

Hydrogen Filling Simulation (H2FillS) User's Manual

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1 H2FillS: Hydrogen Filling Simulation

The Hydrogen Filling Simulation (H2FillS) software is a thermodynamic model designed to track and report on the transient change in hydrogen temperature, pressure, and mass flow when filling a fuel cell electric vehicle (FCEV). H2FillS simulates gas flow from the hydrogen station to the FCEV storage system. Using empirical fueling data sets, the model has been validated over a range of fueling conditions to match common light-duty FCEV fill profiles. Overall, it provides significant benefits to the light-duty fueling market and fill knowledge gaps of the interaction between a hydrogen station and an FCEV.



1.1 Installation

The supported operating system for H2FillS applications is Windows; the applications were tested under Windows 10 (version: 10.0.18363 Build 18363).

1. [Download a software package \(H2FillS_Package.zip\)](#) that includes the following installers:
 - A full-station model (H2FillS_Installer.exe): The simulation starts at a high-pressure ground storage, runs through a dispenser, and ends at a vehicle storage system
 - A partial-station model (H2FillS_Partial_Installer.exe): The simulation starts at a dispenser breakaway and consists solely of dispenser components and a vehicle storage system
2. Execute H2FillS_Installer.exe and/or H2FillS_Partial_Installer.exe to install the application in your system
 - If you have previous versions of software, we recommend to [uninstall it first](#)
3. Install MATLAB Runtime R2018a (9.4): Windows 64-bit
 - [Download the installer from the MATLAB Runtime website](#) for free of charge; a standard MATLAB license is not required to run MATLAB Runtime
 - Follow the instruction of the installer, and we recommend not to change the default root/installation directory of MATLAB Runtime
 - You can install multiple versions of MATLAB Runtime on a single machine, which allows you keep using your existing software. The deployed applications automatically choose the right version of MATLAB Runtime, and this software requires MATLAB Runtime R2018a (9.4)
 - You only need to install MATLAB Runtime once for the full-station and partial-station models
 - After installing MATLAB Runtime, we recommend to restart H2FillS applications

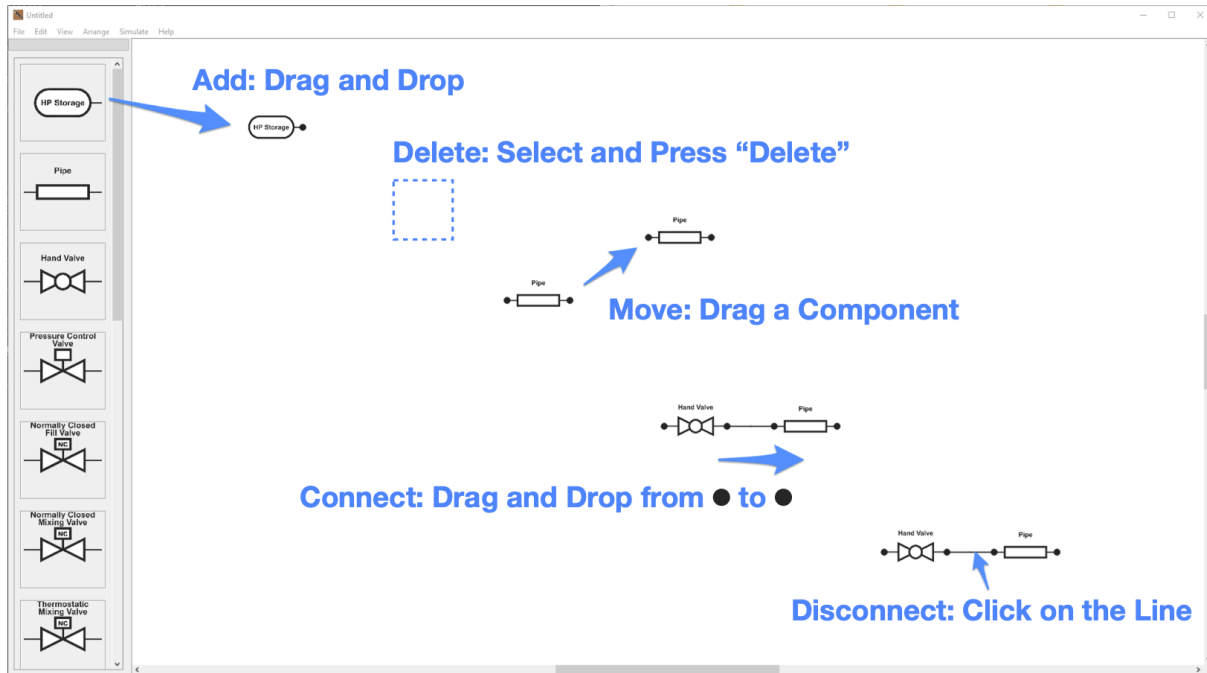
1.2 Uninstallation

The H2FillS software can be uninstalled using **Program Manager** (one of Window's default applications). Note that this process does not uninstall MATLAB Runtime R2018a (9.4): Windows 64-bit.

2 Quick Start

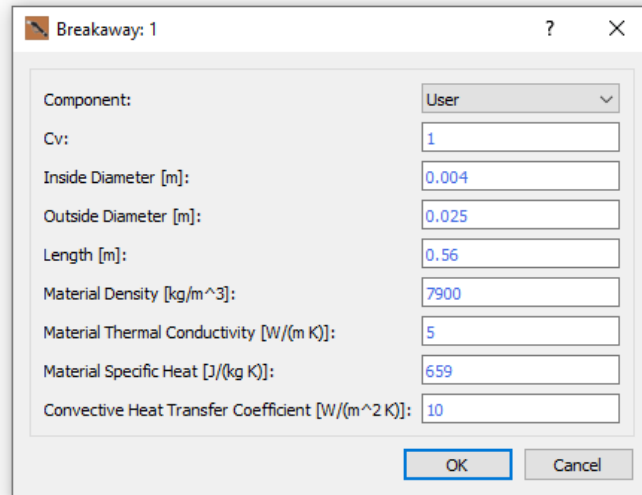
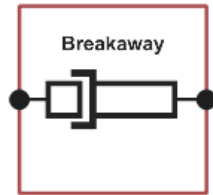
This section provides an overview of the essential features of this software while [the next section](#) demonstrates some of the use cases of this software.

2.1 Add/Delete, Move, and Connect/Disconnect Components



2.2 Specify Component Parameters

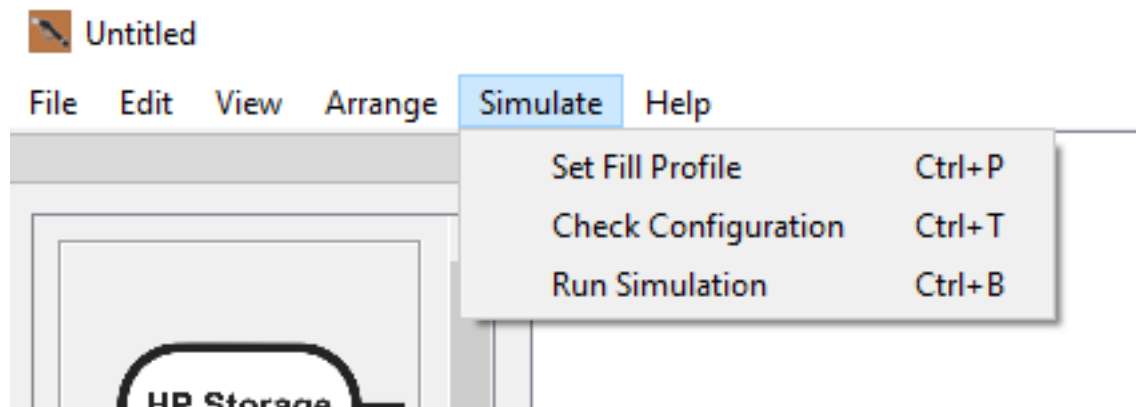
1. Double-click a component, which pops up a property dialog window
 - Note that if the mouse is not held steady during this event, the position of a component might change
2. Specify parameters
3. Press "OK"

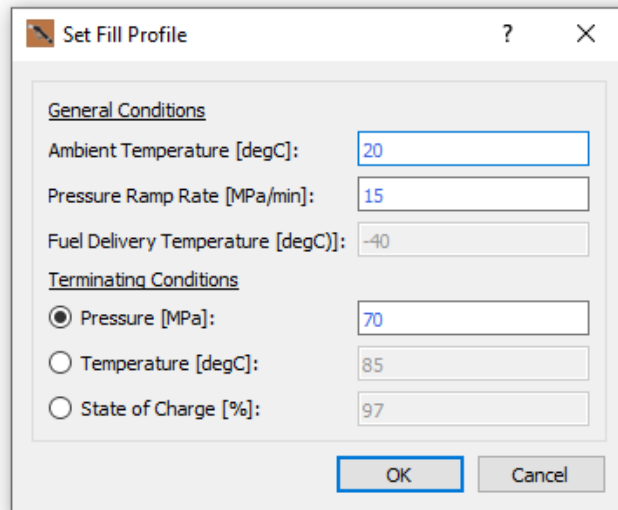
A dialog box titled "Breakaway: 1" with a question mark icon and a close button. It contains several input fields for component properties. The "Component" dropdown is set to "User". The other fields are: Cv (1), Inside Diameter [m] (0.004), Outside Diameter [m] (0.025), Length [m] (0.56), Material Density [kg/m^3] (7900), Material Thermal Conductivity [W/(m K)] (5), Material Specific Heat [J/(kg K)] (659), and Convective Heat Transfer Coefficient [W/(m^2 K)] (10). There are "OK" and "Cancel" buttons at the bottom right.

Property	Value
Component	User
Cv	1
Inside Diameter [m]	0.004
Outside Diameter [m]	0.025
Length [m]	0.56
Material Density [kg/m ³]	7900
Material Thermal Conductivity [W/(m K)]	5
Material Specific Heat [J/(kg K)]	659
Convective Heat Transfer Coefficient [W/(m ² K)]	10

2.3 Specify Filling Parameters

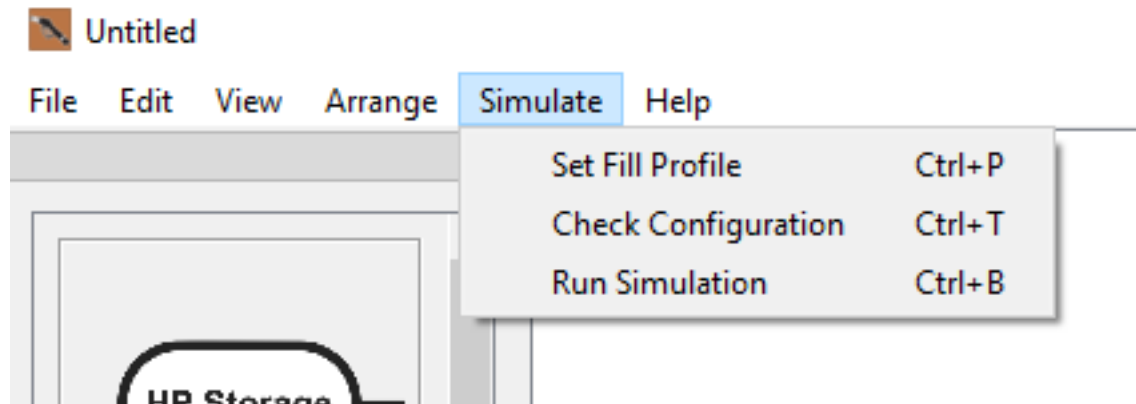
1. Click "Set Fill Profile" from the menu bar (Simulate > Set Fill Profile)
2. Specify parameters
 - For a partial-station model, users can specify the following "Simulation Conditions": 1) [Use Default Values](#) and 2) [Use Supply Condition Data](#)
3. Press "OK"



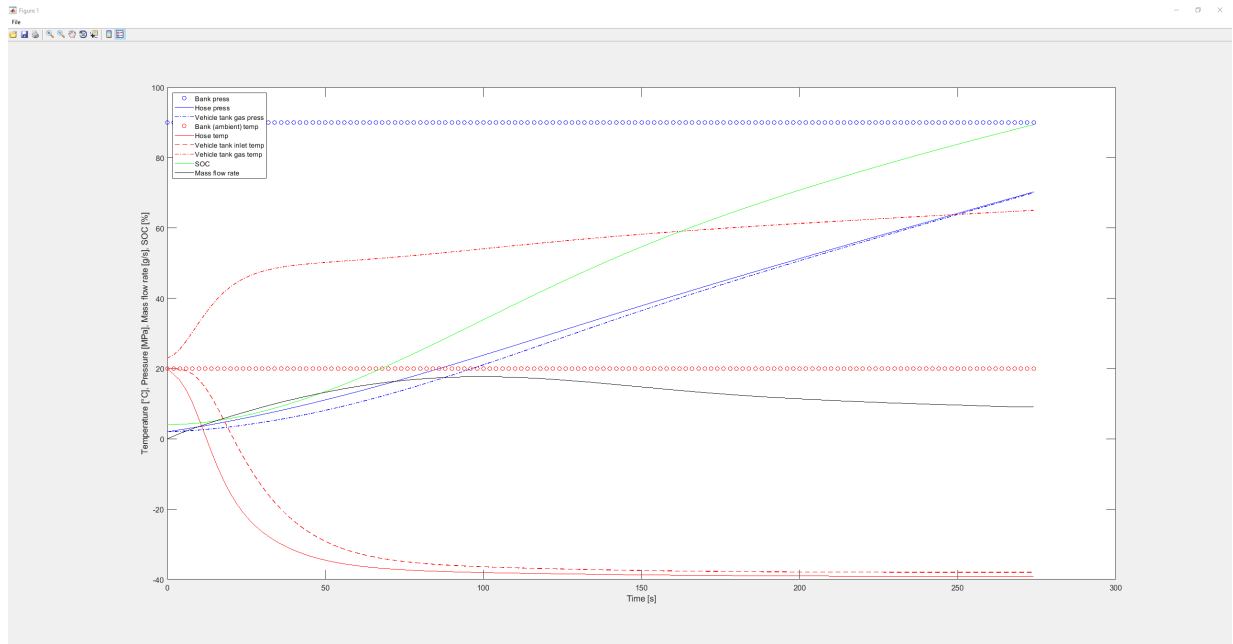


2.4 Run Simulation

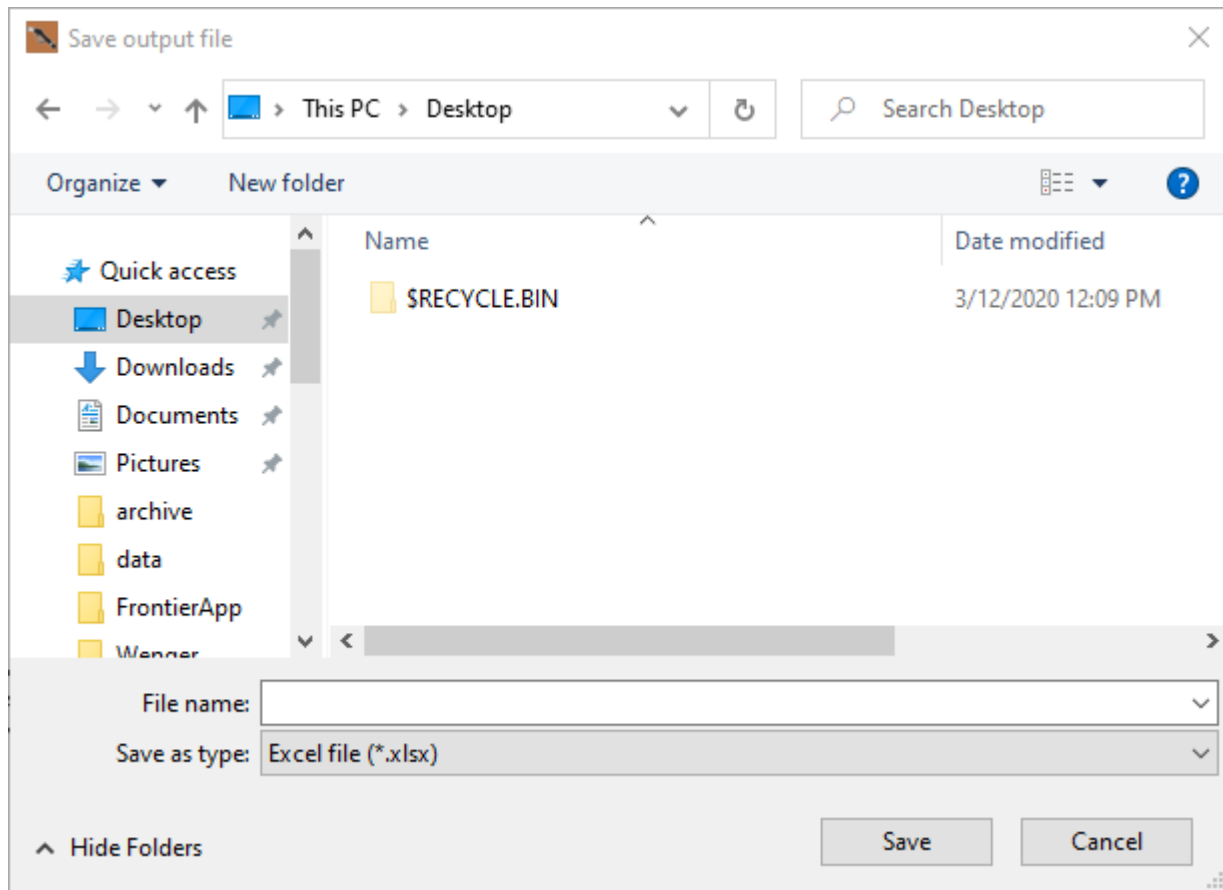
Once you [create a station configuration](#), [specify component parameters](#), and [specify filling parameters](#), you can run the numerical simulation from the menu bar (Simulate > Run Simulation).



