Need for Control: Sensitivity of Polymerization Reactors

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Introduction

Purpose:

- The Low-Density Polyethylene (LDPE) market is very competitive
  - U.S. produces over 3 million metric tons a year [1]
  - Polyethylene products make up 42.9% of the U.S. thermoplastic feedstock [2]
  - LDPE market alone is valued at over US$ 50 billion [3]
- Manufacturers are constantly looking for ways to reduce costs, reduce waste, increase production efficiency, and increase product yield

Problems:

1. Halting a reactor to perform experiments ceases the production of otherwise good product
   - Loss of profit
2. There is no guarantee the experiment will be beneficial
   - Waste of product
   - Potential ramifications of failed experiment
3. The highly exothermic polymerization chemistry of LDPE makes experiments very dangerous
   - Highest adiabatic temperature rise of any commercial monomer [4]
   - 125 kW of energy produced per mole of ethylene decomposed [5]

Solution:

- Computer simulations can perform these experiments without the explosive danger
  - However, many modern simulations assume the mixture is homogeneous [5]
- Computational Fluid Dynamics (CFD) can be used to study the mixing effects in chemical reactors

Objective

- Create a comprehensive CFD simulation of a plant-scale LDPE reactor
  - Improve stability, efficiency, safety, and yield of the industrial process
- It is first necessary to simulate the reactor on a much smaller scale
  - Verify with industry standard homogeneous reactor simulations

Methods

Computational Fluid Dynamics (CFD) Model:

- Mini reactor with mostly uniform mixing
- Coarse tetrahedral mesh
- Low order numerical schemes
- Mixing rate of 10^5 rad/s
- Simple chemistry scheme
  - Initiation
  - Propagation
  - Termination

Stability Testing Metrics:

- Numerical settings
- Startup processes
- Kinetic simplifications
- Reactor design

Without Control

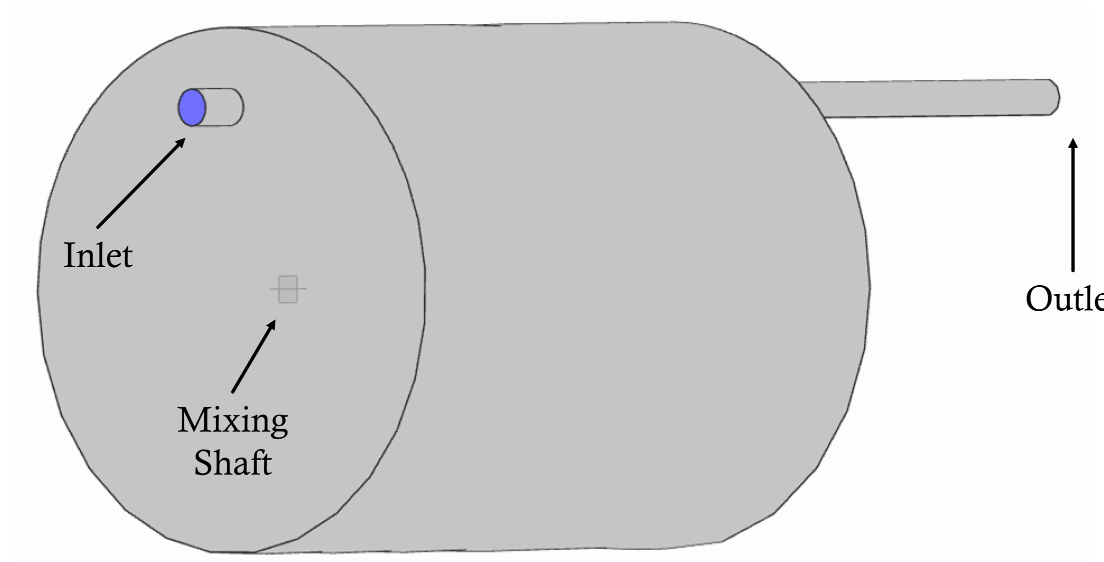

Figure 1 – Geometry of mini reactor. The small shaft on the front side of the reactor is the inlet, the long shaft on the back side is the outlet, and the cross on the inside is the mixing shaft.

