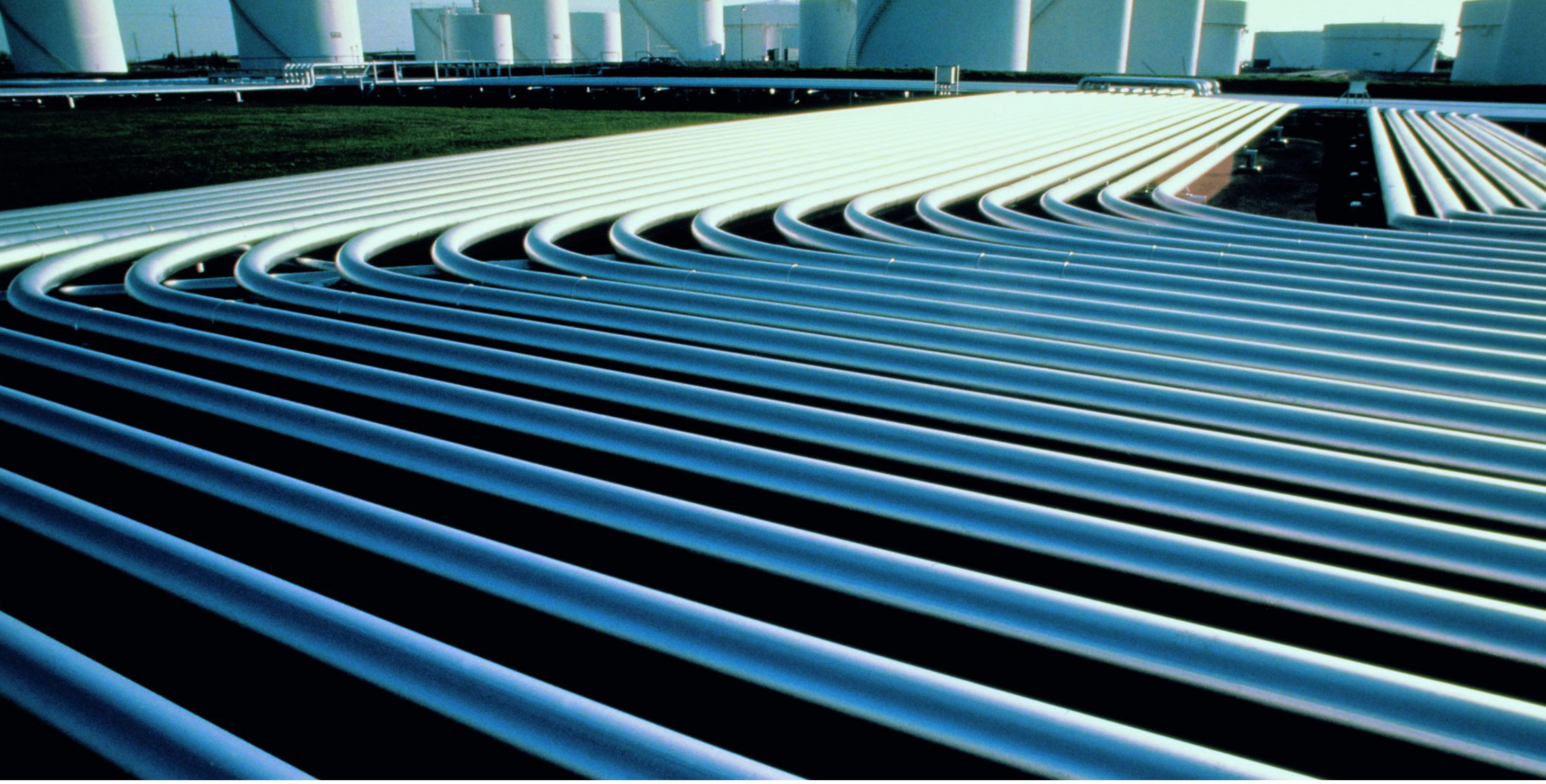

DIGITAL INDUSTRIES SOFTWARE

Leveraging a particle-based approach for 1D CFD

Using Simcenter Flomaster to model transport dynamics in pipes

Executive summary

In fluids engineering, there are times when we expect flow features to remain clear as they move through a pipe or duct, from pipette flows to priming engineering networks. Consider this simple example: would you expect a train to be smeared and undefined when exiting a tunnel? Clearly not, but traditional system computational fluid dynamics (1D CFD) approaches using fixed meshes can lead to numerical dispersion or smearing. This effect is unphysical and undesirable in a simulation in the same way that you would not want the front of a train to look smeared and undefined when exiting a tunnel. Dispersion is an unphysical effect that reduces simulation accuracy and prevents modeling important transport dynamics.