If there are no errors, it will open a command prompt window that shows simulation progress (multi-tank configurations show representative values). After the simulation is completed, it will automatically show a plot window.

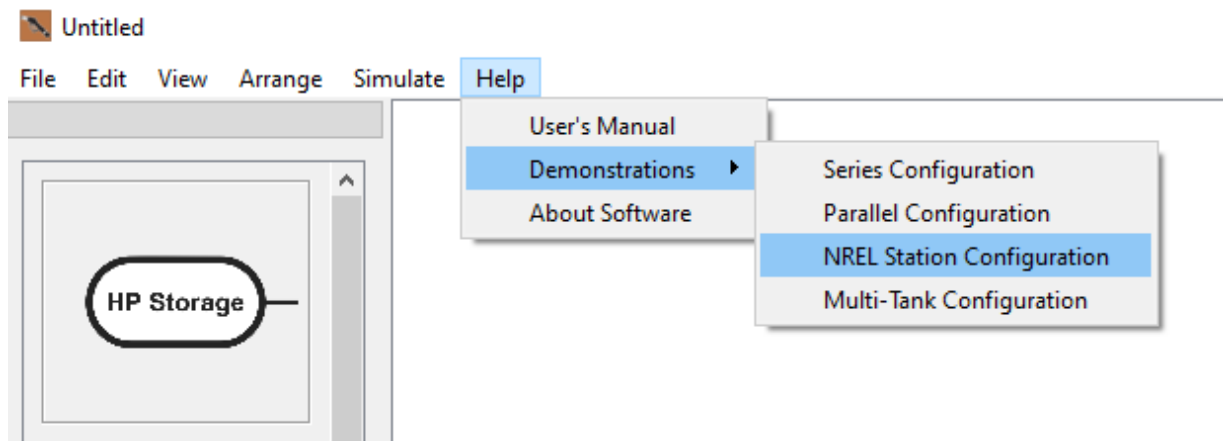


Closing the plot window allows users to save result data as an excel file (.xlsx). A list of data points and their descriptions is provided in the subsequent section, [Data Table for Simulation Results](#).



3 Demonstrations

From the menu bar (Help > Demonstrations), a variety of example configurations is available for H2FillS.exe and H2FillS_Partial.exe.

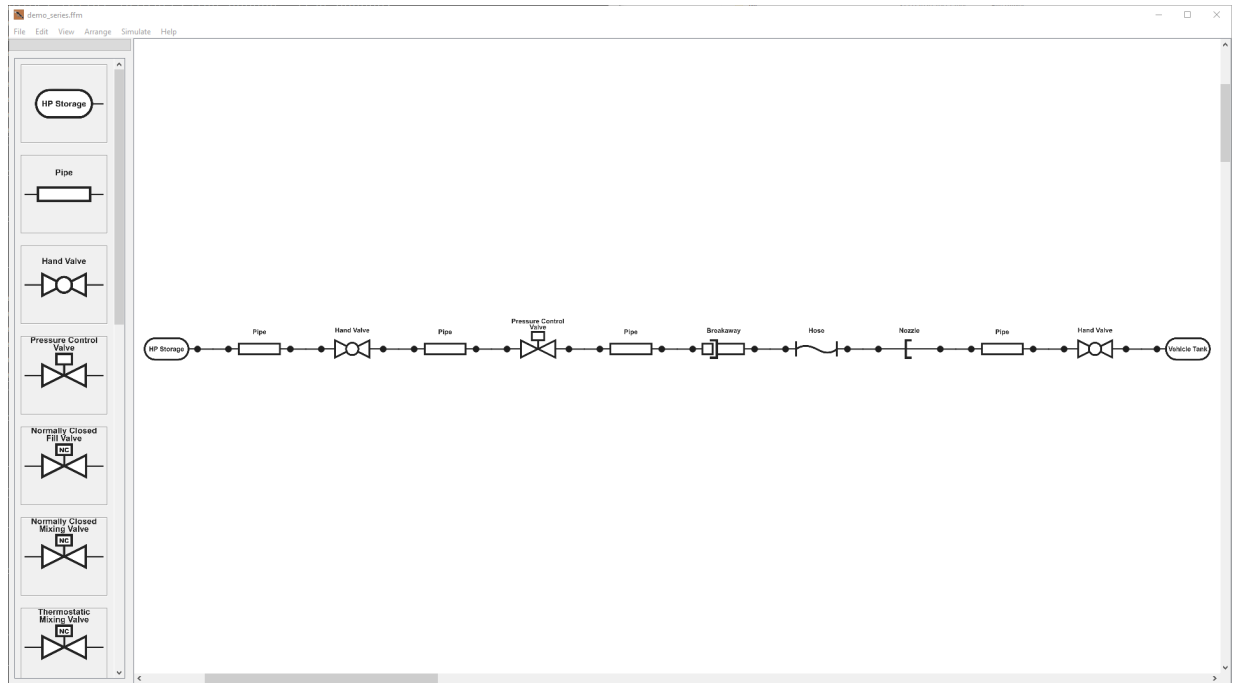


3.1 Full-Station Model (H2FillS.exe)

The full-station model has four configurations available.

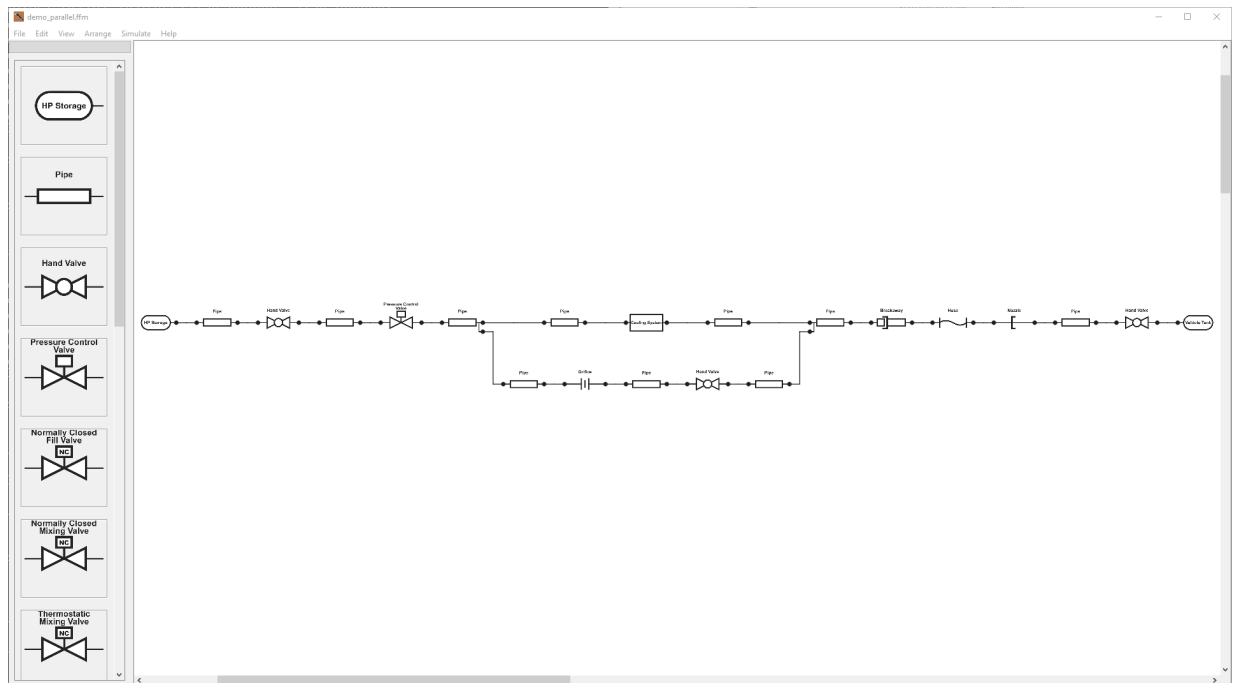
3.1.1 Series Configuration

A series configuration is the simplest configuration for H2FillS.exe, which demonstrates the minimum required components to run the simulation.



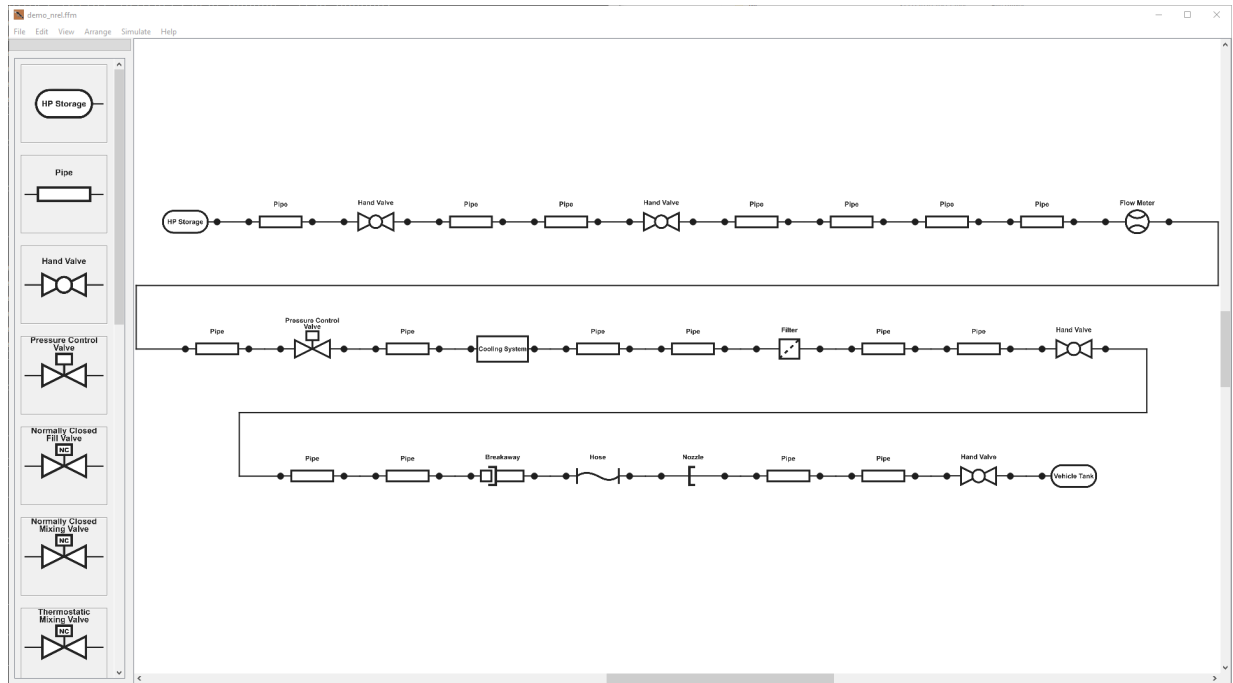
3.1.2 Parallel Configuration

A parallel configuration demonstrates a capability of splitting flows prior and subsequent of a cooling system.



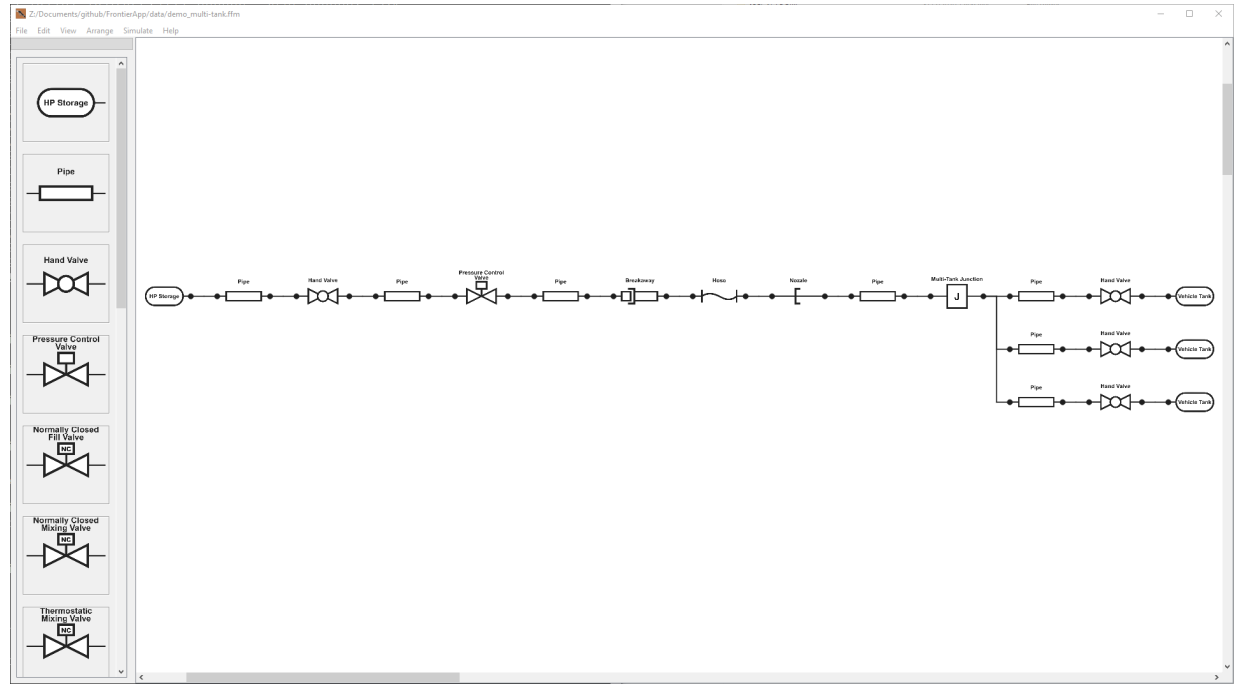
3.1.3 NREL Station Configuration

This demonstration shows a configuration based on [NREL HITRF \(hydrogen infrastructure testing and research facility\)](#).



3.1.4 Multi-Tank Configuration

This demonstration shows a configuration that uses a multi-tank junction to simulate filling multiple vehicle tanks.