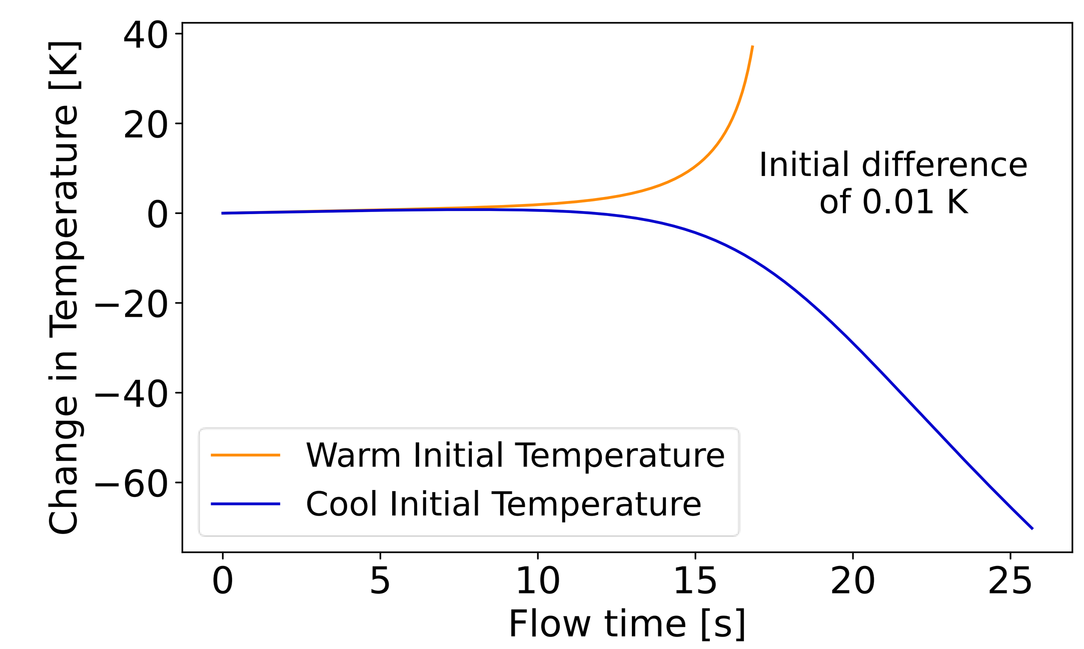

Figure 2 – Temperature change of the mini reactor for cases with an initial temperature that differed by only 0.01 K.

