# 70 MPa Fast-Fill Modeling & Validation Experiments

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**DOE Tank Safety Workshop**

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# Sandia modeling and validation methods can be applied to the 70 MPa Fast Fill Problem

- **Multi year effort to understand flow and heat transfer in compressed gas storage systems**
  - **Vessel Blowdown (supplies)**
  - **Vessel Fillup (receivers)**
  - **Interconnecting systems of tubes, valves and flow branches**
- **Network flow modeling capability – we have developed dedicated software tools**
  - **TOPAZ**
  - **NETFLOW**
  - **Correlations are required for heat transfer & pressure drop**
- **Detailed CFD Modeling – NEW and a work in progress**
  - **Multidimensional**
  - **No correlations are needed**
- **Transient PVT Validation Experiments – provides essential data to validate all models**

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# Presentation Outline

- **Describe modeling approaches (Network & CFD)**
- **Describe methods for obtaining validation data**
- **Present Sandia results**
- **Describe a Sandia Network flow model for 70 MPa Fast – Fill**
  - **Validation using the data of Monde *et. al.***
  - **Validation using the data of Terada *et. al.***
- **Propose validation experiments for 70 MPa Fast – Fill models.**

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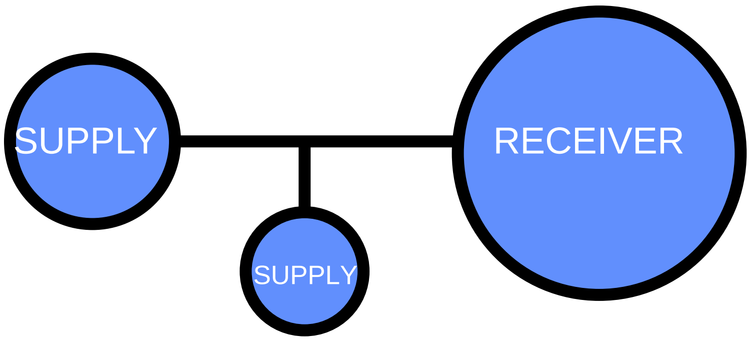
# The Problem

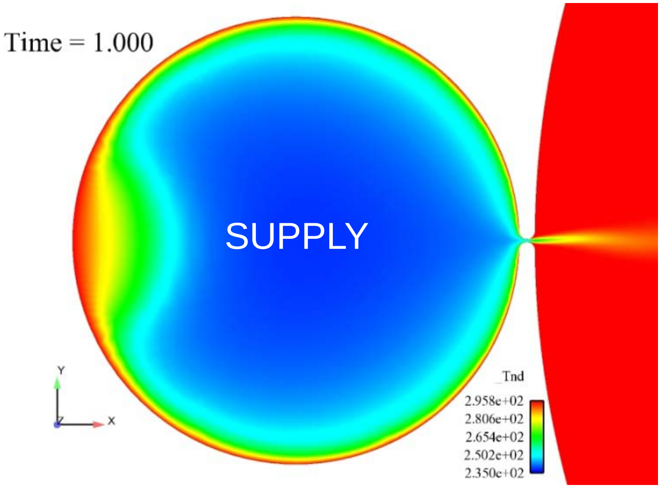
- These high pressure flows exhibit non-ideal gas behavior and are transient, turbulent and compressible (transonic, choking).
- Reservoir/receiver pressure ratios may are high (Ma>6!).
  - 5000:1 Typical for Sandia Systems
  - 1000:1 Typical for 70 MPa Fast-Fill (depending on fill strategy)
- Very limited model validation data is available.

# Two modeling approaches provide a means to predict storage vessel transient pressures and temperatures.

- **NETFLOW models vessel connections (network)**
  - One dimensional flow in tubing
  - Vessels modeled as single control volumes
  - Correlations for tube pressure drop.
  - Correlations for tube & vessel heat transfer
  - Isolates and identifies locations for flow choking and unchoking (high Mach number sonic/super-sonic flow)
  - Advantages
    - Calculations are fast & cheap (seconds & minutes)
    - Transfer times predicted accurately
  - Disadvantages
    - Heat transfer difficult to predict
    - Correlations may not exist or may be "out of range"
    - Temperature gradients in vessels cannot be predicted
- **FUEGO models vessel flows (CFD)**
  - Three dimensional flow and heat transfer
  - Advantages
    - Applicable to any geometry
    - No correlations needed
    - Temperature gradients in vessels predicted
  - Disadvantages
    - Calculations are computer intensive (days & weeks)
    - Transonic flows (receivers) lead to show-stopping instabilities




Network flow model




FUEGO CFD Model

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# Model Validation

We seek to conduct a validation experiment that measures the gas pressure and some representative gas temperature in a vessel as a function of time while it is being filled (or emptied). A model that simulates the experiment and reproduces the measured pressure and temperature can be considered validated (at least for the range of parameters unique to the experiment).

