

Continuous Oscillatory Baffled Reactor Technology

A tubular reactor that can achieve plug flow under *laminar* flow conditions will – it is hoped – help restore chemical engineers' confidence in plug flow and the many benefits it can bring to pharmaceutical processing.



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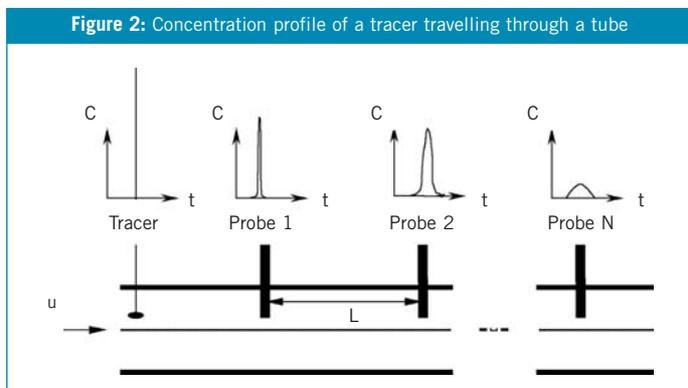
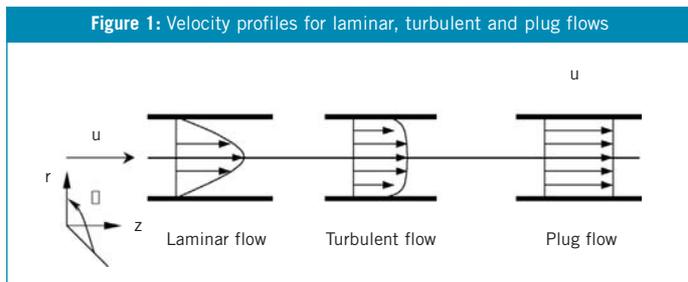
There seems to be a general myth surrounding plug flow at all levels – from plant operators to top management – and it is consistent in small-to-medium enterprises (SMEs) through to multinational corporations. Chemical engineering graduates have learnt the concept, but maybe not in enough depth to convey the idea to their fellow chemists; meanwhile, chemists are vaguely aware of the concept but there are insufficient well-established cases for them to have a real grasp of its magnitude. Between them, they have difficulty convincing company directors of the case for adopting new technologies based on plug flow. In this

article, I intend to unwrap the myth surrounding plug flow – what it is, how to achieve it, how to measure it, its benefits and its limitations.

WHAT IS PLUG FLOW?

Comprehension – or miscomprehension – of the concept of plug flow stems from the way it has been taught; it appears in Chemical Engineering Kinetics/Chemical Reaction Engineering textbooks – but not in Fluids Flow textbooks. In my capacity of teaching Reaction Kinetics and Reaction Engineering for the past 10 years in universities around the UK, I studied no fewer than 15 textbooks – some of which completely avoided giving a definition of plug flow, whilst others assumed plug flow had been achieved so that the prescribed calculations could be performed. Even in the most popular textbooks, the definition of plug flow is not succinct. An added perplexity is the fact that the ideal plug flow cannot be attained; consequently, students don't have any 'feel' in their lab experiments in order to 'visualise' it and so aid their understanding of the subject. By the end of their undergraduate studies, it is not surprising that perhaps only the name is deposited in their knowledge bank.

There is no single accepted concise definition of what constitutes plug flow. In order to appreciate the complex concept of plug flow, it is necessary to introduce velocity profiles in laminar and turbulent tube (pipe) flows. Let us visualise a liquid with a velocity of u flowing from left to right through a long tubular reactor; Figure 1 shows the velocity profiles for laminar, turbulent and plug flows.





Laminar Flows

In laminar flows, the velocity at the centre of the tube (along the dotted line) is equal to that of the incoming flow, u , while the velocity at the wall equals to zero (due to viscosity), giving the well-known parabolic velocity profile. Hence, there is a velocity gradient along the radial direction. As a consequence, the fluid element at the centre would come out of the tube first and that at the wall would come out last – that is, the fluid elements would have different residence times in the tube.