With Control

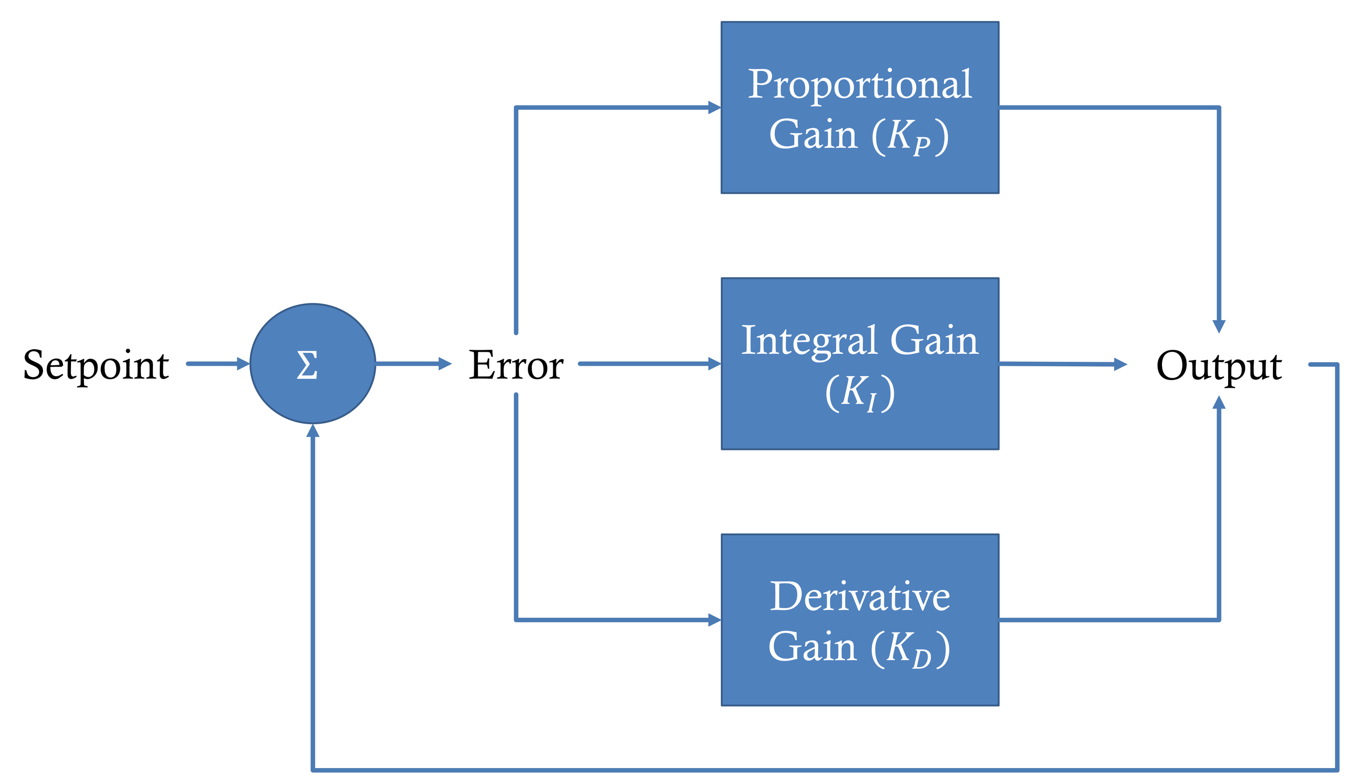

Figure 3 – Graphical explanation of PID Control. The output of a system is compared to a setpoint producing an error. The error is fed into all three gain components which control an aspect of the system, modifying its output.