Contents

Introduction

Figure 1. Pipette flows are important in the pharmaceutical and process industries.

In this white paper, we examine how the multiphysics pipe capability in Simcenter™ Flomaster™ software, which is part of the Siemens Xcelerator business platform of hardware, software and services, to model multiple materials moving and interacting within a pressurized system. When these materials are moving in a pipe or duct system, they move in batches with little axial diffusion. For example, the priming of a sprinkler system as high-pressure water moves through an air-filled network. In the energy industry, engineers send batches of materials through the same pipeline. Additionally, this technique is a way to move slurries from quarry to a shipping point.

The multiphysics pipe allows users to model pipe and duct flows containing multiple material flows in a way that preserves fronts and minimizes numerical dispersion. The method does this by tracking particles in the flow and solving the 1D flow equation in the fluid reference frame. Additionally, the method uses a particle repositioning algorithm to handle particles leaving the domain and ensure a minimum loss in fidelity by trapping key features between particles.

We will also demonstrate how you can use the Simcenter Flomaster system CFD tool and a particle-based approach to model a variety of physical scenarios that are not possible using traditional 1D CFD approaches. This includes batched slurry flows, oscillating columns in a cavitating vertical pipe and pipette flows.

Further, we will demonstrate that we can use this approach with a wide range of fluid types, including liquids, gases and non-Newtonian materials.

Dispersion in 1D CFD models

Using system CFD tools like Simcenter Flomaster, you can solve flow, pressure and temperature distributions in an internal flow system. You can model these flows, which are often dominated by pipes, using the 1D Navier-Stokes equations. By using these equations, you can ensure mass, momentum and energy conservation along the pipe flow.

Typically, these equations are solved using a finite volume (FV), finite difference (FD) or a method of characteristics (MOC) approach. Further, these approaches are all solved using a 1D mesh of points along the pipe. In these cases, transported phenomena such as temperature or concentration suffer from numerical dispersion.

On an engineering level, most fluids are transported along pipes with no significant physical diffusion. Here we expect to maintain the temperature or concentration profile as the fluid flows through the pipe. For example, with hot liquid injection, we expect to see a clear boundary moving through the pipe over time.

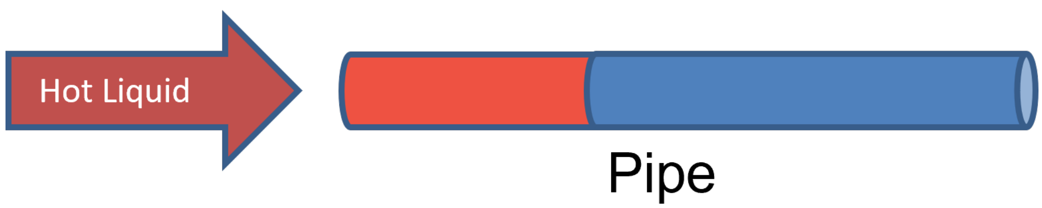

Figure 2. An example showing a temperature propagation when injecting a hot fluid.

However, when we try to model this using a standard FV 1D pipe model, the interface between the hot and cold liquids smears slightly. This can be seen in figure 3. This smearing is not a physical effect; we are not modeling axial diffusion. This smearing is a purely numerical artifact due to the FV approach. To get the low dispersion levels in case one, we must use highly refined timesteps and grids. However, these would not be practical in a real simulation. Coarsening the timestep and segmentation to a practical level can lead to a large dispersion.

