids handling

Acronym: IbD

Grant Agreement No: 680565

Intensified by Design

Deliverable 5.4	IbD® Platform Freemium Version
Associated WP	WP5 IbD® Platform Architecture and Infrastructure
Associated Tasks	T5.1 Platform architecture and programming work organization T5.2 Development of the Platform backend for methodologies, tools and designers T5.3 Development of the Platform Graphic User Interface
Due Date	28/02/2017
Date Delivered	17/10/2017 (updated version)
Prepared by (Lead Partner)	IRIS
Partners involved	All
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Dissemination Level	Public (PU)

STATEMENT FOR OPEN DOCUMENTS

These deliverable results from the IbD project, which is supported by funding Framework Programme Horizon2020 of the European Commission under grant agreement no. 680565.

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Introduction and report summary

The IBD® Platform aims to be a comprehensive working environment that assists the Process Intensification (PI) designer along each stage by providing the most frequent or specific tools in one unique user interface (UI). The PI designer tool is based in eight basic steps: Flow sheeting, Mass/Energy balance, Environmental Performance (containing Life Cycle Assessment - LCA), Knowledge-based Engineering approach (KBE), Process Intensification modules (PIM), Simulations, Optimization and the Theory of Inventive Problem Solving (TRIZ).

Deliverable 5.5 dealt with the IbD platform Freemium release, which embraces all the updates to upgrade the previous Beta version. The main upgrades done are:

- Flow sheeting: The input parameters for each module were added in the Projects view.
- KBE: New updates in the KBE database were done, where several new modules with all their parameters were included.
- LCA: The Process views were added to the platform, and all the process configuration wizards were developed. The mockups for this step, as well as the algorithm, are already done and ready to be coded.
- PI designer: The PI designer was completed for several built in PIMs as: Spinning Disc Reactor (SDR), Oscillatory Baffled Reactor (OBR) and meso-OBR, Miniaturized Reaction Technology (MRT), Coflore Agitated Tube Reactor (ATR), Taylor-Couette Reactor (TCR) and Rotating Fluidised Bed (RFB). All the views, equations and algorithm were developed for each module.
- An error notification system has been implemented to keep the user update with the missing input fields as well as the wrong ones.

The following report is structured as follows:

Section 2 is devoted to the IbD platform Freemium release, and all the intensification steps developed until date: Flow sheeting, KBE, PI designer and LCA. Section 3 deals with the future challenges.

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1. IbD platform Freemium version

In this Freemium version, besides the new upgrade KBE database added to the platform, also the Flowsheet step was upgraded with the possibility to enter all the parameters related to a design module through the UI. The PI designer step was fully developed for seven built in modules, and the foundations to add the remaining PIMs have been fully established. Also, the LCA step was fully designed, the first step named Process view was developed and the final second step which is the LCA comparison is designed and its basis clearly established.

A nice error message system was integrated to the platform, which allows the user to be aware of the wrong/missing input parameters.

1.1. User Interface

The Login view of the Freemium release is depicted in Figure 1.

Figure 1. IbD beta release login view screenshot.

As observed no changes are done in this Freemium version regarding the Login view compared with the Beta version. The same behaviour is guaranteed:

The login will be done by valid users with the right email and password. In case a wrong data is entered, the platform will show a message telling the login failed. Also the right email format is required to can access the platform.

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1.2. Projects and intensification work flow

The format of the project list in the dashboard remains the same in this new version. The list of the intensification projects is placed in the left of the view, as shown in Figure 2.

The tree structure remains as in the beta version and it is the following:

- The user creates the current process to be intensified, (My FlowChart in figure 2).
- Once the flowsheet of the process is drawn, the user can select the module to be intensify and send it to the KBE step. In this moment, a "son" project is created, sharing the same flowsheet of its "father" but with a module sent to intensify (e.g. My Dryer Intensify).
- The user can select another module of the same flowsheet from the "father" flowsheet, and send it to intensify too. In this case, another "son" project with a different device sent to intensify, is created (i.e. My Gran Intensify).

Figure 2. Projects list screenshot.

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Once the device is sent to intensify, the KBE algorithm handles the search of the proper PIMs to substitute the one sent to intensify. The KBE algorithm and database, released in the beta version, would be upgraded and integrated in the Freemium version.

1.3. Flowsheet step

The Flowsheet step was developed and added in the beta release, as shown in Figure 3.

Figure 3. IbD beta release flowsheet view screenshot.

In this view the user has a modules palette, a drawing area and a module configuration area.

In the palette area, all the modules related with industrial processes of end-users, are placed (i.e. dryer, tableting, coating, etc.). The list of devices is open to add new modules, therefore, any new one whose functionality is mapped with one of the KBE functionalities, are able to be added to the palette.

In the grid drawing area, the user is allowed to drag a module from the palette (the list of modules will be updated as the project moves forward) and drop it in the drawing area. The modules can be connected by clicking from one port to the other device's port, and each module can be configured. Their functionalities come by default from the platform, and are mapped with the functionalities given by KBE database.

By using the palette modules, the drawing area and the configuration area, the user can perfectly draw its process flowsheet.

Each module can be configured in the configuration area. At the present moment, only the name can be modified, but more parameters will be added to each module as the project moves forward.

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The new feature added in this Freemium version, is the possibility to enter parameters related to each module, as shown in the Figure 4.

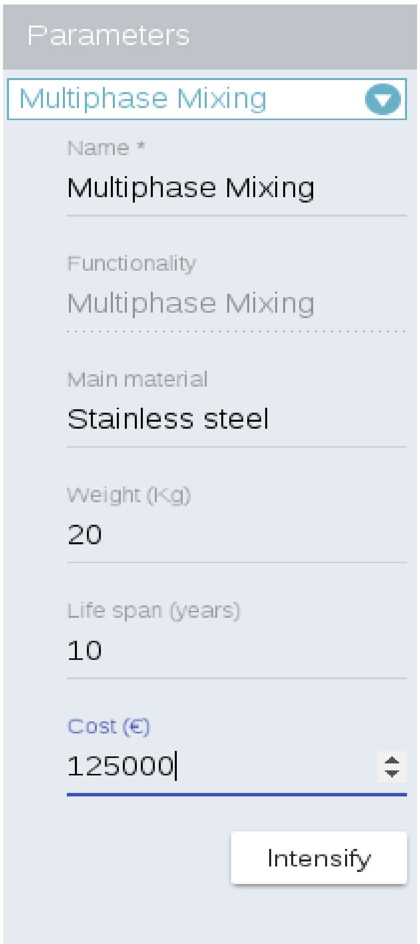

Figure 4. Module parameters view.

