

Two-Phase Flow Simulation Using a 1D Model - Tutorial

V 1.1.X

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Introduction

Welcome to the tutorial for the two-phase flow simulation package using a 1D model (Ngu et al., 2022). This package enables you to model and simulate the behavior of various two-phase flow scenarios. Using this package provides the capability to simulate different flow scenarios and analyze the results.

1 Installation

Before getting started, ensure that Python is installed on your system. You can download Python from the official website. Afterward, install the necessary dependencies by running the following command in your terminal:

```
python -m pip install poetry
poetry install
```

2 Usage

Running a Specific Example

To execute a specific example, use the following command:

```
python -m examples [case number]
```

Replace the [case number] with the number of the example you want to execute. This will initiate the execution of the corresponding example.

Displaying the List of Available Examples

If you want to view the list of available examples, use the following command:

```
python -m examples
```

This command displays the list of examples along with their associated numbers.

2.1 Configuration File

For the program to function correctly, the case name must be specified during execution. Data related to this case, including model and simulation parameters, is stored in the "**Parameters_case.xlsx**" file. Each sheet in this file represents a case to simulate. While it is possible to modify the values in this file, it is recommended not to do so to ensure the proper functioning of the program.

2.2 Model Customization

The main program contains various models that can be simulated. However, if you have specific specifications not covered by these models (different initialization or reaction terms), you have the option to code your own model by replacing the necessary parts. For the needs of the examples, this approach has been utilized (see the technical documentation to understand how to proceed).

3 Bubbly Flow

3.1 Unitary reaction without transfer

In this example, we explore the impact of a constant reaction term and the sensitivity to the initial bubble diameter in a one-dimensional bubbly flow model without phase transfer.

he model considers a single species (H₂) in the gas phase with a constant reaction term set to 1 in both phases. The governing ordinary differential equation (ODE) for each phase is given by:

$$\frac{\partial y}{\partial t} = convection + diffusion + 1$$

In an ideal scenario with constant advection velocity (convection = $u \frac{\partial y}{\partial z}$) and no diffusion, the analytical solution simplifies to

$$y(t, z) = z/u$$

To execute this example, use the following command:

```
python -O -m examples 1
python -O -m examples 2
```

However, the bubbly flow model introduces diffusion as well as velocity dependent on bubble size, influenced by transfer and reaction. Consequently, the analytical solution is not directly applicable, and behavior variations are expected based on the initial bubble diameter. When the velocity depends on the diameter (as illustrated Fig 1), the analytical behavior is altered. In this model, without phase transfer and with a constant reaction term, the diameter changes due to pressure variation along the column. As the pressure decreases with increasing height, the diameter increases linearly. Choosing a diameter resulting in a pseudo-constant velocity approximates the analytical behavior, as both the bubble diameter (db) and velocity (u) remain relatively constant.

Conversely, selecting a diameter leading to significant variations results in bubble acceleration compared to the analytical case (due to the increase in u with db) and deceleration when u decreases with increasing db. Consequently, the "age of the fluid" may be smaller or larger than the analytical case, depending on whether the average velocity is higher or lower.

In summary, this example compares simulations with pseudo-constant velocity Fig 2 , achieved through a carefully chosen initial diameter to the analytical solution, where the two should closely align. Additionally, a comparison is made with non-constant velocity Fig 3 , showcasing significant differences from the analytical solution.

The constant velocity is obtained looking for null derivative of the velocity correlation.

The non-constant velocity profile is achieved by selecting the bubble diameter at the peak of the velocity curve, known as db critical. This specific diameter marks the point where the derivative of velocity with respect to the bubble diameter ($u=f(db)$) is highest, signifying a significant change in velocity concerning variations in bubble diameter.

For db slightly smaller than db critical, the velocity increases as the diameter increases. Conversely, for diameters slightly larger than db critical, the trend is reversed, and the velocity decreases with an increase in diameter. Choosing an initial diameter equal to db critical captures the transition point where bubble behavior changes.

Consequently, with this choice of initial diameter, the simulation exhibits interesting dynamics. As the bubbles ascend in the column, there is an initial acceleration due to the increase in velocity with decreasing bubble diameter. However, as the bubbles reach greater heights, the velocity begins to decrease with increasing bubble diameter, leading to deceleration.