- **Vessel pressures are nearly uniform in time (except near underexpanded inlet jets) so a single transient pressure measurement should be sufficient.**
- **Transient temperature measurements with thermocouples have little value**
  - **It is difficult to prove that thermocouple response times are sufficient**
  - **Temperature distributions in vessels during and shortly after fill/discharge are far from uniform. What does measurement at a single point mean?**
- **The transient mass-averaged temperature is a viable validation measurement.**
  - **This is the temperature predicted by a network flow model**
  - **This temperature can be compared directly to the mass-averaged temperature computed in a CFD simulation.**
  - **It is representative of the total thermal energy of the gas.**

# Two methods can be used to measure $\overline{T}(t)$, the transient mass-averaged temperature.

## Mass Flow Rate Method*

1. Measure transient gas pressure, **P(t).**
2. Measure initial gas mass, $m_o$
3. Measure gas mass flow rate, $\dot{m}(t)$
4. Compute mass-averaged gas density:

$$\overline{\rho}(t) = \left( m_o + \int_0^t \dot{m}(t)\,dt \right) / V$$

5. Compute $\overline{T}(t)$ from the real gas equation of state:

$$\overline{T}(t) = f_T\left(\overline{\rho}(t), P(t)\right)$$

## Transient PVT Method**

1. Measure transient gas pressure, **P(t).**
2. Start a new filling/emptying test.
3. Stop filling/emptying at **t=t*** by closing valve.
4. Wait until temperature of gas and tank walls are uniform at $t = t_\infty$
5. Measure $T(t_\infty)$ and $P(t_\infty)$ with a thermocouple and pressure transducer
6. Use real gas equation of state to compute mass averaged density at **t=t***:

$$\overline{\rho}\left(t_\infty\right) = f_\rho\left(T(t_\infty), P(t_\infty)\right) = \overline{\rho}\left(t^*\right)$$

7. Compute $\overline{T}(t^*)$ from the real gas equation of state:

$$\overline{T}(t^*) = f_T\left(\overline{\rho}(t^*), P(t^*)\right)$$

8. Repeat 2-7 as required.

* Accurate $\dot{m}(t)$ measurements are difficult for compressible flow.

**S. C. Johnston and H. A. Dwyer, "Bulk Gas Temperature Measurement During Vessel Discharge using Transient PVT," Rev. Sci. Instrum., 46, No. 12, December 1975.

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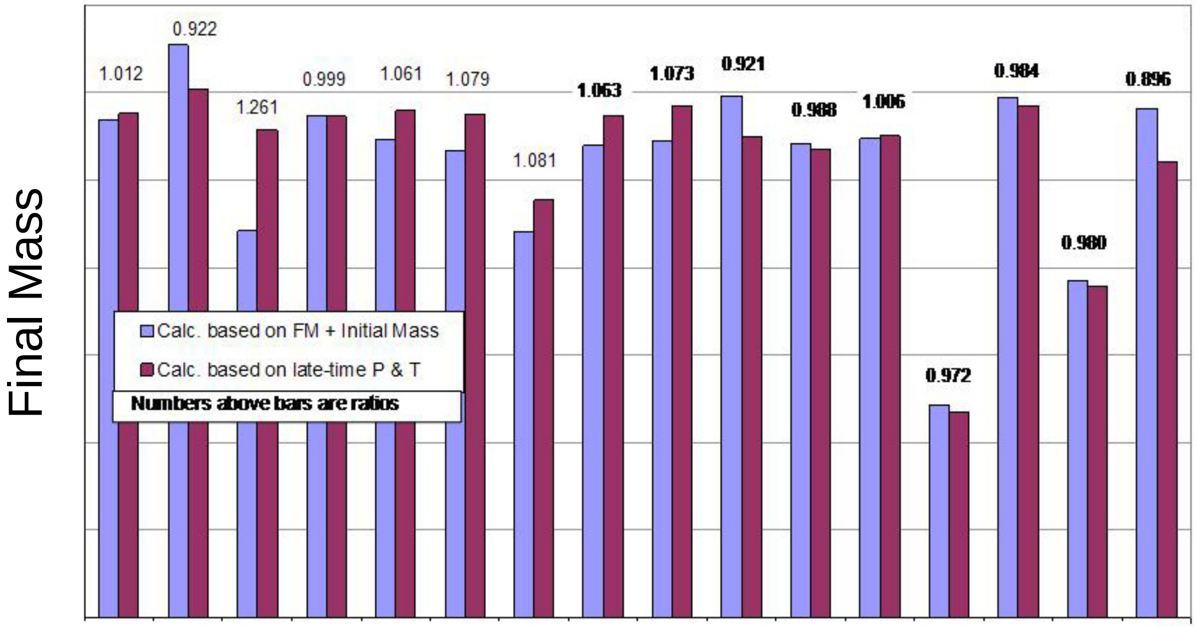
# Determination of transient mass average gas temperature using mass flow meters has be difficult.

- Powertech 70MPa Multi Client Fueling Studies utilized different types of mass flow meters.
- Final mass in tank was determined by integrating mass flow rate data.
- Final mass in tank was also determined from final ($t=t_\infty$) pressure and temperature.
- These measurements seldom matched and produced thermodynamically inconsistent transient mass averaged gas temperatures.