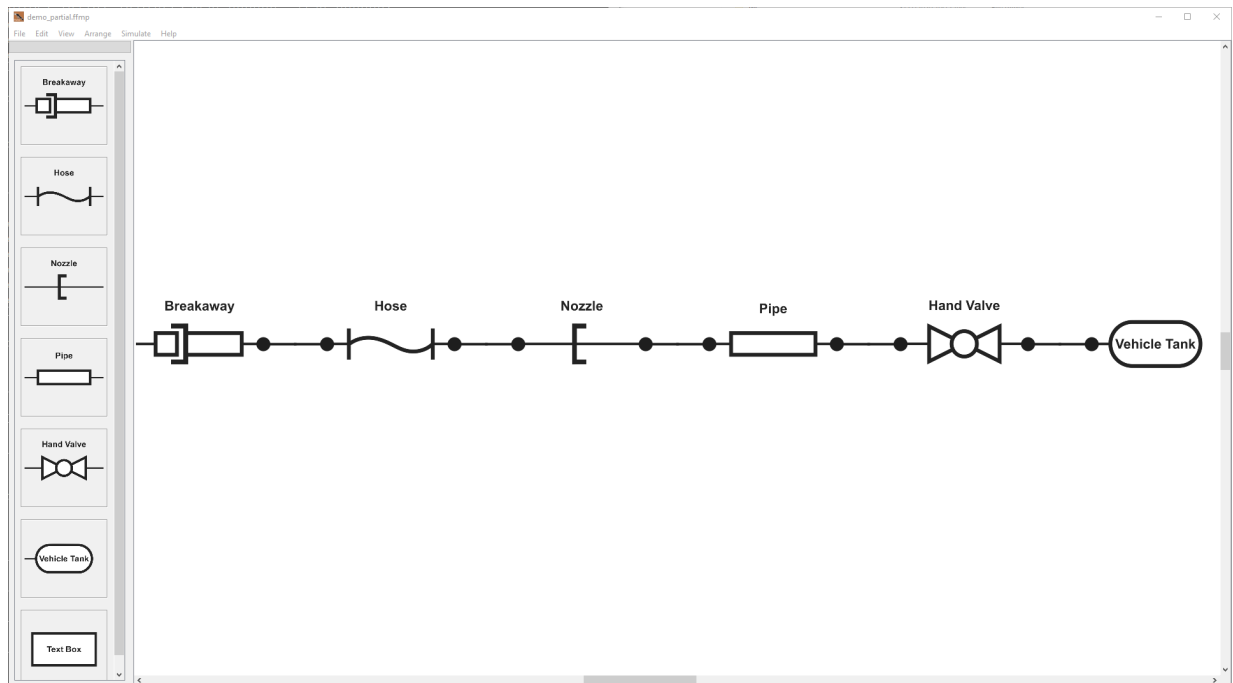


3.2 Partial-Station Model (H2FillS_Partial.exe)

The partial-station model has three configurations available with a capability of running the simulation from [supply condition data](#) in addition to using [default values](#).

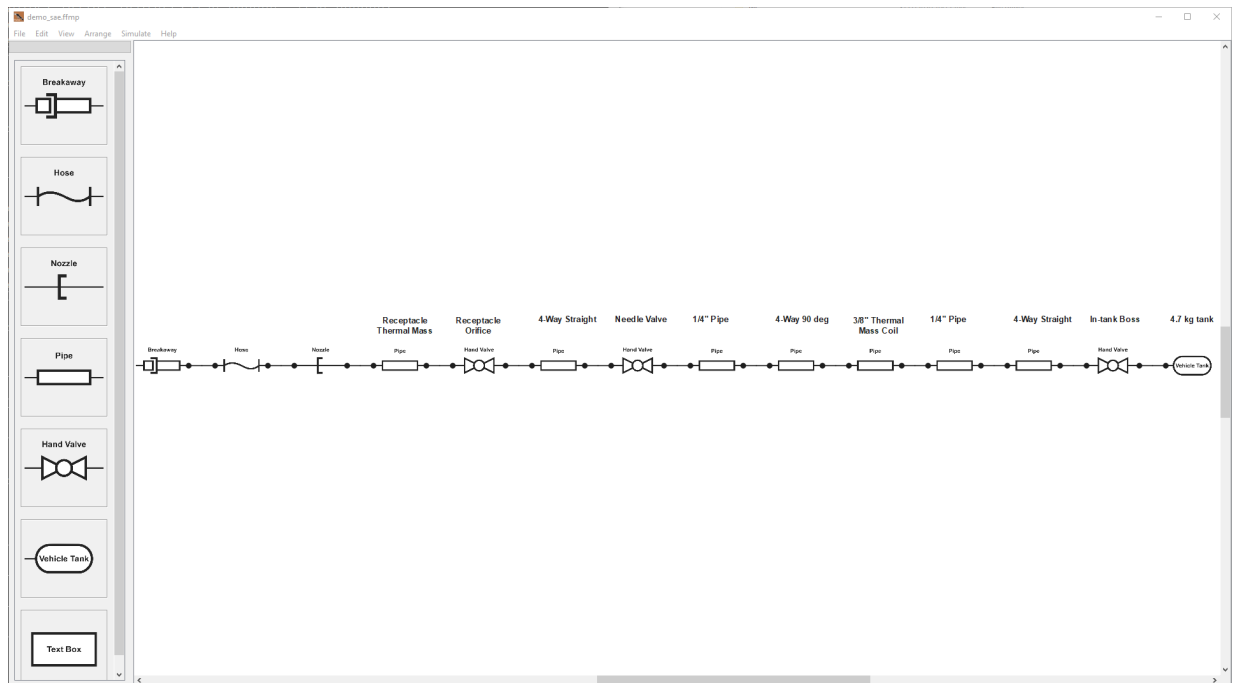
3.2.1 Partial Configuration

A partial configuration is the simplest configuration for H2FillS_Partial.exe, which demonstrates the minimum required components to run the simulation.



3.2.2 SAE Test Configuration

This demonstration shows a configuration that we estimated based on [a report on the SAE J2601 validation tests](#).



3.2.2.1 Use Default Values

- Specify “Pressure Ramp Rate” and “Fuel Delivery Temperature”

Set Fill Profile

General Conditions

Ambient Temperature [degC]: 20

Simulation Conditions

☒ Use the Following Data:

Pressure Ramp Rate [MPa/min]: 15

Fuel Delivery Temperature [degC]: -40

☐ Upload Supply Condition Data:

No file uploaded Upload a file...

Terminating Conditions

☒ Pressure [MPa]: 70

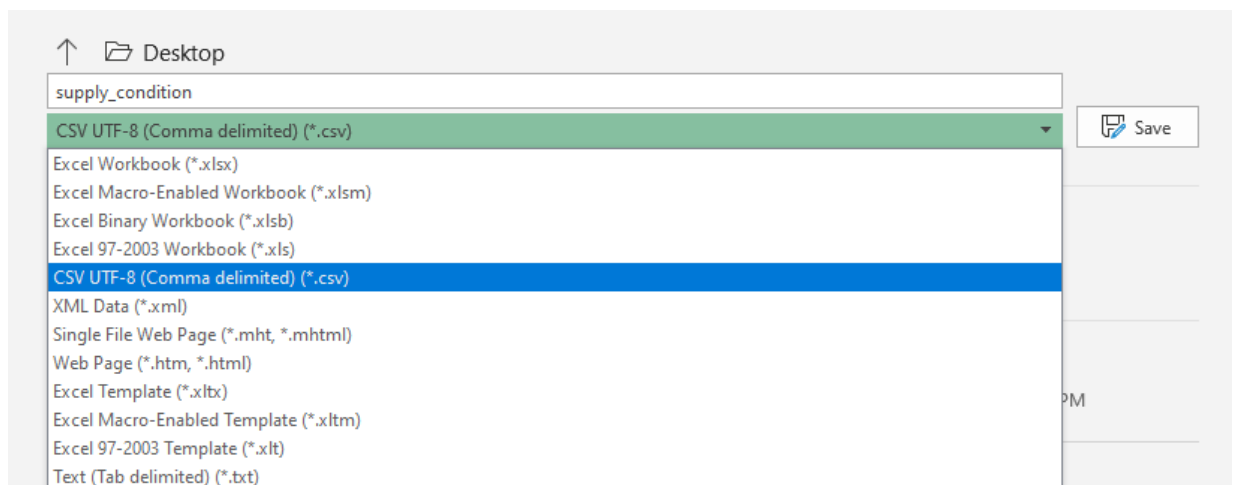
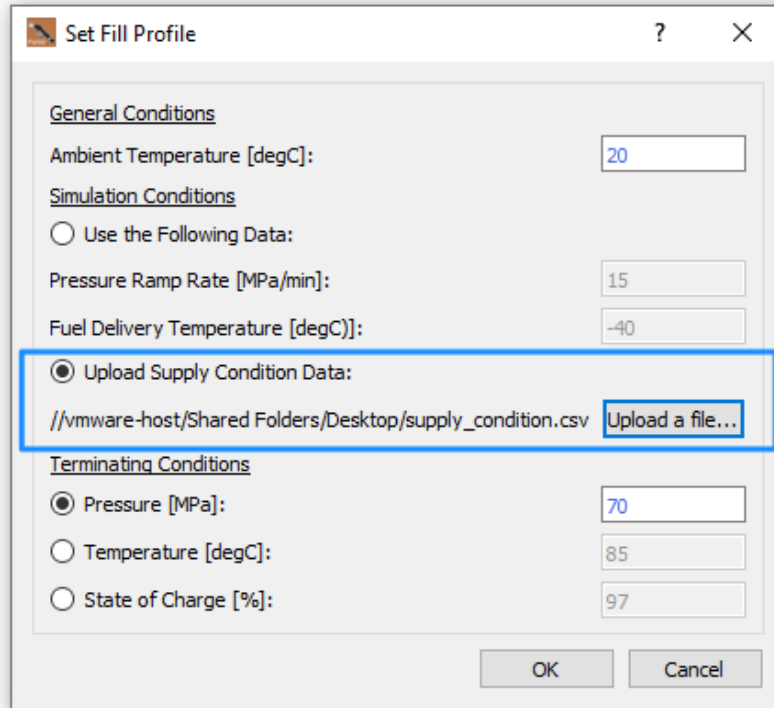
☐ Temperature [degC]: 85

☐ State of Charge [%]: 97

OK Cancel

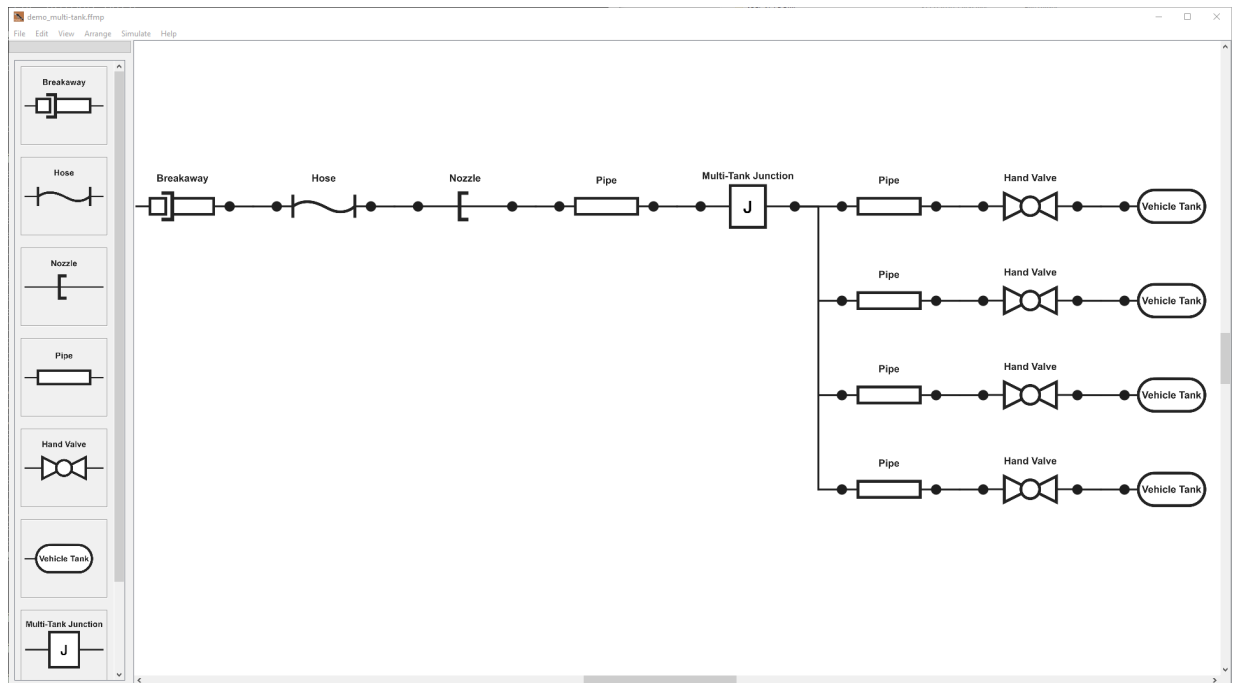
3.2.2.2 Use Supply Condition Data

- An example file is located in the distribution package (H2FillS_Package.zip):
- H2FillS_PackageSupplementalDataSupply_condition.csv
- Select “Upload Supply Condition Data”, click “Upload a file...”, and navigate supply_condition.csv
- **UTF-8** encoding format is supported for this simulation if you create your own supply condition file



3.2.3 Multi-Tank Configuration

This demonstration shows a configuration that uses a multi-tank junction to simulate filling multiple vehicle tanks.

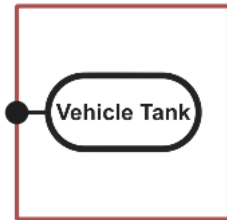


4 Major Features

4.1 Selection of Different Component Parameters

1. Place a component
2. Open a property dialog
3. Select a set of parameters from a pull-down list

Note that the default thermal mass values of the breakaway, hose, and nozzle were estimated based on experimental data, which do not reflect actual specifications guaranteed by manufactures.