In essence, this approach allows us to observe the phenomena of bubble acceleration at lower heights in the column, followed by deceleration at higher heights. This dynamic behavior is a consequence of carefully selecting the initial bubble diameter to coincide with the point of maximum velocity change in the $u=f(db)$ relationship. This behavior cannot be captured by simpler models; the essence of the bubbly flow model is indeed to account for hydrodynamic coupling and thus capture more complex behavior.

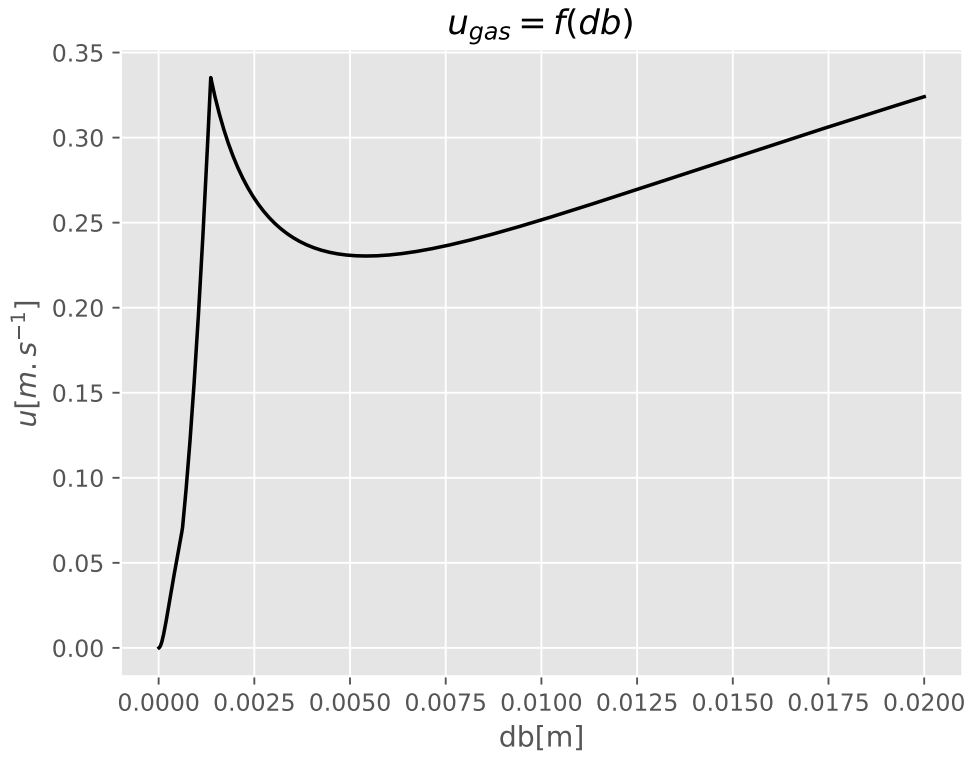


Figure 1: Correlation between gas-liquid relative velocity according to bubble diameter