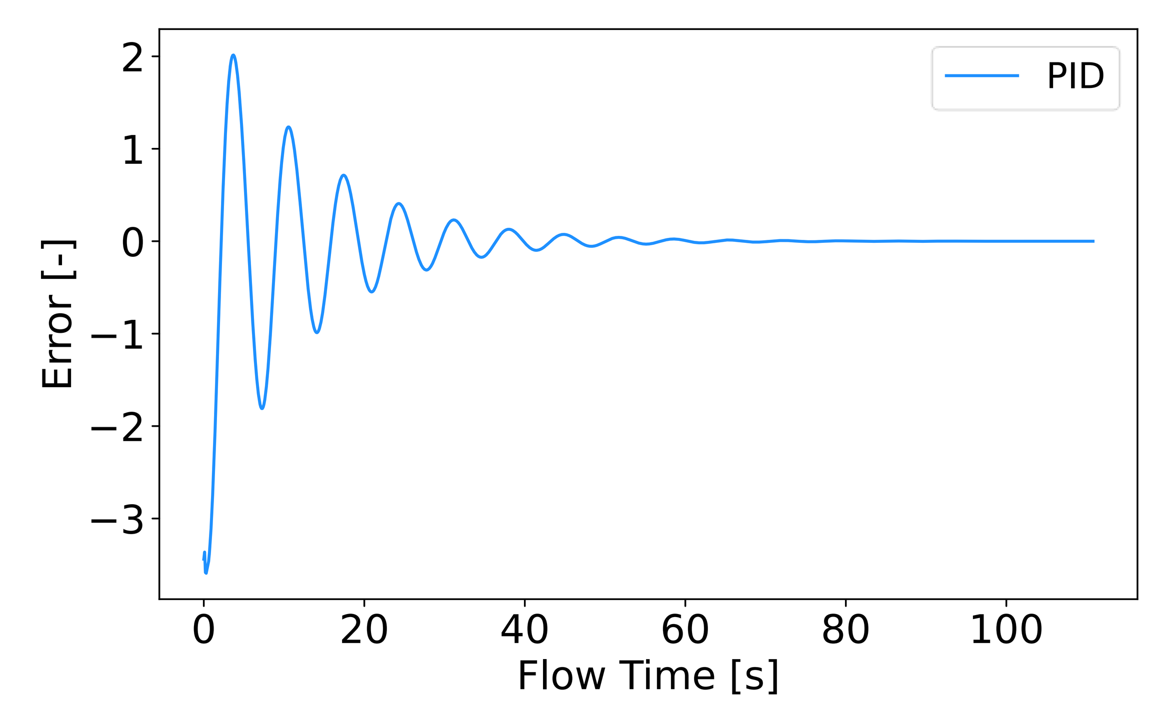

Figure 4 – Temperature response, in the form of error, of the mini reactor with a tuned PID controller.

Fuzzy Logic PID Controller

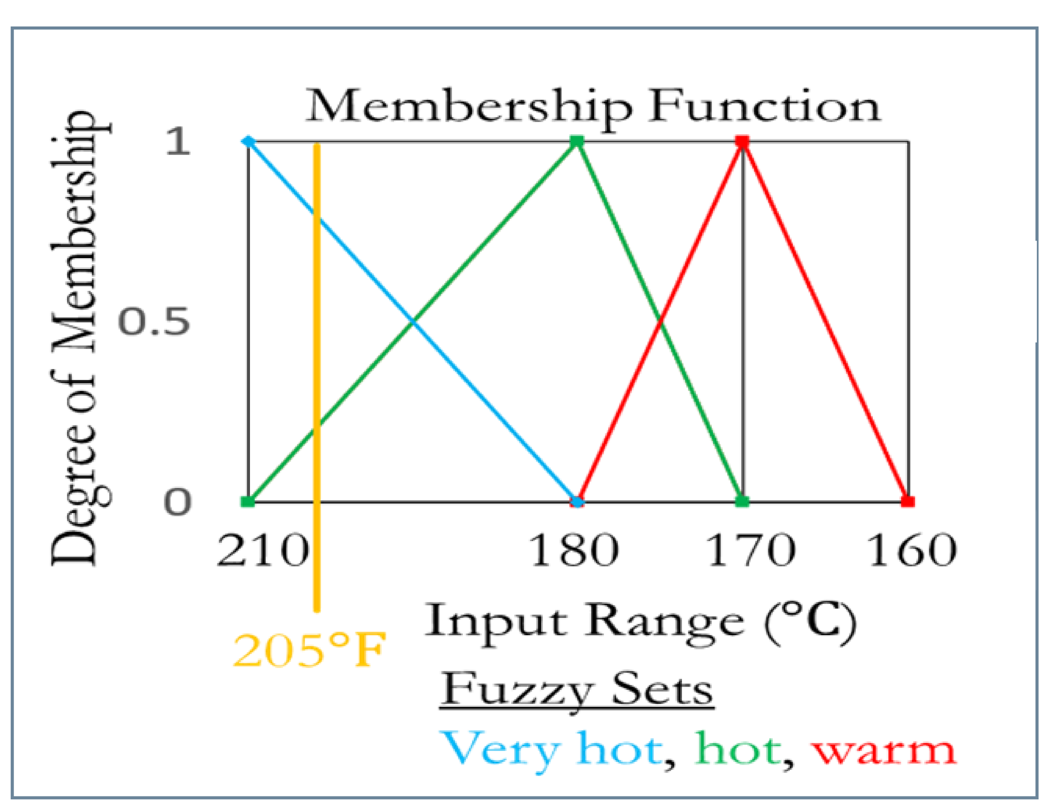

Figure 5 – Example Fuzzy Logic membership function [7]. This is used to classify the error into a fuzzy category, each of which have their own, pre-determined PID constants. This allows the PID controller to tune itself.