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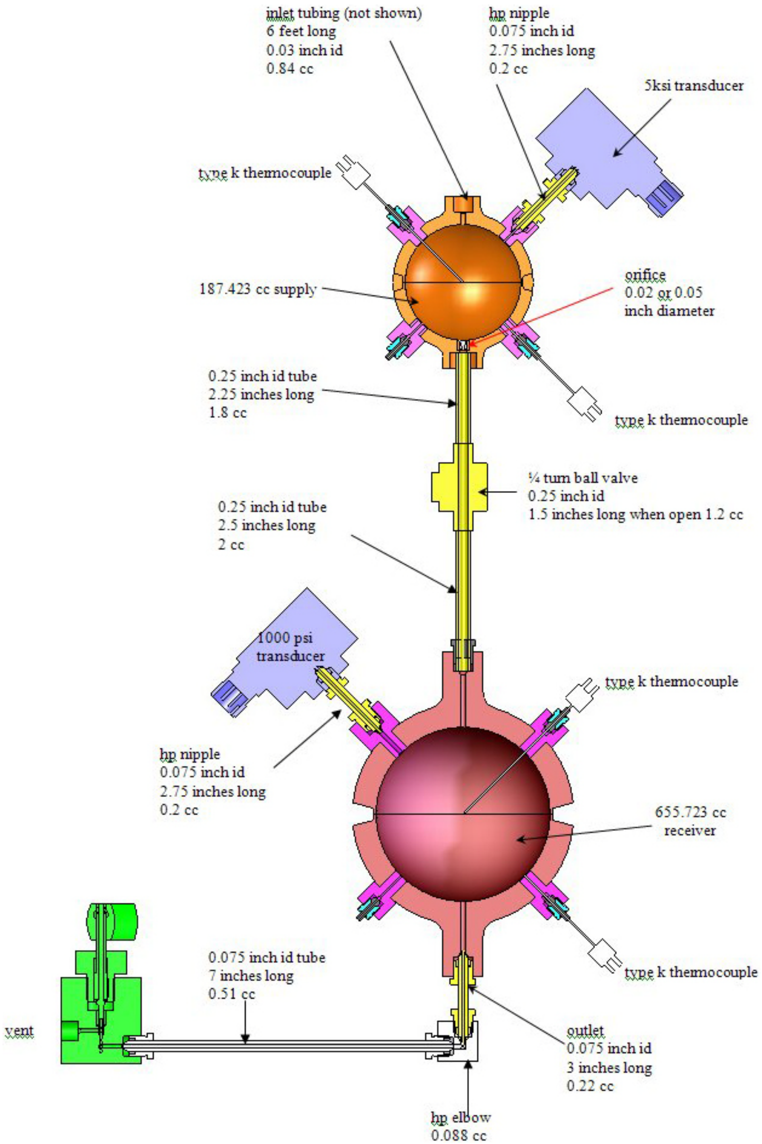
# Sandia has used to Transient PVT method to obtain validation data for supply and receiver fill/discharge models.




- **Transient vessel pressures were measured.**
- **Transient PVT tests determined mass averaged temperature points for the supply and receiver simultaneously.**
- **Mass balances were within 1%**
- **Supply volume 200 cc**
- **Receiver volumes 90, 700, 13000 cc.**
- **Supply pressures: 300, 3000, 6000 PSI**
- **Helium at room temperature**
- **Pressure equilibrium times: seconds**
- **Thermal equilibrium times: 30 seconds**
- **Data collected by S. F. Rice, N. J. Paradiso and T. G. Felver**