Vehicle Tank: 1

Component: User

Internal Parameters

Soak Temperature [degC]:

Initial Pressure [MPa]:

Inside Surface Area [m²]: 1.1

Volume [m³]: 0.099

Length [m]: 0.855

Diameter [m]: 0.42

Liner Parameters

Thickness [m]: 0.005

Material Density [kg/m³]: 945

Material Thermal Conductivity [W/(m K)]: 0.5

Material Specific Heat [J/(kg K)]: 2100

Composite Parameters

Thickness [m]: 0.0316

Material Density [kg/m³]: 1494

Material Thermal Conductivity [W/(m K)]: 0.5

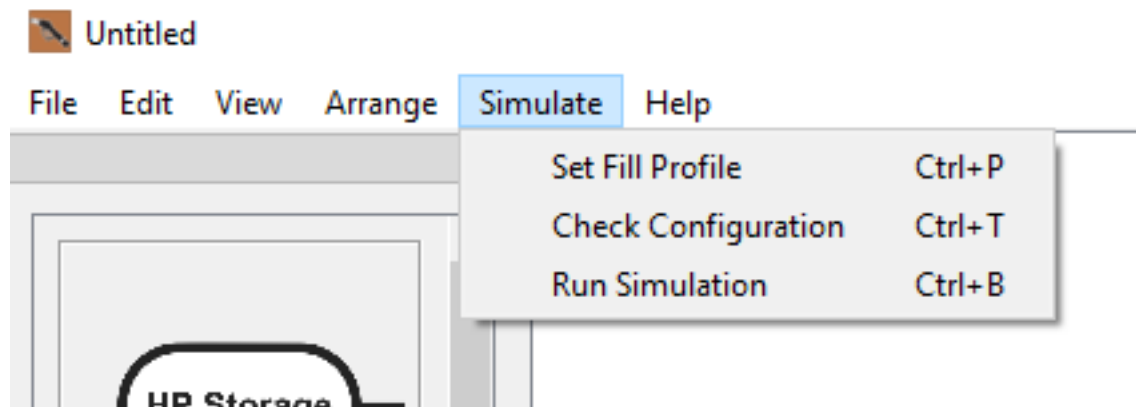
Material Specific Heat [J/(kg K)]: 1120

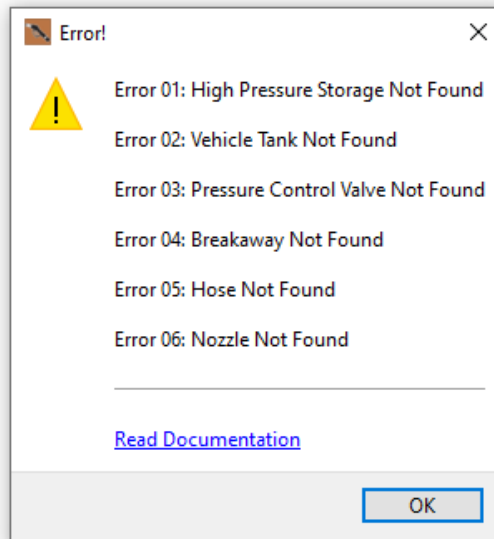
Convective Heat Transfer Coefficient [W/(m² K)]: 8

OK Cancel

4.2 Configuration Verification

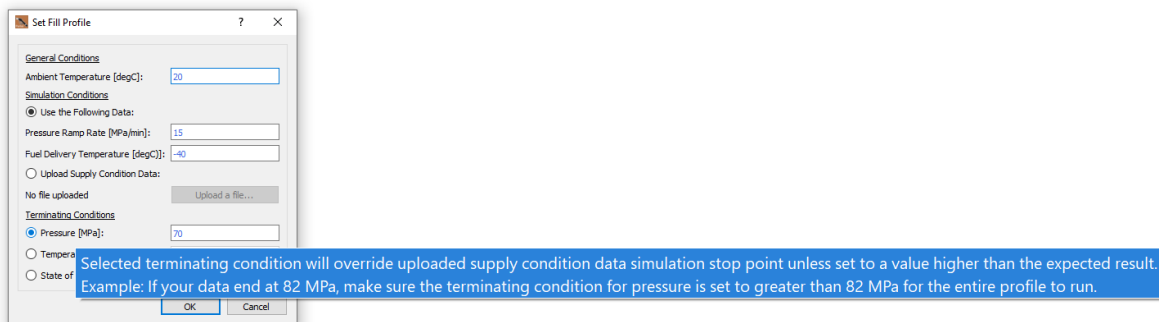
- Users can check a system configuration from the menu bar: Simulate > Check Configuration
- This feature notifies users if the system configuration has errors for the simulation. The section, [Error Messages](#), lists all the errors that needed to be addressed before running the simulation



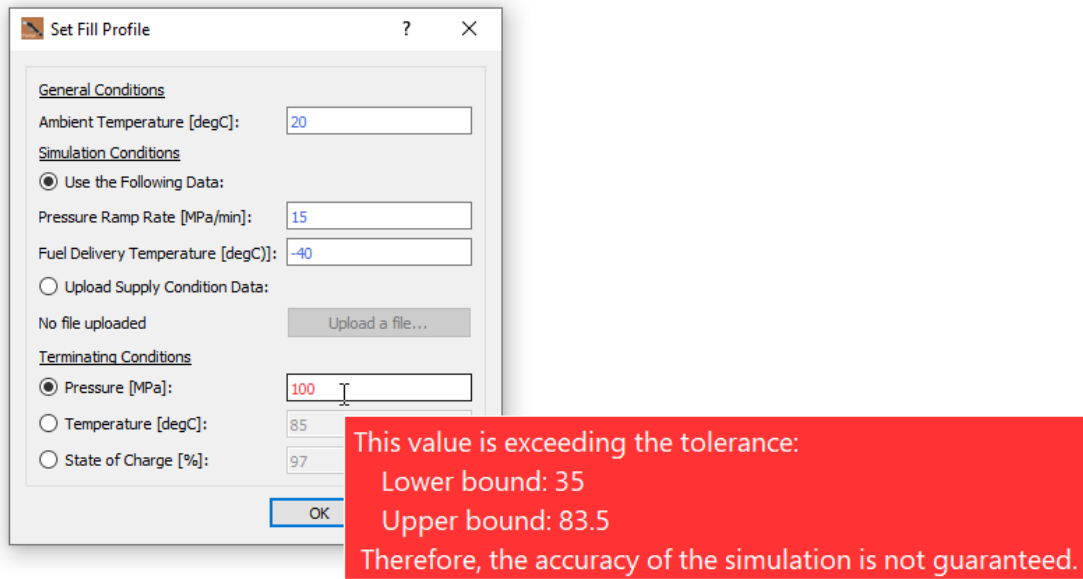


4.3 Tooltips: Parameter Description and Input Warning

If you put your cursor to the parameter description on the left side (e.g. “Pressure [MPa]” in an example below), selected parameters show a tooltip description to provide better understanding how this value is taken care of in the simulation.



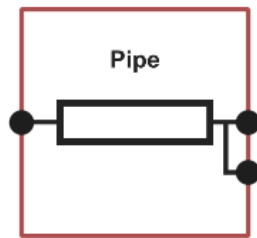
To eliminate unnecessary simulation errors, parameter entry is dynamically validated; users can only put values in an appropriate format (negative values, nonnegative values, no alphabets, etc.). Numbers in blue indicate the parameters are within the simulation tolerance range while numbers in red give a warning message when a cursor is on the number, showing an appropriate range of each parameter.



4.4 Parallel Connection

4.4.1 Diverging/Converging Pipe Components

1. Place a pipe component
 2. Open a property dialog
 3. Select either “Diverging” or “Converging”
- Note that this feature is only available for H2FillS.exe, solely for a [configuration that has a cooling system](#)



Parameter	Value
Component:	User
Inside Diameter [m]:	0.00516
Outside Diameter [m]:	0.00956
Pipe Length [m]:	3
# of 90-deg Bends:	0
Material Density [kg/m ³]:	8000
Material Thermal Conductivity [W/(m K)]:	16.3
Material Specific Heat [J/(kg K)]:	500
Convective Heat Transfer Coefficient [W/(m ² K)]:	5
Parallel Connection:	Diverging

4.4.2 Specific Parameters for Parallel Connection

As default, the following parameters are grayed out, but it is allowed to set when [a configuration is in parallel connection](#)

- Fuel delivery temperature in “Set Fill Profile”
- Transferred heat rate in “Heat Exchanger Component”

4.5 Control Criteria for Pre-Cooling Temperature

The H2FillS model meets the pre-cooling temperature if specified in the fuel delivery temperature in the fill profile and/or in the outlet temperature at the heat exchanger (Component: Cooling System). The descriptions below explain controlling criteria based on each configuration.

4.5.1 Full-Station Model (H2FillS.exe)

- [Series configuration without the heat exchanger](#): The model does not control the pre-cooling temperature, which means the model starts filling with the ambient temperature initially set in the fill profile
- [Series configuration with the heat exchanger](#): The model uses the outlet temperature at the heat exchanger as the pre-cooling temperature
- [Parallel configuration](#): The model controls the mass flow rate so that the temperature at the heat exchanger outlet reaches the outlet temperature at the heat exchanger. If the change in the mass flow rate is significant and unexpected, the temperature at the heat exchanger outlet may decrease below the outlet temperature at the heat exchanger (e.g. due to the capacity specified as the heat energy transferred in the heat exchanger). In that case, the model tolerates the temperature decrease down to the fuel delivery temperature in the fill profile, which means that the fuel delivery temperature in the fill profile is used as the lower limit of the hose temperature. Even if the hydrogen temperature

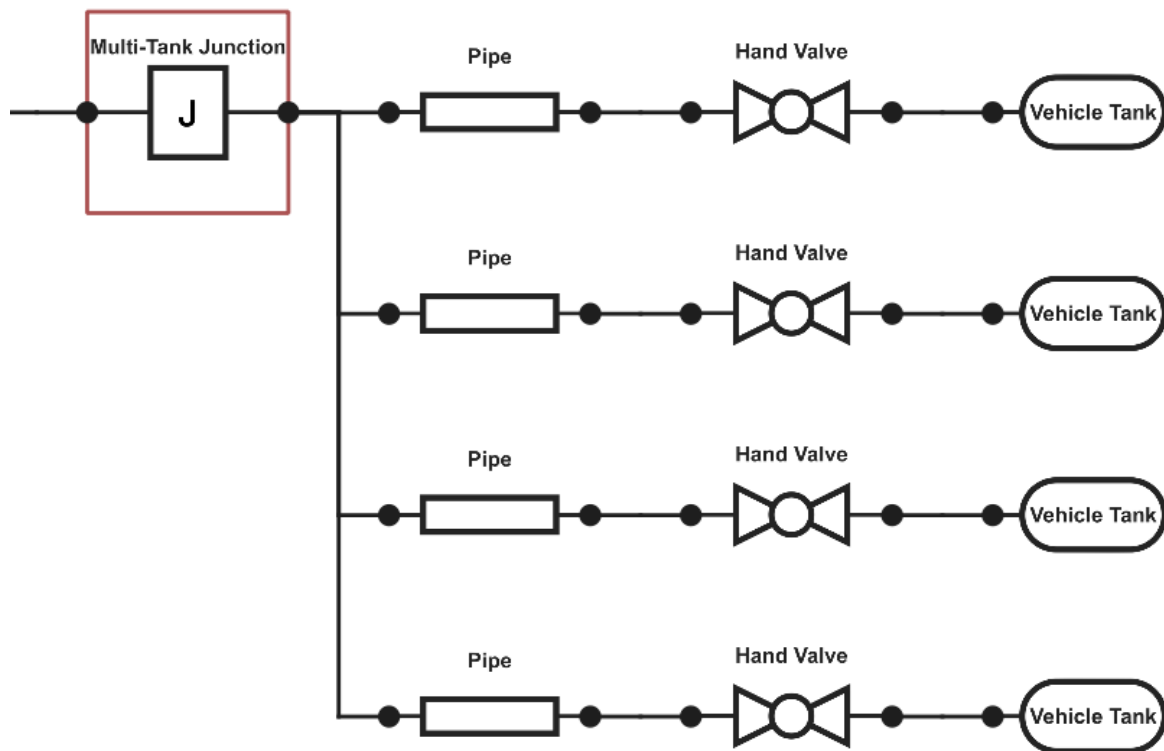
reaches the lower limit, the model will continue to dispense hydrogen into the vehicle tank(s) at the lower limit temperature

4.5.2 Partial-Station Model (H2FillS_Partial.exe)

- [Configuration that uses the pressure ramp rate and fuel delivery temperature](#): The model uses the fuel delivery temperature in the fill profile as the pre-cooling temperature
- [Configuration that uses supply_condition.csv](#): The model follows the values in the `supply_condition.csv` that consists of the gas temperature and other values

4.6 Multi-Tank Modeling

A multi-tank junction can be used for multi-tank modeling. For multi-tank configurations, the simulation model takes into account of initial vehicle tank temperatures (soak temperatures) for each vehicle tank. However, for initial pressures, the model finds and utilizes the lowest vehicle tank pressure among the multiple vehicle tanks to initialize all the vehicle tank pressures.



4.7 Data Table for Simulation Results

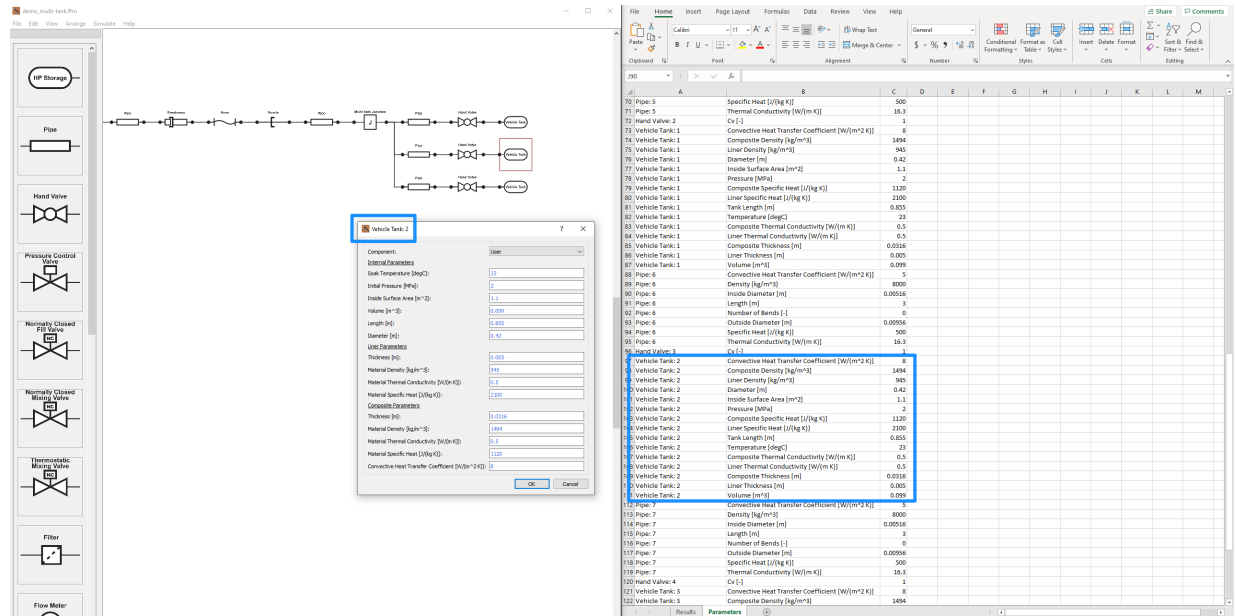
With successful simulation, an exported excel (.xlsx) file contains the following data points in “Results” tab. The data points with an asterisk symbol (*) can have multiple sets of values if the system configuration

has multiple vehicle tanks.

Data Point	H2FillS	H2FillS_Partial	Description
Time [s]	X	X	Simulation time.
Mass flow [g/s]	X	X	Dispensed mass flow rate.
Tamb [deg C]	X	X	Ambient temperature.
Bank press [MPa]	X		Pressure of the high pressure storage.
Bank temp [deg C]	X		Temperature of the high pressure storage.
PCV inlet press [MPa]	X		Inlet pressure of the pressure control valve (PCV).
PCV inlet temp [deg C]	X		Inlet temperature of the pressure control valve (PCV).
PCV outlet press [MPa]	X		Outlet pressure of the pressure control valve (PCV).
PCV outlet temp [deg C]	X		Outlet temperature of the pressure control valve (PCV).
Set target press [MPa]	X		Ideal pressure rise that is defined based on the set average pressure ramp rate (APRR).
Heat exchanger outlet temp [deg C]	X		Outlet temperature of the heat exchanger.
Required Q [J]	X		Heat transfer rate required to cool hydrogen down to the target temperature. Note that this value is not exported for the parallel configuration.
Hose (breakaway) press [MPa]	X	X	Pressure of the hose/breakaway.
Hose (breakaway) temp [deg C]	X	X	Temperature of the hose/breakaway.
Receptacle press [MPa]	X	X	Pressure of the receptacle/nozzle.
Receptacle temp [deg C]	X	X	Temperature of the receptacle/nozzle.
*Vehicle tank inlet press [MPa]	X	X	Inlet pressure of the vehicle tank.
*Vehicle tank inlet temp [deg C]	X	X	Inlet temperature of the vehicle.
*Vehicle tank press [MPa]	X	X	Pressure of the vehicle tank.
*Vehicle tank temp [deg C]	X	X	Temperature of the vehicle tank.
*Liner inner surface temp [deg C]	X	X	Surface temperature of the liner.
*Boundary temp between liner and CFRP [deg C]	X	X	Boundary temperature between linear and carbon fiber reinforced plastic (CFRP).
*CFRP outer surface temp [deg C]	X	X	Outer surface temperature of carbon fiber reinforced plastic (CFRP).
*SOC [-]	X	X	State of charge (SOC) of the vehicle tank.

“Parameters” tab includes fill conditions and component parameters. As shown in the figure below,

component name in “Parameters” tab is matched with the property window of a component in the graphical user interface, which is especially important for analyzing multi-tank configurations.