Turbulent Flows

In turbulent flows, the laminar parabolic velocity front is significantly flattened; however, there is still a laminar sub-layer remaining in the velocity profile. For a given fluid (ρ and μ) and tube diameter (d), the main criterion that separates laminar from turbulent flow is the fluid velocity – generally the net flow Reynolds number, Re_n .

Plug Flow

In plug flow, all the velocity components in the tube equal that of the incoming flow, u ; hence there is no velocity gradient in the radial direction, indicating complete mixing across the tube. Also, because of the velocity profile, all fluid elements travelling through the vessel will have an equal residence time. From the illustrations and descriptions, plug flow is a type of flow that satisfies the following criteria:

- ◆ The velocity profile in the direction of flow (axial) is flat and $u_r = u$
- ◆ There is no mixing in the axial direction
- ◆ There is complete mixing in the radial direction

Fundamentally, any plug flow system is made up of two essential components: a) a tubular configuration, and b) a net flow. Thus, plug flow cannot be achieved in a batch reactor, as there is no net flow.

HOW CAN PLUG FLOW BE MEASURED?

Plug flow is easier to identify than to define, and use of a tracer is the most commonly used method. In a tubular reactor, a tracer (for example, NaCl or KNO_3) with a known concentration and density can be injected at some point along the reactor; conductivity probes placed downstream to the injection point register the concentration of the tracer changing with time (the so-called ‘C’ curve), as shown in Figure 2. The C-curve spreads out gradually until an infinite length is reached where it completely levels off. For plug flow, the area under the C curve is equal to 1, and the width of the

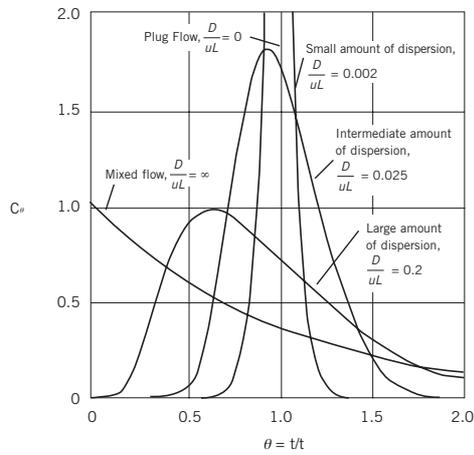
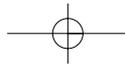


Figure 3: Trace concentration as a function of a dimension-less time as predicted by the dispersion model (Levenspiel, 1999 (1))

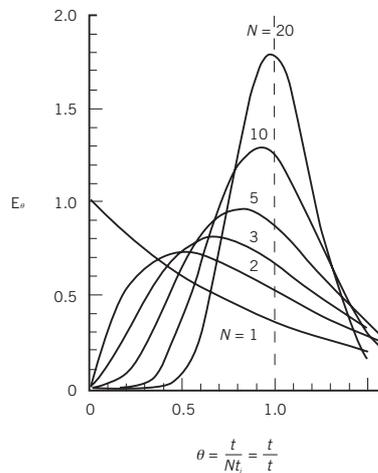


Figure 4: Residence time distribution curves for tanks-in-series model (Levenspiel, 1999 (1))

curve to 0. In the real world, this is not possible, which is why the ideal plug flow cannot be achieved.

Using the measured concentration profiles, the degree of deviation from the true plug flow (that is, the spread) or the axial dispersion coefficient (D) can be quantified. Generally, the smaller the value of D , the closer to the plug flow it is. Figure 3 shows concentration as a function of a dimension-less time for various axial dispersions. When the dimension-less group of D/uL equals zero, it is a true plug flow; when D/uL approaches infinity, the system behaves as a single continuous stirred tank.

