Next generation batch reactor productivity and efficiency: An introduction to the PI QFlux™ Batch Reactor System – Form, function and results

PTSC (Process Technology Strategic Consultancy Ltd) has completed performance testing of its PI QFlux™ batch reactor system vs an equivalent industry standard batch reactor and confirmed it achieved more than four times the heat transfer performance to that of a standard batch reactor, whilst utilizing 50% less primary energy in the process. These tests were carried out jointly with KOBELCO ECO-SOLUTIONS CO. LTD. Japan who constructed a purpose-built test facility, in order to host the back-to-back trials.

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The history of chemical batch processing

It is an often-overlooked fact, that the current industrial scale chemical batch reactor differs little from that produced in the late 19th century albeit with a few more improvements around the edges. Even with the introduction of stainless reactors and other alloys beginning in the mid 20th century, the basic design and performance of the batch reactor varies little from those first introductions.

The industrial batch reactor covers many material forms including glass lined, stainless, high alloy as well as others, and all are designed to operate with some or all of the following features – corrosion resistance, pressure containment, mixing, heat transfer capability and process product ingress and egress. There are of course additional features that can be added such as containment, CIP, safety systems, etc. but these play no role in the basic operation of the current reactor form.

In the well-established terminology of "form follows function" the basic premise of the batch reactor has followed the 6 overriding "functional" requirements being corrosion, pressure, heat transfer, mixing, and containment. It may be somewhat of a surprise but at no point has productivity or efficiency ever come into the "functional" requirement either from the supply base or the end users outside perhaps adding some exterior insulation to the batch reactor. This is all the more surprising when you consider the dismal productivity and energy efficiency of the standard batch reactor, which is often overlooked on the basis that it has "always been this way" and it is the universal accepted norm. Despite such wide use of batch reactors in the global fine, specialty and pharma sectors the level of understanding and analysis available on batch reactor operational efficiency is very small.

In one of the most detailed surveys carried out, the Swiss Federal Office of Energy (Analysis and modelling of Energy consumption of Batch Chemical plants March 2004) reviewed over an extended period of time multiple production buildings, and products with the report undertaking a monitoring and modelling exercise of the utilization of energy across numerous process plant equipment types.

The findings are sobering reading and go some way to explaining why the chemicals industry is one of the top global industry CO_2 emitters. One of the more noted measures in the report was the assessment that for every tonne of fine chemical product produced the primary energy consumption was equivalent to 22,500 kWh or 22.5kWh per Kg which is an extraordinary energy cost of conversion, in what is a relatively low process temperature environment.

The PI QFlux™ Reactor Design Concept

The PI QFlux™ reactor system has also been developed as a "form following function" technology, however the sequence and identification of the "function" is very different, focusing on – productivity, efficiency, heat transfer, corrosion, mixing, containment. The PI QFlux™ Reactor is designed not from the basis of a piece of process equipment but as an integrated production system. In developing a reactor process system, it was vital to combine the method of achieving the transfer of energy as well as the process unit itself to enable a higher productivity, this lead both PTSC and TFS to develop a specialized Thermal Control Unit (TCU) specifically for this task.

The PI QFlux™ reactor system differs from other mass transfer reaction technologies such a "flow chemistry" in that it is not aimed at a radical revision of the chemical process methodology, but one in which the flexibility of batch can approach the kinetic speed of larger flow processing. Unlike flow however, the PI QFlux™ reactor system is designed to be fully integrated into existing plant infrastructure with the chemistry and SoP's performed in the same way as current batch technology only significantly faster, it also provides the same level of in-process flexibility in terms of multi-phase material mixing, evaporation, and crystallization just significantly faster and more accurately.

The development of this integrated technology follows some 4 years of R&D and with a specific target at the outset of being the development of the fastest batch reactor system utilizing conventional materials of construction, as well as the most energy efficient; this being before its relevance was fully appreciated. During the development stage of the technology PTSC utilized powerful computer thermodynamic modelling of the new reactor design and TCU options whilst combining with the extensive mixing modelling and FEA of the reactor vessel and components. This work enabled a very high

The following link provides an introduction to the technology infrastructure: https://www.youtube.com/watch?v=PzRmtHKJwpo

degree of design adjustment and tuning even before the first materials were fully specified or cut. This fully integrated computer design modelling combination allowed PTSC to go from conceptual design to full scale detail design without passing through an intermediate scaled or prototype step.