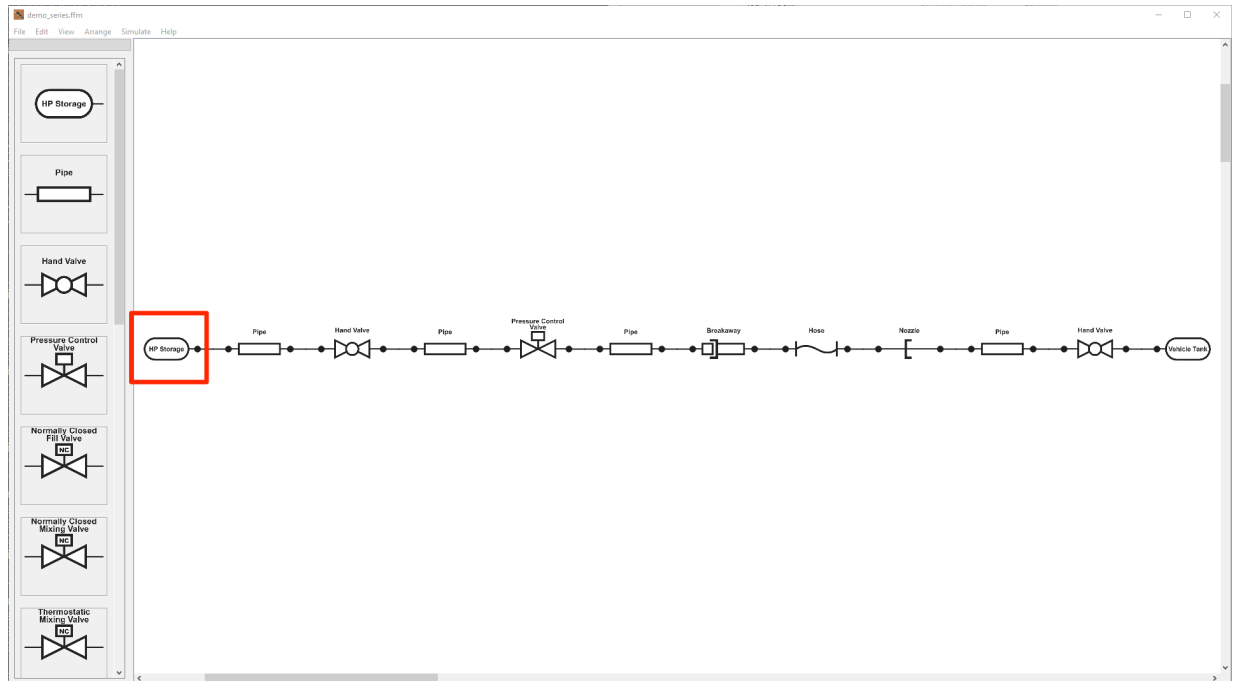


5 Error Messages

The following errors describe the required connections for H2FillS.exe and H2FillS_Partial.exe. Users must resolve these errors to run the simulation.

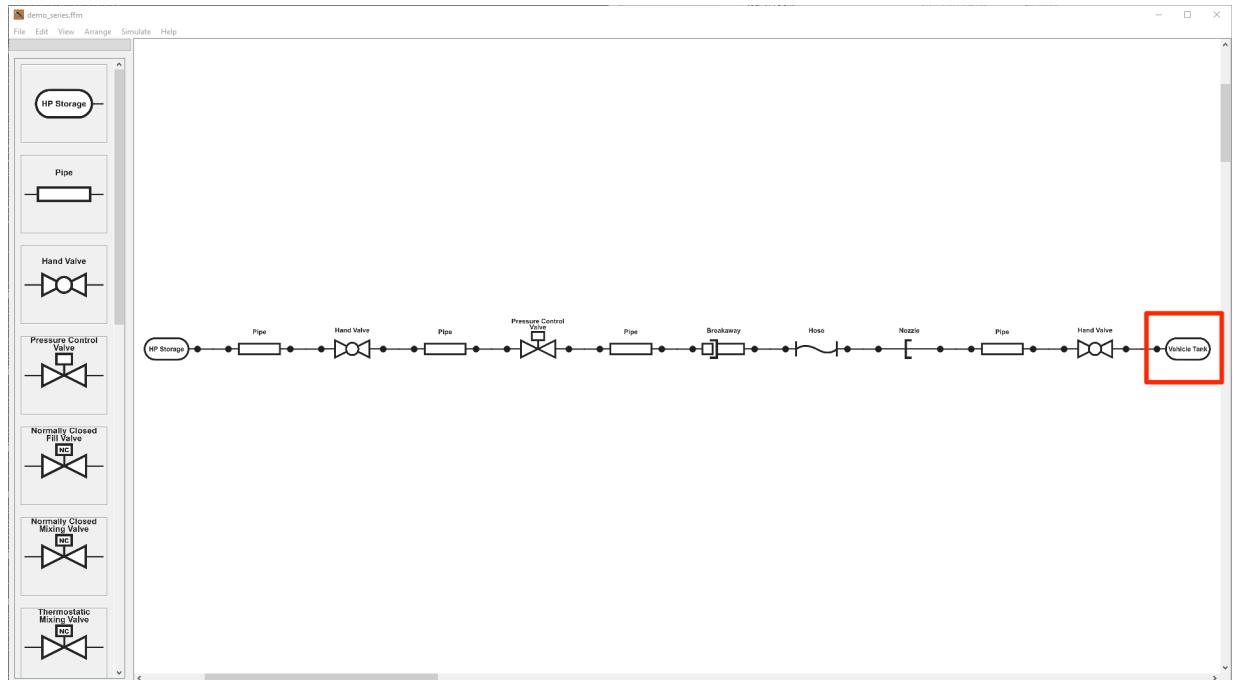
5.1 Error 01: High Pressure Storage Not Found/Connected

The system does not have a high pressure storage. [Add it to the system, and connect it with another component.](#)



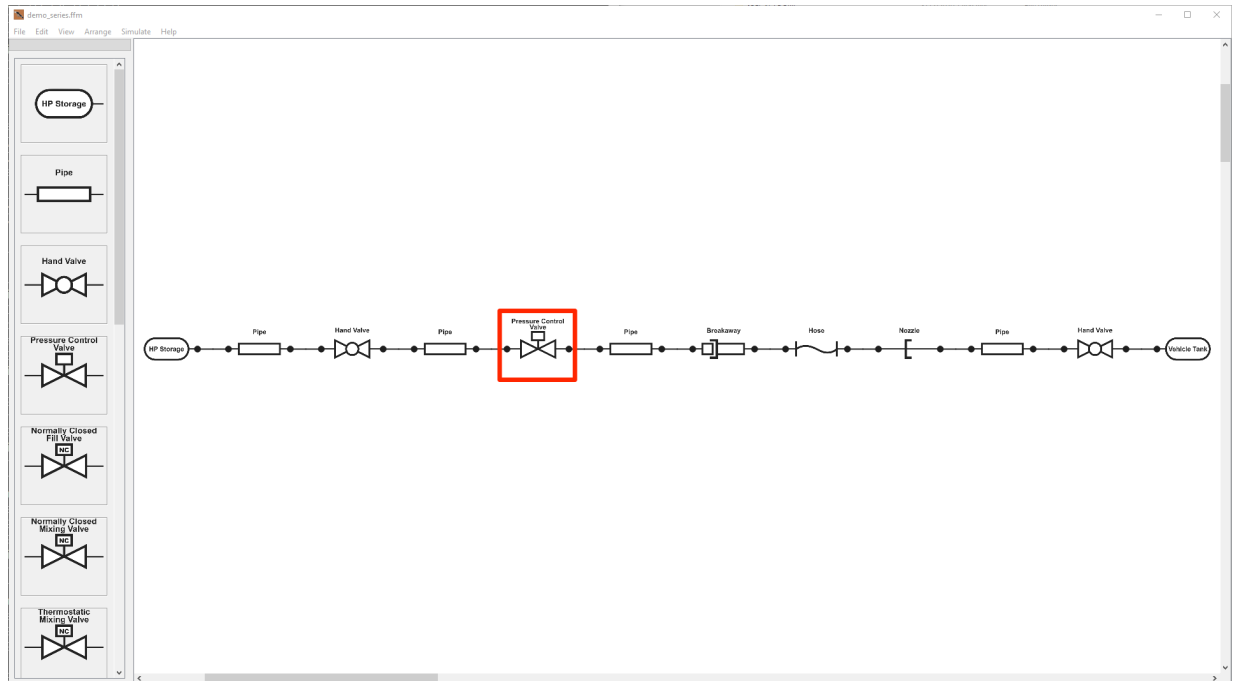
5.2 Error 02: Vehicle Tank Not Found/Connected

The system does not have a vehicle tank. [Add it to the system, and connect it with another component.](#)



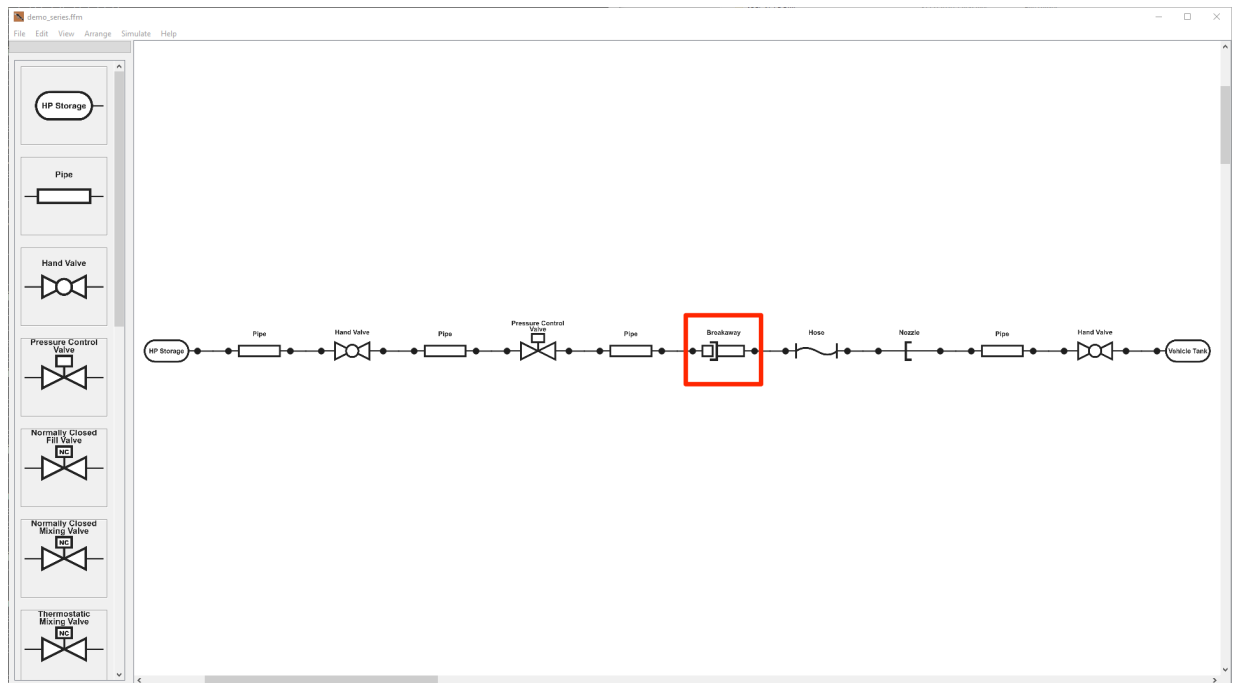
5.3 Error 03: Pressure Control Valve Not Found/Connected

The system does not have a pressure control valve. [Add it to the system, and connect it with another component.](#)



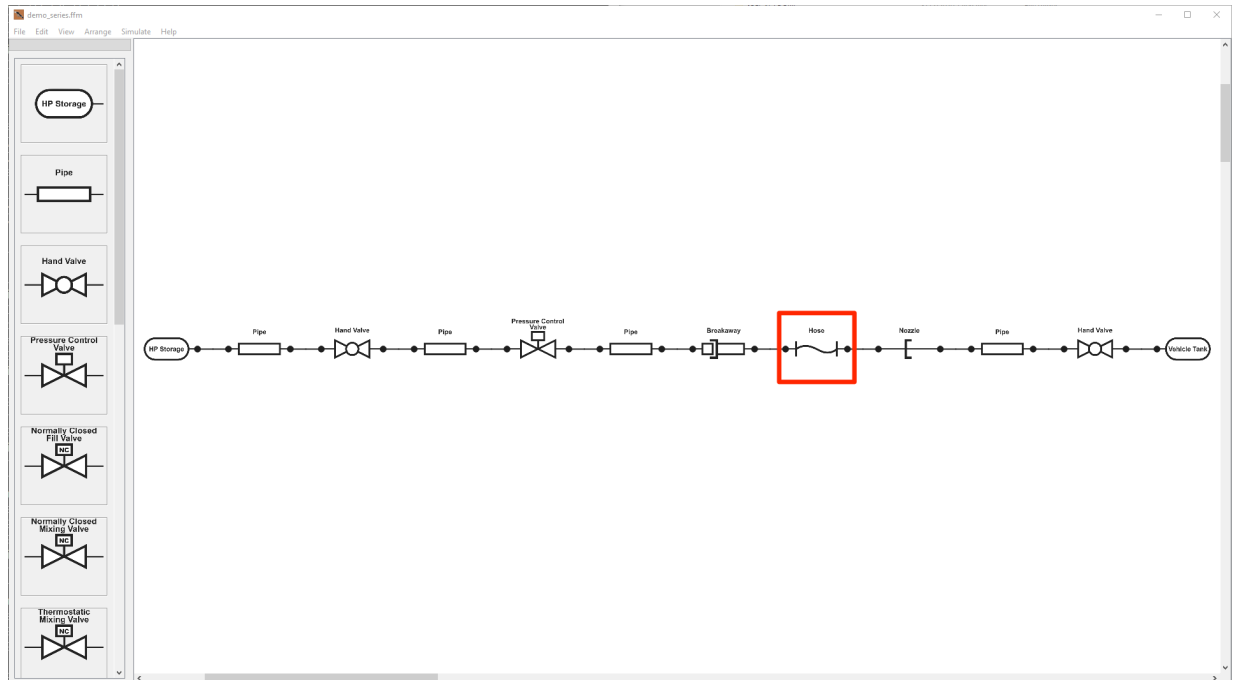
5.4 Error 04: Breakaway Not Found/Connected

The system does not have a breakaway. [Add it to the system, and connect it with another component.](#)