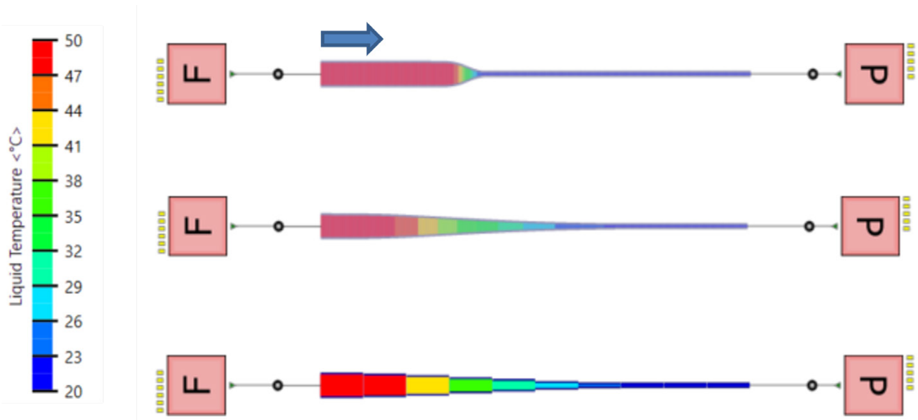

Figure 3. A diagram showing the temperature dispersion in a FV pipe model.

Even with a highly refined timestep and grid, there is still numerical dispersion, leading to a sigmoid shape, which is typical of numerical dispersion. You can reduce the smearing width, but you cannot eliminate it and recover the step change that we expect to see.

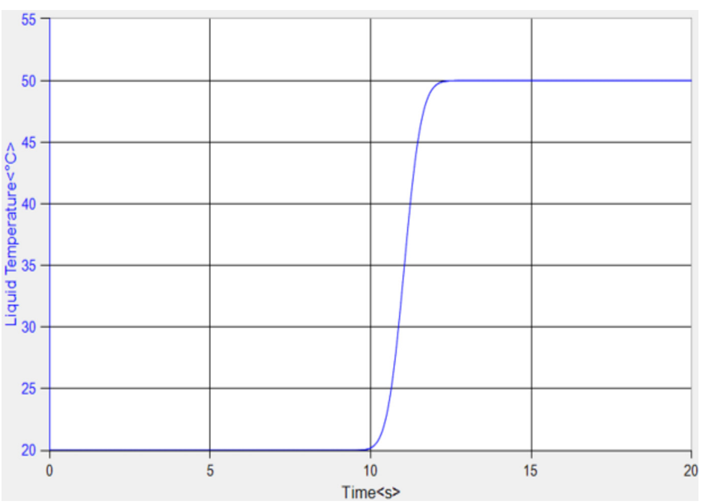

Figure 4. A graph showing the temperature profile at the outflow (dt: 0.01, 1,000 segments).

Using a particle-based pipe model

In some cases, you need to accurately predict the temperature or concentration front of a fluid, for instance when modeling the liquid priming of a network like a fire suppression system.

For most simulations, the level of grid and timestep refinement required to capture the temperature or concentration front moving through a pipe system using a fixed mesh approach is expensive.

To address this problem with minimal concentration or temperature front dispersion, you can use the particle-based pipe model. Using this novel methodology, you can model the internal solution with a 1D series of particles in the pipe that are moving with the fluid. A particle can be thought of as a moving segment.

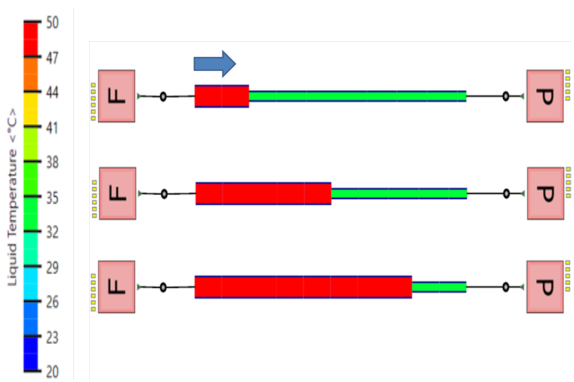

Figure 5. A diagram showing temperature dispersion in a particle-based pipe model (dt: 1s, 10 particles).