The TCU was specifically developed by PTSC sister company, Thermal Fluid Systems Ltd to integrate seamlessly with the new PI QFlux™ reactor as well as provide the opportunity to run the reactor as an electric only heat source which could operate on a zero-carbon basis with green electric supply. This has provided the PI QFlux™ with a 50% reduction in energy requirements in conventional steam supplies, additionally the system has been designed to further reduce its energy demand by integrating within the TCU an electric heating module due to its higher source and transmission efficiency.

PI QFlux™ Innovations

From the outset the integration of the PI QFlux™ system technology with existing chemical plant and infrastructure had been considered both in terms of process connections and integration but importantly services, safety, and maintenance requirements. Some examples of the unique features of the PI QFlux™ technology include increased vessel process openings for ease of flow and the number of utilities that can be connected, the "cool to touch" top head, primary and secondary balanced seals on main flange closures thus preventing fugitive emissions and same performance options utilizing both low and high shear mixers.

One of the many patented features of PI QFlux™ and a core technology differentiator is its heated baffle design which in addition to providing ideal mixing, operates completely independently mechanically and thermally from the vessel heat transfer zones. This technology allows very rapid heat flux changes due to its lower thermal mass and high thermal conductivity.

A further unique feature of the many in the PI QFlux™ batch reactor is that the complete reactor is supported from the top head and not the vessel body, this has two important functions in that it alleviates expansion effects on the vessel overheads, but it also enables maintenance and vessel/mixer removal to take place without ever having to remove the overheads from the top head.

The PI QFlux™ reactor system enables multiple options for production flexibility which include using 75% smaller capacity vessels for the same overall output or similar vessel capacity for 300% output increase, with the reactor in turn capable of operating at any percentage level or capacity fill.

Scalability and thermal flux capability are given problems when moving from lab and pilot plant scale up to production scale and Q_{max} /V (kWm^{-3}) [1] for various lab and plant with 1 m^3 reactor typically being 12 times lower than a 1ltr reactor. This requires a significant de-tuning of the lab scale performance to meet with the production scale requirements. The PI QFlux™ is designed to achieve Q_{max} /V in the range of 650 kW m^{-3} which is some 50% of that performed at 1ltr scale, allowing higher kinetics and reagent addition improving yield quality by compressing the reagent addition period.

It is also worth noting that some 75% of all production time of a batch reactor involves heat transfer either through content heating, exothermic/endothermic reaction control, crystallization, cool down, evaporation/reflux and CIP.

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PI QFlux™ Test Centre

The only true way to compare performance claims is to provide a benchmark with a back-to-back testing utilizing the same services and infrastructure between both technologies. To provide such a comparative test PTSC in collaboration with KOBELCO ECO-SOLUTIONS CO.,LTD Japan constructed a bespoke test facility in which PTSC supplied the PI QFlux™ reactor, TCU and PLC including software algorithms as part of the overall controls package for both batch reactors.

In terms of the test regime both reactors were connected to the same TCU with both being serviced by the same primary resources of steam boiler, cooler and chiller. Both reactor vessels were constructed in glass-lined steel and the same heat transfer thermal fluid as well as product fluid type, volume and atmospheric pressure was maintained throughout both units' tests. Thermodynamic modelling of both reactors had been carried out prior to testing in order to assess where the empirical test results fell in terms of the calculated values.

Prior to starting the test program, the system was extensively commissioned to ensure controls, valves, mixers, pumps and instrument calibrations were operating within specification for the TCU and reactors as well as ensuring that the boiler, cooler, chiller pump systems and power generations for the services were operating reliably and to duty requirements.