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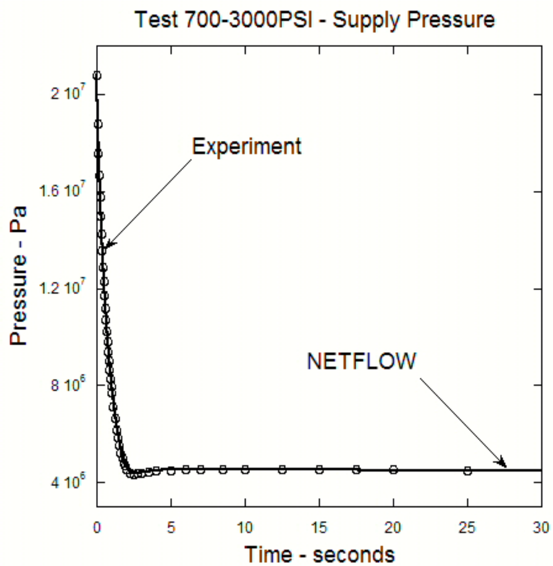
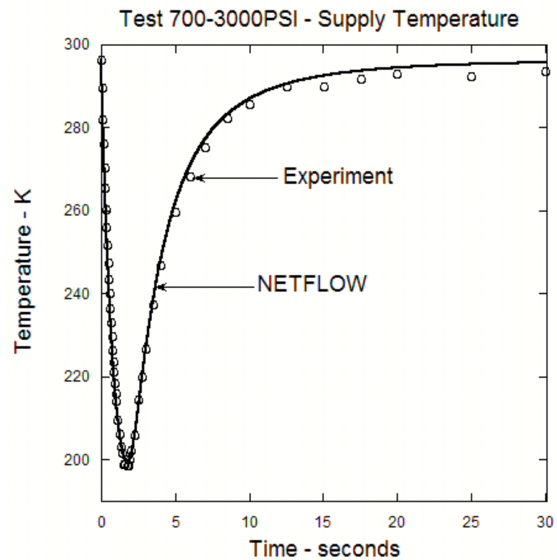
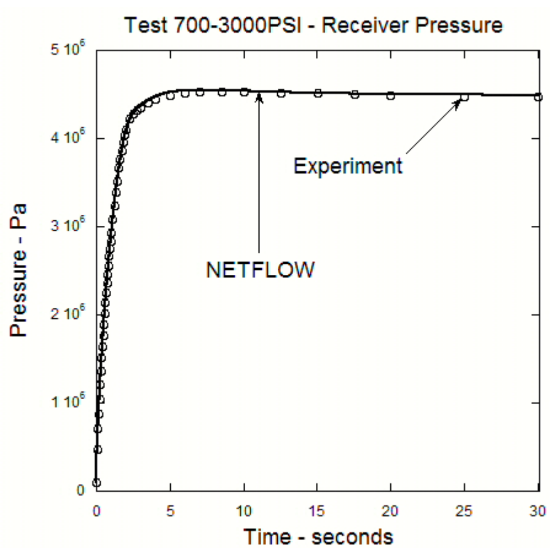
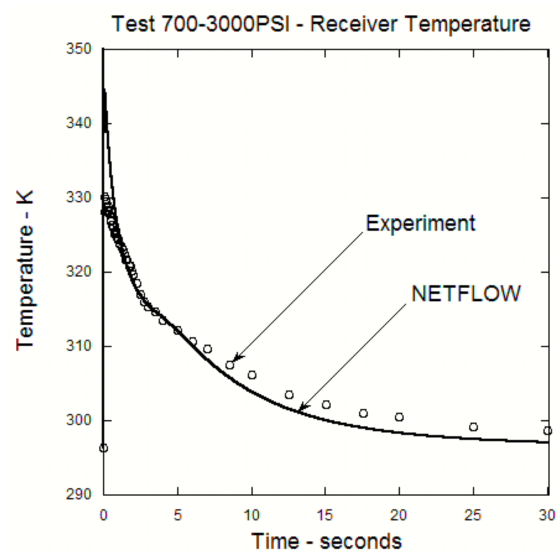
# NETFLOW network models were validated with Sandia transient PVT data.




- **NETFLOW models were validated for 6 high precision transient PVT simulations (tests).**
- **Validation demonstrated the accuracy of existing supply heat transfer correlations.**
- **Improvements were made to receiver heat transfer correlations but more work is needed to capture early time behavior.**

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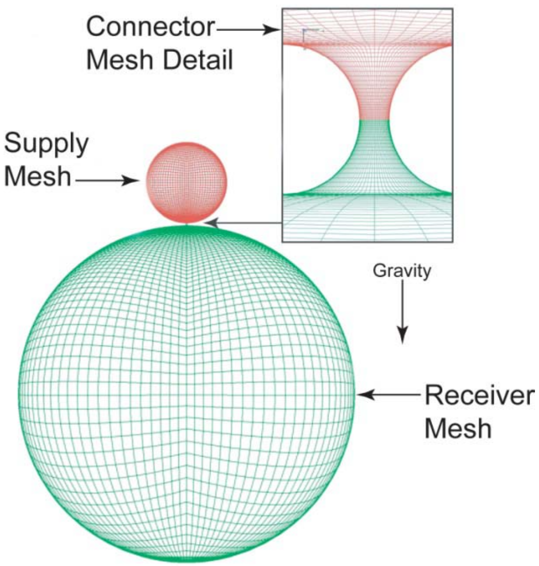
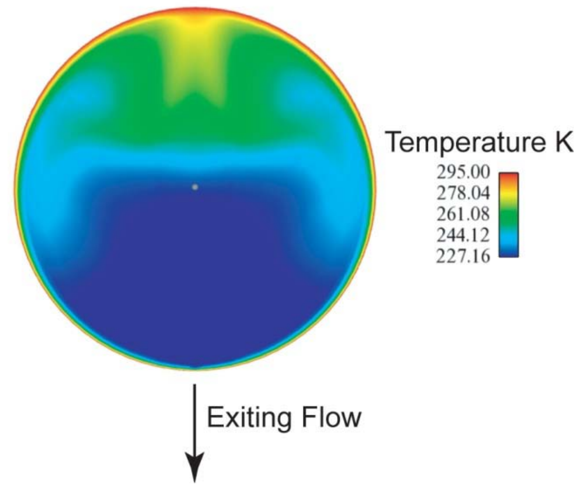
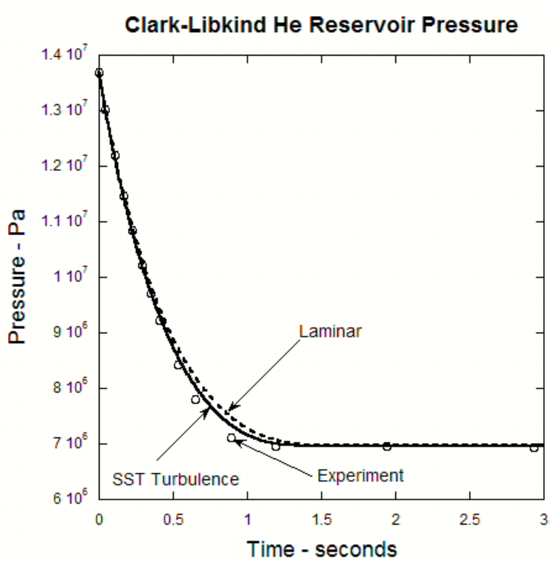
# FUEGO simulations demonstrate the value of CFD in predicting vessel flow and heat transfer.