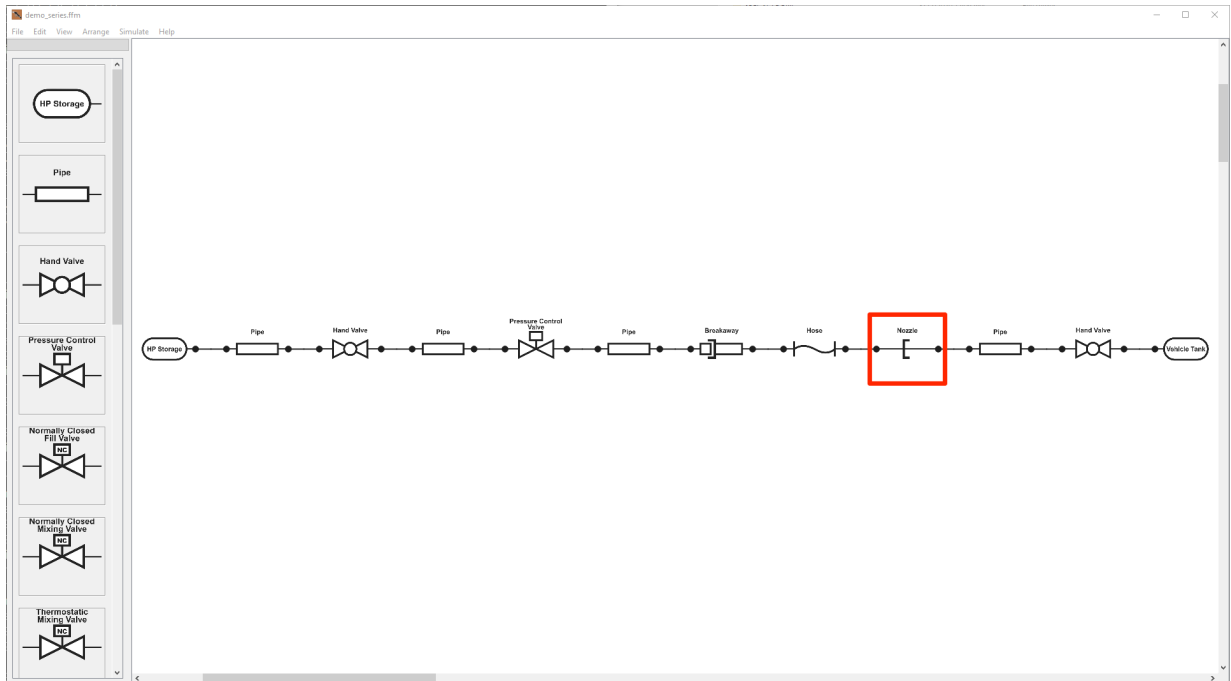
5.5 Error 05: Hose Not Found/Connected

The system does not have a hose. [Add it to the system, and connect it with another component.](#)



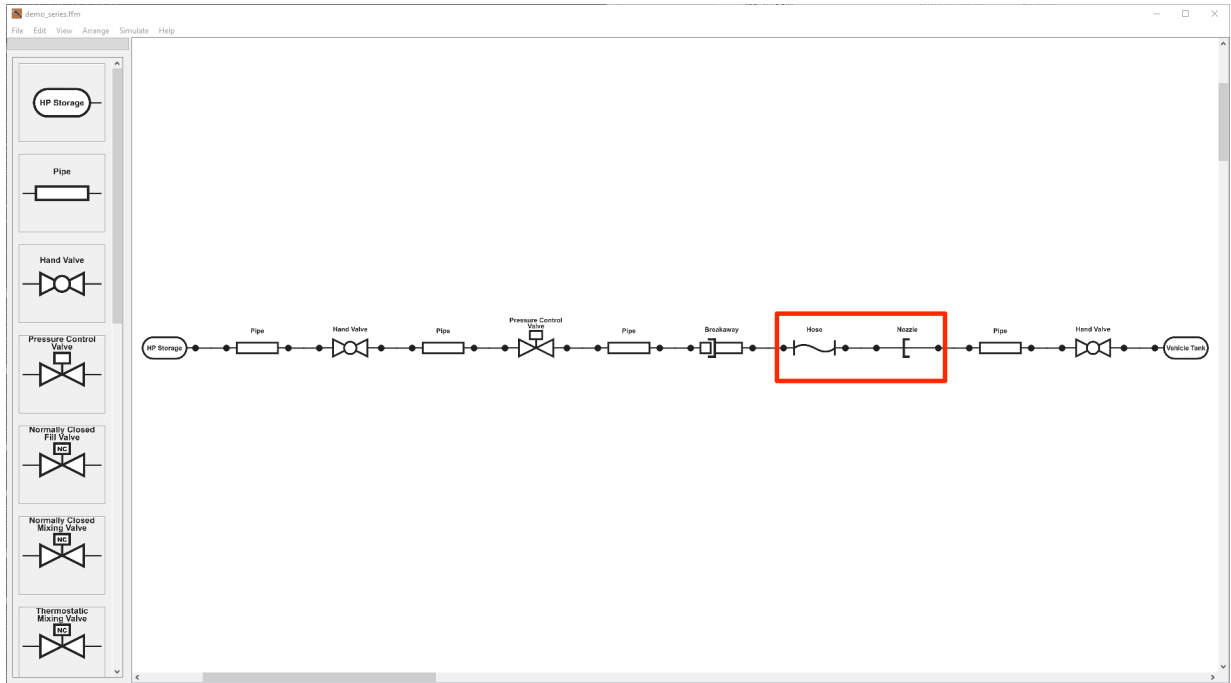
5.6 Error 06: Nozzle Not Found/Connected

The system does not have a nozzle. [Add it to the system, and connect it with another component.](#)



5.7 Error 07: Hose and Nozzle Must Be Connected

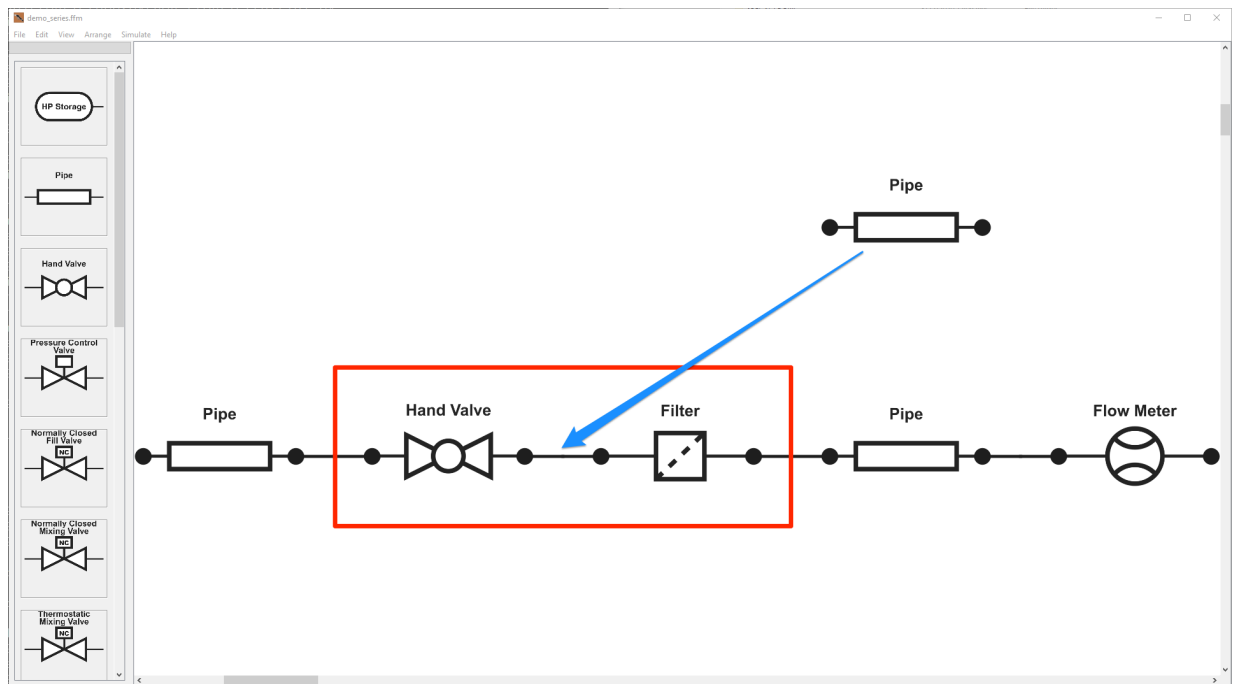
The hose and nozzle must be connected.



5.8 Error 08: Insert a Pipe Component Between Components

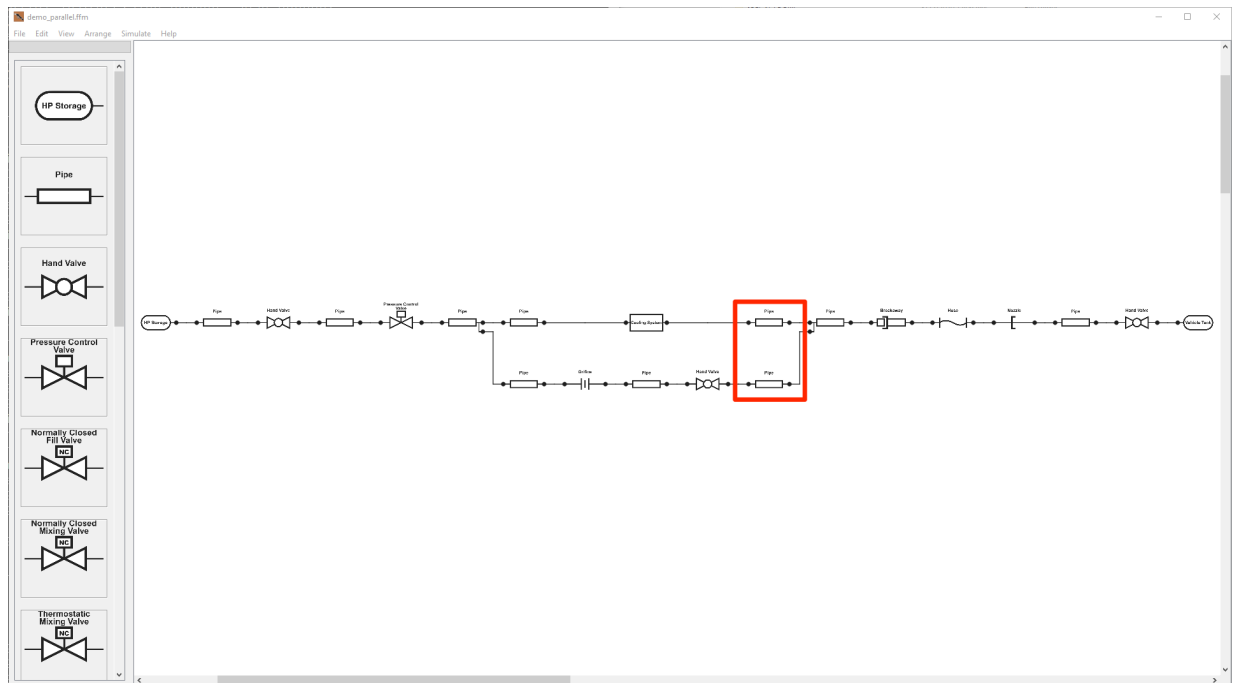
Insert a pipe component between the combination of the following components:

- Pressure Control Valve
- Hand Valve
- Normally Closed Fill Valve
- Normally Closed Mixing Valve
- Proportional Thermostatic Mixing Valve
- Cooling System
- Orifice
- Breakaway
- Flow Meter
- Filter
- Nozzle
- Multi-Tank Junction



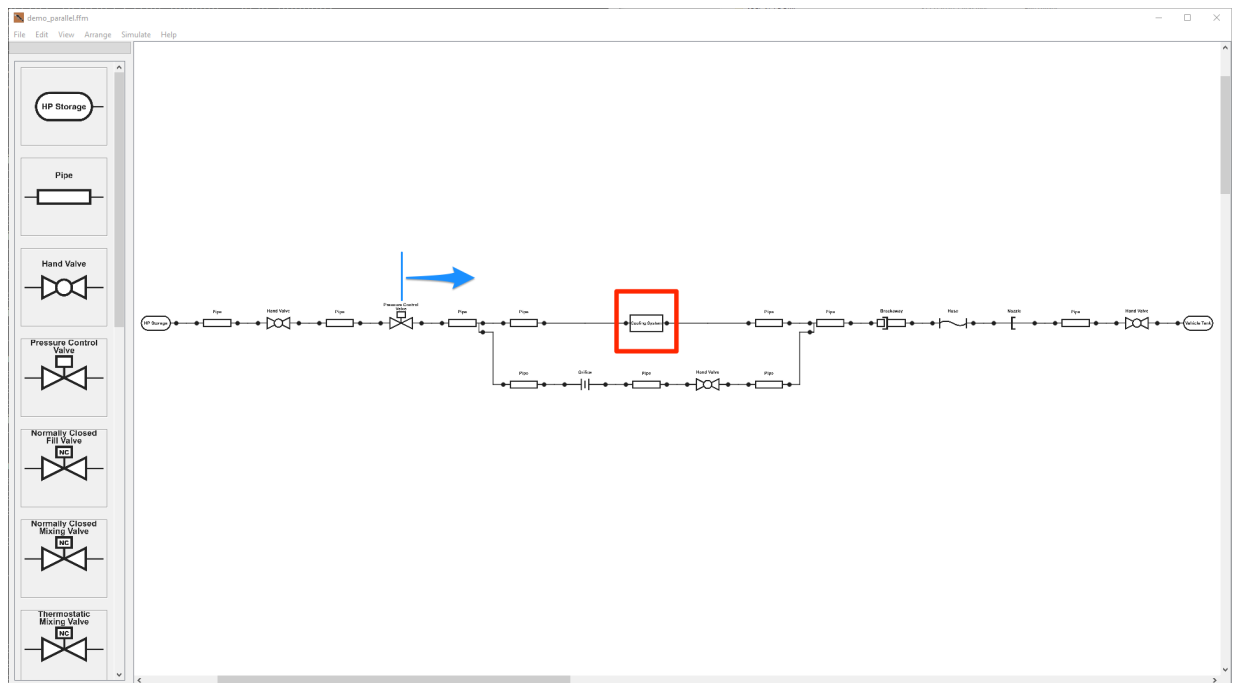
5.9 Error 09: Insert a Pipe Component in the End of the Parallel Stream

Insert a pipe component in the end of the parallel stream.



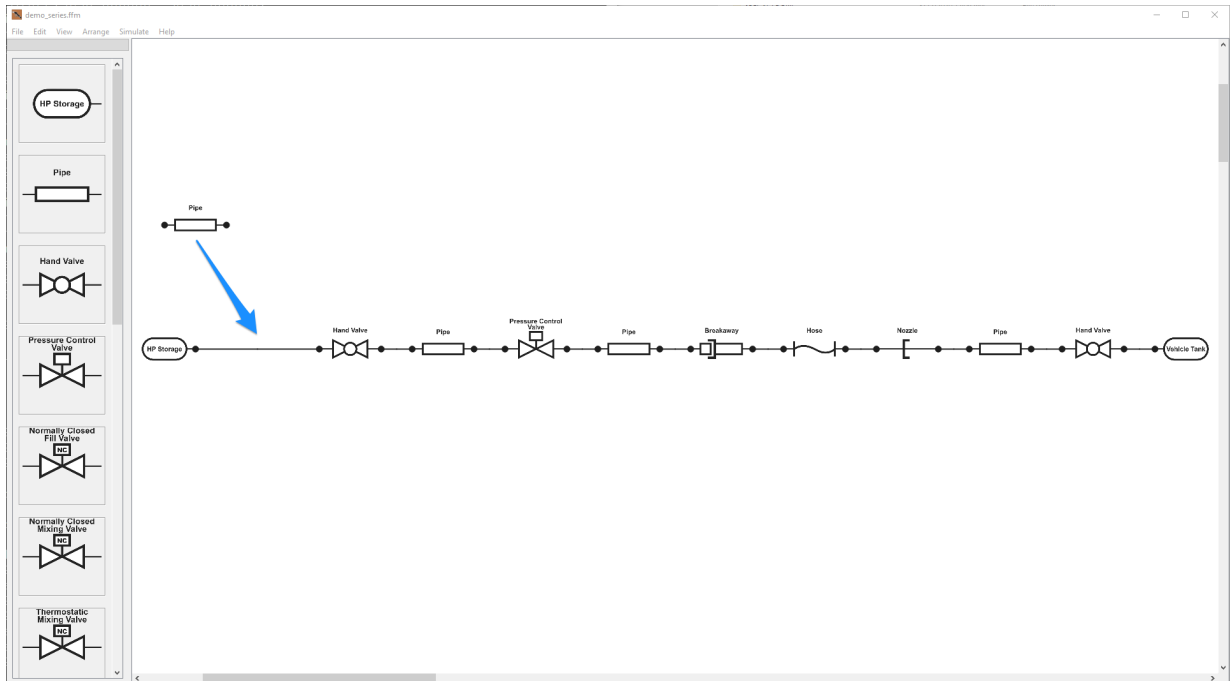
5.10 Error 10: Cooling System Must Be Located After the Pressure Control Valve

Make sure to place the cooling system after the pressure control valve (the low pressure side).