It was determined that the standard reactor would be tested first with a 1000Ltr charge of water and provide the benchmark before carrying out the same tests with the PI QFlux™ reactor. The standard reactor was fitted with a 3-blade retreat curve agitator running at 90 rpm, and ambient air temperature ranged from 28 to 34 °C. Each test started from a set product temperature, in the case of water being 5 °C to 95 °C and comparative heating and cooling performances were taken along with primary fuel consumptions for the boiler. The same trial was undertaken using corn oil as the product over a temperature range of 10 °C to 160 °C.

PI QFlux™ Test Results

Charts 1&2 below provide in startling detail the "real time" performance difference between the PI QFlux™ reactor and a standard batch reactor of equivalent volume, over differing temperature ranges and vessel internal product material specifications. Unlike product brochures or partial material conductivities the tests performed provide a true end to end comparison of the overall heat transfer rate and efficiency from primary heat source to product. By comparing the energy consumption of the primary heat source in order to reach comparable temperatures an overall energy efficiency could be measured for both reactors on alternative product contents.

The test results were plotted over numerous trial runs with some 750,000 data points taken measuring services flow rates, individual zonal temperatures, pressures, motor powers, as well as product side multi-point temperatures.

In chart 1, below the blue line plots the standard batch reactor actual performance and the orange being the PI QFlux™ under the same heating operating conditions. The PI QFlux™ is designed to utilize higher primary temperatures as indicated by the red line, which is some 5.5 times faster at higher temperatures than a standard batch reactor at 8 barg equivalent steam pressure temperatures. During these trials the heating rate for internal contents reached above 5 °C per minute and despite this the temperature variation across the vessel contents was within 0.3 °C. As all services to the point of both reactors were the same the only variation was related to the individual reactor performance.

During testing when operating at some 70% of its maximum mean services operating temperature potential the PI QFlux™ system was able to provide up to 329 kW (0.33kWkg^{-1}) of energy flux in heating directly to the product contents of the PI QFlux™ vessel this being in addition to the commensurate heat added to the general system mass. This is hugely more than the maximum heat flux able to be imparted to the standard reactor product contents which was only 82 kW (0.082kWkg^{-1}) when both were operating on the same heat services conditions.

When the PI QFlux™ operating temperature range was increased to 75% of its maximum mean operating services temperature potential, the heat flux increased due to this 5% services temperature profile produced a further 20% increase to 394 kW (0.39kWkg^{-1}) of energy flux directly to the vessel product, whilst still maintaining a temperature profile of 0.3 °C across the reactor contents. This being a comparable temperature profile to that of the slower standard reactor.

It should be noted that during these trials the PI QFlux™ reactor was still only operating at a restricted 75% operating design capability, with additional heat flux increases still available to utilize.

This superior heat flux capability potential of the PI QFlux™ in addition to its massive overall productivity advantage has a significant effect on the accuracy and rate of change available to operational control and product quality, this effect was easily observed in that the PI

Test center layout

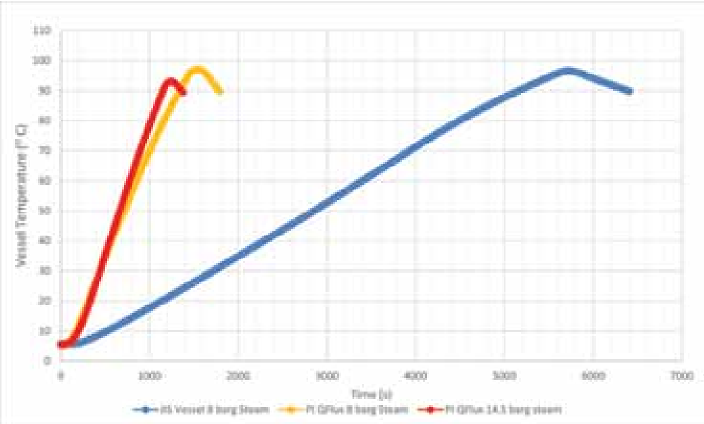

Chart 1: Comparison of heating rates for PI QFlux Reactor™ and JIS Reactor for 1000l water