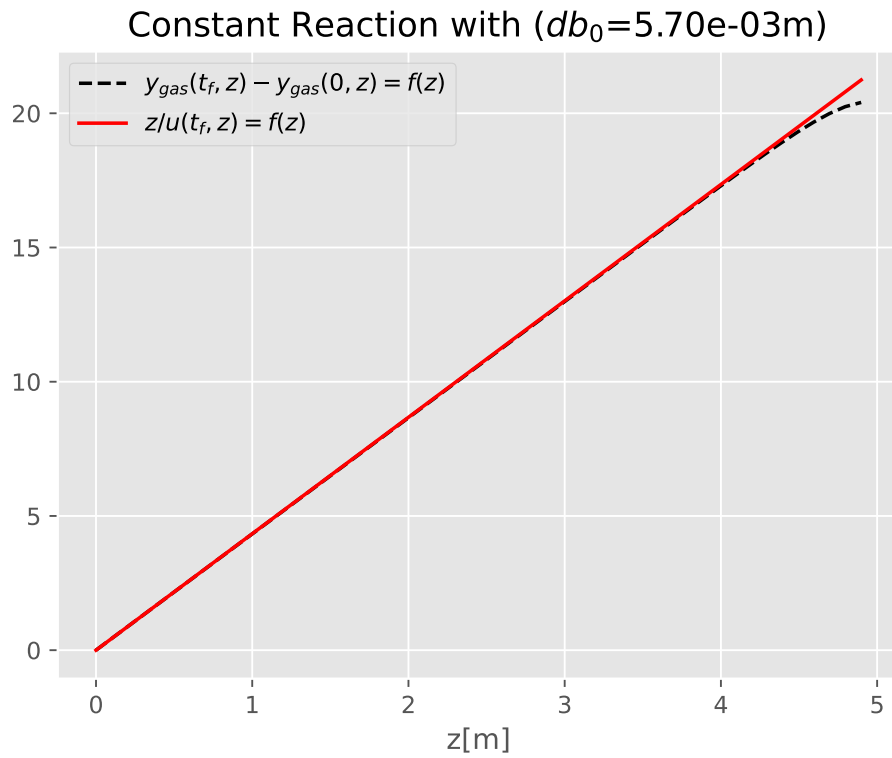


Figure 2: Comparison between analytical solution and simulation with almost constant gas velocity

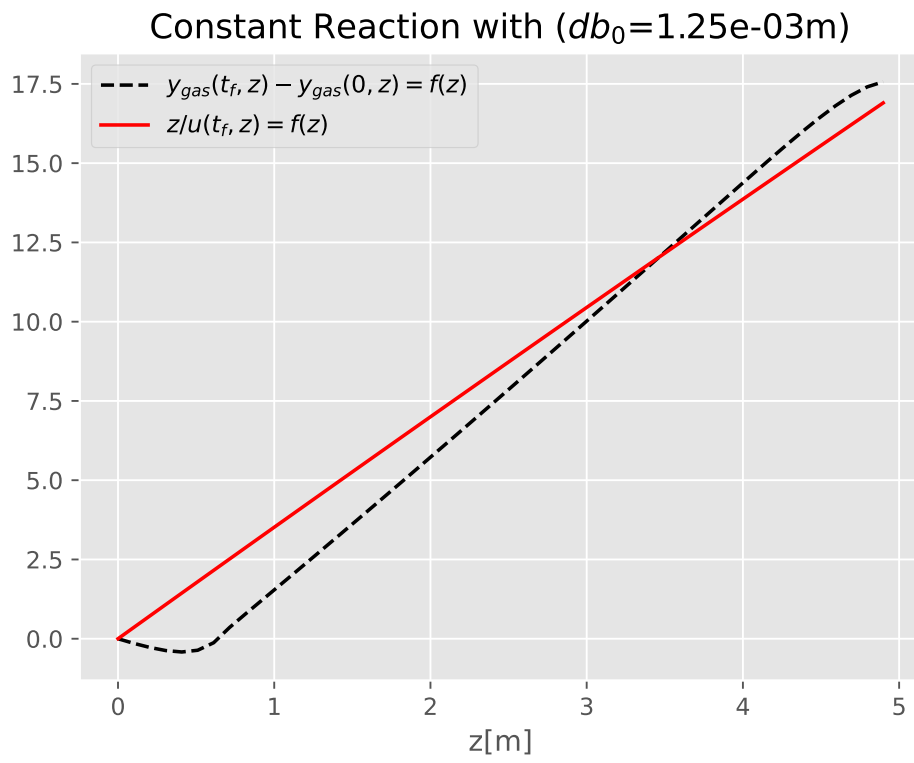


Figure 3: Comparaision between analytical solution and simulation with non constant gas velocity

3.2 Transfer of Gaseous Hydrogen in a Bubble Column

This example illustrates the simulation of a bubble column for bubbling gaseous dihydrogen into water to observe mass transfer from the gas phase to the aqueous phase. A feed of $10 \text{ Nm}^3/h$ of pure dihydrogen is introduced. Two models are simulated: one with a uniform initialization at $t=0$ (uniform gas rate throughout the column) and another with an initialization where the gas rate follows a normal distribution centered around a mean value.

The main objective of this example is to demonstrate how to customize the initialization and show solution stability in a steady state for different initializations.