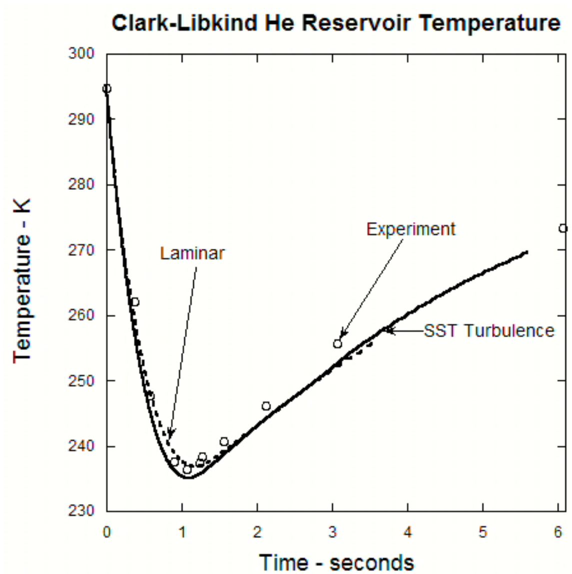



**Supply temperature distribution at t=2 s.**

- **Supply mass averaged temperature and pressure were predicted.**
- **No heat transfer correlations were necessary.**
- **Calculations demonstrate transition free convection to be the dominant heat transfer mode.**
- **Transient PVT data from G. Clark & M. Libkind 1983.**




$$\overline{T} = \frac{\int_V T \rho \, dv}{\int_V \rho \, dv}$$

**FUEGO mass averaged T.**

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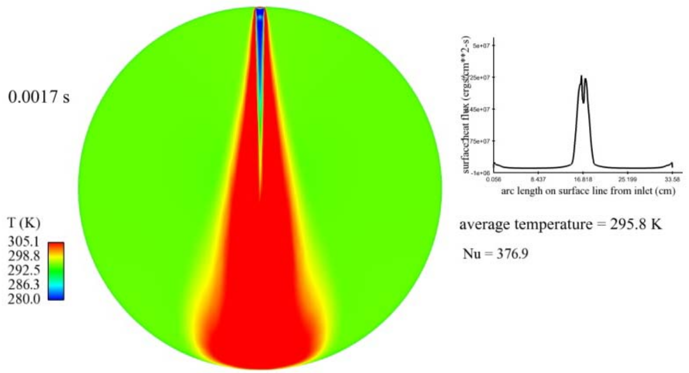
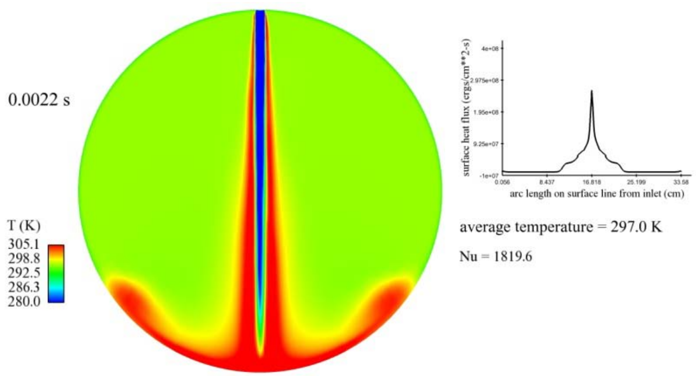
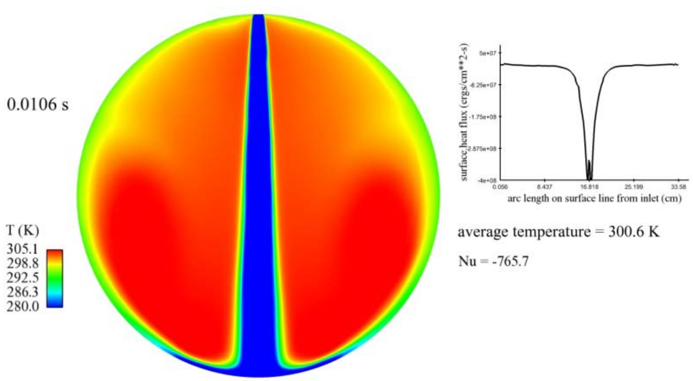
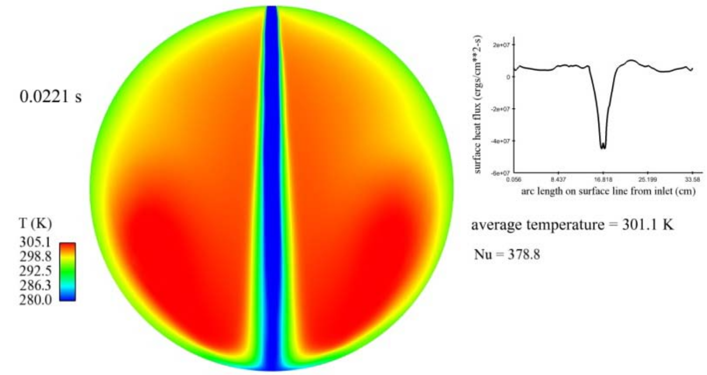
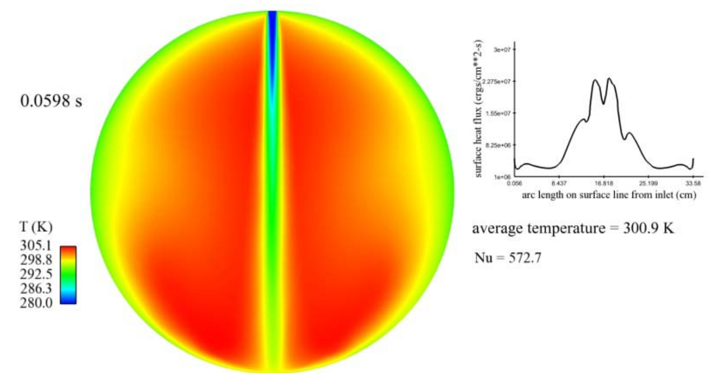
# Preliminary FUEGO CFD calculations demonstrate the complexity of receiver heat transfer.