Figure 5 shows the same scenario as figure 4 but instead uses a particle-based pipe model with minimal segmentation and a large timestep (dt: 1s, 10 segments). The temperature is shown at varying times and the temperature front propagates downstream with no dispersion.

Figure 6 shows the temperature profile at the outflow. Here the temperature changes without any smearing between the two adjacent timesteps at time (t) = 10 seconds (s) and t = 11s.

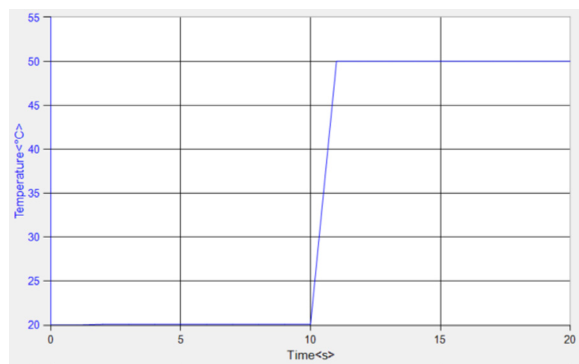

Figure 6. A graph showing the temperature profile at the outflow (dt: 1s, 10 particles).

Using a particle-based method, you can track temperature and concentration profiles through the pipe and preserve discontinuities. Figure 7 shows the effects of applying a repeating temperature gradient and plateau at the inflow. As the fluid flows from left to right, it transports the temperature at the inflow with the fluid. This preserves the temperature profile without dispersion.

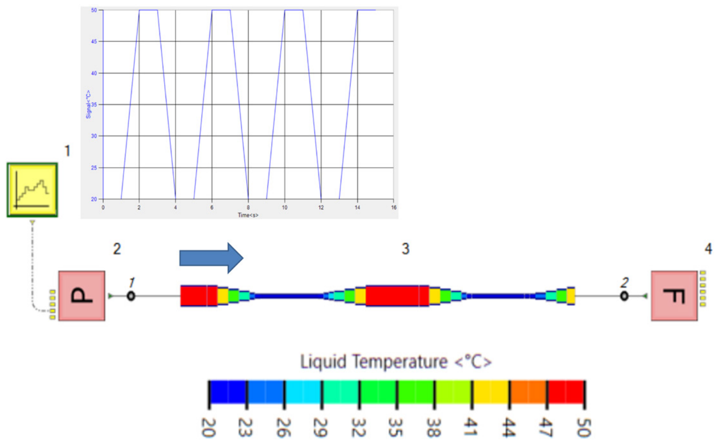

Figure 7. A diagram of a pipe flow with a specific temperature variation.

Modeling pipette flows

A particle-based pipe model can also preserve concentrations as they are transported in multispecies simulations. This is particularly important in simulations where gas and liquid slugs pass through the same pipe. Examples include:

- Priming a lubrication system
- Starting up a sprinkler system
- Using a pipette with air pockets potentially separating liquid slugs

The ability to model the movement of these phases without dispersion is essential.

Using the network shown in figure 9, you can replicate the operation of a Pasteur pipette or an eye dropper. Further, you can model the pipette using a particle-based pipe with a flow boundary condition at the top to represent the piston's motion. The network simulates drawing in water, holding it at the same level for a period of time and then expelling it back through the same entry point. The concentration surface shows that the particle-based pipe can track the fluid front accurately, even in zero flow or reverse flow conditions. This can be beneficial when modeling priming situations, especially in safety systems. A safety system might not always be in an active state; however, it requires a rapid response during an emergency scenario. To avoid catastrophic failures, it is essential to monitor the operating fluids and track the mixtures.