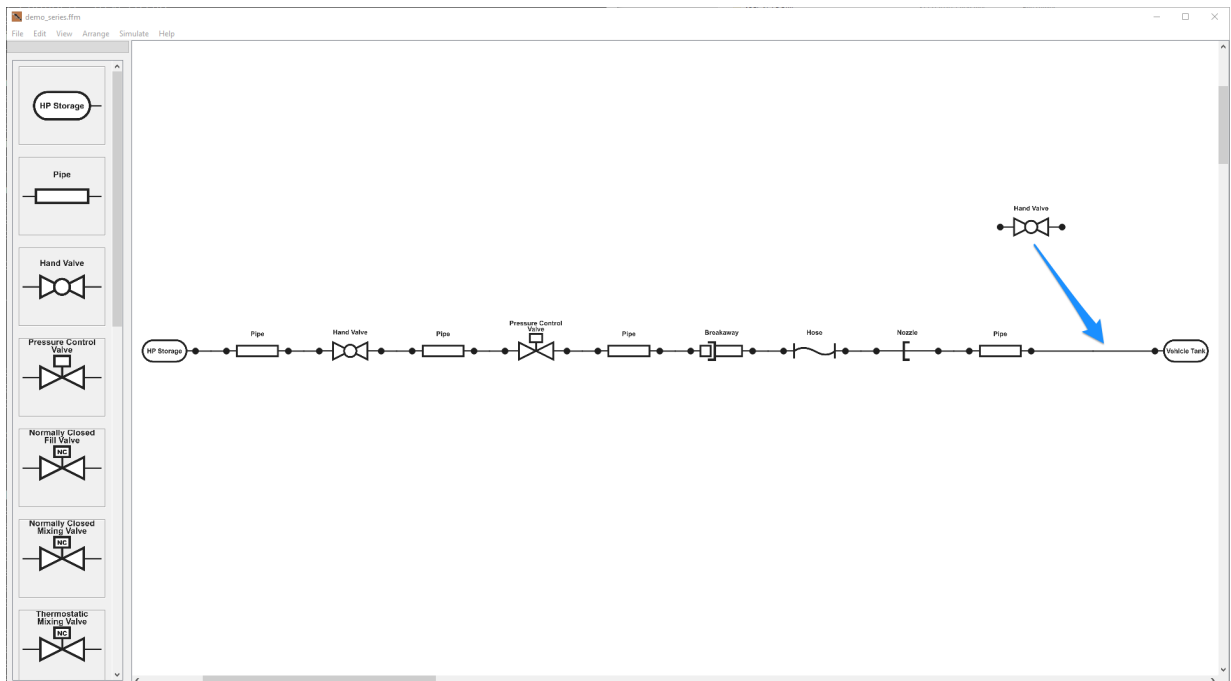
5.11 Error 11: Insert a Pipe Component After the High Pressure Storage

Insert a pipe component after the high pressure storage.



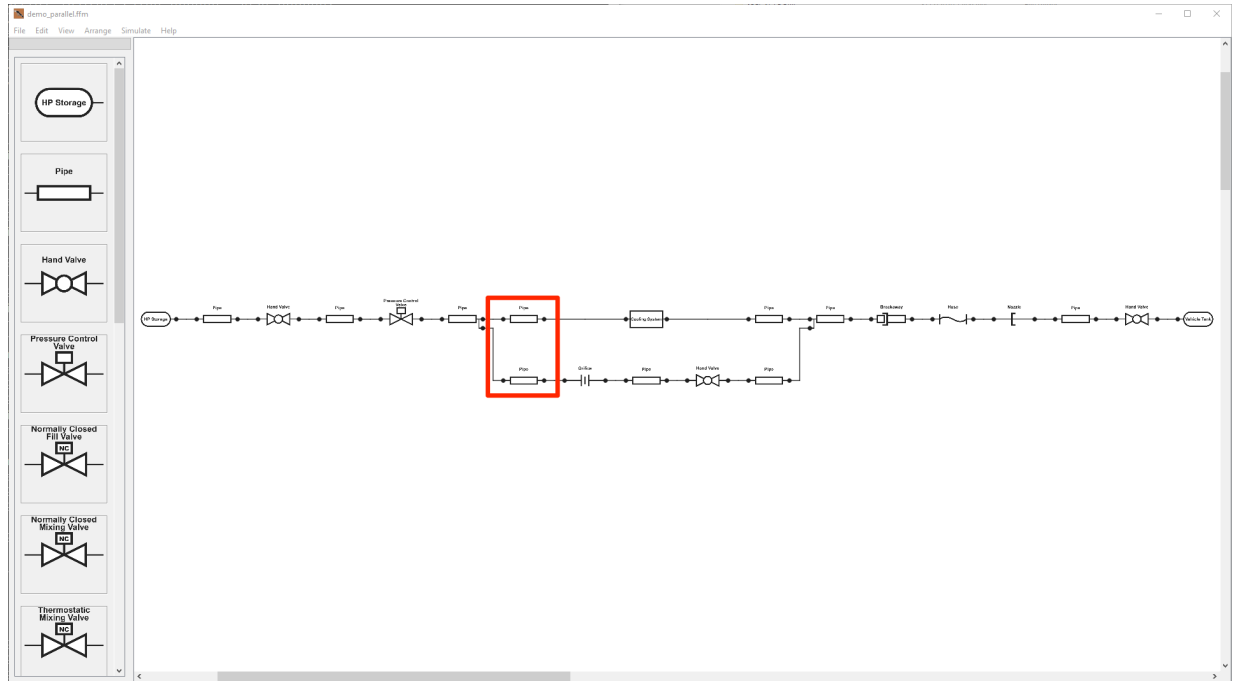
5.12 Error 12: Insert a Valve Component Before the Vehicle Tank

Insert a valve component (that has a CV value) before the vehicle tank.



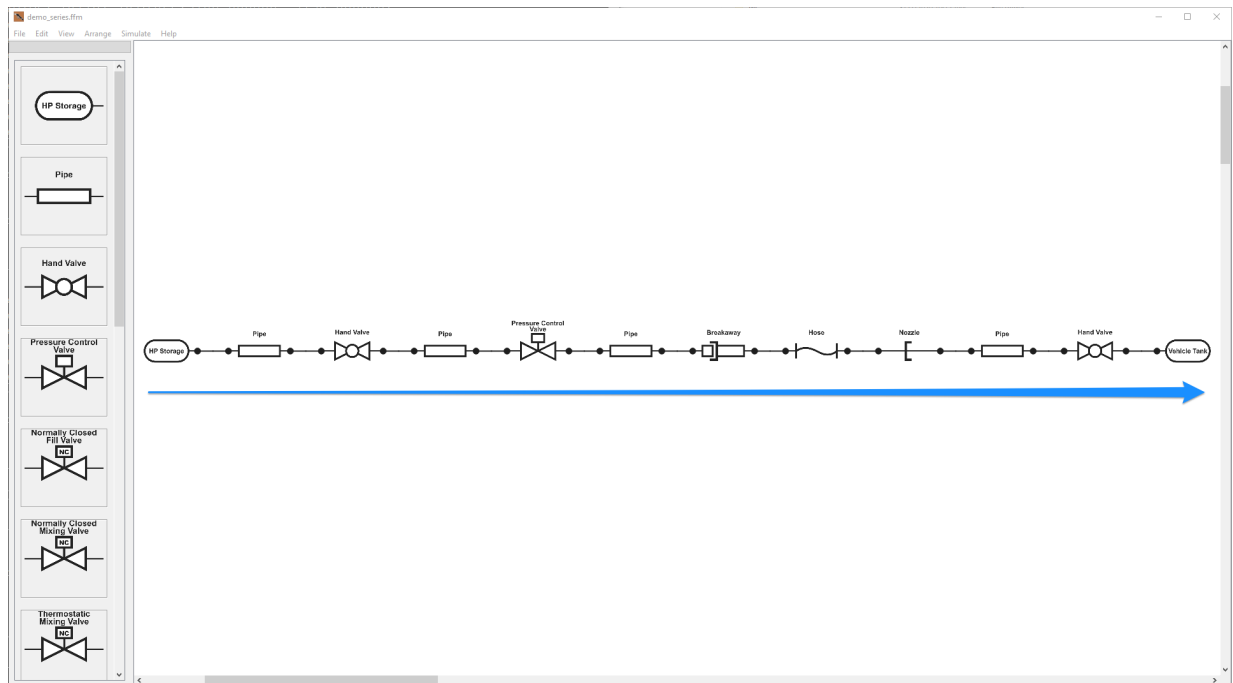
5.13 Error 13: Insert a Pipe Component in the Beginning of the Parallel Stream

Insert a pipe component in the beginning of the parallel stream.



5.14 Error 14: Connect All the Components

Make sure to [connect all the components](#).



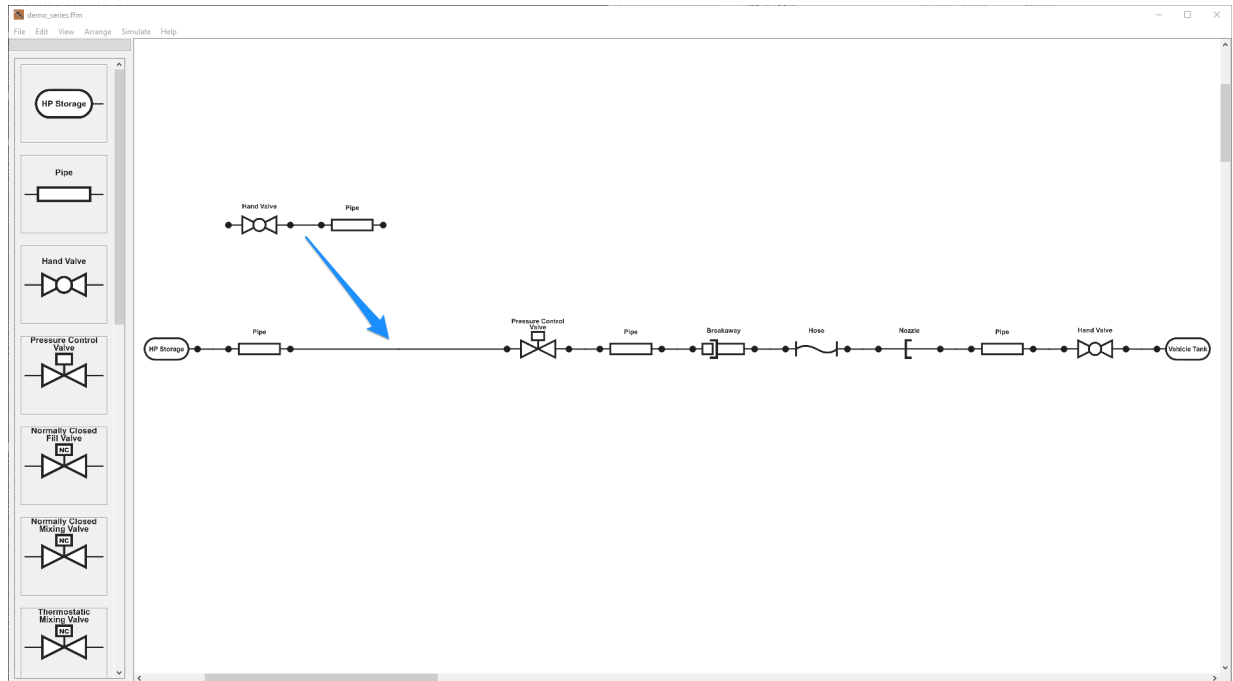
5.15 Error 15: Duplicates Found

The system allows to include only one of each component in the following list:

- High Pressure Tank Storage
- Vehicle Tank
- Pressure Control Valve
- Breakaway
- Hose
- Nozzle

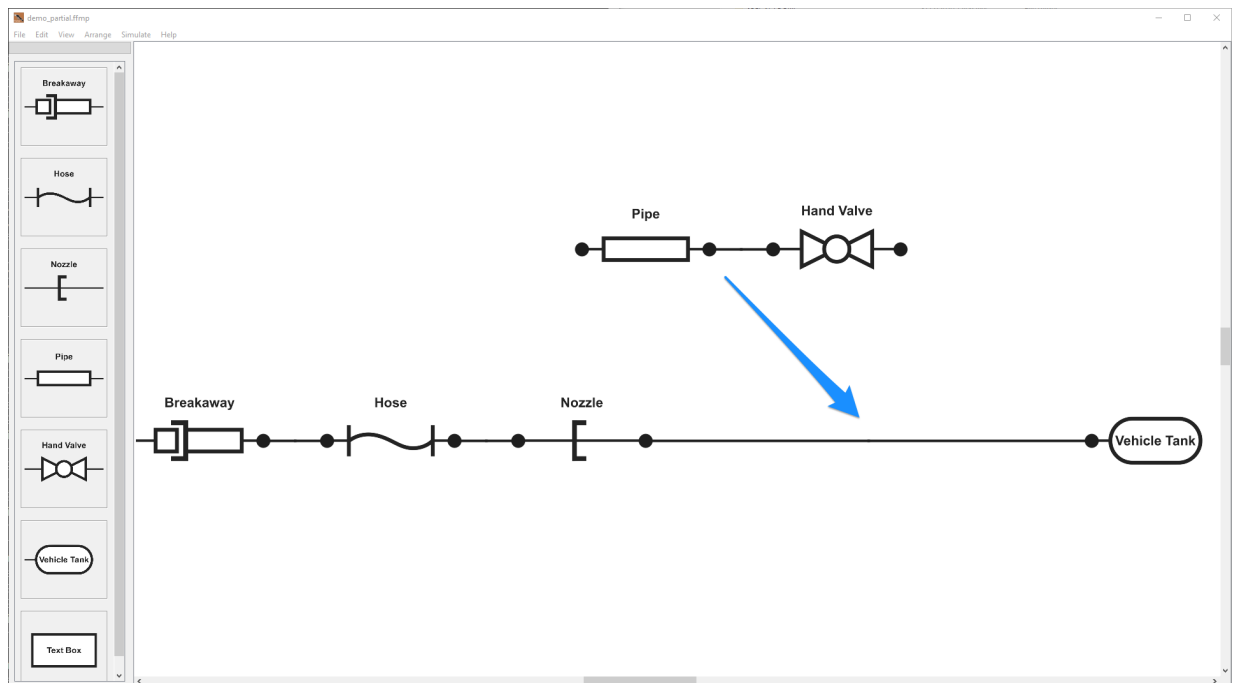
5.16 Error 16: Add Hand Valve and Pipe Component Pair before Pressure Control Valve

From the upstream, the system must have the series of High Pressure Storage Tank, Pipe, and **Hand Valve**.