- **700 cc receiver**
- **2:1 pressure ratio**
- **Jet is slightly underexpanded**
- **Early forced convection heat transfer**

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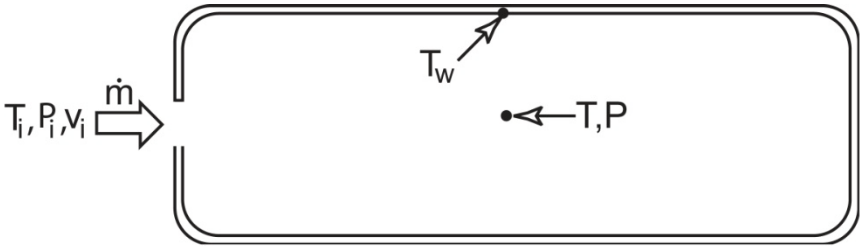
# A Network Model for Tank Filling




## Hydrogen Gas

Continuity: $V\frac{d\rho}{dt} = \begin{cases} +\dot{m} \\ -\dot{m} \end{cases}$

Energy: $VC_v\frac{d(\rho T)}{dt} + hA(T - T_w) = \begin{cases} +\dot{m}\left(C_p T_i + \frac{1}{2}v_i^2\right) \\ -\dot{m}C_p T \end{cases}$

## Heat Transfer Correlations

**Forced:** $\mathrm{Nu} = a\left[\mathrm{Re}_D \,\mathrm{Pr}\left(\frac{d}{D}\right)^2\right]^b$

**Free:** $\mathrm{Nu} = c\mathrm{Ra}^n$

$\mathrm{Nu} = \frac{hD}{k} \qquad \mathrm{Re}_D = \frac{\rho v_i D}{\mu} \qquad \mathrm{Pr} = \frac{C_p \mu}{k}$

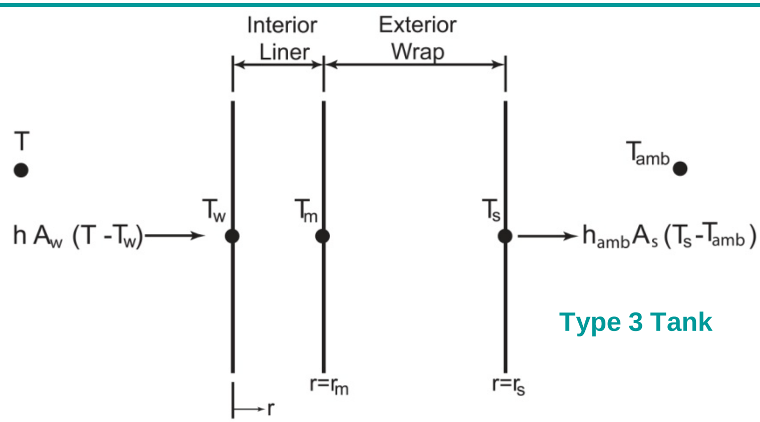
$\mathrm{Ra} = \mathrm{Gr}\,\mathrm{Pr} = \frac{g\beta(T - T_w)\rho^2 D^3}{\mu^2}\frac{C_p \mu}{k}$