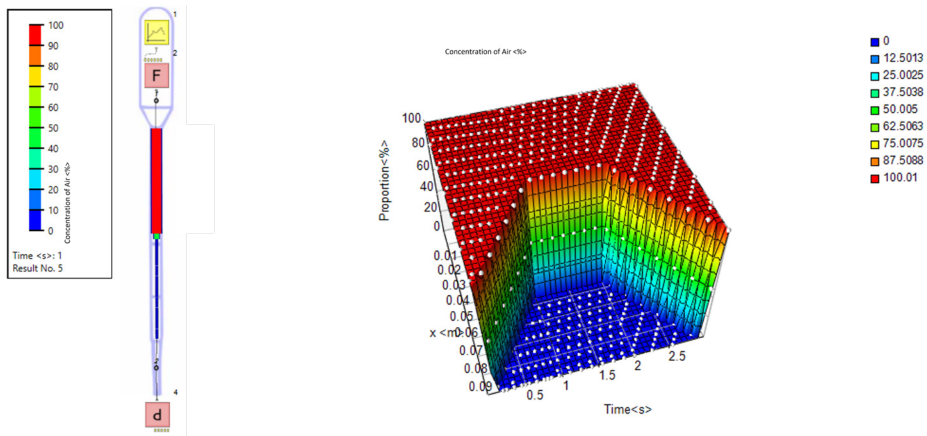

Figure 8. A graph showing the air concentration as a water slug is sucked into and expelled from a pipette.

Using the network shown in figure 8, you can replicate the operation of a Pasteur pipette or an eye dropper. Further, you can model the pipette using a particle-based pipe with a flow boundary condition at the top to represent the piston's motion. The network simulates drawing in water, holding it at the same level for a period of time and then expelling it back through the same entry point. The concentration surface shows that the particle-based pipe can track the fluid front accurately, even in zero flow or reverse flow conditions. This can be beneficial when modeling priming situations, especially in safety systems. A safety system might not always be in an active state; however, it requires a rapid response during an emergency scenario. To avoid catastrophic failures, it is essential to monitor the operating fluids and track the mixtures.

The ability to model both priming and de-priming is a significant step forward in 1D CFD modeling capabilities. Previously, they could only be used to model priming.

Oscillating column flows

Gravity is an important factor in multicomponent pipe flows where the materials have differing densities. This can be important in pipelines moving over mountains or in subsea terrains. Gravitational forces dominate flows in these types of pipes, and accurate concentration front modeling without dispersion is essential.

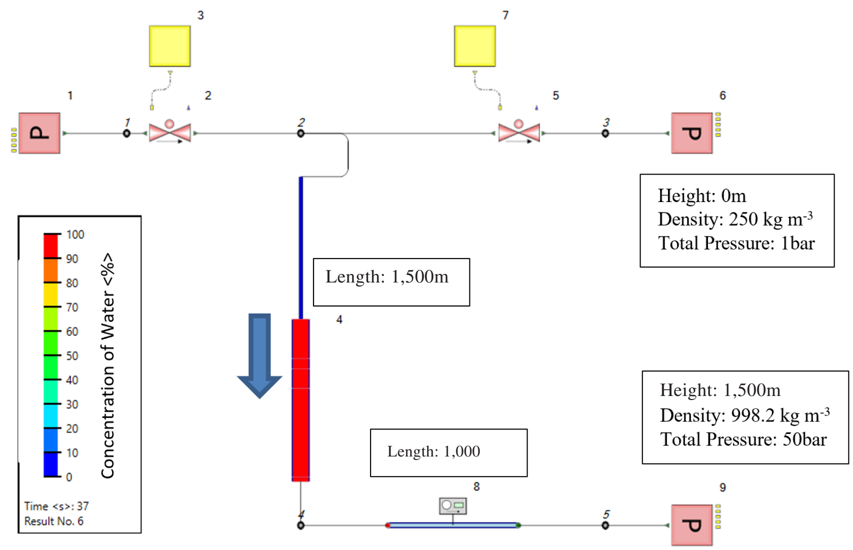

Figure 9. A pipe network diagram showing how two components flow in a long vertical pipe.

In figure 9, the network models a long vertical pipe that is initially full of water and then later connects to a lower-density liquid at the top. Initially, the left-hand valve is open, and the right-hand valve is closed. Water flows from the top-left down a 1,500-meter (m) vertical pipe. The pressure at the bottom right boundary is 50 bar.

