

Table 3.1 Specific surface area calculations.

| Diameter (m) | Area (m ²) | Height (m) | Volume (m ³) | Surface area (m ²) | Specific surface area (m ² m ⁻³) |
|--------------|------------------------|------------|--------------------------|--------------------------------|---|
| 0.05 | 0.0020 | 0.5 | 0.001 | 0.08 | 80 |
| 0.75 | 0.4418 | 2.3 | 1 | 5.33 | 5.33 |
| 1.51 | 1.7857 | 5.6 | 10 | 8.44 | 0.84 |

At the same time, the mixing worsens, leading to concentration and temperature gradients that would have randomly altered the width of metastable zone within the crystalliser. Spontaneous nucleation would have occurred whenever the metastable zone has been crossed, leading to nucleation dominated crystals that do not grow, which in turn gives wide crystal size distributions. Precisely due to this, prolonged filtration time and lower purity due to solvent entrapment are often the expected outcomes. It is thus the combination of the mixing and temperature control that is problematic in scaling up batch crystallisation processes.

I realized in 2004 that continuous crystallisation was an elegant way forward, as plug flow can deliver the consistent and scale independent mixing environment. At the same time, mass and heat transfer constraints are minimized due to the achievement of plug flow, the two unique elements required by crystallisation, which cannot be attainable *simultaneously* in traditional batch crystallisers. There were however a number of interesting experimental observations that were hard to explain, for example,

- Why were nucleation temperatures higher in the oscillatory baffled crystalliser (OBC) than in stirred tank crystallisers?
- Why/how did OBC allow consistent crystal morphology?
- Why/how did OBC achieve better purities while using faster cooling rates than benchmark cases?
- How did nucleation take place in OBC without seeds, while seeding was essential in benchmarking cases?

3.2 Plug Flow

3.2.1 The Definition

Plug flow is regarded as the “holy grail” of chemical engineering, however the concept of plug flow is generally poorly understood by chemical engineers and chemists. There is no simple accepted concise definition for 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 longitudinal tubular reactor, Figure 3.1 shows the velocity profiles for laminar, turbulent and plug 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