To execute this example, use the following command:

```
python -0 -m examples 0
```

This will display three figures representing:

1. The profile of gaseous hydrogen in different initializations.
2. The profile of liquid hydrogen in different initializations.
3. The evolution of hydrogen concentration in the liquid for both simulations over time, with two different abscissa scales.

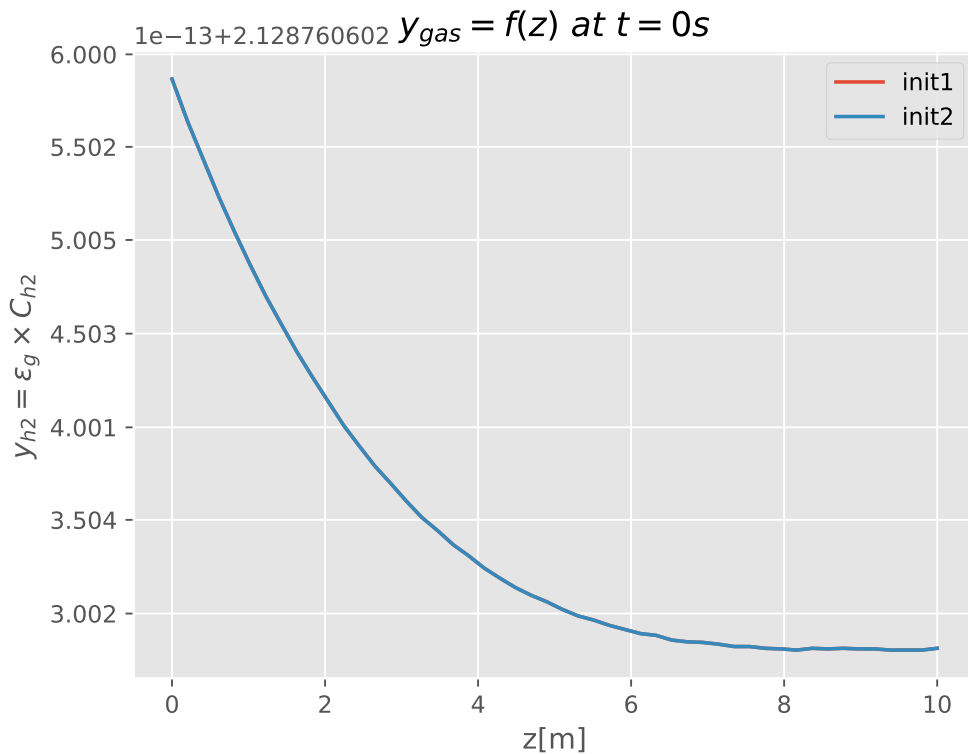


Figure 4: Hydrogen gas initialization profile

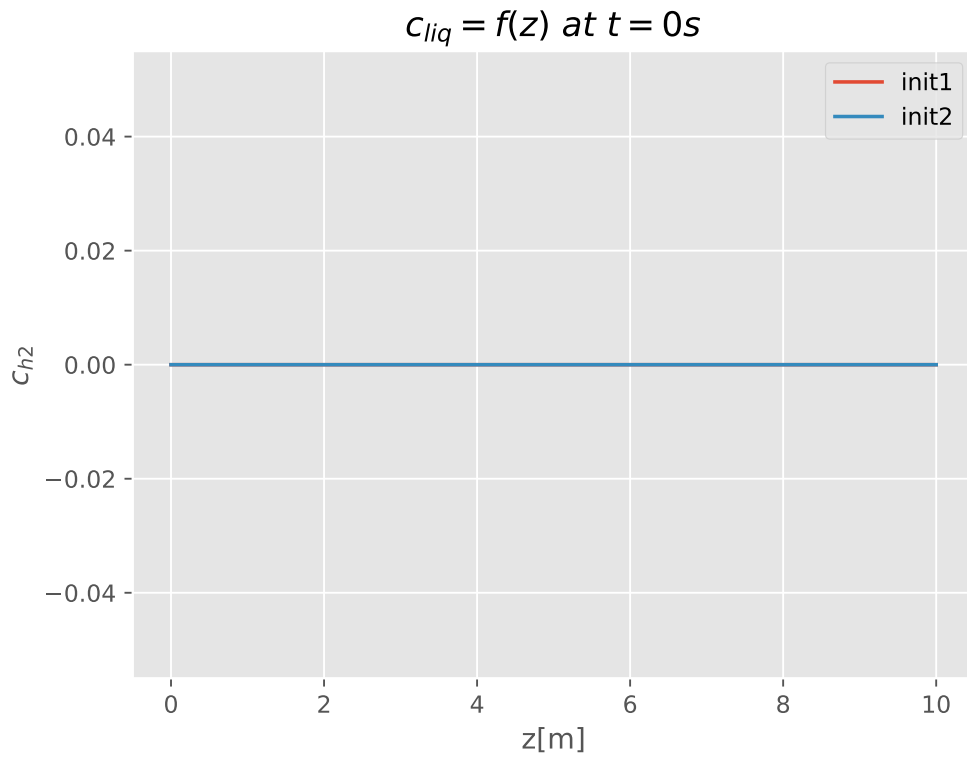


Figure 5: Hydrogen liquid initialization profile

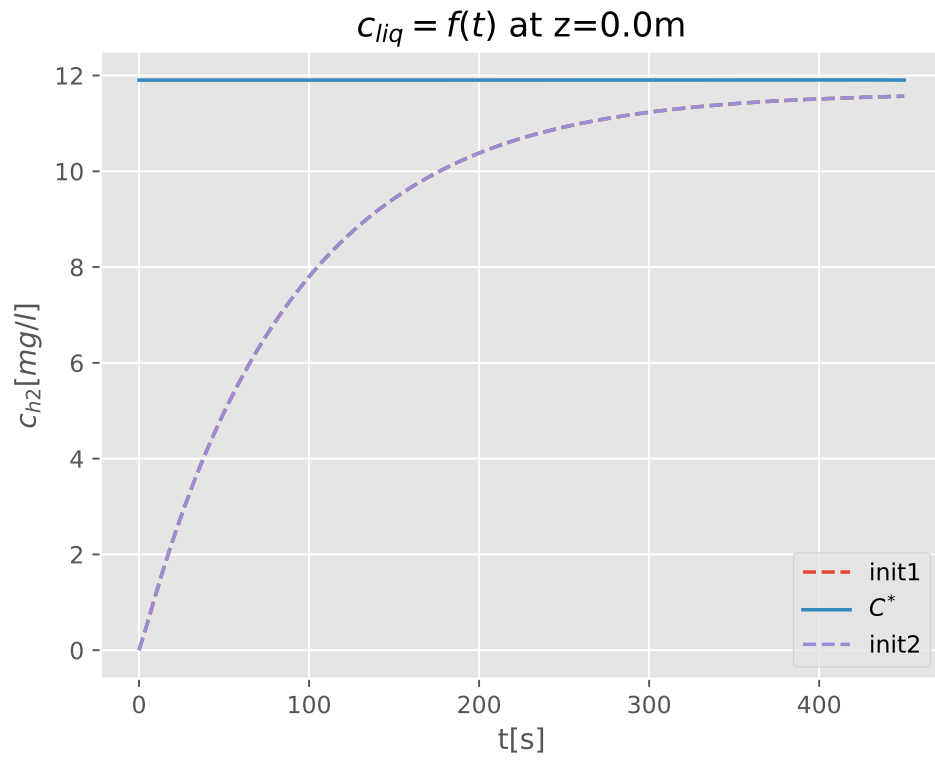


Figure 6: Hydrogen liquid evolution

3.3 gas recycling

Users can customize boundary conditions for a given problem, adjusting parameters like feed and recycling rates. In this scenario, we focus on a high gas recycling rate without transfer or reaction, illustrating the possibility of recycling without these elements. The recycling is instantaneous and its behavior can be adjusted by changing the recycling flow rate function. While liquid recycling is currently not implemented in the bubbling flow model, it remains a potential future addition.

In this scenario, a 90% gas recycling rate is directed to the bottom of the column, accentuating effects for enhanced visibility during simulation. The initial state entails an empty bottom column with high gas retention at the top, creating a gas pocket that will undergo recycling. The feed is halted at $t=0$, simulating a scenario with no feed during the simulation. Despite might not be a real-world situations, it serves to magnify observable effects.