The user can easily select the main material, the weight in Kg, the life span in years and the cost in euros for their Flow sheeting module. These parameters are stored in database and will be helpful to apply the LCA step.

1.4. KBE step

The KBE view remains the same as in the beta version. The changes in this step are related to an upgrade of the KBE database by adding new PIMs and updating several ones.

Once the user has sent the device to be intensified, the KBE step shows up with the selected functionality (i.e. blending), and the user can select the performance criteria and score it, as shown in Figure 5.

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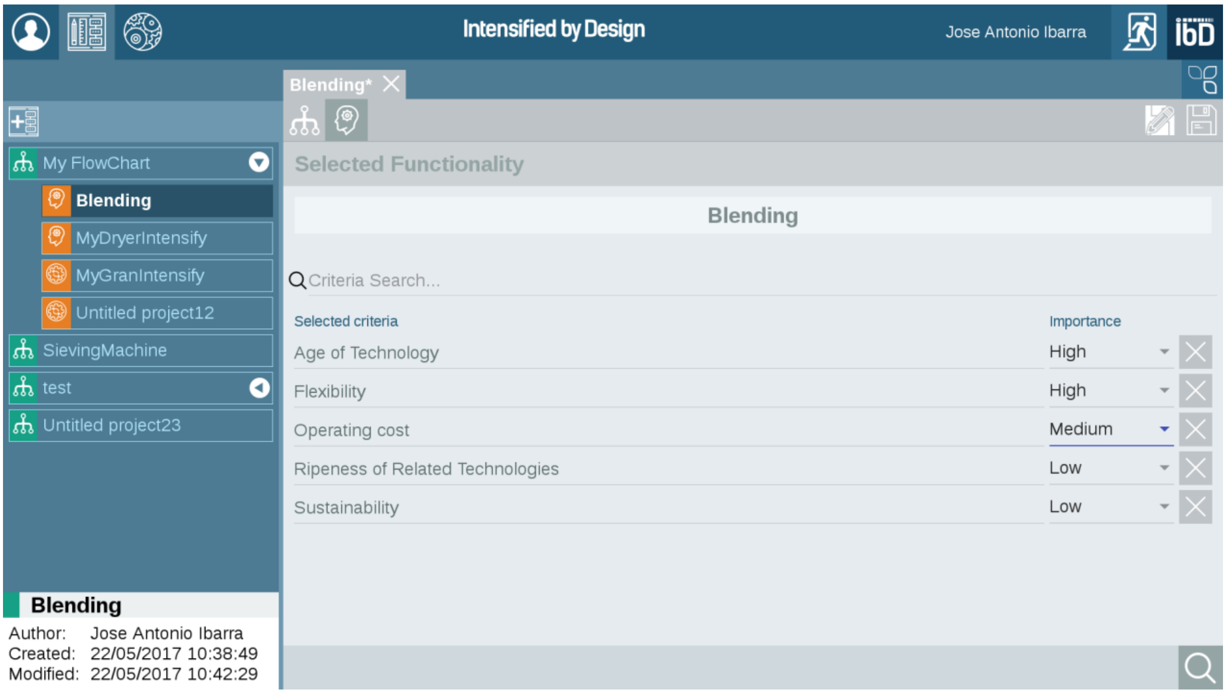

Figure 5. KBE screenshot. Scoring the performing criteria

Then the user can search for a PIM solution, as shown in Figure 6, where a list of suitable PI units is offered by the KBE algorithm, sorted by the best performance related to the functionality the user wants to intensify, and later by the scored criteria.