At 20 seconds, the left-hand valve closes, and the right-hand valve opens. A new fluid then flows into the pipe with a lower density of 250 kilograms per cubic meter (kg/m3) and is at a pressure of 1 bar. The weight of the fluid in the pipe causes it to move downward until it reaches an equilibrium height where the pressure from the fluid's gravity in the pipe is equal to 49 bars. However, as the fluid moves downward, the momentum causes it to overshoot and then oscillate around the equilibrium point until the pipe wall's friction dampens the motion. Figure 10 shows the results of the simulation. The rate at which the water column falls is a sensitive balance between the fluid's weight in the pipe, the upstream pressure and the wall friction. Figure 10 demonstrates the multiphysics pipe can be used to model the physics, including mass, momentum and energy transients.

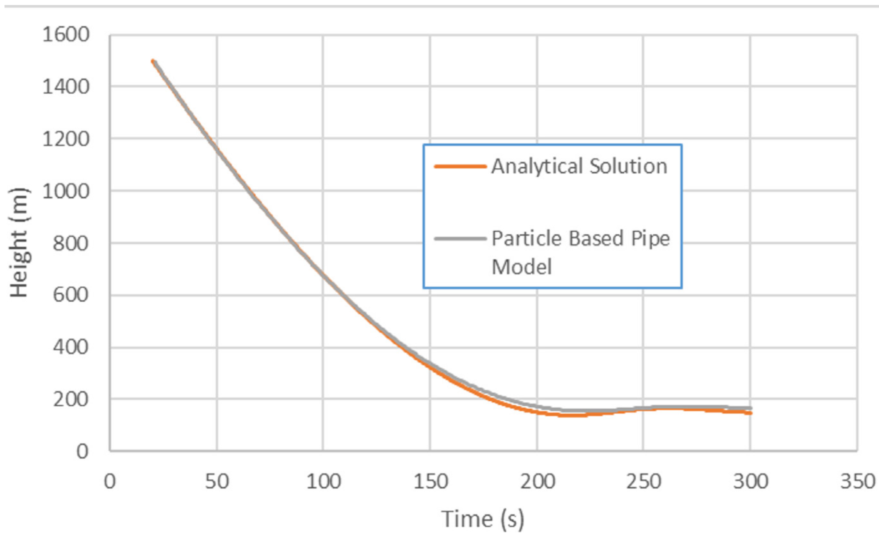

Figure 10. A line graph of the water column's height in the vertical pipe over time

Batching slurry flows

Batching is an important process on pipelines and production lines. It involves moving various materials along the same pipe with a slug of neutral fluid – typically water – between the materials. For example, moving slurries from a quarry to a port or moving petroleum grades from place to place. Often, these batches move tens or hundreds of kilometers. Gravity and wall friction effects are important for predicting system dynamics. Non-Newtonian materials – including those found in slurries – can have excessive wall friction, and even a small slug can have a large effect on flow rates and pressure drops.

Using a particle-based model allows for accurate simulation of this type of batching scenario. Further, an important simulation aspect is modeling the wall friction for each fluid since each fluid may have unique wall friction behaviors. This is important when modeling non-Newtonian fluids, as they need an appropriate friction model such as the power law. Additionally, the water around a slurry is a Newtonian fluid, and we can find its wall friction by using a more specific model such as the Colebrook-White equation.

Figure 11 shows a network for simulating batches in a process plant. The line draws water from its supply with valves 4 and 6 open and 3 and 7 closed. You

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Figure 11 shows a network for simulating batches in a process plant. The line draws water from its supply with valves 4 and 6 open and 3 and 7 closed. You can introduce a batch by closing valve 4 on the water supply and opening valve 3 on the material supply. The valves switch again after 1s. This introduces a slug of fluid with non-Newtonian properties typical of the process industry. For example, shear-thinning properties are found in food products like apple sauce.

As the slug reaches the end of the pipe, valves 6 and 7 switch open to allow the material to reach the consumer endpoint. The valves then switch back when all material exits the pipe. Figure 11 also shows the water concentration at t = 4s and the batch of material is clearly visible in the center of the pipe. Figure 12 shows the material's effect on the pressure drops along the pipe. The introduction of the material at this flow rate leads to a tenfold increase in pressure drop.