The expectation is that a portion of the gas compounds from the column's top (output) to the bottom (input). The observed oscillations in Fig 7 are not numerical artifacts but the result of actual recycled flow injected at the bottom causing retention oscillations. Note that the frequency relates to the residence time of the gas phase in the column¹.

While the depicted oscillations in Fig 7 may vary with specific initialization and flow rate choices, it is recognized that in practical cases, these oscillations might not be as visibly apparent. Nevertheless, this behavior occurs in real scenarios, emphasizing the significance of recycling dynamics.

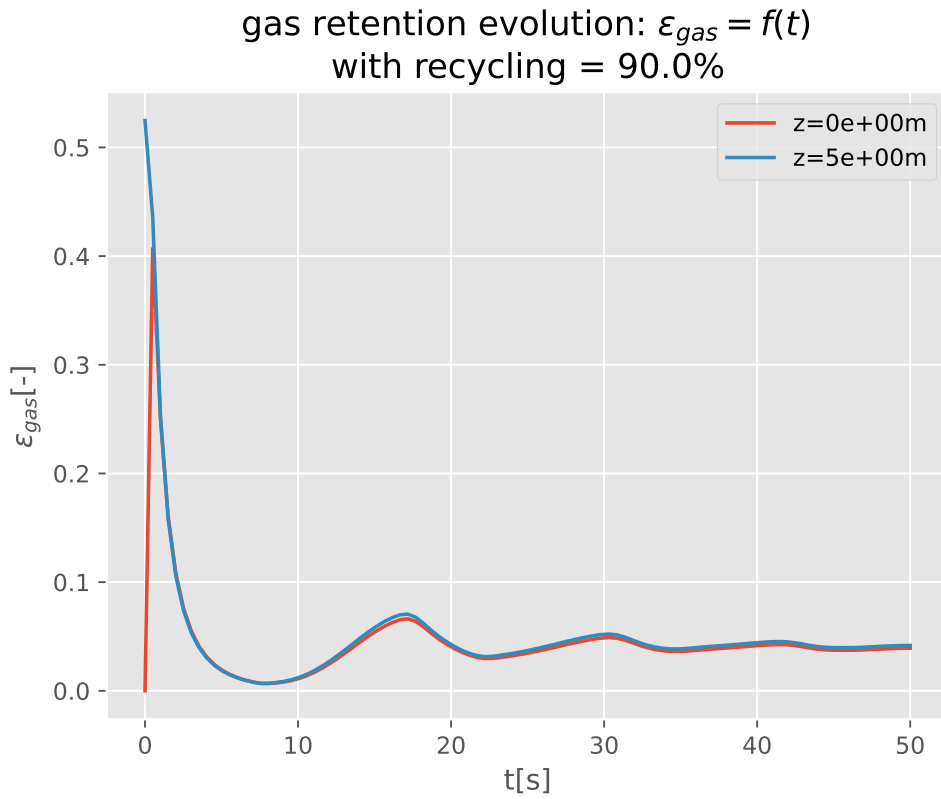


Figure 7: gas retention evolution

Note that in this scenario, it takes over 50 seconds to empty the entire column even without feed, whereas the process should ideally take less than 10 seconds if recycling is not involved. As expected, the gas retention is higher when recycling is set up

¹As depicted in Fig 1 we can estimate the relative velocity of the gas bubble to be approximately 0.3 m/s (considering the liquid to be static in our example). Additionally, we simulate a 5 m high column, the residence time can be roughly calculated as $t_{residence} = \frac{H}{v} = \frac{5}{0.3} \approx 16 \text{ seconds}$ which roughly corresponds to the period of oscillations.

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Ngu, Vincent et al. (2022). “Spatio-temporal 1D gas-liquid model for biological methanation in lab scale and industrial bubble column”. In: *Chemical Engineering Science* 251, p. 117478. ISSN: 0009-2509. DOI: <https://doi.org/10.1016/j.ces.2022.117478>. URL: <https://www.sciencedirect.com/science/article/pii/S0009250922000628>.