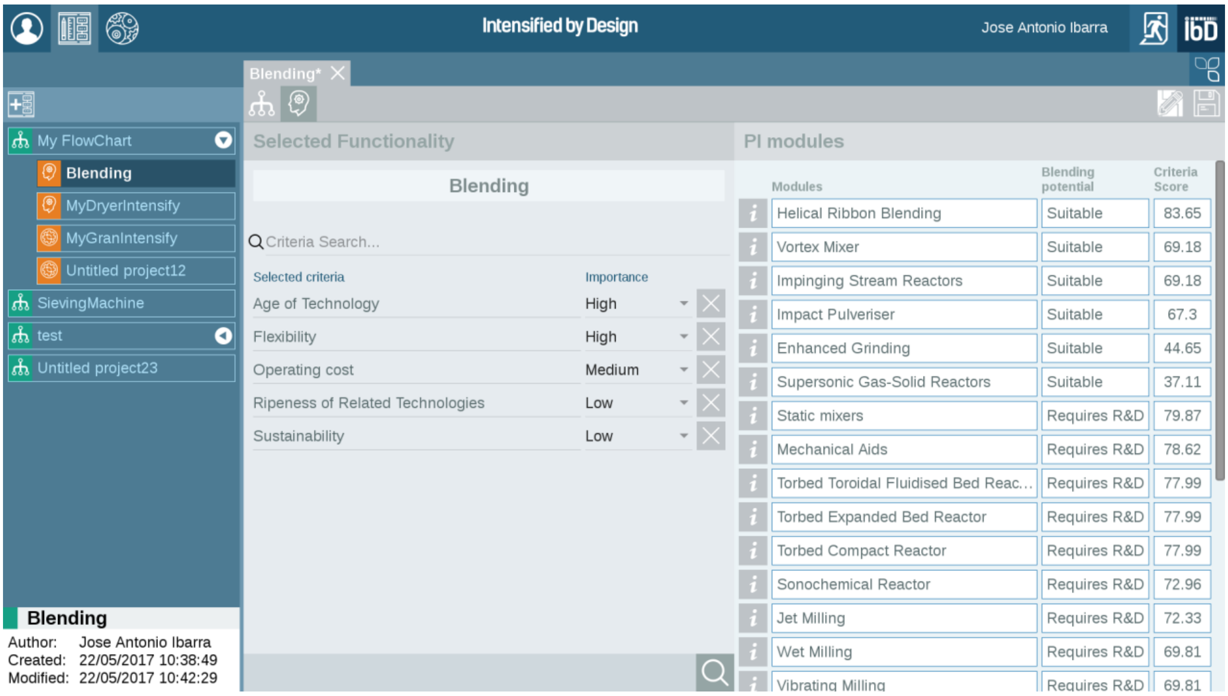

Figure 6. Displaying the PIMs suitable for the intensification process.

As shown, the PIMs available have been sorted first by functionality (Optimum, Suitable and Requires R&D), and later by criteria score. Each module has an information button where the technology is described. Also, the PIM row is clickable, to show each criteria score given by KBE.

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1.5. TRIZ step

TRIZ step discussions and implementations in the case studies are ongoing, in order to obtain a standard way to include it within the platform to fulfill all industrial sectors in a generic way.

1.6. PI Designer step

The PIMs can be classified as built in or novel modules. The built ones have a set of equations and design algorithms which allow to have some output designs. The novel PIMs are under development and currently don't have a set of equations, and are being analyzing by the expert partners.

The PI designer step was fully developed for several built in PIMs. The developed PIMs, as starting point, are:

- Spinning Disc Reactor (SDR).
- Oscillatory Baffled Reactor (OBR).
- meso-OBR.
- Miniaturized Reaction Technology (MRT).
- Coflore Agitated Tube Reactor (ATR).
- Taylor-Couette reactor (TCR).
- Rotating Fluidised Bed (RFB).

The following figure shows the example of the PI designer step within the platform for the TCR.

Figure 7. View of the PI designer within the platform

The PI designer view is composed by an index and the content. The user can use the index to move within the content by clicking in the desired topic, see Figure 8.

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Taylor-Couette Reactor

1. DESCRIPTION OF TECHNOLOGY
2. APPLICATIONS
3. SWOT ANALYSIS
4. MATERIAL INPUT PARAMETERS
5. FLOW REGIME OF TAYLOR-COUETTE REACTOR
5.1. TAYLOR-COUETTE PARAMETERS
5.2. TAYLOR-COUETTE OUTPUT PARAMETERS
5.2.1. ROTATIONAL REYNOLDS NUMBER VS. ROTATIONAL SPEED OF THE INNER CYLINDER
6. CUSTOMIZED TAYLOR-COUETTE DESIGN
6.1. CUSTOMIZED DESIGN OUTPUTS
7. CONTROL FOR TCR
8. FOULING CONTROL FOR TCR

Figure 8. Index of the PI designer for the TCR.

All the built in PIMs have the more or less the same sections: Description of technology, applications, SWOT analysis, the designing which embraces the input and output section, the control and fouling sections.

The content part is composed for the content of all the sections listed in the index part. Figures 9 and 10, show the "description of technology" and "applications" section within the TCR designer, respectively.

1. DESCRIPTION OF TECHNOLOGY

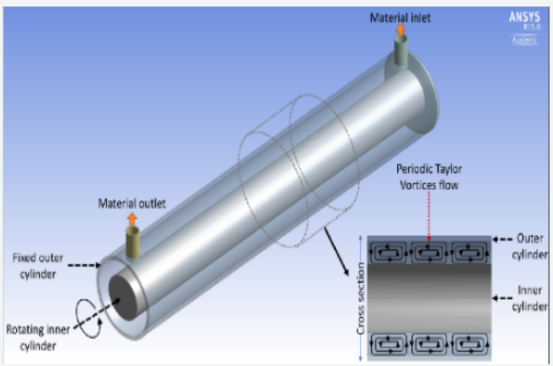
The Taylor-Couette reactor technology imposes high centrifugal acceleration and high shear rate to liquids flowing between the gap of the two differentially rotating cylinders. The Taylor-Couette reactor could be either a batch reactor or a continuous reactor. The fluid is supplied from one end of the cylinder and driven by the rotational cylinder. Several flow regimes occur with different rotational speed:

Flow regimes of Taylor-Couette reactor:

1. Laminar circular Couette flow (0 < ReTC < ReTCc)
2. Taylor vortex flow (ReTCc < ReTC < 5.5ReTCc)
3. Wavy vortex flow (5.5ReTCc ≤ ReTC ≤ 17ReTCc)
4. Modulated wavy vortex flow (17ReTCc < ReTC < 24ReTCc)
5. Turbulent Taylor vortex flow (24ReTCc < ReTC)

Where ReTC is the rotational Reynolds number and ReTCc is the critical rotational Reynolds number.

In most applications, the aim is to operate under the Taylor vortex regime.



3D view of a Taylor-Couette system with inset showing Taylor vortices formed in fluid flowing in annular space.

Figure 9. Description of technology section for the TCR.

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2. APPLICATIONS

Reaction	TCR characteristics of relevance to reaction	Phases involved	References
Photocatalysis	- Photocatalysis particles travel in the gap by vortex motion. - Controlled periodic illumination by flow regime.	Liquid/Solid	[1]
Emulsion polymerization	- Pre-reactor for the continuous emulsion polymerization. - Control the steady-state conversion and particle number. Stable long-term operation without shear-induced coagulation and polymer deposition.	Liquid/Solid	[2]
Crystallization	- Efficient mixing and heat transfer enhance the crystal size distribution and crystal product recovery.	Liquid/Solid	[3 - 9]
Mixing	Ideal plug flow with good mixing.	Liquid/Solid	[10 - 12]

References

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Figure 10. Applications section for the TCR.