Another popular method for quantifying the state of plug flow is to use the Tanks-in-Series model, which views the fluid as flowing through a series of equal-size ideal continuous stirred tank reactors (CSTRs). The number of tanks (N) can be evaluated experimentally; Figure 4 shows the correlation between the number of tanks and the state of plug flow being achieved. When N



→ ∞, it is a true plug flow; when N = 1, it is a CSTR system. This reiterates that the state of plug flow can never be obtained in a single tank.

HOW COULD 'NEAR PLUG FLOW' BE ACHIEVED IN THE REAL WORLD?

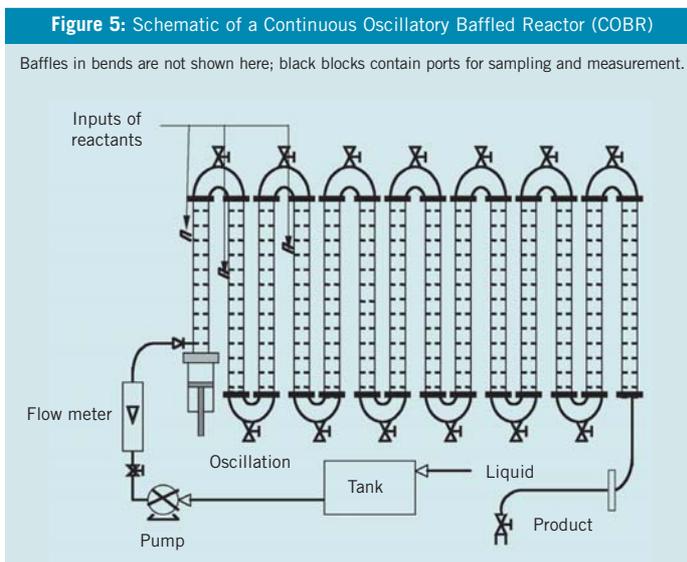
Plug flow can be achieved by two methods: a) using a number of CSTRs in series, and b) operating high net flow Reynolds numbers in a tubular reactor.

Ideal plug flow would require an infinite number of CSTRs, which is impossible. In practice, five to 10 CSTRs in series is the norm for the model chemical industries – at least in my experience. Imagine 10 identical CSTRs connected in series, each with an identical control/input/output unit. This set-up alone would require large running operations and storage space, and hence high capital and energy costs – not to mention the fact that it would still be far from a true plug flow.

An alternative is to use a tubular type of reactor with its main bulk phase flowing through the reactor and other reactants added in at different stages. Without going into too much detail, such an arrangement would be simpler in terms of the inventory requirement. A critical drawback for this type of reactor is, however, that it must run at turbulent flow regimes – meaning significantly high net flow Reynolds numbers, translating into very long pipes for even low to moderate residence times. In reality, only reactions with very short reaction times (<<5mins) would be feasible; consequently, there have been few continuous operations with regard to the production of fine, speciality chemicals and APIs.

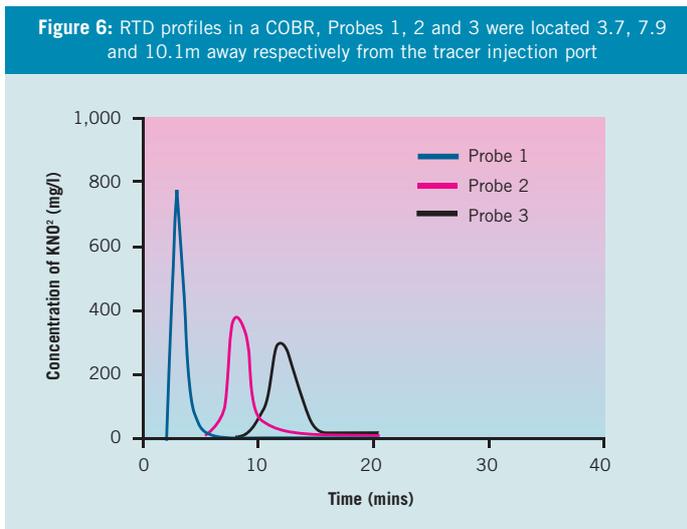
Companies such as NiTech Solutions Ltd have developed a tubular reactor that can achieve plug flow under *laminar* flow conditions. Figure 5 shows the basic configuration of a Continuous Oscillatory Baffled Reactor (COBR); it consists of a tubular device with periodically spaced orifice baffles superimposed with fluid oscillation. The key features for this type of system are as follows:

- ◆ Mixing is achieved by the generation and cessation of eddies; each baffled cell acts as a CSTR, and hence a very high number of tanks in series can be readily accommodated simply by arranging baffle cells as shown in Figure 5



- ◆ Mixing in the COBR is independent of net flow, so laminar flows can be operated, maintaining much longer residence times that cannot be achieved in turbulent flow systems
- ◆ Mixing in the COBR can be controlled to a very high degree of precision, providing a wide range of mixing conditions from 'soft' mixing (exhibiting plug flow characteristics) to the most intense (approaching mixed flow conditions)

Figure 6 shows the residence time distributions in a COBR, and the plug flow characteristics are clearly seen here.



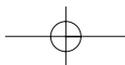
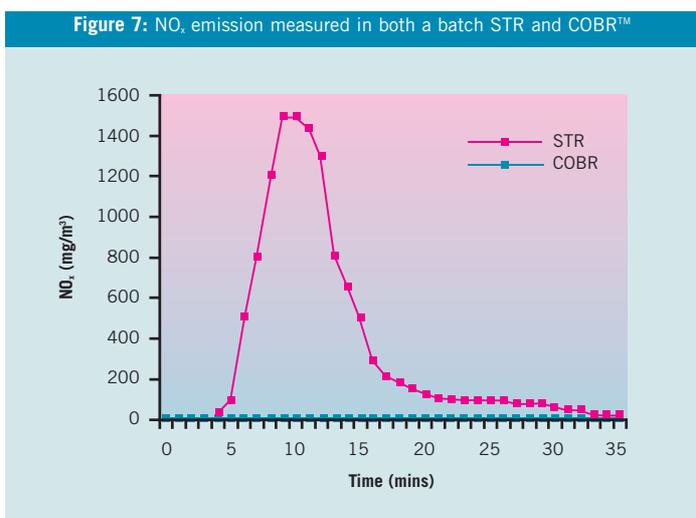


Table 1: Comparison of overall reaction times

Process	Batch STR	COBR™
A fine chemical	6 hrs	30 mins
A polymer	8 hrs	45 mins
A speciality chemical	12 hrs	40 mins
One stage reaction of an API	10 hrs	20 mins
A sugar based product	30 mins	15 mins
Coagulation	1 hr	10 secs



WHAT ARE THE BENEFITS OF PLUG FLOW?

Significantly Smaller Footprint

With plug flow, there is complete mixing in a radial direction; this eliminates any mass gradients of reactants building up and allows instant contact

between reactants – leading to faster reactions, and much smaller footprints.

Much Safer Operation

The implementation of COBR™ means that there is no longer a need to use large pumps and storage tanks for the transportation of acids and reactants in the plant; supplies of acid and reactants can now be in the form of beer-sized drums. This reduces hazards and the evaporation of acids during the plant operation, and provides for much safer operating conditions. It also results in great savings in energy utilisation.

Shorter Reaction Times

Most organic syntheses involve multi-stage reactions. As each stage can take a number of hours, the overall reaction time can be very long. In industry, this overall reaction time generally consists of the intrinsic and the external reaction time. The latter largely results from mass and/or heat gradients built up in a given batch reactor, and is often much longer than the intrinsic reaction time given in reaction engineering textbooks. The mass gradients have two effects: first, they give rise to a strong mass transfer-controlled reaction process; and second, they slow down the main reaction, which in turn encourages side reactions (see below). Removing the mass/heat gradients considerably reduces the overall reaction time (see Table 1 for a time comparison between a batch STR and a COBR).