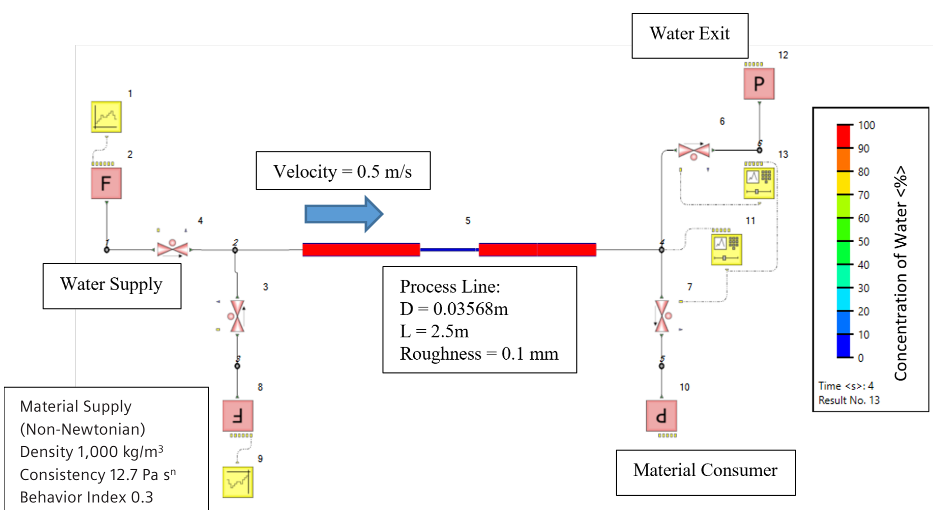

Figure 11. A diagram showing the water concentration along a pipe when a batch moves through it.

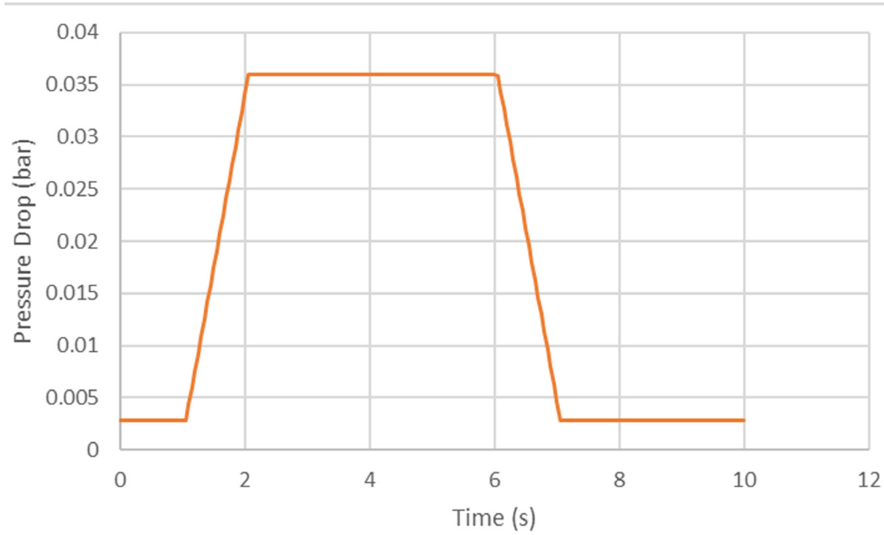

Figure 13. A line graph showing the pressure drop across the pipe as the slurry batch moves along it.

Conclusion

By implementing the multiphysics pipe in Simcenter Flomaster, we can model fast and complex transport dynamics within a pipe using a novel particle-based approach. Compared with traditional mesh-based system CFD approaches, a particle-based approach has advantages, including:

- Using a small number of particles to define temperature and concentration features
- Achieving zero or low dispersion
- Running simulations with large timesteps

These advantages help you use system CFD for a range of applications, including batched slurry flows, oscillating columns in a vertical pipe and pipette flows. Additionally, you can use this approach with a wide range of fluid types, including liquids, gases and non-Newtonian materials.

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