The SWOT analysis section is shown in the following figure.

3. SWOT ANALYSIS

STRENGTH	WEAKNESS
- High level of heat and mass transfer rates. - Near ideal plug flow behaviour which gives good mixing. - High crystal size distribution. - A continuous reactor technology offering opportunities for efficient light activated reactions.	- Lack of awareness of TCR technology in the industry. - Lack of understanding of the application of turbulent flow regime of the technology in reactions.
OPPORTUNITY	**THREATS**
- Modification of the shape of inner cylinder enhancing mixing for reactions. - Decomposition ability offering opportunities for granulation reaction. - Anti-fouling for the rotating filtration.	- Industry reluctance to adopt rotating technologies for safety reasons. - Lack of online nonintrusive measurement technique.

Figure 11. Swot analysis of the TCR.

These three sections are common for all the built in PIMs. The design section involving the input and output parameters in inherent to each PIM. The user should enter a determined group of input parameters to obtain the outputs desired. In the middle a set of equations and algorithm are running behind in the platform's backend to transform the inputs in outputs.

Figure 12, shows the input parameters sections, where the user has to enter the material and the device input parameters to plot the regimes of the TCR to allow the user to choose the desired work

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regime. Figure 13 displays the value to be entered by the user depending of the regime selected, and the output parameters.

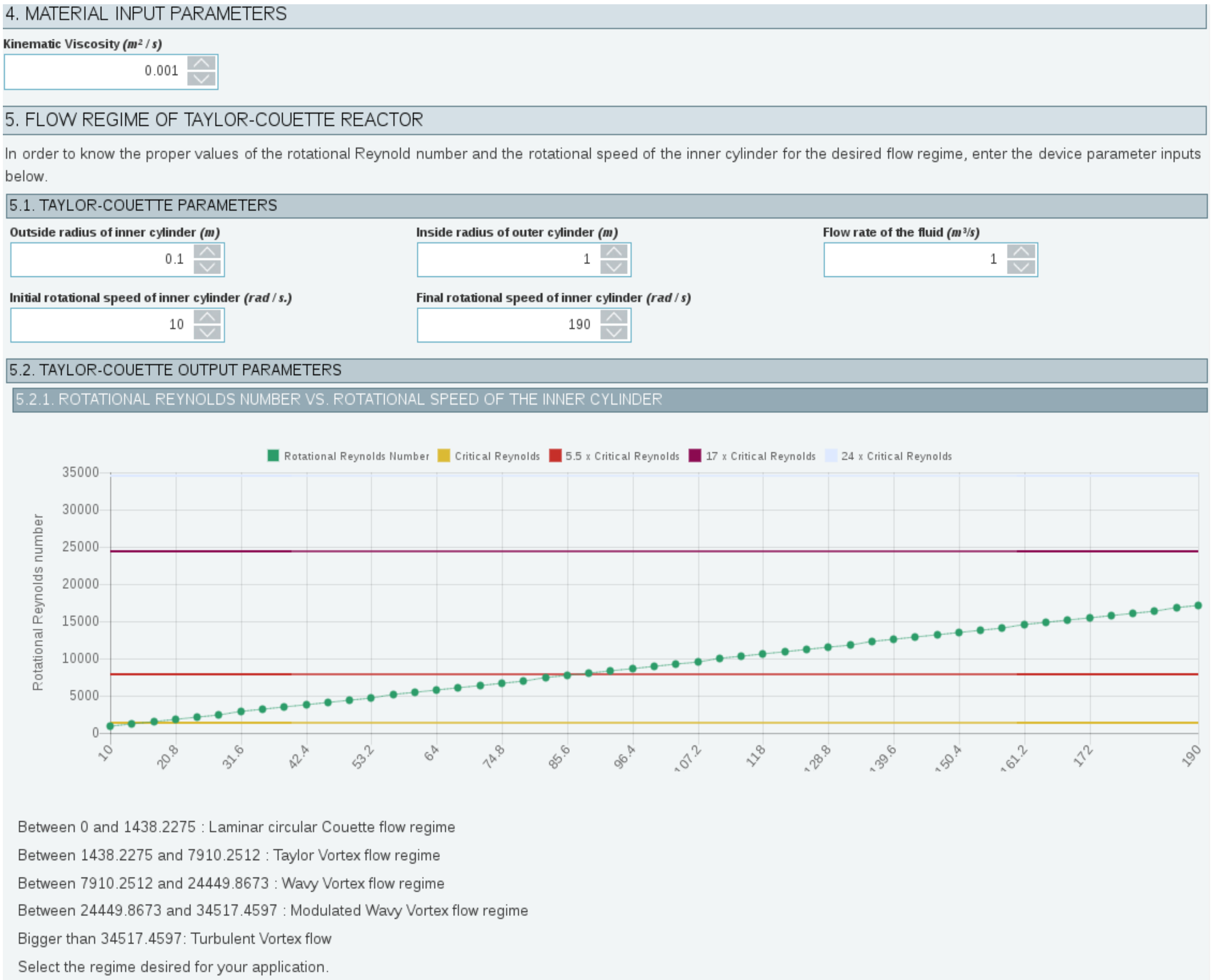

Figure 12. Several design sections for the TCR.

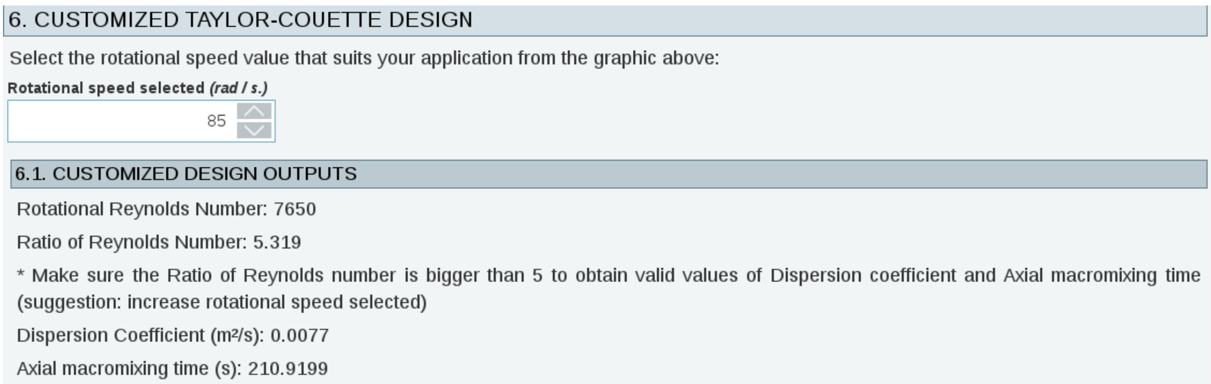

Figure 13. Output parameters.