Reduced Emissions

Reducing unwanted side reactions cuts emissions. Figure 7 shows NO_x emissions in the production of a speciality chemical in both a batch STR and a COBR. The plug flow reactor completely stops the emission of NO_x.

Solid Suspension And Conveying

In a similar vein to the discussions above, the excellent radial mixing in a COBR™ has the ability to uniformly suspend and convey solids along the tubular reactor. One of our projects involved mixing a toxic solid powder of yellow colour (d_{mean} ≈ 150µm) with an aqueous phase. In the batch operation, the mixing process took 12 hours to complete in a 3,000 litre STR. This was reduced to less than 10 minutes in a COBR™ at a volumetric rate of 6 l/min. Within the





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same 12 hour period, 4,320 litres of solid-liquid slurry are produced, giving a 144% increase over the batch operation.

In another project involving the mixing of a sugar-based material, the COBR™ had the capability to transport 50% v/v solids while maintaining plug flow characteristics, compared with about 10% v/v using traditional devices.

OVERCOMING LIMITATIONS

No system in the world is perfect – as is the case with plug flow. In order to achieve plug flow, a tubular device with a net flow is essential. This may not be practical for chemists in their labs, which may be why they are still using small STRs for these initial innovative and discovery experiments. When a molecule or compound is discovered and made in the lab, the scale-up protocol often duplicates what was achieved in small vessels, as it is regarded as easy – or is it? In scaling up either a chemical or biological process, one is dealing with a net result from several independent, but interrelated, steps. A mixing vessel is three-dimensional, so that as the linear dimensions increase, the capacity of the system increases as the cube of the linear dimension. With this increase in scale, other variables increase on a linear scale with different exponents, which may vary from negative to zero to three and higher. As a result, the scale-up of STRs has always been very troublesome. In addition, there is no agreement as to the set of parameters to be kept constant during scale-up.

This has led to some of the problems existing in the chemical industry today: large velocity gradients in plant-scale reactors and, in turn, large mass and heat gradients in systems (which may not have been there in the first place); reactions that are either incomplete or too slow with unwanted reactions proceeding actively; and the need for more downstream separation/isolation stages in order to extract the product – leading to lower efficiency and higher cost operations.

With the help of the COBR™, such problems would be eliminated, as mixing in the COBR™ is independent of net flow; experiments in small *batch* oscillatory baffled reactors (OBRs) can be incorporated into the scale-up COBRs by connecting a series of baffled cells together. This would allow chemists to create their ideas in the lab using batch OBRs, and then linearly transfer them to plant-scale operations. As a true plug flow can never be achieved, the degree of deviation from it is strongly affected by a number of factors, including both physical and operational conditions. A better understanding of the specific chemistry in each process, the physical attributes of reactants, catalysts and products, the operational conditions, the throughput, the thermal loading and so on, can lead to an optimised plug flow device that can significantly speed up the pace of scale-up; otherwise, either a significantly longer time is required or plug flow is hardly attainable. The failures of reactions in self-tuning COBRs in the early 1990s should serve as a reminder to us all today.

CONCLUSION

In this article, I have attempted to unravel the myth surrounding the concept of plug flow – from the fundamentals in textbooks to applications in the real world. I hope to help chemical engineers regain their confidence in plug flow, while assisting them in establishing a clearer understanding of the concept, and helping them realise the significance of plug flow and the benefits it can bring to processes. It is clear that the benefits offered by plug flow have wide implications for the fine, speciality, pharmaceutical and process industries. The technology is ready and viable, and NiTech has already been working with major pharmaceutical companies to assist them in gaining competitive advantage in the manufacturing of APIs. I also hope that an understanding of plug flow will result in a renewed confidence to create innovative molecules or compounds, and identify new, useful – and perhaps unexpected – pharmaceutical applications using plug flow reactors.

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References

1. Levenspiel O, "Chemical Reaction Engineering", 3rd Edition, 1999. John Wiley & Sons, New York.