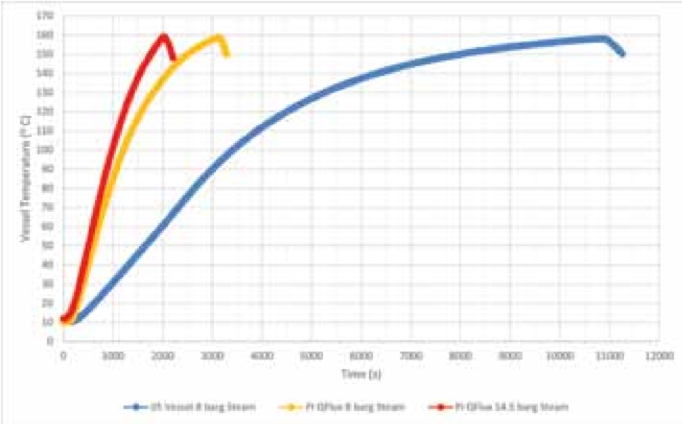

Chart 2: Comparison of heating rates for PI QFlux™ Reactor and JIS Reactor for 1000l of corn oil

QFlux™ being able to cool product temperatures by 3 °C in 250 seconds or 5 °C in 300 seconds whereas the standard batch reactor took more than 640 second for a 3 °C product temperature change and over 810 seconds for a 5 °C product temperature change. In terms of heat flux the performance of the PI QFlux™ reactor was restricted and only operating at less than 55 % of its operational cooling capacity temperature range, this being due to the higher ambient cooling water temperatures and limited chiller capacity available for the test, this did not affect the standard vessel as its heat flux was not limited to the same extent by the services. Despite this the PI QFlux™ maximum heat flux on cooling of the products was 170kW (0.17kWkg^{-1}) vs the standard reactor of 55kw (0.055kWkg^{-1}). With a higher available cooling capacity, the PI QFlux™ reactor will achieve well in excess of 300kW in cooling capacity.

One of the design features of the PI QFlux™ is its lack of Delta T restrictions; even on the glassed vessel, this allows a much higher than normal services and product temperature differential in both heating and cooling, enabling rapid and instantaneous temperature control changes.

Conclusion

The adoption of single thermal fluids for heating and cooling applications varies between different sectors of the chemical production industries and the use of conventional mixed services such as steam and cooling water remains.

A contributing factor to this has been the non-availability of process production equipment which has been designed from the off-set to utilize thermal fluid services and so those using thermal fluids have been constrained, by lack of alternatives, to use process equipment designed for steam and cooling water services.

PTSC has launched the next generation batch reactor, the PI QFlux™ reactor, available in glass steel or alloy, which has been designed for integration with thermal fluids, stepping out in a completely different direction from what has been available for chemical producers. The reduced "U values" historically present when using thermal fluid in place of steam that chemical producers have had to consider has been overcome by the novel design of the PI QFlux™.

In summer of 2022, a purpose built test centre was constructed for performance testing of a 1m^3 PI QFlux™ in a back to back basis against a conventional batch, where all of the site service infrastructure driving both vessels was the same. In these tests the PI QFlux™ achieved a heat flux of four times that of the conventional batch reactor, whilst using up to 50% less primary fuel consumption; the results from this are shown in the above charts 1 and 2.

The PI QFlux™ "fast batch" concept is challenging the industrial trend towards flow chemistry, offering a solution that has the comfort of batch processing coupled with radical productivity improvement.

References

1. Table 12.10. Novel Concepts in Catalysis and Chemical reactions – Andrezej Cybulski, Moulijn, Stankiewicz

De Dietrich PROCESS SYSTEMS

PTSC LTD PROCESS TECHNOLOGY INNOVATION

PTSC and De Dietrich Process Systems are partnering in North America to provide specialized expertise in the design, construction and execution of high productivity batch and continuous thermal transfer process equipment and systems, within the chemical, pharmaceutical and industrial segments. DDPS's extensive capabilities in systems design and integration combined with their manufacturing expertise complements PTSC's design and innovation in batch reactor and thermal fluid control packages to provide locally-based advance batch reactor system technology.