Each PIM has its own design process and therefore, inherent sections for this.

The control and fouling sections are common for all built in PIMs, and they are shown in Figures 14 and 15.

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7. CONTROL FOR TCR

The variables relevant to advanced process control and process monitoring for the TCR are presented in the following qualitative interaction table. The table is aimed for filling the purpose of early stage control design, and to facilitate integrated process design and control design. The variables listed in the interaction table are considered as a set of possible inputs and outputs for process modelling, sensitivity analysis and controllability analysis.

The input (manipulated and disturbance) variables can be found from the columns and the output (controlled and observed) variables from the rows. The power/magnitude and the speed/dynamic response of the control qualitative indicated for some of the known interactions.

Taylor-Couette Reactor			Input variables		
			Design		Application
			Rotational speed	Axial liquid flow rate	Temperature[1]
Output variables	Design	Flow regime (measured by ratio of rotational Re to critical Re)	Large Fast	Large Fast	Moderate Fair-Fast
		Dispersion	Large Fast	Large Fast	Moderate Fair-Fast
	Application	Particle size and distribution	Large Fast	Moderate Fast	Moderate Fair-Fast
		Particle classification	Large Fair	Moderate Fast	Moderate Fair-Fast

The speed/dynamic responses are defined for the SDR as:

- Fast: seconds
- Fair: minutes
- Slow: hours
- Nil: not applicable/no effect

Notes:

[1] Temperature affects density and viscosity of working fluid which in turn affect the controlled parameters.

Figure 14. Control section for the TCR.

8. FOULING CONTROL FOR TCR

Key features of technology in fouling prevention/reduction	Important Parameters	Remedies
Taylor-Couette reactor is normally used as a rotating filtration technology, which has potential to control of flux decline related to concentration polarization and membrane fouling. Based on a numerical study [Ref.2], particles in the TCR typically have a trend to form a thin cake on the inner porous cylinder due to the radial flow in the laminar circular Couette flow. If the rotational speed of inner cylinder increases above the critical point, the particles are swept off the inner cylinder to resuspend them in the vortical flow. The vortical motion in the annulus carries the particles across the annulus further reducing the particle concentration near the inner cylinder.	Rotational speed of the inner cylinder (Increasing the rotational speed beyond the that for the laminar flow regime increases vortex formation which aids in the displacement of solid deposits from the inner and outer cylinder surfaces)**.	Surfaces in contact with particularly fouling solids can be coated with a non-stick material.

Notes:

* Have direct effect on fouling (increase in parameter value reduces fouling).

** Have inverse effect on fouling (increase in parameter value increases fouling).

References

[1] Crastes, Misha; Lagkaditi, Lydia; Ball, Jonathan; Yang, Junfeng; Coletti, Francesco; Macchietto, Sandro; Matar, Omar, Numerical study of crude oil fouling in a Taylor-Couette-type reactor, APS Division of Fluid Dynamics (Fall) 2015, abstract #D14.007 (2015).

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Figure 15. Fouling section for the TCR.

Any new built in PIM can be included into the platform in a very straightforward way, as an intermediate template done in .xml format can be easily translated into the platform.

1.7. Control Solution and Simulation Step

The Control Solution and Simulation steps are still under discussion by the partners. The Simulation step is performed for novel PIMs, as they have no equations to provide the proper outputs to the user.

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Once a simulation is performed by the partner involved in this task, a radial basis equation will be built by another partner, and the development team will include it within the PI designer step. Therefore, the user will have a set of equations to design the PIM, by using these expressions.

The Control solution step is still under discussion as the case studies are ongoing.

1.8. LCA Step

In this step, the user can analyze how its current process and the intensify processes perform in terms of environmental indicator. The first step is to enter the data related with the industrial sector (e.g. pharmaceutical), measurement units related to this sector, etc.

For doing so, a Process tab has been enabled to organize all the process related to a project, as shown in Figure 16.