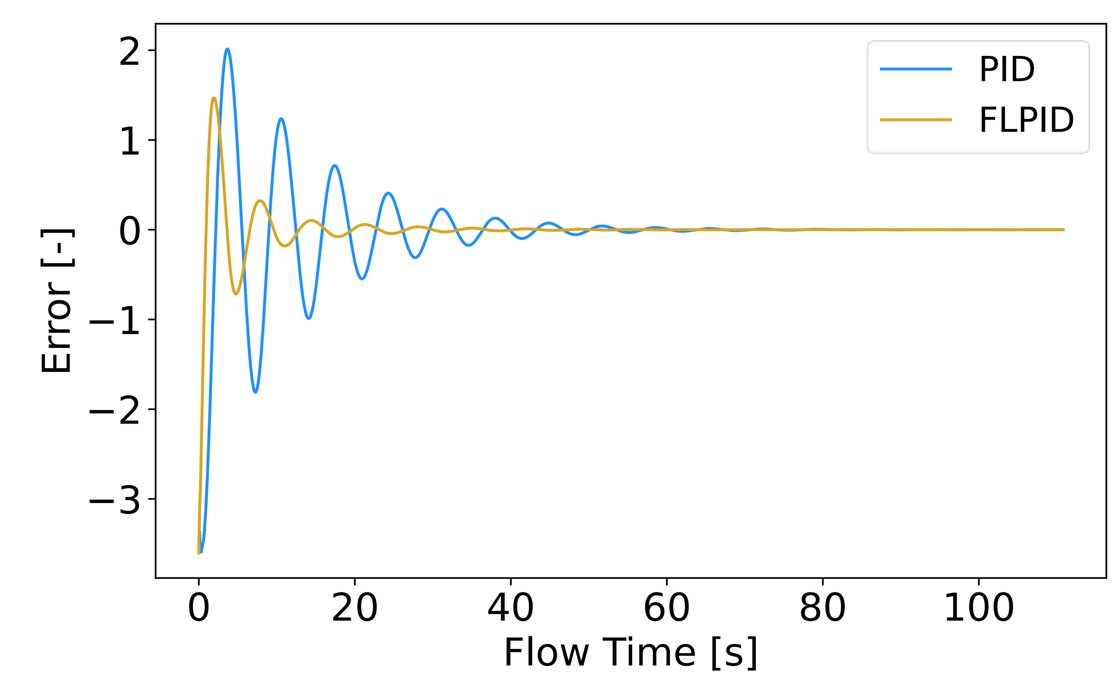

Figure 6 – Temperature response, in the form of error, of the mini reactor with a tuned PID and FLPID controller.

	Overshoot	Settling Time	Total Error
PID	2.01	66.2	248
FLPID	1.47	42.1	75.2

Figure 7 – Control metrics for the PID and FLPID controllers, respectively. Overshoot is the maximum error in the response, settling time the is time required for the error to never exceed 1%, and the total error is the cumulative sum of the error over the entire response.

Results and Conclusion

Results:

- Stiff chemistry makes stable solution difficult to obtain, even with a simple chemistry scheme
  - Too much reaction can cause a reactor to explode
  - Too little reaction will not sustain polymer production
  - There is a narrow band through which LDPE can be created economically [6]
- Numerical instability further complicates this
- There were no combinations of initial conditions, numerical settings, and chemistry that produced a stable solution
  - A reactor with an initial temperature difference of 0.01 K produced vastly different temperature responses

Conclusion:

- Active control is necessary for the simulation of an LDPE reactor
  - Moreover, a Fuzzy Logic PID controller provided a faster response time with less overshoot
- The industrial process also utilizes PID controllers

Future Work

1. Complex chemistry in the mini reactor
2. Complex chemistry in the mini reactor at different operating conditions
3. Complex chemistry in a plant-scale reactor model
   1. Variable material properties
   2. Molecular Weight Distribution (MWD) reconstruction
4. Study mixing effects on MWD properties

References

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