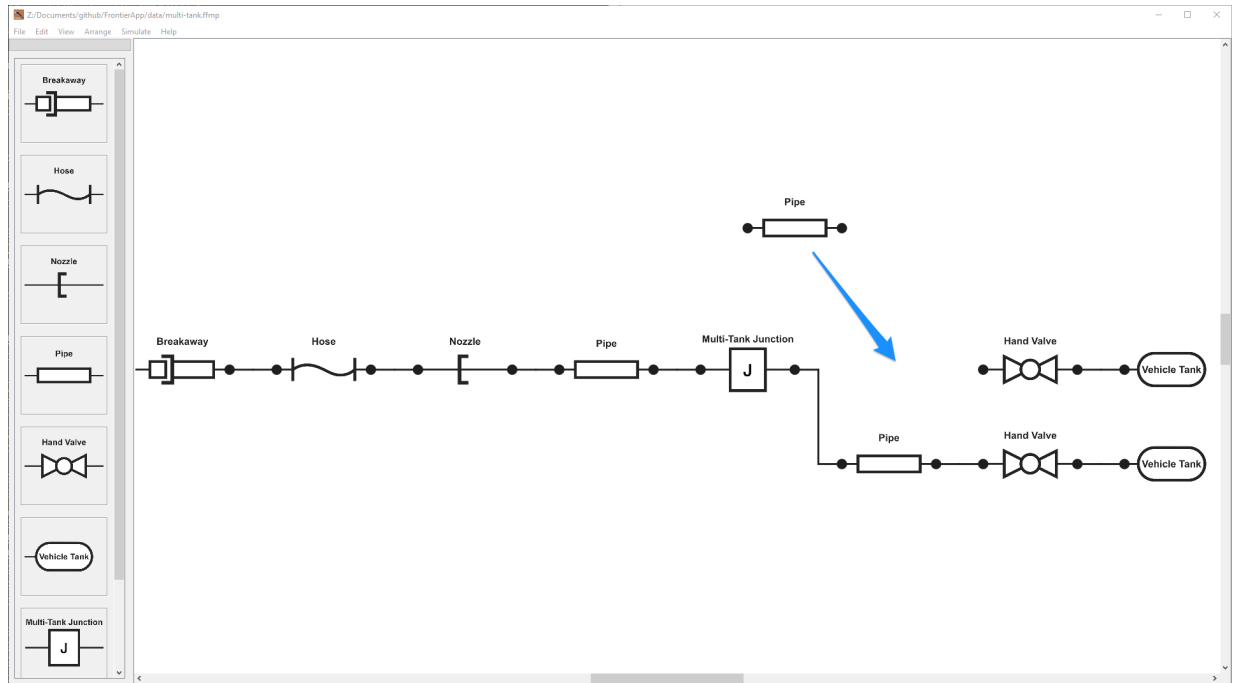
5.17 Error 17: Add Pipe and Hand Valve Component Pair between Vehicle Tank and Nozzle

Between the vehicle tank and nozzle, add a valve and at least one pipe component.



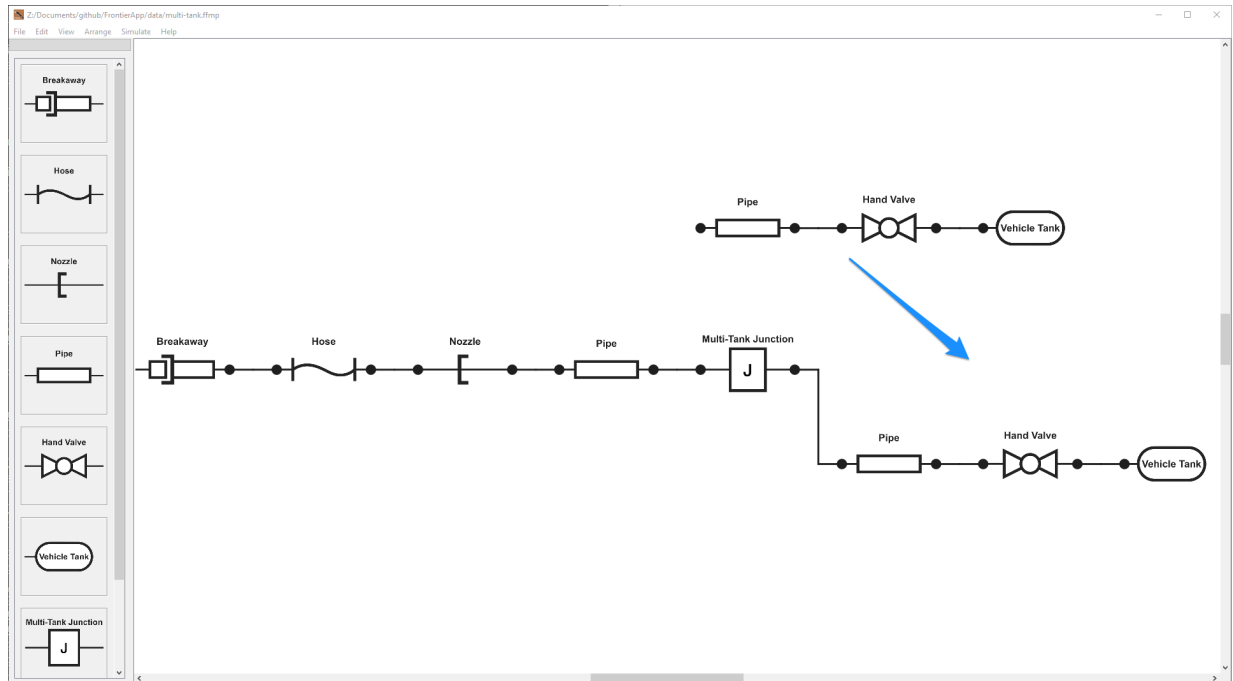
5.18 Error 18: Add Pipe Component after Multi-Tank Junction

Insert a pipe component right after the multi-tank junction.



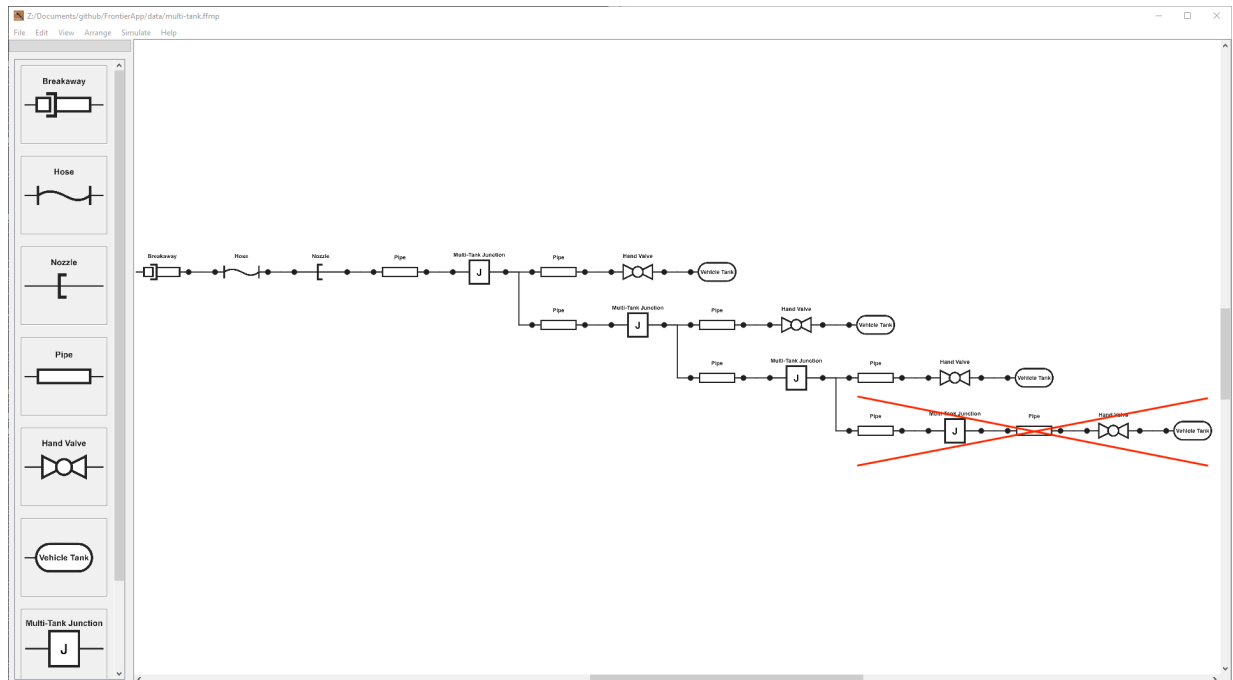
5.19 Error 19: Add at Least Two Multi-Tank Paths or Eliminate Multi-Tank Junction

A multi-tank junction is specifically used for the multi-tank configuration; for simulating the configuration with only one vehicle tank, eliminate multi-tank junctions. And, the multi-tank configuration needs to have at least two multi-tank paths.



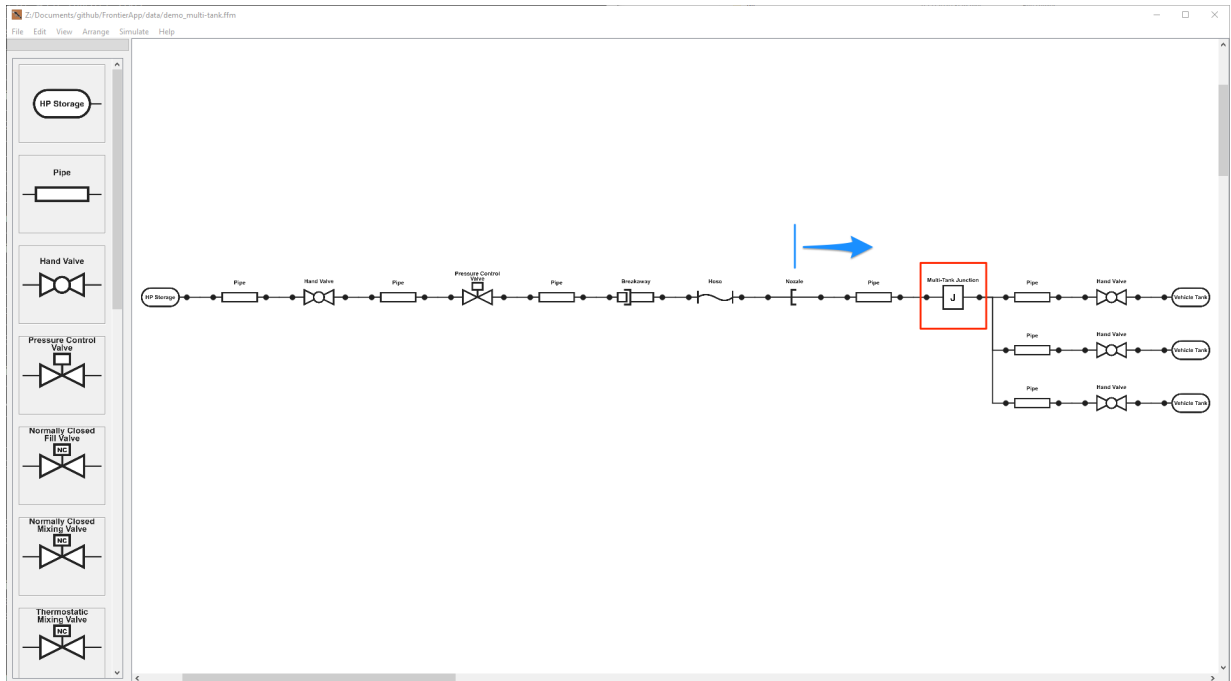
5.20 Error 20: Remove Excess Multi-Tank Junction(s)

The configuration can have three multi-tank junctions at most. Remove excess multi-tank junction(s).



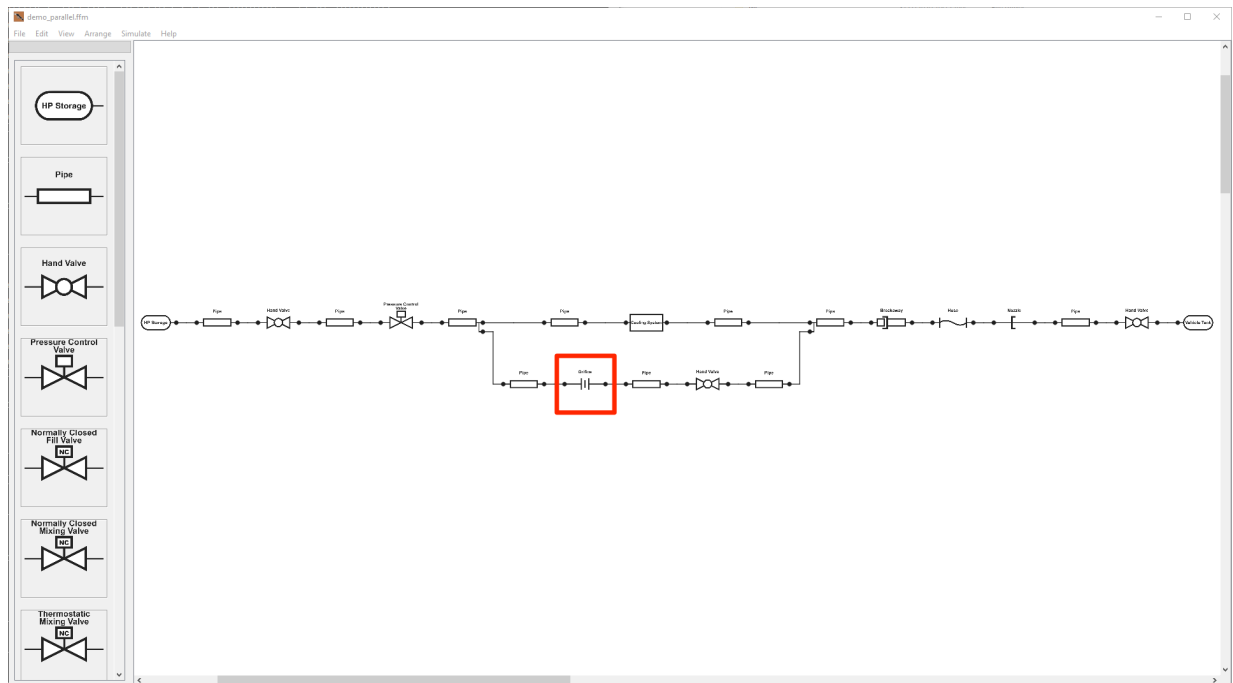
5.21 Error 21: Multi-Tank Junction Must Be Located After the Nozzle

Make sure to place the multi-tank junction(s) after the nozzle.



5.22 Error 22: Orifice Must Be Located Only the Other Parallel Side of the Cooling System

A parallel configuration only allows to place an orifice, and it must be located only the other parallel side of the cooling system.



5.23 Error 50: Incorrect Data Format

Make sure the order of data columns with the following header names:

- 1st column: Time_second
- 2nd column: PressureSupply_MPa
- 3rd column: TemperatureSupply_degC

	A	B	C
1	Time_second	PressureSupply_MPa	TemperatureSupply_degC
2	0	90.7363	32.4023
3	1	57.0387	36.9235
4	2	21.659	0.194798
5	3	10.3402	-3.97395
6	4	5.50775	-4.47351
7	5	3.7244	-3.2953
8	6	3.46559	-1.71179
9	7	3.49795	0.0942574

5.24 Error 51: Supply Condition File Not Found

Upload the supply condition file. See [how to upload supply condition data](#).

6 How to Cite H2FillS

If you use H2FillS software for work described in a publication, please [notify us](#) and include a citation consistent with the following format:

T. Kuroki, K. Nagasawa, M. Peters, D. Leighton, J. Kurtz, N. Sakoda, M. Monde, Y. Takata. Forthcoming. “Thermodynamic Modeling of Hydrogen Fueling Process from High Pressure Storage Tanks to Vehicle Tank.”

7 Acknowledgments

Institutional sponsors and an advisory council supported the development of H2FillS.

7.1 Sponsors

The U.S. Department of Energy's Hydrogen and Fuel Cell Technologies Office within the Office of Energy Efficiency and Renewable Energy was a sponsor along with the following industry and corporate sponsors:

- Ford Motor Company
- General Motors LLC
- Honda R&D Americas
- Hyundai-Kia America Technical Center
- Ivys Energy Solutions
- Shell
- Toyota.

7.2 Advisory Council

The advisory council includes Frontier Energy, which oversaw project management, along with a technical committee:

- Argonne National Laboratory
- Kyushu University
- Saga University
- Sandia National Laboratories
- Zero Carbon Energy Solutions, Inc.

8 Contact

While NREL does not provide technical support for H2FillS software, we welcome your feedback on the tool. To provide feedback or report any problems, contact h2fills@nrel.gov.

9 Changelog

Version 2.0 (August 31, 2020)

- Implemented multi-tank modeling capability

- Added multi-tank demonstrations
- Added a component name in the property window
- Improved the result export function. Changed a file extension from csv to xlsx to include results and parameter data with tabs
- Added error handling for multi-tank modeling
- Fixed some error handling bugs. Revised some error statements
- Fixed hyperlinks in the User's Manual

Version 1.0 (May 15, 2020)

- Released the first version of H2FillS Software