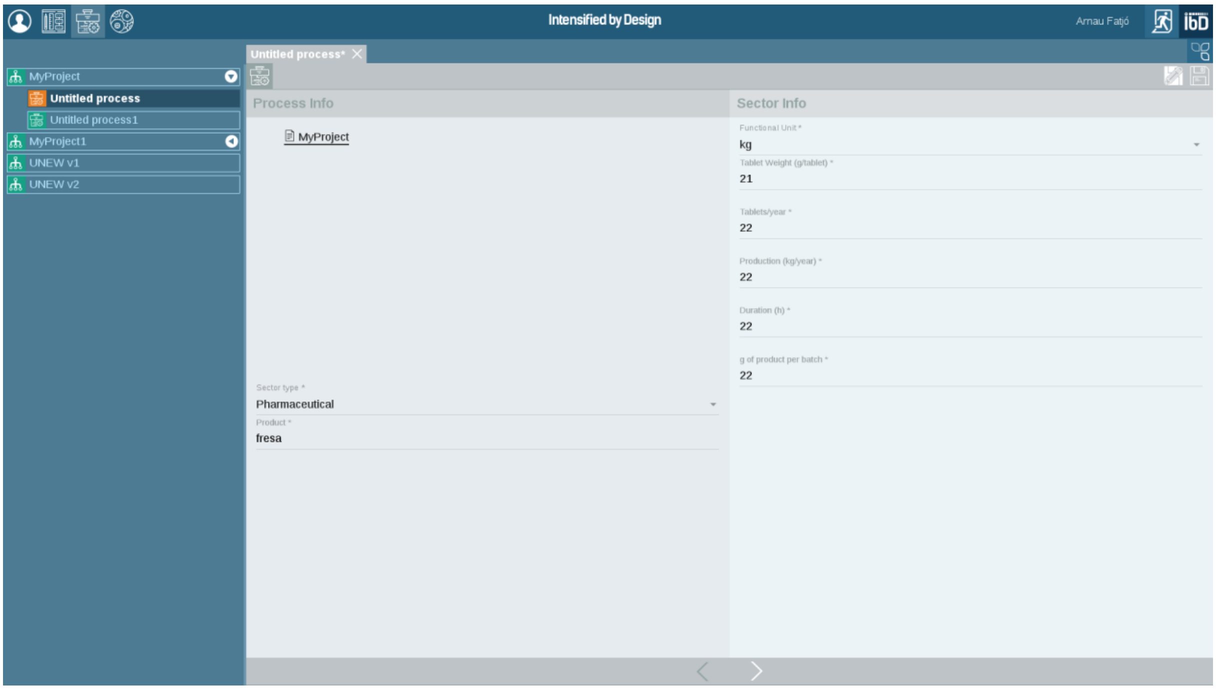

Figure 16. Process view.

In the process view, a project list with related process are listed and the left of the view. In the right, all the process input field data are placed, in order the user can fulfill them. The process info, as shown in Figure 17, is divided in:

- Process info
- Sector info

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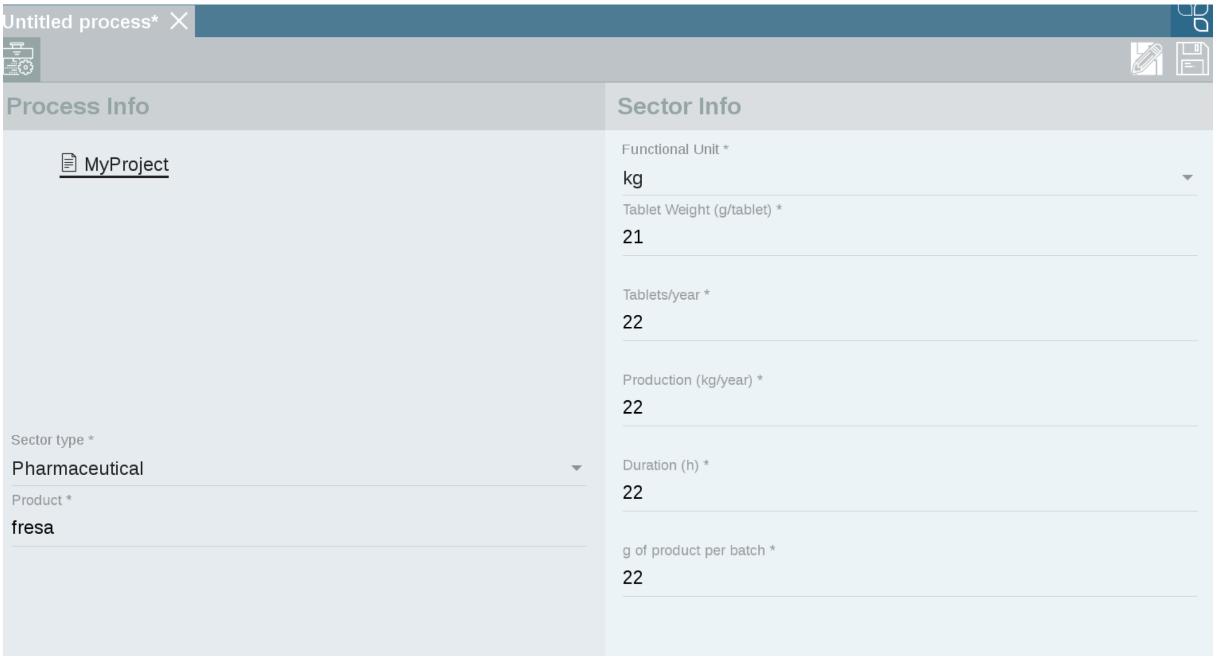

Figure 17. input parameters for My process view.

Next step within the LCA, is to enter the parameter related with the product fabrication, as can be the raw material energy consumption, and also the output parameters as can be emission to air, effluent treated, etc. This will be done through a Wizard, where the main views are shown in the mockups of Figures:

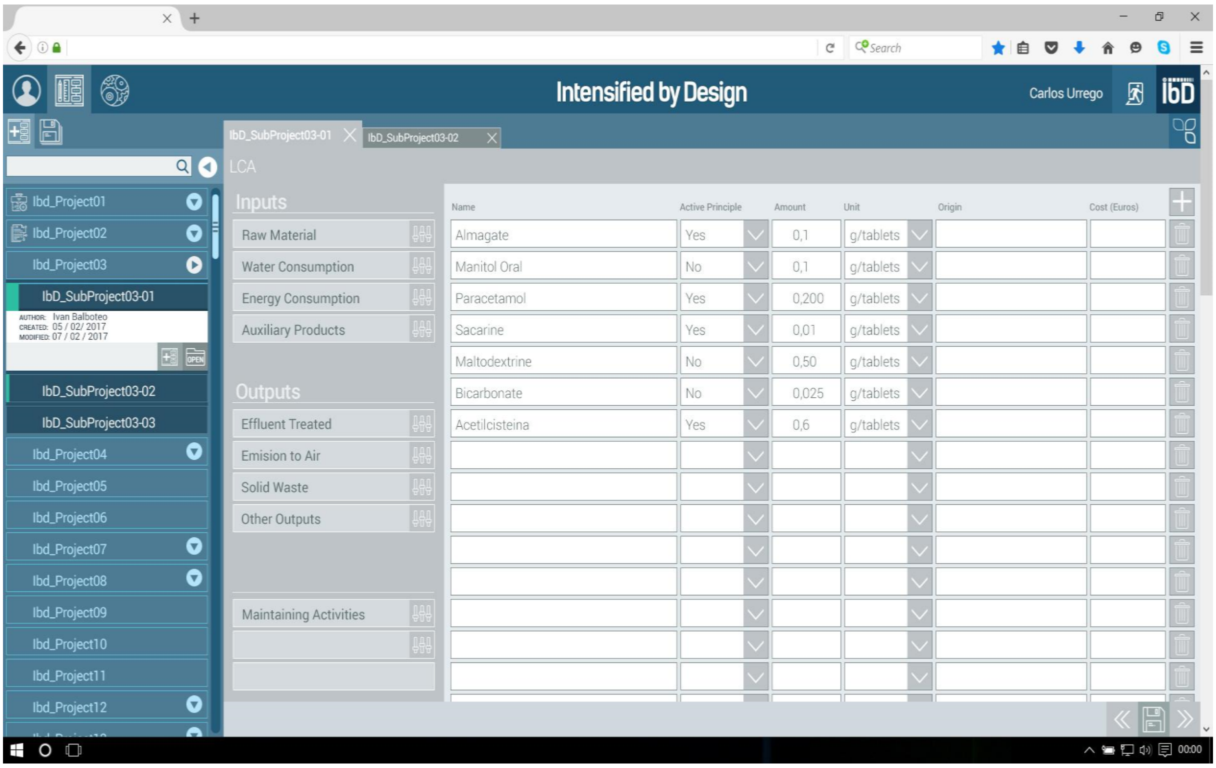

Figure 18. LCA input and outputs parameters to be filled by the user.

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Once all the input/output data are entered by the user, the next step is to select the intensification projects to be compared in terms of environmental indicators with the non-intensified project, as depicted in Figure 19. The results of such comparison are displayed in Figure 20.

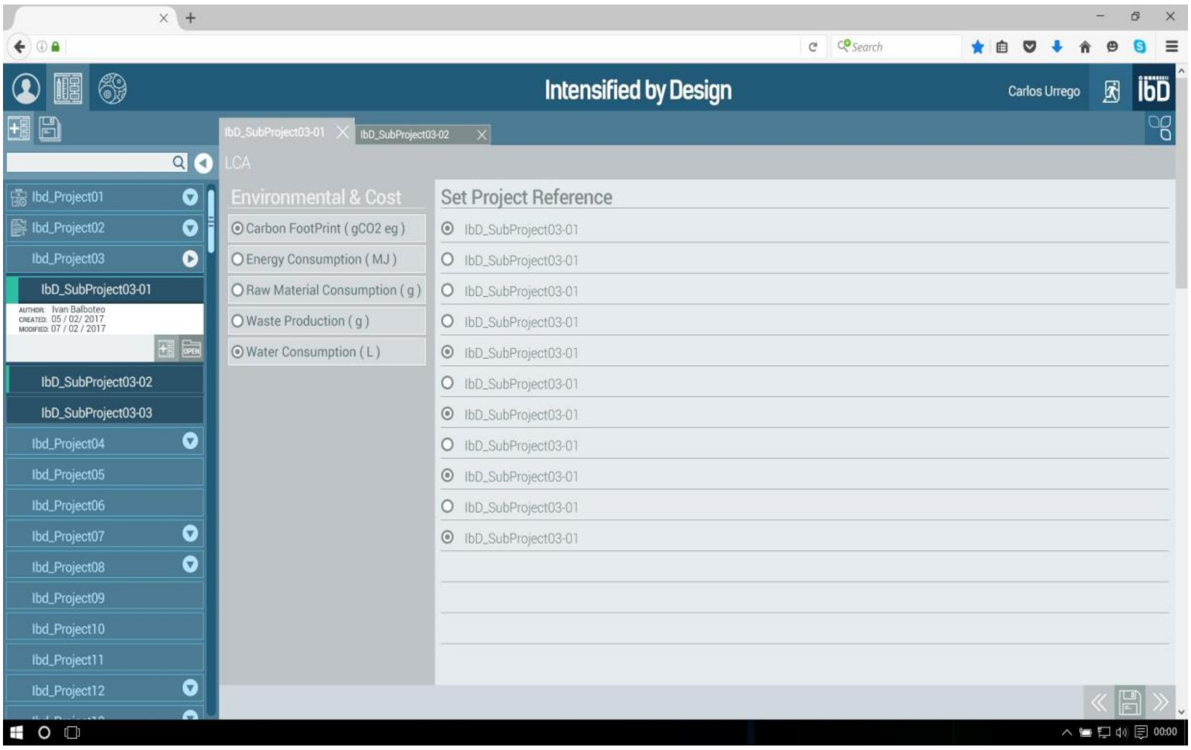

Figure 19. LCA environmental indicators and projects to be compared through a LCA analysis.