## Abel-Nobel Equation of State:

$P = \frac{\rho RT}{1 - B\rho}$

B=.007691 $m^3$ for Hydrogen

## Tank Wall Heat Transfer




$$\rho_* C_* A_*(r)\frac{\partial T_*}{\partial t} = \frac{\partial}{\partial r}\left(k_* A_*(r)\frac{\partial T_*}{\partial r}\right)$$

$$h\left(T - T_w\right) = -k_* \left.\frac{\partial T_*}{\partial r}\right|_{r=0}$$

$$h_{amb}\left(T_s - T_{amb}\right) = -k_* \left.\frac{\partial T_*}{\partial r}\right|_{r=r_s}$$

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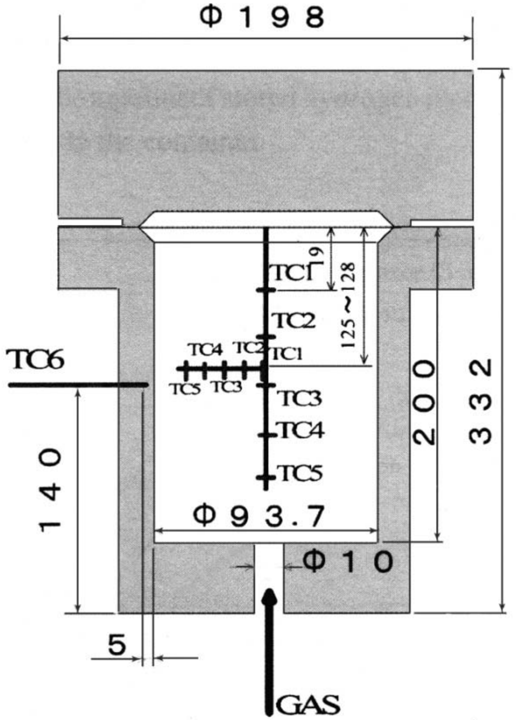
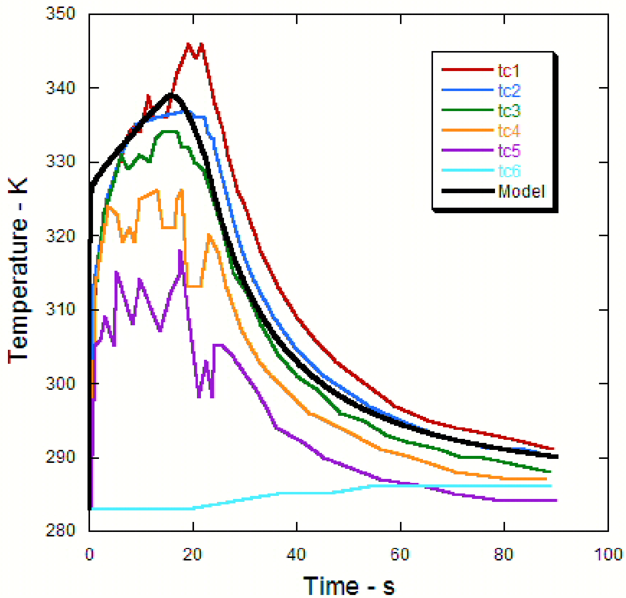
# Model Validation with Monde et. al.* data.

Dimensions are in mm

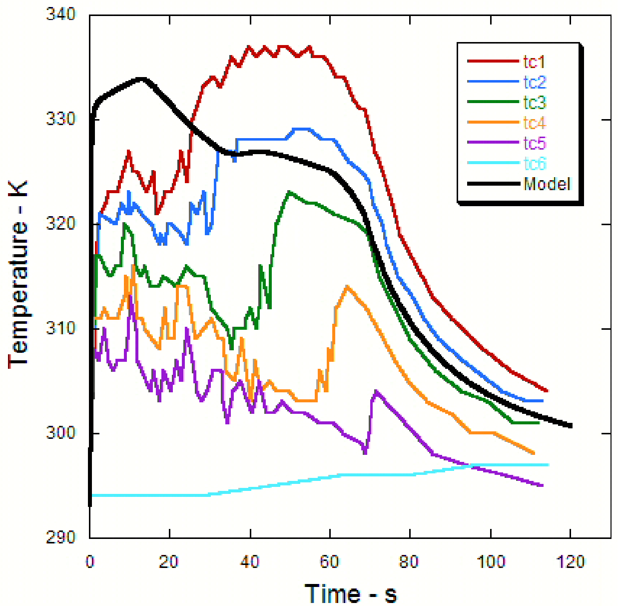



Instrumented 1.38 L
H2 Pressure Vessel

Comparisons of thermocouple measurements to predicted mass-averaged gas temperature.




170 g/min Test




45 g/min Test

* M. Monde, Y. Mitsutake, P. L. Woodfield and S. Maruyama, "Characteristics of Heat Transfer and Temperature Rise of Hydrogen during Rapid Hydrogen Filling at High Pressure," Heat Transfer-Asian Research, Vol. 36, No. 1, 2007.