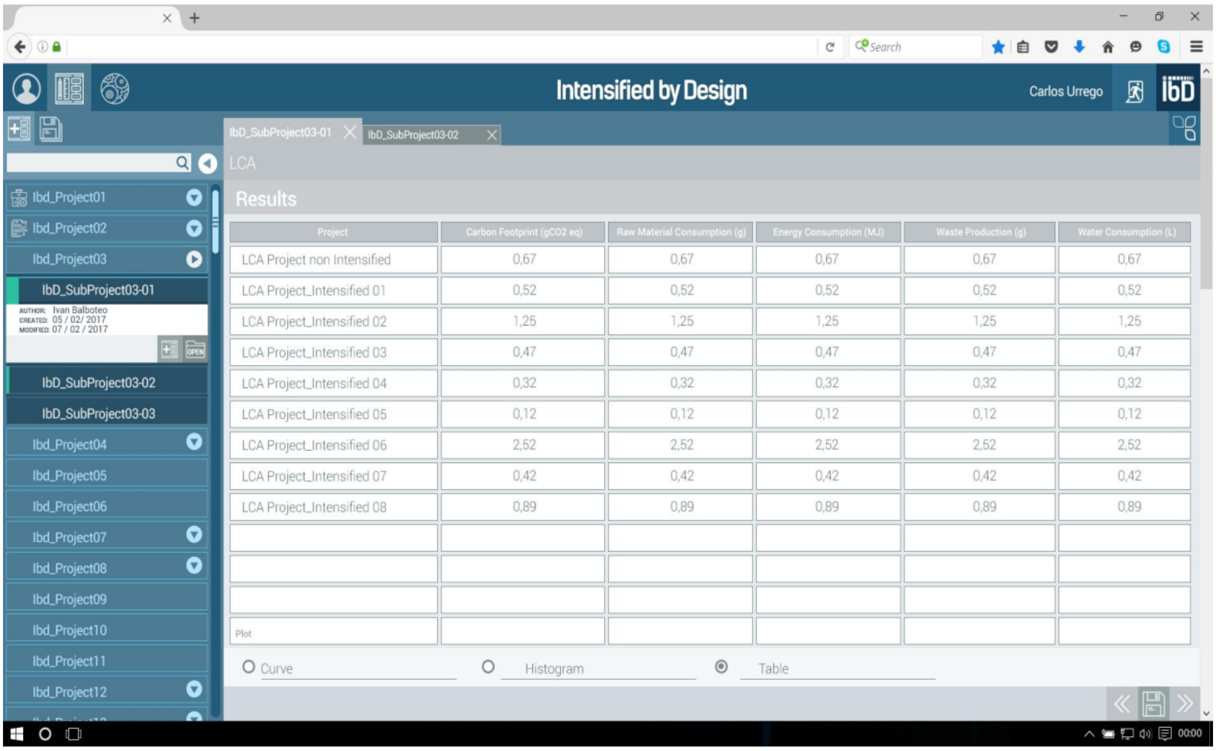

Figure 20. LCA comparison results between projects (non-intensified and intensified).

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As the case studies are ongoing, the project is receiving feedback for different industrial sectors, and the conversion factors related to each sector would be updated in the database, and provide the proper output by sector.

1.9. Error messaging and control

An error messaging system, to warn the user about the errors present in the form, was developed. As observed in Figure 21, when the user forgets or enter an invalid value, the error icon placed in the right top of the view show in red the number of errors. When clicked, a pop up shows up displaying all the errors and where they are within any of the form used in the platform.

When the user corrects each error, it will disappear from the errors list and the error counter will be updated. Once the forms have no error, the error icon will disappear which can be translated to the user as no error is found.

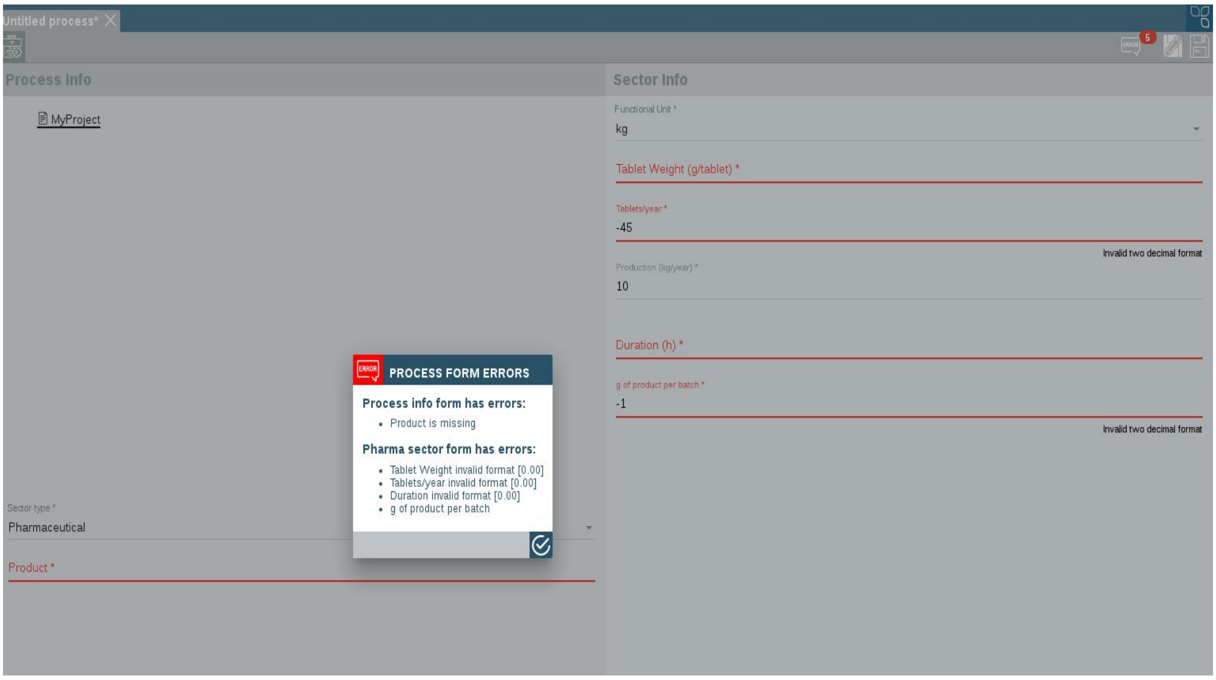

Figure 21. Errors messaging to alert the user.

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2. Future work

The IbD beta release platform is available for all partners in the following link: http://ibd.iris.cat/. Each user has been provided with a login user and a password to access the platform, where they can create their own projects, and "play" with the platform in order to provide feedback to the development team. The new platform has been tested in the Chrome browser version 53.0.2785.101, and Firefox browser version 45.4, working properly in both cases.

Future work is to implement and to include within the platform the remaining steps of the intensification process and continue updating and improving the already developed steps along the industry is giving feedback of the usage of the platform.

The goal of this deliverable has been achieved. A Freemium IbD version has been released. The platform was previously tested in the most common browsers nowadays.

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