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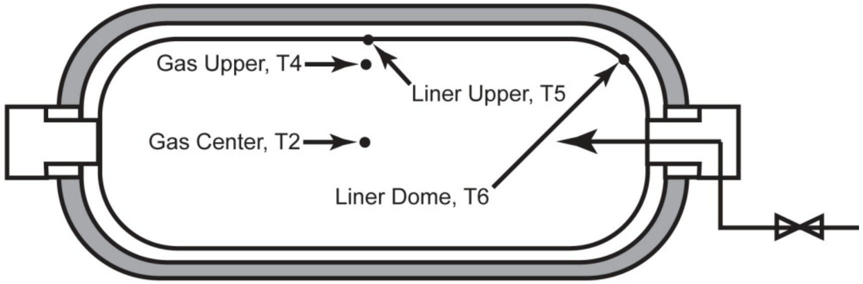
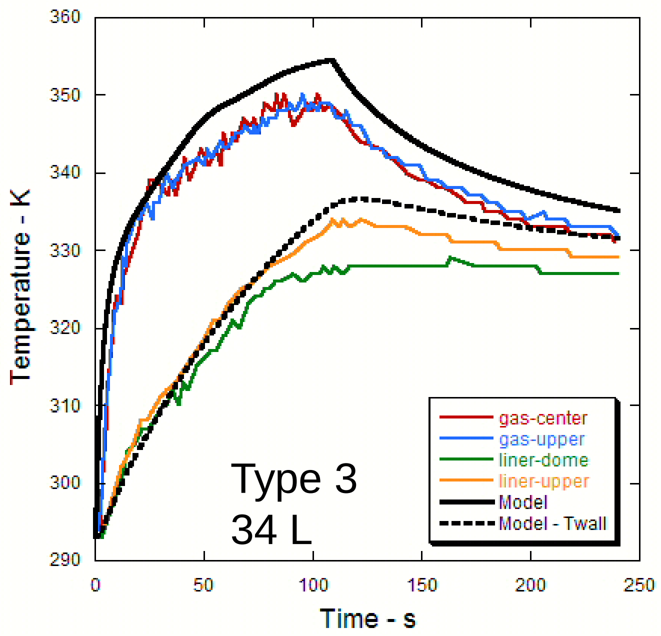
# Model Validation with Terada et. al.* data.

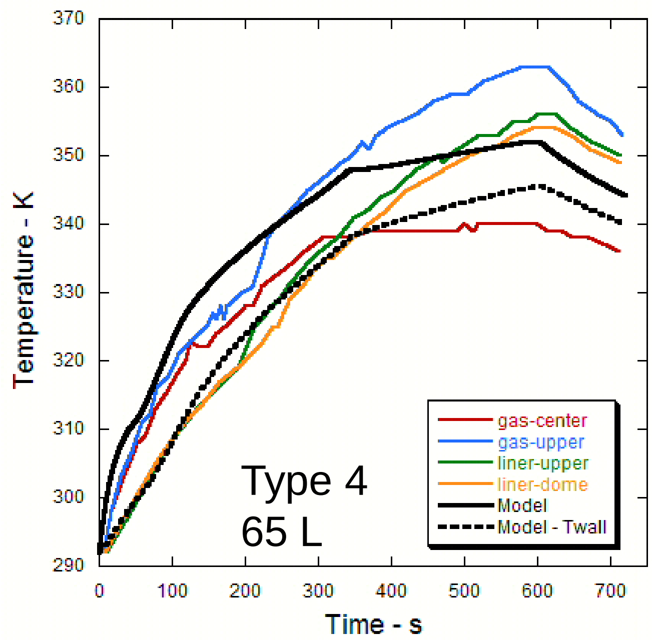



Thermocouple Locations

Test Matrix

| Tank type | TYPE 3 | TYPE 4 |
|---|---|---|
| Filling time (sec) | 60<br>120<br>300 | 300<br>600 |
| Filling pattern | Constant rate of pressure rise | |
| Start pressure | 2MPa | |
| Filling pressure | 35MPa | |
| Ambient temp. | 20°C | |
| Filling gas temp. | Ambient | |




Comparisons of thermocouple measurements to predicted mass-averaged gas temperature and wall temperature.

* T. Terada, H. Yoshimura, Y. Tamura, H. Mitsuishi and S. Watanabe, "Thermal Behavior in Hydrogen Storage Tank for FCV on Fast Filling (2nd Report)," SAE Technical Paper 2008-01-0463, 2008 World Congress, Detroit, MI, April 14-17, 2008.

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# High quality data is needed for 70 MPa Fast Fill model validation.

- Data would benefit both “network” and CFD models.
- Validation data must include (but not be limited to) transient tank pressure and transient mass average temperatures.
- Transient tank pressure should be measured using a transducer in the tank.
- Transient mass-averaged temperature data should be obtained from transient PVT method or from a well-calibrated mass flow meter and a transient pressure measurement. Transient thermocouple measurements should NOT be used.
- Model validation would be accomplished by simulating the experiment
  - Time dependent boundary conditions must be measured experimentally
    - » Pressure/Temperature Inlet BC – Measure incoming total temperature and pressure
    - » Mass Flow Rate Inlet BC – Measure mass flow rate and incoming total temperature
  - Tank wall thermal properties should be well characterized (thickness, thermal conductivity, heat capacity, for all layers)
- Tank sizes and design should be relevant to 70 MPa fast fill (Type 3 and Type 4 tanks)
- The tank design must not be proprietary.